Full wwPDB NMR Structure Validation Report

Aug 10, 2026 – 10:27 AM EDT

PDB ID	:	9Q30 / pdb_00009q30
BMRB ID	:	52074
Title	:	Solution Structure of T35S mutant of KRAS4b-GppNHp
Authors	:	Sharma, A.K.; Maciag, A.E.
Deposited on	:	2025-08-15

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

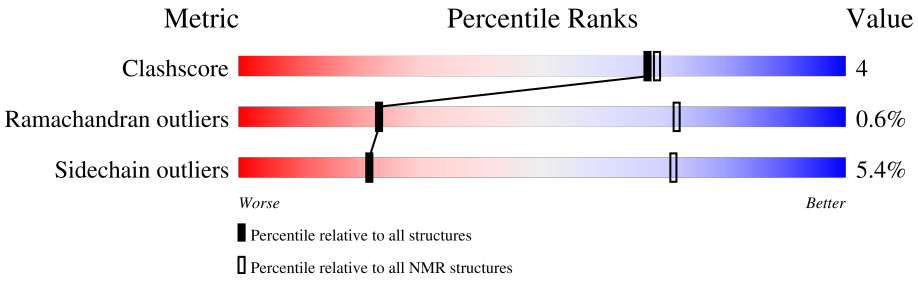
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 59%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	170	90% 7% • •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:166 (165)	0.77	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 5, 6, 7, 9, 10, 12, 13, 14, 17, 18
2	2, 3, 4, 8, 11, 15, 16, 19, 20

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2730 atoms, of which 1347 are hydrogens and 0 are deuteriums.

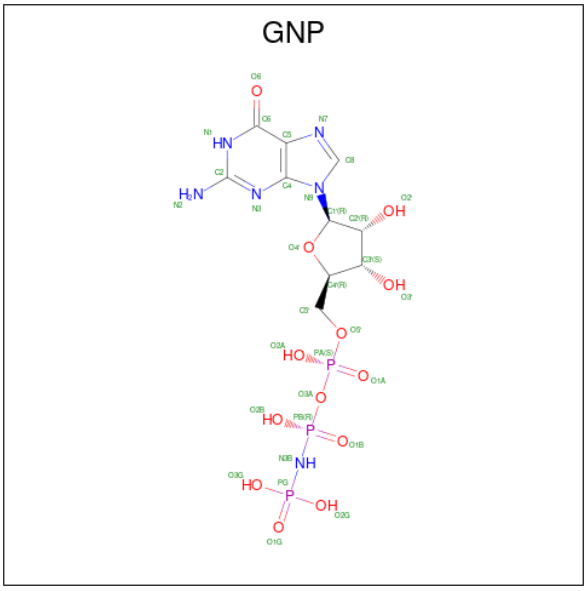
- Molecule 1 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	169	2684	844	1334	232	268	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	35	SER	THR	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	45	10	13	6	13	3

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
			Total	Mg
3	A	1	1	1

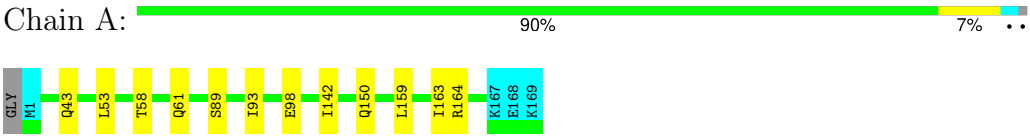
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Isoform 2B of GTPase KRas

Chain A:



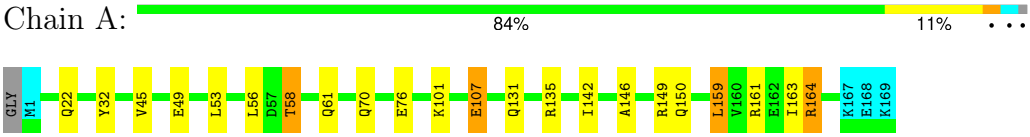
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Isoform 2B of GTPase KRas

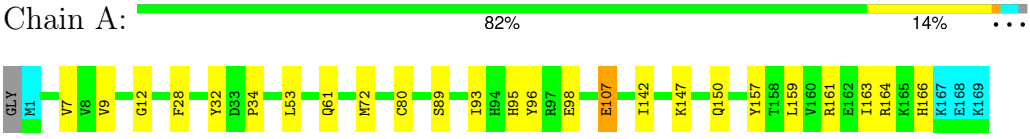
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Isoform 2B of GTPase KRas

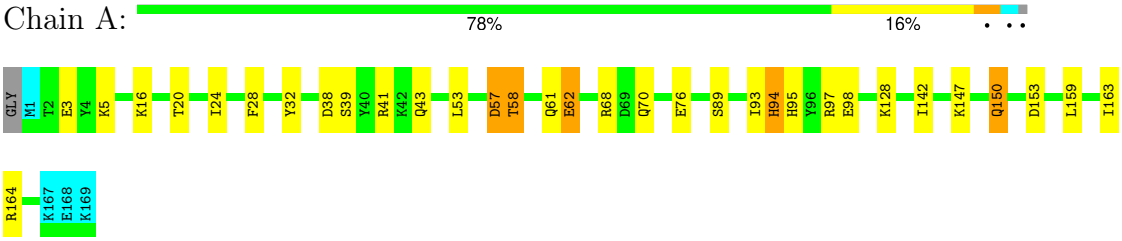
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Isoform 2B of GTPase KRas

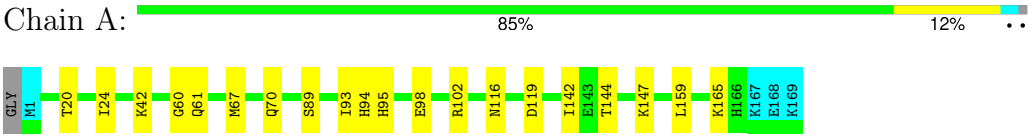
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Isoform 2B of GTPase KRas

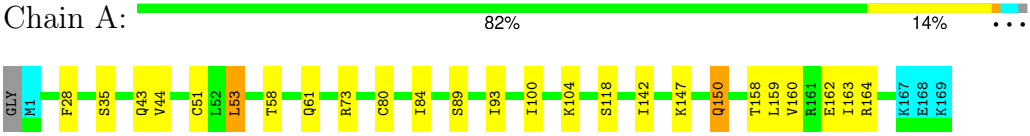
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Isoform 2B of GTPase KRas

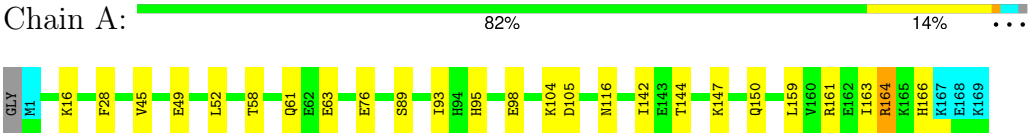
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Isoform 2B of GTPase KRas

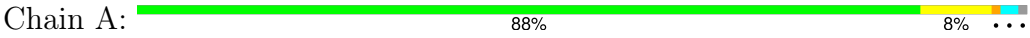
Chain A:

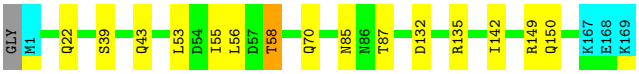


4.2.7 Score per residue for model 7

• Molecule 1: Isoform 2B of GTPase KRas

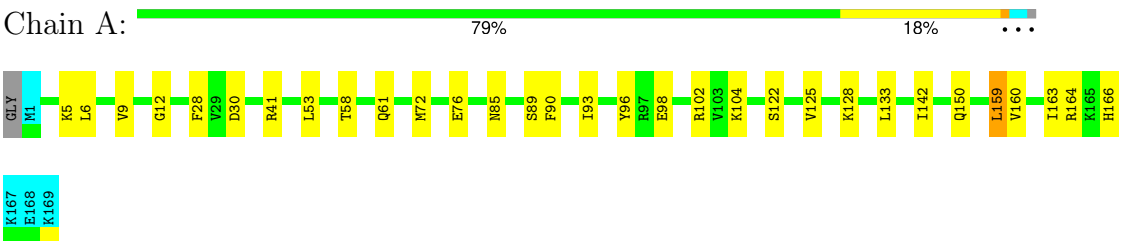
Chain A:





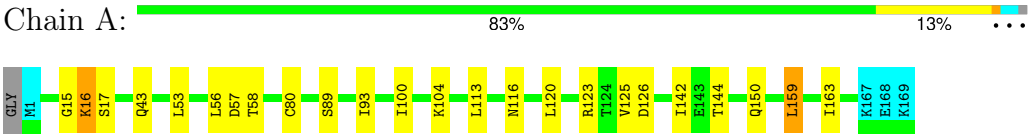
4.2.8 Score per residue for model 8

• Molecule 1: Isoform 2B of GTPase KRas



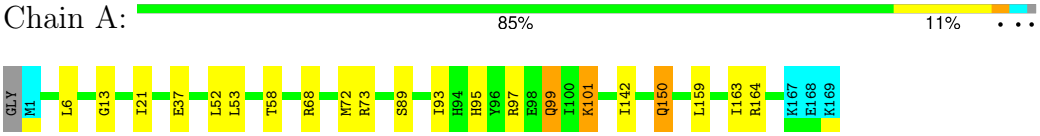
4.2.9 Score per residue for model 9

• Molecule 1: Isoform 2B of GTPase KRas



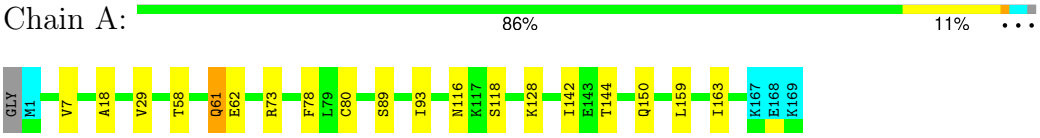
4.2.10 Score per residue for model 10

• Molecule 1: Isoform 2B of GTPase KRas



4.2.11 Score per residue for model 11

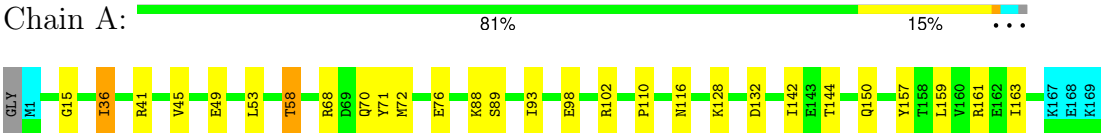
• Molecule 1: Isoform 2B of GTPase KRas



4.2.12 Score per residue for model 12

• Molecule 1: Isoform 2B of GTPase KRas

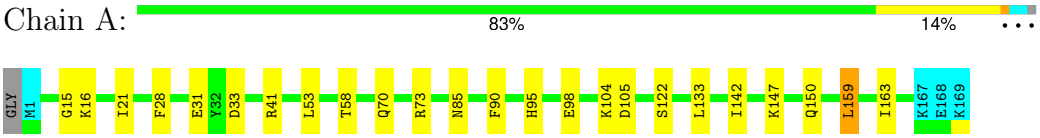
Chain A:



4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Isoform 2B of GTPase KRas

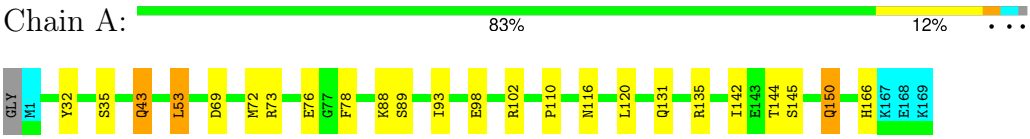
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Isoform 2B of GTPase KRas

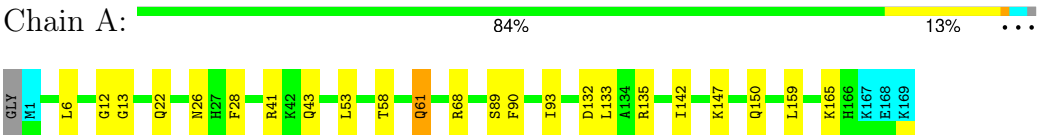
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Isoform 2B of GTPase KRas

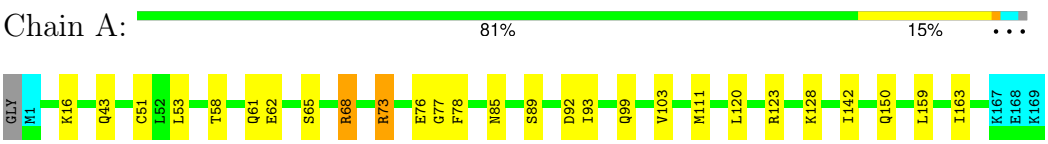
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Isoform 2B of GTPase KRas

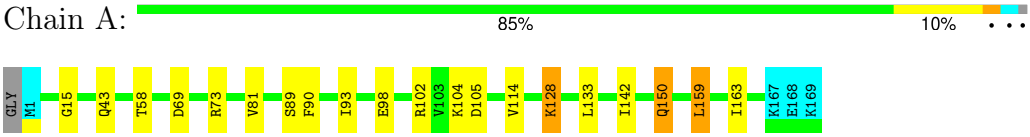
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Isoform 2B of GTPase KRas

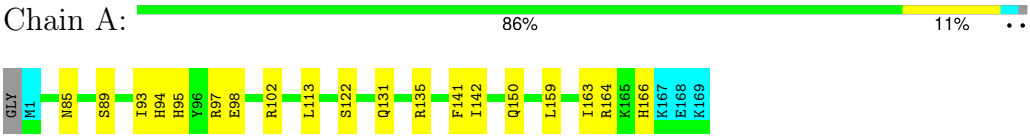
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Isoform 2B of GTPase KRas

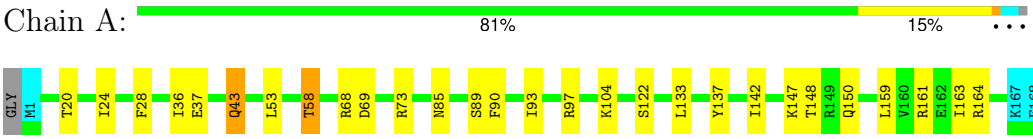
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Isoform 2B of GTPase KRas

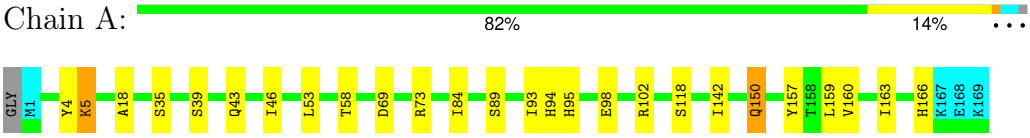
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Isoform 2B of GTPase KRas

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.98.15
CNS	refinement	1.3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2114
Number of shifts mapped to atoms	2114
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	59%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1314	1293	1289	10±3
2	A	32	13	13	1±1
All	All	26940	26120	26037	199

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:THR:HB	1:A:68:ARG:NH2	0.62	2.09	3	3
1:A:39:SER:HB3	1:A:55:ILE:O	0.60	1.95	7	1
1:A:159:LEU:O	1:A:163:ILE:HG12	0.59	1.97	5	14
1:A:94:HIS:O	1:A:97:ARG:HG2	0.58	1.99	3	1
1:A:95:HIS:O	1:A:98:GLU:HG2	0.57	1.99	3	7
1:A:68:ARG:O	1:A:72:MET:HG2	0.57	1.99	10	2
1:A:98:GLU:O	1:A:102:ARG:HG3	0.57	1.99	14	7
1:A:80:CYS:SG	1:A:93:ILE:HD12	0.57	2.39	5	2
1:A:5:LYS:HE3	1:A:76:GLU:OE2	0.57	2.00	8	1
1:A:116:ASN:HA	1:A:144:THR:O	0.56	1.99	11	6
1:A:41:ARG:HA	1:A:53:LEU:O	0.56	1.99	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:SER:O	1:A:93:ILE:HG12	0.56	2.01	3	17
1:A:18:ALA:HB2	2:A:201:GNP:O2'	0.55	2.02	11	2
1:A:15:GLY:CA	2:A:201:GNP:H5'2	0.55	2.31	9	4
1:A:73:ARG:NH2	1:A:103:VAL:HG23	0.54	2.17	16	1
1:A:9:VAL:HG11	1:A:80:CYS:SG	0.54	2.41	2	1
1:A:62:GLU:CD	1:A:62:GLU:H	0.54	2.09	16	2
1:A:80:CYS:SG	1:A:113:LEU:HA	0.53	2.44	9	1
1:A:157:TYR:O	1:A:161:ARG:HG3	0.52	2.04	2	2
1:A:69:ASP:OD1	1:A:73:ARG:HD3	0.52	2.05	17	2
1:A:100:ILE:O	1:A:104:LYS:HB2	0.51	2.04	9	2
1:A:28:PHE:CD1	1:A:147:LYS:HA	0.51	2.40	2	2
1:A:32:TYR:CE2	2:A:201:GNP:H3'	0.51	2.41	2	3
1:A:53:LEU:HD12	1:A:53:LEU:O	0.50	2.07	1	4
1:A:161:ARG:O	1:A:164:ARG:HG2	0.49	2.08	6	2
1:A:73:ARG:NE	1:A:73:ARG:HA	0.48	2.23	11	2
1:A:45:VAL:HA	1:A:49:GLU:O	0.48	2.08	12	3
1:A:20:THR:O	1:A:24:ILE:HG22	0.48	2.09	19	3
1:A:22:GLN:NE2	1:A:149:ARG:HG2	0.48	2.23	7	1
1:A:9:VAL:HG13	1:A:96:TYR:CG	0.48	2.43	2	1
1:A:94:HIS:O	1:A:97:ARG:HB3	0.48	2.09	18	1
1:A:12:GLY:HA3	1:A:61:GLN:NE2	0.48	2.24	2	1
1:A:85:ASN:HB3	1:A:122:SER:O	0.47	2.09	8	4
1:A:43:GLN:C	1:A:43:GLN:HE21	0.47	2.17	14	2
1:A:131:GLN:O	1:A:135:ARG:HG3	0.47	2.09	14	2
1:A:107:GLU:CD	1:A:107:GLU:H	0.47	2.17	1	1
1:A:61:GLN:N	1:A:61:GLN:HE21	0.47	2.08	11	1
1:A:90:PHE:CE1	1:A:133:LEU:HD22	0.47	2.45	19	5
1:A:95:HIS:O	1:A:99:GLN:HB3	0.47	2.10	10	1
1:A:131:GLN:O	1:A:135:ARG:HG2	0.46	2.10	1	1
1:A:22:GLN:O	1:A:26:ASN:HA	0.46	2.11	15	1
1:A:16:LYS:HD2	1:A:57:ASP:OD1	0.46	2.11	3	1
1:A:84:ILE:HD13	1:A:118:SER:HA	0.46	1.86	20	1
1:A:28:PHE:CE1	1:A:147:LYS:HA	0.45	2.46	15	4
1:A:12:GLY:H	1:A:61:GLN:NE2	0.45	2.08	8	1
1:A:88:LYS:HA	1:A:88:LYS:HE2	0.45	1.89	12	2
1:A:72:MET:SD	1:A:78:PHE:HE2	0.45	2.35	14	1
1:A:76:GLU:O	1:A:163:ILE:HD12	0.45	2.11	6	2
1:A:113:LEU:O	1:A:141:PHE:HA	0.45	2.11	18	1
1:A:5:LYS:HD3	1:A:5:LYS:N	0.45	2.26	20	1
1:A:61:GLN:H	1:A:61:GLN:CD	0.45	2.19	1	1
1:A:3:GLU:HG3	1:A:41:ARG:NH2	0.45	2.26	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ASP:O	1:A:73:ARG:HG2	0.45	2.12	14	3
1:A:101:LYS:NZ	1:A:107:GLU:HA	0.44	2.26	1	1
1:A:120:LEU:HD21	2:A:201:GNP:N2	0.44	2.27	9	2
1:A:128:LYS:C	1:A:128:LYS:HD3	0.44	2.37	17	1
1:A:81:VAL:HA	1:A:114:VAL:O	0.44	2.13	17	1
1:A:158:THR:O	1:A:162:GLU:HG2	0.44	2.13	5	1
1:A:5:LYS:O	1:A:76:GLU:HB2	0.43	2.13	3	1
1:A:119:ASP:OD1	1:A:147:LYS:HB3	0.43	2.12	4	1
1:A:36:ILE:HD12	1:A:36:ILE:O	0.43	2.14	19	1
1:A:132:ASP:HA	1:A:135:ARG:NE	0.43	2.29	7	1
1:A:16:LYS:HD2	1:A:17:SER:N	0.43	2.29	9	1
1:A:9:VAL:HB	1:A:96:TYR:CE2	0.43	2.49	8	1
1:A:15:GLY:HA2	2:A:201:GNP:H5'2	0.43	1.89	9	1
1:A:60:GLY:HA3	1:A:67:MET:SD	0.43	2.53	4	1
1:A:46:ILE:HG12	1:A:157:TYR:CE2	0.43	2.48	20	1
1:A:38:ASP:CG	1:A:39:SER:H	0.43	2.21	3	1
1:A:41:ARG:HD3	1:A:53:LEU:O	0.43	2.14	8	1
1:A:76:GLU:O	1:A:110:PRO:HG2	0.43	2.14	14	2
1:A:53:LEU:H	1:A:53:LEU:HD23	0.42	1.74	2	1
1:A:150:GLN:CA	1:A:150:GLN:HE21	0.42	2.27	3	2
1:A:150:GLN:HE21	1:A:150:GLN:N	0.42	2.12	3	1
1:A:29:VAL:HG13	2:A:201:GNP:O2'	0.42	2.14	11	1
1:A:132:ASP:O	1:A:135:ARG:HG2	0.42	2.14	15	1
1:A:147:LYS:HE3	2:A:201:GNP:N2	0.42	2.30	4	1
1:A:123:ARG:HD3	1:A:125:VAL:O	0.42	2.14	9	1
1:A:97:ARG:O	1:A:101:LYS:HB2	0.42	2.14	10	1
1:A:97:ARG:HD2	1:A:137:TYR:CE2	0.42	2.49	19	1
1:A:104:LYS:O	1:A:105:ASP:HB3	0.42	2.13	13	3
2:A:201:GNP:O3G	2:A:201:GNP:O1B	0.42	2.38	4	1
1:A:150:GLN:HE21	1:A:150:GLN:HA	0.42	1.74	17	4
1:A:72:MET:O	1:A:104:LYS:HD3	0.42	2.14	8	1
1:A:16:LYS:HE3	1:A:57:ASP:OD1	0.42	2.14	9	1
1:A:7:VAL:HG11	1:A:72:MET:SD	0.42	2.55	2	1
1:A:28:PHE:CZ	1:A:147:LYS:HA	0.41	2.49	19	1
1:A:4:TYR:CE1	1:A:160:VAL:HG13	0.41	2.50	20	1
1:A:58:THR:HG23	1:A:71:TYR:CD1	0.41	2.50	12	1
1:A:78:PHE:O	1:A:111:MET:HA	0.41	2.16	16	1
1:A:149:ARG:HG2	1:A:149:ARG:O	0.41	2.16	1	1
1:A:7:VAL:O	1:A:78:PHE:HA	0.41	2.15	11	1
1:A:77:GLY:HA3	1:A:163:ILE:CD1	0.41	2.46	16	1
1:A:44:VAL:HG23	1:A:51:CYS:SG	0.41	2.56	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:VAL:O	1:A:164:ARG:HD3	0.41	2.16	5	1
1:A:160:VAL:O	1:A:164:ARG:HG2	0.41	2.16	8	1
1:A:161:ARG:O	1:A:164:ARG:HB2	0.40	2.17	1	1
1:A:61:GLN:NE2	1:A:61:GLN:H	0.40	2.14	15	1
1:A:159:LEU:O	1:A:163:ILE:HG13	0.40	2.15	8	1
1:A:107:GLU:H	1:A:107:GLU:CD	0.40	2.24	2	1
1:A:123:ARG:C	1:A:123:ARG:HD2	0.40	2.41	9	1
1:A:22:GLN:OE1	1:A:146:ALA:HA	0.40	2.16	1	1
1:A:84:ILE:CD1	1:A:118:SER:HA	0.40	2.47	5	1
1:A:28:PHE:CZ	1:A:30:ASP:HB2	0.40	2.51	8	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	165/170 (97%)	158±2 (96±1%)	6±2 (4±1%)	1±1 (1±0%)	23	72
All	All	3300/3400 (97%)	3156 (96%)	123 (4%)	21 (1%)	23	72

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	58	THR	15
1	A	13	GLY	2
1	A	34	PRO	1
1	A	36	ILE	1
1	A	12	GLY	1
1	A	65	SER	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	145/149 (97%)	137±2 (95±2%)	8±2 (5±2%)	21	71
All	All	2900/2980 (97%)	2744 (95%)	156 (5%)	21	71

All 50 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	142	ILE	20
1	A	150	GLN	19
1	A	53	LEU	9
1	A	159	LEU	8
1	A	43	GLN	8
1	A	61	GLN	7
1	A	70	GLN	6
1	A	164	ARG	6
1	A	166	HIS	6
1	A	128	LYS	6
1	A	16	LYS	4
1	A	56	LEU	3
1	A	94	HIS	3
1	A	35	SER	3
1	A	73	ARG	3
1	A	6	LEU	3
1	A	58	THR	2
1	A	107	GLU	2
1	A	62	GLU	2
1	A	85	ASN	2
1	A	21	ILE	2
1	A	37	GLU	2
1	A	99	GLN	2
1	A	68	ARG	2
1	A	32	TYR	1
1	A	57	ASP	1
1	A	153	ASP	1
1	A	42	LYS	1
1	A	165	LYS	1
1	A	52	LEU	1
1	A	63	GLU	1
1	A	87	THR	1
1	A	125	VAL	1
1	A	126	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	101	LYS	1
1	A	118	SER	1
1	A	36	ILE	1
1	A	132	ASP	1
1	A	31	GLU	1
1	A	33	ASP	1
1	A	120	LEU	1
1	A	145	SER	1
1	A	51	CYS	1
1	A	76	GLU	1
1	A	92	ASP	1
1	A	123	ARG	1
1	A	104	LYS	1
1	A	148	THR	1
1	A	5	LYS	1
1	A	39	SER	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	GNP	A	201	3	34,34,34	2.16±0.02	5±1 (13±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	GNP	A	201	3	47,54,54	1.95±0.01	13±1 (26±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNP	A	201	3	-	0±0,18,38,38	0±0,3,3,3

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	GNP	PG-O1G	10.11	1.61	1.46	1	20
2	A	201	GNP	PB-O2B	3.56	1.47	1.56	9	20
2	A	201	GNP	PG-O3G	3.29	1.48	1.56	19	20
2	A	201	GNP	C5-N7	3.09	1.32	1.39	18	20
2	A	201	GNP	C8-N9	2.39	1.32	1.37	11	4
2	A	201	GNP	PA-O3A	2.10	1.61	1.59	7	4
2	A	201	GNP	PB-O3A	2.07	1.61	1.59	20	2
2	A	201	GNP	PG-O2G	2.01	1.62	1.56	9	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	201	GNP	C2-N3-C4	5.39	121.58	112.30	10	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	201	GNP	C5-C4-N3	5.01	120.42	128.39	20	20
2	A	201	GNP	O2B-PB-O1B	4.30	119.09	109.87	5	20
2	A	201	GNP	O1G-PG-N3B	4.14	105.67	111.77	20	20
2	A	201	GNP	N9-C4-N3	3.50	132.94	125.95	13	20
2	A	201	GNP	C2-N1-C6	3.46	118.83	125.11	9	20
2	A	201	GNP	O2G-PG-O1G	3.25	105.31	113.45	11	20
2	A	201	GNP	O1B-PB-N3B	2.50	108.09	111.77	1	19
2	A	201	GNP	C3'-C2'-C1'	2.47	96.79	101.46	9	3
2	A	201	GNP	O6-C6-C5	2.31	120.43	126.53	12	20
2	A	201	GNP	C8-N7-C5	2.25	108.27	104.26	20	20
2	A	201	GNP	C5-C6-N1	2.24	118.95	113.25	9	20
2	A	201	GNP	O4'-C1'-N9	2.21	113.37	108.36	11	1
2	A	201	GNP	C4-C5-N7	2.20	107.18	110.67	11	20
2	A	201	GNP	O2G-PG-O3G	2.05	113.11	107.59	11	5
2	A	201	GNP	N9-C8-N7	2.05	109.60	113.40	9	2
2	A	201	GNP	C5'-C4'-C3'	2.02	107.92	115.21	4	2

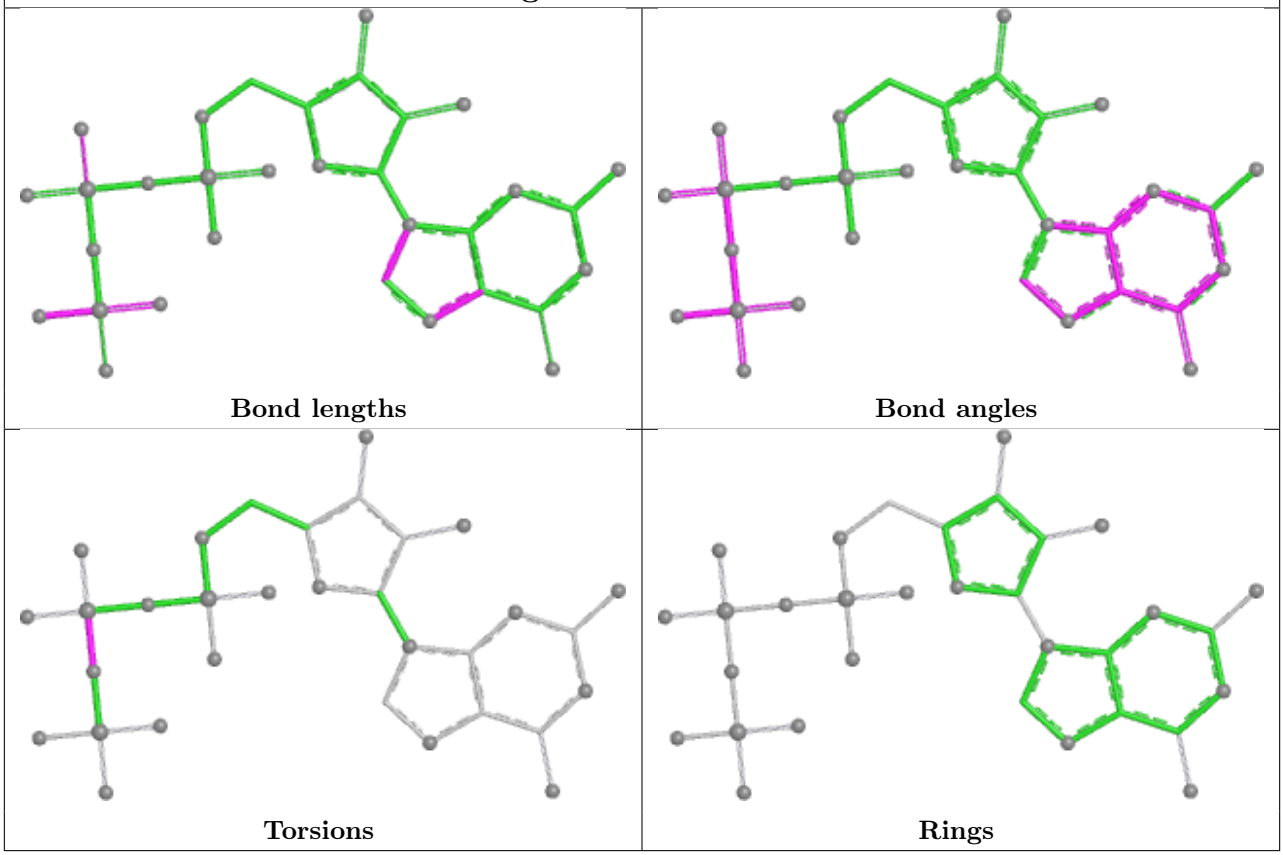
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP A 201



6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 59% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2114
Number of shifts mapped to atoms	2114
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

- Can not parse the chemical shift value. All 743 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HB2	1.891	0.003	.
1	A	1	MET	HB3	1.946	0.005	.
1	A	1	MET	HG2	2.347	0.002	.
1	A	1	MET	HG3	2.389	0.005	.
1	A	3	GLU	HB2	1.861	0.000	.
1	A	3	GLU	HB3	1.777	0.000	.
1	A	3	GLU	HG2	2.012	0.011	.
1	A	3	GLU	HG3	2.187	0.000	.
1	A	4	TYR	HB2	2.646	0.000	.
1	A	4	TYR	HB3	2.646	0.000	.
1	A	4	TYR	HD1	6.889	0.001	.
1	A	4	TYR	HD2	6.889	0.001	.
1	A	4	TYR	HE1	6.634	0.003	.
1	A	4	TYR	HE2	6.634	0.003	.
1	A	4	TYR	CD1	132.967	0.012	.
1	A	4	TYR	CE1	118.118	0.014	.
1	A	5	LYS	HB2	1.784	0.011	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LYS	HB3	1.913	0.013	.
1	A	5	LYS	HD2	1.606	0.007	.
1	A	5	LYS	HD3	1.606	0.000	.
1	A	5	LYS	HE2	2.889	0.002	.
1	A	5	LYS	HE3	2.889	0.000	.
1	A	5	LYS	HG2	1.408	0.000	.
1	A	5	LYS	HG3	1.464	0.000	.
1	A	6	LEU	HB2	1.886	0.013	.
1	A	6	LEU	HB3	1.178	0.000	.
1	A	6	LEU	HD11	0.667	0.001	.
1	A	6	LEU	HD12	0.667	0.001	.
1	A	6	LEU	HD13	0.667	0.001	.
1	A	6	LEU	HD21	0.948	0.002	.
1	A	6	LEU	HD22	0.948	0.002	.
1	A	6	LEU	HD23	0.948	0.002	.
1	A	6	LEU	CD1	24.391	0.028	.
1	A	6	LEU	CD2	26.578	0.063	.
1	A	7	VAL	HG11	0.714	0.000	.
1	A	7	VAL	HG12	0.714	0.000	.
1	A	7	VAL	HG13	0.714	0.000	.
1	A	7	VAL	HG21	0.992	0.000	.
1	A	7	VAL	HG22	0.992	0.000	.
1	A	7	VAL	HG23	0.992	0.000	.
1	A	7	VAL	CG1	22.010	0.000	.
1	A	7	VAL	CG2	22.260	0.000	.
1	A	8	VAL	HG11	0.944	0.001	.
1	A	8	VAL	HG12	0.944	0.001	.
1	A	8	VAL	HG13	0.944	0.001	.
1	A	8	VAL	HG21	0.934	0.000	.
1	A	8	VAL	HG22	0.934	0.000	.
1	A	8	VAL	HG23	0.934	0.000	.
1	A	8	VAL	CG1	20.516	0.029	.
1	A	8	VAL	CG2	22.350	0.000	.
1	A	9	VAL	HG11	0.856	0.014	.
1	A	9	VAL	HG12	0.856	0.014	.
1	A	9	VAL	HG13	0.856	0.014	.
1	A	9	VAL	HG21	1.001	0.000	.
1	A	9	VAL	HG22	1.001	0.000	.
1	A	9	VAL	HG23	1.001	0.000	.
1	A	9	VAL	CG1	20.925	0.080	.
1	A	9	VAL	CG2	22.277	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	GLY	HA2	2.941	0.006	.
1	A	10	GLY	HA3	4.641	0.014	.
1	A	12	GLY	HA2	3.706	0.004	.
1	A	12	GLY	HA3	4.798	0.000	.
1	A	13	GLY	HA2	3.915	0.010	.
1	A	13	GLY	HA3	4.201	0.000	.
1	A	14	VAL	HG11	0.961	0.000	.
1	A	14	VAL	HG12	0.961	0.000	.
1	A	14	VAL	HG13	0.961	0.000	.
1	A	14	VAL	HG21	1.164	0.000	.
1	A	14	VAL	HG22	1.164	0.000	.
1	A	14	VAL	HG23	1.164	0.000	.
1	A	14	VAL	CG1	17.725	0.000	.
1	A	14	VAL	CG2	22.108	0.000	.
1	A	15	GLY	HA2	4.608	0.011	.
1	A	15	GLY	HA3	4.301	0.004	.
1	A	16	LYS	HB2	2.457	0.000	.
1	A	16	LYS	HB3	1.662	0.000	.
1	A	17	SER	HB2	3.705	0.006	.
1	A	17	SER	HB3	3.705	0.006	.
1	A	19	LEU	HB2	1.313	0.003	.
1	A	19	LEU	HB3	2.227	0.005	.
1	A	19	LEU	HD11	0.631	0.006	.
1	A	19	LEU	HD12	0.631	0.006	.
1	A	19	LEU	HD13	0.631	0.006	.
1	A	19	LEU	HD21	0.795	0.000	.
1	A	19	LEU	HD22	0.795	0.000	.
1	A	19	LEU	HD23	0.795	0.000	.
1	A	19	LEU	CD1	26.821	0.064	.
1	A	19	LEU	CD2	24.568	0.000	.
1	A	21	ILE	HG12	1.086	0.005	.
1	A	21	ILE	HG13	1.327	0.000	.
1	A	22	GLN	HB2	2.020	0.000	.
1	A	22	GLN	HB3	2.359	0.004	.
1	A	22	GLN	HE21	6.624	0.042	.
1	A	22	GLN	HE22	7.754	0.001	.
1	A	22	GLN	HG2	2.376	0.000	.
1	A	22	GLN	HG3	2.602	0.000	.
1	A	23	LEU	HB2	0.972	0.006	.
1	A	23	LEU	HB3	1.570	0.004	.
1	A	23	LEU	HD11	-0.230	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	LEU	HD12	-0.230	0.001	.
1	A	23	LEU	HD13	-0.230	0.001	.
1	A	23	LEU	HD21	0.622	0.005	.
1	A	23	LEU	HD22	0.622	0.005	.
1	A	23	LEU	HD23	0.622	0.005	.
1	A	23	LEU	CD1	24.064	0.016	.
1	A	23	LEU	CD2	22.756	0.128	.
1	A	24	ILE	HG12	1.540	0.006	.
1	A	24	ILE	HG13	1.106	0.008	.
1	A	25	GLN	HB2	2.171	0.000	.
1	A	25	GLN	HB3	1.823	0.000	.
1	A	25	GLN	HE21	6.945	0.002	.
1	A	25	GLN	HE22	7.491	0.000	.
1	A	25	GLN	HG2	2.243	0.015	.
1	A	25	GLN	HG3	2.421	0.007	.
1	A	26	ASN	HB2	2.775	0.002	.
1	A	26	ASN	HB3	3.071	0.001	.
1	A	26	ASN	HD21	6.733	0.002	.
1	A	26	ASN	HD22	7.461	0.004	.
1	A	27	HIS	HB2	3.004	0.010	.
1	A	27	HIS	HB3	3.121	0.003	.
1	A	28	PHE	HB2	3.065	0.003	.
1	A	28	PHE	HB3	2.828	0.000	.
1	A	28	PHE	HD1	7.029	0.001	.
1	A	28	PHE	HD2	7.029	0.001	.
1	A	28	PHE	HE1	6.581	0.030	.
1	A	28	PHE	HE2	6.581	0.030	.
1	A	28	PHE	CD2	131.943	0.057	.
1	A	29	VAL	HG11	0.622	0.001	.
1	A	29	VAL	HG12	0.622	0.001	.
1	A	29	VAL	HG13	0.622	0.001	.
1	A	29	VAL	HG21	0.709	0.002	.
1	A	29	VAL	HG22	0.709	0.002	.
1	A	29	VAL	HG23	0.709	0.002	.
1	A	29	VAL	CG1	19.700	0.013	.
1	A	29	VAL	CG2	21.429	0.083	.
1	A	30	ASP	HB2	2.588	0.000	.
1	A	30	ASP	HB3	2.510	0.004	.
1	A	31	GLU	HB2	1.873	0.000	.
1	A	31	GLU	HB3	1.956	0.008	.
1	A	31	GLU	HG2	2.111	0.006	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	GLU	HG3	2.111	0.006	.
1	A	32	TYR	HB2	2.882	0.006	.
1	A	32	TYR	HB3	2.882	0.006	.
1	A	32	TYR	HD1	7.059	0.002	.
1	A	32	TYR	HD2	7.059	0.002	.
1	A	32	TYR	HE1	6.777	0.000	.
1	A	32	TYR	HE2	6.777	0.000	.
1	A	32	TYR	CD1	132.933	0.039	.
1	A	32	TYR	CE1	118.227	0.000	.
1	A	33	ASP	HB2	2.462	0.000	.
1	A	33	ASP	HB3	2.720	0.000	.
1	A	34	PRO	HB2	2.282	0.003	.
1	A	34	PRO	HB3	1.997	0.009	.
1	A	34	PRO	HD2	3.549	0.003	.
1	A	34	PRO	HD3	3.746	0.002	.
1	A	34	PRO	HG2	1.967	0.010	.
1	A	34	PRO	HG3	1.967	0.010	.
1	A	35	SER	HB2	3.855	0.006	.
1	A	35	SER	HB3	3.893	0.002	.
1	A	36	ILE	HG12	1.154	0.001	.
1	A	36	ILE	HG13	1.420	0.009	.
1	A	37	GLU	HB2	1.792	0.006	.
1	A	37	GLU	HB3	1.979	0.008	.
1	A	37	GLU	HG2	2.184	0.000	.
1	A	37	GLU	HG3	1.184	0.000	.
1	A	38	ASP	HB2	2.544	0.005	.
1	A	38	ASP	HB3	2.704	0.003	.
1	A	39	SER	HB2	3.640	0.002	.
1	A	39	SER	HB3	3.640	0.020	.
1	A	40	TYR	HB2	2.712	0.000	.
1	A	40	TYR	HB3	2.910	0.000	.
1	A	40	TYR	HD1	6.995	0.001	.
1	A	40	TYR	HD2	6.995	0.001	.
1	A	40	TYR	HE1	6.760	0.002	.
1	A	40	TYR	HE2	6.760	0.002	.
1	A	40	TYR	CD2	133.242	0.019	.
1	A	40	TYR	CE2	117.917	0.035	.
1	A	41	ARG	HB2	1.678	0.003	.
1	A	41	ARG	HB3	1.678	0.003	.
1	A	41	ARG	HD2	3.082	0.003	.
1	A	41	ARG	HD3	3.121	0.007	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	ARG	HG2	1.564	0.003	.
1	A	41	ARG	HG3	1.541	0.007	.
1	A	42	LYS	HB2	1.474	0.003	.
1	A	42	LYS	HB3	1.679	0.004	.
1	A	42	LYS	HD2	1.397	0.002	.
1	A	42	LYS	HD3	1.731	0.006	.
1	A	42	LYS	HE2	3.057	0.000	.
1	A	42	LYS	HE3	3.057	0.000	.
1	A	42	LYS	HG2	1.255	0.004	.
1	A	42	LYS	HG3	1.471	0.000	.
1	A	43	GLN	HB2	1.942	0.003	.
1	A	43	GLN	HB3	1.942	0.003	.
1	A	43	GLN	HE21	7.260	0.001	.
1	A	43	GLN	HE22	6.783	0.001	.
1	A	43	GLN	HG2	2.123	0.001	.
1	A	43	GLN	HG3	2.231	0.001	.
1	A	44	VAL	HG11	0.706	0.001	.
1	A	44	VAL	HG12	0.706	0.001	.
1	A	44	VAL	HG13	0.706	0.001	.
1	A	44	VAL	HG21	0.849	0.003	.
1	A	44	VAL	HG22	0.849	0.003	.
1	A	44	VAL	HG23	0.849	0.003	.
1	A	44	VAL	CG1	19.966	0.045	.
1	A	44	VAL	CG2	21.677	0.045	.
1	A	45	VAL	HG11	0.636	0.001	.
1	A	45	VAL	HG12	0.636	0.001	.
1	A	45	VAL	HG13	0.636	0.001	.
1	A	45	VAL	HG21	0.880	0.001	.
1	A	45	VAL	HG22	0.880	0.001	.
1	A	45	VAL	HG23	0.880	0.001	.
1	A	45	VAL	CG1	20.866	0.019	.
1	A	45	VAL	CG2	20.964	0.009	.
1	A	46	ILE	HG12	-0.322	0.002	.
1	A	46	ILE	HG13	0.910	0.000	.
1	A	47	ASP	HB2	2.784	0.004	.
1	A	47	ASP	HB3	2.884	0.004	.
1	A	48	GLY	HA2	4.140	0.005	.
1	A	48	GLY	HA3	3.452	0.007	.
1	A	49	GLU	HB2	1.816	0.000	.
1	A	49	GLU	HB3	2.049	0.000	.
1	A	49	GLU	HG2	2.269	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	GLU	HG3	2.098	0.000	.
1	A	51	CYS	HB2	2.840	0.005	.
1	A	51	CYS	HB3	2.903	0.010	.
1	A	52	LEU	HB2	1.461	0.004	.
1	A	52	LEU	HB3	1.554	0.002	.
1	A	52	LEU	HD11	0.782	0.000	.
1	A	52	LEU	HD12	0.782	0.000	.
1	A	52	LEU	HD13	0.782	0.000	.
1	A	52	LEU	CD1	24.588	0.000	.
1	A	53	LEU	HB2	1.930	0.000	.
1	A	53	LEU	HB3	1.172	0.003	.
1	A	53	LEU	HD11	0.774	0.001	.
1	A	53	LEU	HD12	0.774	0.001	.
1	A	53	LEU	HD13	0.774	0.001	.
1	A	53	LEU	HD21	0.783	0.000	.
1	A	53	LEU	HD22	0.783	0.000	.
1	A	53	LEU	HD23	0.783	0.000	.
1	A	53	LEU	CD1	25.418	0.057	.
1	A	53	LEU	CD2	24.190	0.000	.
1	A	54	ASP	HB2	2.438	0.000	.
1	A	54	ASP	HB3	2.789	0.000	.
1	A	55	ILE	HG12	1.034	0.000	.
1	A	55	ILE	HG13	1.314	0.000	.
1	A	56	LEU	HB2	1.369	0.000	.
1	A	56	LEU	HB3	1.369	0.000	.
1	A	56	LEU	HD11	0.526	0.001	.
1	A	56	LEU	HD12	0.526	0.001	.
1	A	56	LEU	HD13	0.526	0.001	.
1	A	56	LEU	HD21	0.604	0.001	.
1	A	56	LEU	HD22	0.604	0.001	.
1	A	56	LEU	HD23	0.604	0.001	.
1	A	56	LEU	CD1	25.009	0.017	.
1	A	56	LEU	CD2	23.924	0.033	.
1	A	57	ASP	HB2	2.889	0.000	.
1	A	57	ASP	HB3	2.553	0.000	.
1	A	60	GLY	HA2	3.825	0.004	.
1	A	60	GLY	HA3	4.326	0.012	.
1	A	61	GLN	HB2	2.088	0.000	.
1	A	61	GLN	HB3	2.229	0.008	.
1	A	61	GLN	HE21	7.631	0.002	.
1	A	61	GLN	HE22	7.062	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	GLN	HG2	2.428	0.001	.
1	A	61	GLN	HG3	2.428	0.001	.
1	A	62	GLU	HB2	2.081	0.002	.
1	A	62	GLU	HB3	2.008	0.000	.
1	A	62	GLU	HG2	2.321	0.000	.
1	A	62	GLU	HG3	2.321	0.000	.
1	A	63	GLU	HB2	1.889	0.003	.
1	A	63	GLU	HB3	1.889	0.003	.
1	A	63	GLU	HG2	2.098	0.000	.
1	A	63	GLU	HG3	2.125	0.000	.
1	A	64	TYR	HB2	2.940	0.006	.
1	A	64	TYR	HB3	3.087	0.002	.
1	A	64	TYR	HD1	7.085	0.001	.
1	A	64	TYR	HD2	7.085	0.001	.
1	A	64	TYR	HE1	6.784	0.000	.
1	A	64	TYR	HE2	6.784	0.000	.
1	A	64	TYR	CD1	133.008	0.057	.
1	A	64	TYR	CE1	118.257	0.000	.
1	A	65	SER	HB2	3.781	0.002	.
1	A	65	SER	HB3	3.968	0.003	.
1	A	67	MET	HB2	1.902	0.003	.
1	A	67	MET	HB3	1.979	0.005	.
1	A	67	MET	HG2	2.436	0.005	.
1	A	67	MET	HG3	2.521	0.002	.
1	A	68	ARG	HB2	1.947	0.009	.
1	A	68	ARG	HB3	1.947	0.009	.
1	A	68	ARG	HD2	3.360	0.007	.
1	A	68	ARG	HD3	3.360	0.007	.
1	A	68	ARG	HG2	1.689	0.000	.
1	A	68	ARG	HG3	1.733	0.010	.
1	A	69	ASP	HB2	2.632	0.002	.
1	A	69	ASP	HB3	2.759	0.009	.
1	A	70	GLN	HB2	2.120	0.008	.
1	A	70	GLN	HB3	2.168	0.006	.
1	A	70	GLN	HE21	6.886	0.001	.
1	A	70	GLN	HE22	7.442	0.002	.
1	A	70	GLN	HG2	2.360	0.006	.
1	A	70	GLN	HG3	2.360	0.006	.
1	A	71	TYR	HB2	2.990	0.005	.
1	A	71	TYR	HB3	3.209	0.006	.
1	A	71	TYR	HD1	7.014	0.002	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	TYR	HD2	7.014	0.002	.
1	A	71	TYR	HE1	6.818	0.002	.
1	A	71	TYR	HE2	6.818	0.002	.
1	A	71	TYR	CD2	132.485	0.073	.
1	A	71	TYR	CE2	118.358	0.017	.
1	A	72	MET	HB2	1.958	0.008	.
1	A	72	MET	HB3	2.365	0.008	.
1	A	72	MET	HG2	2.961	0.001	.
1	A	72	MET	HG3	2.469	0.004	.
1	A	73	ARG	HB2	1.948	0.000	.
1	A	73	ARG	HB3	1.948	0.000	.
1	A	73	ARG	HD2	3.201	0.008	.
1	A	73	ARG	HD3	3.284	0.000	.
1	A	73	ARG	HG2	1.682	0.000	.
1	A	73	ARG	HG3	1.794	0.010	.
1	A	75	GLY	HA2	3.510	0.005	.
1	A	75	GLY	HA3	3.223	0.005	.
1	A	76	GLU	HB2	2.154	0.000	.
1	A	76	GLU	HB3	2.374	0.012	.
1	A	76	GLU	HG2	2.396	0.001	.
1	A	76	GLU	HG3	2.482	0.007	.
1	A	77	GLY	HA2	4.914	0.018	.
1	A	77	GLY	HA3	3.155	0.004	.
1	A	78	PHE	HB2	2.746	0.000	.
1	A	78	PHE	HB3	2.746	0.000	.
1	A	78	PHE	HD1	7.085	0.003	.
1	A	78	PHE	HD2	7.085	0.003	.
1	A	78	PHE	HE1	7.066	0.001	.
1	A	78	PHE	HE2	7.066	0.001	.
1	A	78	PHE	CD2	132.699	0.074	.
1	A	78	PHE	CE2	130.582	0.045	.
1	A	79	LEU	HB2	1.184	0.000	.
1	A	79	LEU	HB3	1.623	0.004	.
1	A	79	LEU	HD11	0.113	0.001	.
1	A	79	LEU	HD12	0.113	0.001	.
1	A	79	LEU	HD13	0.113	0.001	.
1	A	79	LEU	HD21	0.161	0.001	.
1	A	79	LEU	HD22	0.161	0.001	.
1	A	79	LEU	HD23	0.161	0.001	.
1	A	79	LEU	CD1	25.027	0.029	.
1	A	79	LEU	CD2	25.609	0.012	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	CYS	HB2	2.665	0.001	.
1	A	80	CYS	HB3	2.957	0.002	.
1	A	81	VAL	HG11	0.556	0.000	.
1	A	81	VAL	HG12	0.556	0.000	.
1	A	81	VAL	HG13	0.556	0.000	.
1	A	81	VAL	HG21	0.663	0.010	.
1	A	81	VAL	HG22	0.663	0.010	.
1	A	81	VAL	HG23	0.663	0.010	.
1	A	81	VAL	CG1	22.779	0.000	.
1	A	81	VAL	CG2	22.090	0.010	.
1	A	82	PHE	HB2	2.932	0.000	.
1	A	82	PHE	HB3	3.683	0.000	.
1	A	84	ILE	HG12	1.267	0.000	.
1	A	84	ILE	HG13	1.028	0.000	.
1	A	85	ASN	HB2	3.308	0.000	.
1	A	85	ASN	HB3	2.394	0.000	.
1	A	85	ASN	HD21	6.848	0.001	.
1	A	85	ASN	HD22	7.773	0.000	.
1	A	86	ASN	HB2	2.488	0.000	.
1	A	86	ASN	HB3	3.201	0.000	.
1	A	86	ASN	HD21	7.187	0.000	.
1	A	86	ASN	HD22	8.059	0.000	.
1	A	88	LYS	HB2	1.958	0.000	.
1	A	88	LYS	HB3	2.054	0.000	.
1	A	88	LYS	HD2	1.821	0.000	.
1	A	88	LYS	HD3	1.691	0.000	.
1	A	88	LYS	HE2	3.076	0.000	.
1	A	88	LYS	HE3	3.076	0.000	.
1	A	88	LYS	HG2	1.545	0.000	.
1	A	88	LYS	HG3	1.545	0.000	.
1	A	89	SER	HB2	4.064	0.000	.
1	A	89	SER	HB3	4.495	0.000	.
1	A	90	PHE	HB2	2.720	0.000	.
1	A	90	PHE	HB3	3.263	0.000	.
1	A	90	PHE	HD1	6.000	0.001	.
1	A	90	PHE	HD2	6.000	0.001	.
1	A	90	PHE	HE1	6.779	0.000	.
1	A	90	PHE	HE2	6.779	0.000	.
1	A	90	PHE	CD1	131.544	0.020	.
1	A	90	PHE	CE1	130.381	0.000	.
1	A	91	GLU	HB2	2.120	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	GLU	HB3	2.248	0.000	.
1	A	91	GLU	HG2	2.546	0.000	.
1	A	91	GLU	HG3	2.325	0.000	.
1	A	92	ASP	HB2	2.899	0.000	.
1	A	92	ASP	HB3	2.899	0.000	.
1	A	93	ILE	HG12	2.231	0.000	.
1	A	93	ILE	HG13	1.392	0.000	.
1	A	94	HIS	HB2	3.132	0.003	.
1	A	94	HIS	HB3	3.255	0.007	.
1	A	95	HIS	HB2	3.034	0.004	.
1	A	95	HIS	HB3	3.034	0.004	.
1	A	96	TYR	HB2	2.882	0.000	.
1	A	96	TYR	HB3	2.882	0.000	.
1	A	96	TYR	HD1	7.078	0.000	.
1	A	96	TYR	HD2	7.078	0.000	.
1	A	96	TYR	HE1	6.887	0.001	.
1	A	96	TYR	HE2	6.887	0.001	.
1	A	96	TYR	CD1	132.479	0.000	.
1	A	96	TYR	CE1	118.581	0.018	.
1	A	97	ARG	HB2	1.381	0.000	.
1	A	97	ARG	HB3	1.774	0.000	.
1	A	97	ARG	HD2	2.024	0.000	.
1	A	97	ARG	HD3	2.231	0.000	.
1	A	97	ARG	HG2	1.095	0.000	.
1	A	97	ARG	HG3	1.145	0.000	.
1	A	98	GLU	HB2	2.012	0.000	.
1	A	98	GLU	HB3	2.012	0.000	.
1	A	98	GLU	HG2	2.246	0.000	.
1	A	98	GLU	HG3	2.205	0.000	.
1	A	99	GLN	HB2	2.005	0.000	.
1	A	99	GLN	HB3	2.005	0.000	.
1	A	99	GLN	HE21	7.223	0.001	.
1	A	99	GLN	HE22	6.673	0.000	.
1	A	99	GLN	HG2	2.168	0.000	.
1	A	99	GLN	HG3	2.278	0.000	.
1	A	100	ILE	HG12	-0.110	0.004	.
1	A	100	ILE	HG13	1.571	0.000	.
1	A	101	LYS	HB2	1.685	0.000	.
1	A	101	LYS	HB3	1.773	0.000	.
1	A	101	LYS	HD2	1.525	0.000	.
1	A	101	LYS	HD3	1.549	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	LYS	HE2	2.831	0.000	.
1	A	101	LYS	HE3	2.831	0.000	.
1	A	101	LYS	HG2	1.346	0.000	.
1	A	101	LYS	HG3	1.346	0.000	.
1	A	102	ARG	HB2	1.937	0.000	.
1	A	102	ARG	HB3	1.877	0.000	.
1	A	102	ARG	HD2	3.175	0.000	.
1	A	102	ARG	HD3	3.241	0.000	.
1	A	102	ARG	HG2	1.545	0.000	.
1	A	102	ARG	HG3	1.663	0.000	.
1	A	103	VAL	HG11	1.040	0.000	.
1	A	103	VAL	HG12	1.040	0.000	.
1	A	103	VAL	HG13	1.040	0.000	.
1	A	103	VAL	HG21	0.940	0.000	.
1	A	103	VAL	HG22	0.940	0.000	.
1	A	103	VAL	HG23	0.940	0.000	.
1	A	103	VAL	CG1	22.349	0.000	.
1	A	103	VAL	CG2	21.641	0.000	.
1	A	104	LYS	HB2	1.861	0.000	.
1	A	104	LYS	HB3	1.861	0.000	.
1	A	104	LYS	HD2	1.917	0.000	.
1	A	104	LYS	HD3	1.835	0.000	.
1	A	104	LYS	HE2	3.220	0.000	.
1	A	104	LYS	HE3	3.265	0.000	.
1	A	104	LYS	HG2	1.589	0.000	.
1	A	104	LYS	HG3	1.422	0.000	.
1	A	105	ASP	HB2	3.113	0.000	.
1	A	105	ASP	HB3	2.360	0.000	.
1	A	106	SER	HB2	3.233	0.005	.
1	A	106	SER	HB3	3.802	0.002	.
1	A	107	GLU	HB2	1.886	0.000	.
1	A	107	GLU	HB3	2.169	0.000	.
1	A	107	GLU	HG2	2.208	0.000	.
1	A	107	GLU	HG3	2.325	0.000	.
1	A	108	ASP	HB2	2.537	0.000	.
1	A	108	ASP	HB3	2.760	0.000	.
1	A	109	VAL	HG11	0.743	0.000	.
1	A	109	VAL	HG12	0.743	0.000	.
1	A	109	VAL	HG13	0.743	0.000	.
1	A	109	VAL	HG21	0.956	0.000	.
1	A	109	VAL	HG22	0.956	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	VAL	HG23	0.956	0.000	.
1	A	109	VAL	CG1	21.599	0.000	.
1	A	109	VAL	CG2	21.202	0.000	.
1	A	110	PRO	HB2	1.826	0.000	.
1	A	110	PRO	HB3	2.125	0.000	.
1	A	110	PRO	HD2	3.572	0.002	.
1	A	110	PRO	HD3	3.781	0.004	.
1	A	110	PRO	HG2	2.228	0.000	.
1	A	110	PRO	HG3	1.506	0.000	.
1	A	111	MET	HB2	2.099	0.003	.
1	A	111	MET	HB3	2.119	0.000	.
1	A	111	MET	HG2	2.607	0.006	.
1	A	111	MET	HG3	2.695	0.015	.
1	A	112	VAL	HG11	0.748	0.000	.
1	A	112	VAL	HG12	0.748	0.000	.
1	A	112	VAL	HG13	0.748	0.000	.
1	A	112	VAL	HG21	0.783	0.000	.
1	A	112	VAL	HG22	0.783	0.000	.
1	A	112	VAL	HG23	0.783	0.000	.
1	A	112	VAL	CG1	21.177	0.000	.
1	A	112	VAL	CG2	22.706	0.000	.
1	A	113	LEU	HB2	2.491	0.000	.
1	A	113	LEU	HB3	1.476	0.000	.
1	A	113	LEU	HD11	1.339	0.000	.
1	A	113	LEU	HD12	1.339	0.000	.
1	A	113	LEU	HD13	1.339	0.000	.
1	A	113	LEU	HD21	1.068	0.000	.
1	A	113	LEU	HD22	1.068	0.000	.
1	A	113	LEU	HD23	1.068	0.000	.
1	A	113	LEU	CD1	25.402	0.000	.
1	A	113	LEU	CD2	27.262	0.000	.
1	A	114	VAL	HG11	0.609	0.000	.
1	A	114	VAL	HG12	0.609	0.000	.
1	A	114	VAL	HG13	0.609	0.000	.
1	A	114	VAL	HG21	0.699	0.000	.
1	A	114	VAL	HG22	0.699	0.000	.
1	A	114	VAL	HG23	0.699	0.000	.
1	A	114	VAL	CG1	23.073	0.000	.
1	A	114	VAL	CG2	23.404	0.000	.
1	A	115	GLY	HA2	2.414	0.003	.
1	A	115	GLY	HA3	2.899	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	ASN	HB2	2.182	0.000	.
1	A	116	ASN	HB3	2.543	0.000	.
1	A	116	ASN	HD21	8.842	0.002	.
1	A	116	ASN	HD22	7.454	0.001	.
1	A	117	LYS	HB2	1.647	0.000	.
1	A	117	LYS	HB3	2.395	0.000	.
1	A	118	SER	HB2	3.653	0.000	.
1	A	118	SER	HB3	3.881	0.000	.
1	A	119	ASP	HB2	2.592	0.000	.
1	A	119	ASP	HB3	2.592	0.000	.
1	A	120	LEU	HB2	1.948	0.000	.
1	A	120	LEU	HB3	1.431	0.000	.
1	A	120	LEU	HD11	0.892	0.000	.
1	A	120	LEU	HD12	0.892	0.000	.
1	A	120	LEU	HD13	0.892	0.000	.
1	A	120	LEU	HD21	0.923	0.000	.
1	A	120	LEU	HD22	0.923	0.000	.
1	A	120	LEU	HD23	0.923	0.000	.
1	A	120	LEU	CD1	27.211	0.000	.
1	A	120	LEU	CD2	22.390	0.000	.
1	A	121	PRO	HB2	2.115	0.000	.
1	A	121	PRO	HB3	2.264	0.000	.
1	A	121	PRO	HD2	3.833	0.002	.
1	A	121	PRO	HD3	3.894	0.010	.
1	A	121	PRO	HG2	2.129	0.000	.
1	A	121	PRO	HG3	1.985	0.000	.
1	A	122	SER	HB2	3.806	0.000	.
1	A	122	SER	HB3	3.988	0.000	.
1	A	123	ARG	HB2	1.659	0.000	.
1	A	123	ARG	HB3	1.890	0.000	.
1	A	123	ARG	HD2	3.120	0.000	.
1	A	123	ARG	HD3	3.468	0.000	.
1	A	123	ARG	HG2	1.468	0.000	.
1	A	123	ARG	HG3	1.435	0.000	.
1	A	125	VAL	HG11	-0.125	0.001	.
1	A	125	VAL	HG12	-0.125	0.001	.
1	A	125	VAL	HG13	-0.125	0.001	.
1	A	125	VAL	HG21	0.703	0.000	.
1	A	125	VAL	HG22	0.703	0.000	.
1	A	125	VAL	HG23	0.703	0.000	.
1	A	125	VAL	CG1	19.346	0.013	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	VAL	CG2	20.295	0.000	.
1	A	126	ASP	HB2	2.664	0.000	.
1	A	126	ASP	HB3	2.664	0.000	.
1	A	128	LYS	HB2	1.805	0.000	.
1	A	128	LYS	HB3	1.805	0.000	.
1	A	128	LYS	HD2	1.620	0.000	.
1	A	128	LYS	HD3	1.708	0.000	.
1	A	128	LYS	HE2	3.006	0.000	.
1	A	128	LYS	HE3	3.006	0.000	.
1	A	128	LYS	HG2	1.396	0.000	.
1	A	128	LYS	HG3	1.434	0.000	.
1	A	129	GLN	HB2	1.918	0.000	.
1	A	129	GLN	HB3	2.034	0.000	.
1	A	129	GLN	HE21	6.911	0.001	.
1	A	129	GLN	HE22	7.574	0.001	.
1	A	129	GLN	HG2	2.293	0.000	.
1	A	129	GLN	HG3	2.368	0.000	.
1	A	131	GLN	HB2	2.233	0.000	.
1	A	131	GLN	HB3	2.018	0.000	.
1	A	131	GLN	HE21	7.552	0.002	.
1	A	131	GLN	HE22	6.960	0.001	.
1	A	131	GLN	HG2	2.518	0.000	.
1	A	131	GLN	HG3	2.518	0.000	.
1	A	132	ASP	HB2	2.562	0.000	.
1	A	132	ASP	HB3	2.751	0.000	.
1	A	133	LEU	HB2	1.753	0.000	.
1	A	133	LEU	HB3	1.449	0.000	.
1	A	133	LEU	HD11	0.424	0.001	.
1	A	133	LEU	HD12	0.424	0.001	.
1	A	133	LEU	HD13	0.424	0.001	.
1	A	133	LEU	HD21	0.463	0.000	.
1	A	133	LEU	HD22	0.463	0.000	.
1	A	133	LEU	HD23	0.463	0.000	.
1	A	133	LEU	CD1	26.185	0.024	.
1	A	133	LEU	CD2	22.873	0.000	.
1	A	135	ARG	HB2	1.957	0.000	.
1	A	135	ARG	HB3	2.016	0.000	.
1	A	135	ARG	HD2	3.271	0.000	.
1	A	135	ARG	HD3	3.271	0.000	.
1	A	135	ARG	HG2	1.660	0.000	.
1	A	135	ARG	HG3	1.803	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	SER	HB2	3.925	0.000	.
1	A	136	SER	HB3	3.925	0.000	.
1	A	137	TYR	HB2	3.076	0.000	.
1	A	137	TYR	HB3	3.269	0.000	.
1	A	137	TYR	HD1	6.801	0.000	.
1	A	137	TYR	HD2	6.801	0.000	.
1	A	137	TYR	HE1	6.593	0.002	.
1	A	137	TYR	HE2	6.593	0.002	.
1	A	137	TYR	CD1	130.255	0.000	.
1	A	137	TYR	CE1	118.153	0.019	.
1	A	138	GLY	HA2	4.175	0.013	.
1	A	138	GLY	HA3	4.014	0.004	.
1	A	139	ILE	HG12	1.413	0.000	.
1	A	139	ILE	HG13	1.691	0.000	.
1	A	140	PRO	HB2	2.533	0.000	.
1	A	140	PRO	HB3	1.669	0.000	.
1	A	140	PRO	HD2	3.974	0.003	.
1	A	140	PRO	HD3	4.068	0.004	.
1	A	140	PRO	HG2	1.957	0.000	.
1	A	140	PRO	HG3	1.783	0.000	.
1	A	141	PHE	HB2	2.788	0.000	.
1	A	141	PHE	HB3	3.099	0.000	.
1	A	141	PHE	HD1	7.168	0.001	.
1	A	141	PHE	HD2	7.168	0.001	.
1	A	141	PHE	HE1	7.287	0.003	.
1	A	141	PHE	HE2	7.287	0.003	.
1	A	141	PHE	CD1	131.842	0.021	.
1	A	141	PHE	CE1	131.193	0.075	.
1	A	142	ILE	HG12	1.024	0.000	.
1	A	142	ILE	HG13	1.253	0.000	.
1	A	143	GLU	HB2	1.744	0.000	.
1	A	143	GLU	HB3	1.873	0.000	.
1	A	143	GLU	HG2	2.123	0.000	.
1	A	143	GLU	HG3	2.280	0.000	.
1	A	145	SER	HB2	3.995	0.000	.
1	A	145	SER	HB3	3.995	0.000	.
1	A	147	LYS	HB2	0.391	0.007	.
1	A	147	LYS	HB3	1.071	0.011	.
1	A	147	LYS	HD2	1.210	0.000	.
1	A	147	LYS	HD3	1.338	0.000	.
1	A	147	LYS	HE2	2.733	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	LYS	HE3	2.785	0.000	.
1	A	147	LYS	HG2	0.434	0.000	.
1	A	147	LYS	HG3	0.676	0.000	.
1	A	149	ARG	HB2	1.671	0.000	.
1	A	149	ARG	HB3	2.218	0.000	.
1	A	149	ARG	HD2	3.118	0.000	.
1	A	149	ARG	HD3	3.118	0.000	.
1	A	149	ARG	HG2	1.166	0.005	.
1	A	149	ARG	HG3	1.935	0.000	.
1	A	150	GLN	HB2	1.929	0.000	.
1	A	150	GLN	HB3	1.752	0.000	.
1	A	150	GLN	HE21	7.342	0.002	.
1	A	150	GLN	HE22	6.927	0.001	.
1	A	150	GLN	HG2	2.192	0.000	.
1	A	150	GLN	HG3	2.306	0.000	.
1	A	151	GLY	HA2	3.804	0.009	.
1	A	151	GLY	HA3	4.058	0.007	.
1	A	152	VAL	HG11	0.929	0.000	.
1	A	152	VAL	HG12	0.929	0.000	.
1	A	152	VAL	HG13	0.929	0.000	.
1	A	152	VAL	HG21	0.766	0.000	.
1	A	152	VAL	HG22	0.766	0.000	.
1	A	152	VAL	HG23	0.766	0.000	.
1	A	152	VAL	CG1	20.933	0.000	.
1	A	152	VAL	CG2	24.145	0.000	.
1	A	153	ASP	HB2	1.846	0.000	.
1	A	153	ASP	HB3	2.204	0.000	.
1	A	154	ASP	HB2	2.428	0.000	.
1	A	154	ASP	HB3	2.481	0.000	.
1	A	156	PHE	HB2	2.652	0.000	.
1	A	156	PHE	HB3	2.845	0.000	.
1	A	156	PHE	HD1	7.377	0.003	.
1	A	156	PHE	HD2	7.377	0.003	.
1	A	156	PHE	HE1	6.931	0.000	.
1	A	156	PHE	HE2	6.931	0.000	.
1	A	156	PHE	CD2	132.363	0.048	.
1	A	156	PHE	CE2	131.174	0.000	.
1	A	157	TYR	HB2	2.931	0.000	.
1	A	157	TYR	HB3	3.286	0.000	.
1	A	157	TYR	HD1	6.910	0.000	.
1	A	157	TYR	HD2	6.910	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	157	TYR	HE1	6.676	0.001	.
1	A	157	TYR	HE2	6.676	0.001	.
1	A	157	TYR	CD1	131.155	0.000	.
1	A	157	TYR	CE1	117.546	0.036	.
1	A	159	LEU	HB2	1.241	0.000	.
1	A	159	LEU	HB3	2.131	0.000	.
1	A	159	LEU	HD11	0.691	0.000	.
1	A	159	LEU	HD12	0.691	0.000	.
1	A	159	LEU	HD13	0.691	0.000	.
1	A	159	LEU	HD21	0.826	0.000	.
1	A	159	LEU	HD22	0.826	0.000	.
1	A	159	LEU	HD23	0.826	0.000	.
1	A	159	LEU	CD1	27.425	0.000	.
1	A	159	LEU	CD2	21.665	0.000	.
1	A	160	VAL	HG11	0.078	0.001	.
1	A	160	VAL	HG12	0.078	0.001	.
1	A	160	VAL	HG13	0.078	0.001	.
1	A	160	VAL	HG21	0.704	0.000	.
1	A	160	VAL	HG22	0.704	0.000	.
1	A	160	VAL	HG23	0.704	0.000	.
1	A	160	VAL	CG1	19.849	0.006	.
1	A	160	VAL	CG2	23.950	0.000	.
1	A	161	ARG	HB2	1.869	0.000	.
1	A	161	ARG	HB3	2.069	0.000	.
1	A	161	ARG	HD2	3.142	0.000	.
1	A	161	ARG	HD3	3.142	0.000	.
1	A	161	ARG	HG2	1.551	0.000	.
1	A	161	ARG	HG3	1.793	0.000	.
1	A	162	GLU	HB2	2.428	0.000	.
1	A	162	GLU	HB3	2.242	0.000	.
1	A	162	GLU	HG2	2.160	0.000	.
1	A	162	GLU	HG3	2.506	0.000	.
1	A	163	ILE	HG12	0.851	0.000	.
1	A	163	ILE	HG13	1.825	0.000	.
1	A	164	ARG	HB2	1.991	0.000	.
1	A	164	ARG	HB3	1.936	0.000	.
1	A	164	ARG	HD2	3.116	0.000	.
1	A	164	ARG	HD3	3.051	0.000	.
1	A	164	ARG	HG2	1.845	0.000	.
1	A	164	ARG	HG3	1.845	0.000	.
1	A	165	LYS	HB2	1.897	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	165	LYS	HB3	1.931	0.000	.
1	A	165	LYS	HD2	1.708	0.000	.
1	A	165	LYS	HD3	1.708	0.000	.
1	A	165	LYS	HE2	2.923	0.000	.
1	A	165	LYS	HE3	2.923	0.000	.
1	A	165	LYS	HG2	1.590	0.000	.
1	A	165	LYS	HG3	1.590	0.000	.
1	A	166	HIS	HB2	3.617	0.005	.
1	A	166	HIS	HB3	3.313	0.007	.
1	A	167	LYS	HB2	1.956	0.000	.
1	A	167	LYS	HB3	2.002	0.000	.
1	A	167	LYS	HD2	1.782	0.000	.
1	A	167	LYS	HD3	1.749	0.000	.
1	A	167	LYS	HE2	2.999	0.000	.
1	A	167	LYS	HE3	2.999	0.000	.
1	A	167	LYS	HG2	1.736	0.000	.
1	A	167	LYS	HG3	1.568	0.000	.
1	A	168	GLU	HB2	2.020	0.000	.
1	A	168	GLU	HB3	2.154	0.000	.
1	A	168	GLU	HG2	2.436	0.000	.
1	A	168	GLU	HG3	2.333	0.000	.
1	A	169	LYS	HB2	1.762	0.000	.
1	A	169	LYS	HB3	1.846	0.000	.
1	A	169	LYS	HD2	1.446	0.000	.
1	A	169	LYS	HD3	1.691	0.000	.
1	A	169	LYS	HE2	3.004	0.000	.
1	A	169	LYS	HE3	3.004	0.000	.
1	A	169	LYS	HG2	1.445	0.000	.
1	A	169	LYS	HG3	1.445	0.000	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	169	-0.30 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	158	0.32 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	169	0.09 ± 0.19	None needed (< 0.5 ppm)
^{15}N	165	0.03 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 59%, i.e. 1335 atoms were assigned a chemical shift out of a possible 2258. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	806/828 (97%)	315/337 (93%)	330/330 (100%)	161/161 (100%)
Sidechain	504/1266 (40%)	193/817 (24%)	288/396 (73%)	23/53 (43%)
Aromatic	25/164 (15%)	13/78 (17%)	12/78 (15%)	0/8 (0%)
Overall	1335/2258 (59%)	521/1232 (42%)	630/804 (78%)	184/222 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 1371 atoms were assigned a chemical shift out of a possible 2321. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	826/848 (97%)	323/345 (94%)	338/338 (100%)	165/165 (100%)
Sidechain	520/1309 (40%)	196/844 (23%)	301/410 (73%)	23/55 (42%)
Aromatic	25/164 (15%)	13/78 (17%)	12/78 (15%)	0/8 (0%)
Overall	1371/2321 (59%)	532/1267 (42%)	651/826 (79%)	188/228 (82%)

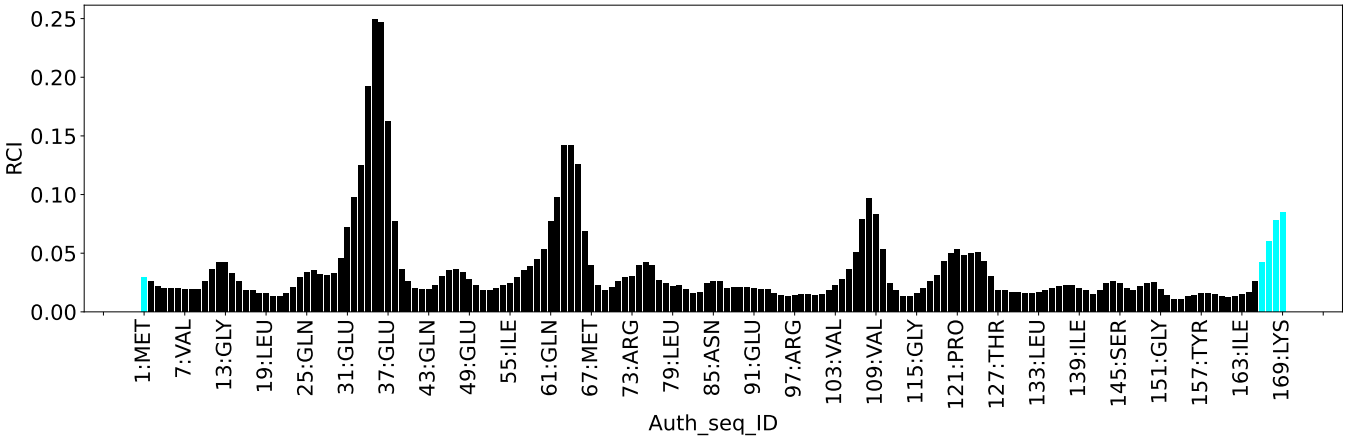
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
7:VAL
13:GLY
19:LEU
25:GLN
31:GLU
37:GLU
43:GLN
49:GLU
55:ILE
61:GLN
67:MET
73:ARG
79:LEU
85:ASN
91:GLU
97:ARG
103:VAL
109:VAL
115:GLY
121:PRO
127:THR
133:LEU
139:ILE
145:SER
151:GLY
157:TYR
163:ILE
169:LYS
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	3341
Intra-residue (|i-j|=0)	795
Sequential (|i-j|=1)	859
Medium range (|i-j|>1 and |i-j|<5)	583
Long range (|i-j|≥5)	1063
Inter-chain	35
Hydrogen bond restraints	3
Disulfide bond restraints	0
Total dihedral-angle restraints	268
Number of unmapped restraints	0
Number of restraints per residue	21.0
Number of long range restraints per residue[1]	6.2

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	71.2	0.2
0.2-0.5 (Medium)	165.8	0.5
>0.5 (Large)	24.8	0.57

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

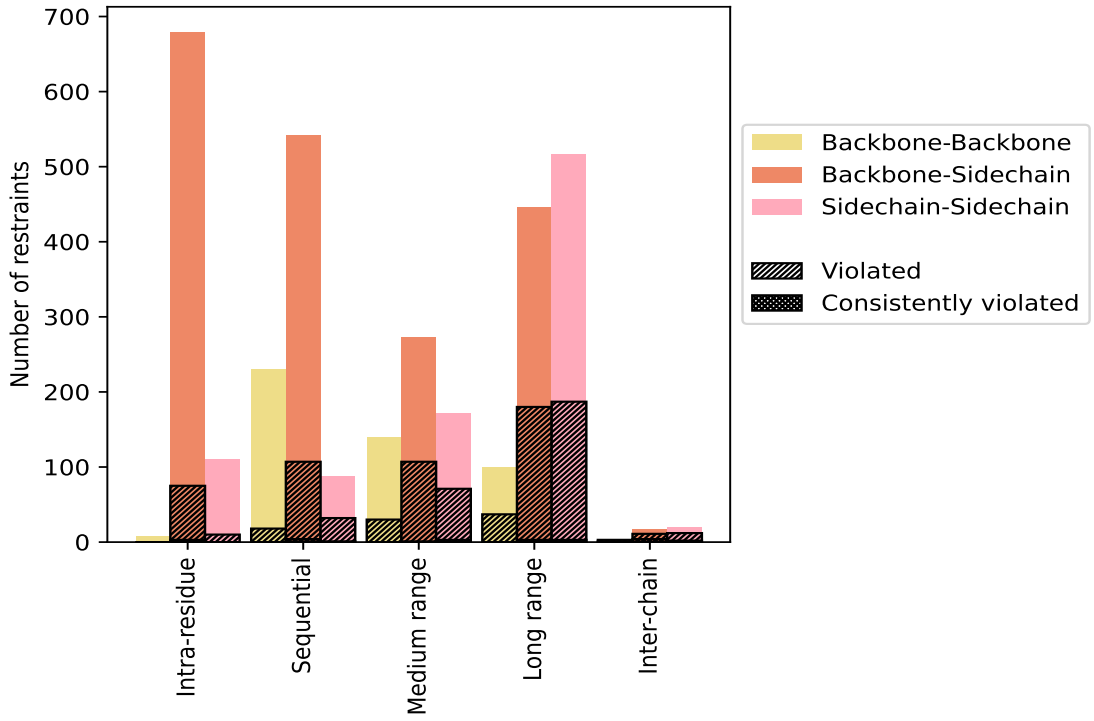
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	795	23.8	85	10.7	2.5	3	0.4	0.1
Backbone-Backbone	7	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	679	20.3	75	11.0	2.2	3	0.4	0.1
Sidechain-Sidechain	109	3.3	10	9.2	0.3	0	0.0	0.0
Sequential (|i-j|=1)	859	25.7	157	18.3	4.7	5	0.6	0.1
Backbone-Backbone	230	6.9	18	7.8	0.5	0	0.0	0.0
Backbone-Sidechain	542	16.2	107	19.7	3.2	4	0.7	0.1
Sidechain-Sidechain	87	2.6	32	36.8	1.0	1	1.1	0.0
Medium range (|i-j|>1 & |i-j|<5)	583	17.4	208	35.7	6.2	4	0.7	0.1
Backbone-Backbone	139	4.2	30	21.6	0.9	0	0.0	0.0
Backbone-Sidechain	273	8.2	107	39.2	3.2	1	0.4	0.0
Sidechain-Sidechain	171	5.1	71	41.5	2.1	3	1.8	0.1
Long range (|i-j|≥5)	1063	31.8	404	38.0	12.1	6	0.6	0.2
Backbone-Backbone	100	3.0	37	37.0	1.1	0	0.0	0.0
Backbone-Sidechain	446	13.3	180	40.4	5.4	3	0.7	0.1
Sidechain-Sidechain	517	15.5	187	36.2	5.6	3	0.6	0.1
Inter-chain	35	1.0	24	68.6	0.7	7	20.0	0.2
Backbone-Backbone	4	0.1	3	75.0	0.1	1	25.0	0.0
Backbone-Sidechain	17	0.5	11	64.7	0.3	4	23.5	0.1
Sidechain-Sidechain	14	0.4	10	71.4	0.3	2	14.3	0.1
Hydrogen bond	3	0.1	1	33.3	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3341	100.0	880	26.3	26.3	25	0.7	0.7
Backbone-Backbone	480	14.4	88	18.3	2.6	1	0.2	0.0
Backbone-Sidechain	1957	58.6	480	24.5	14.4	15	0.8	0.4
Sidechain-Sidechain	904	27.1	312	34.5	9.3	9	1.0	0.3

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å
are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	21	45	59	105	19	249	0.34	0.57	0.13	0.36
2	19	52	61	114	19	265	0.31	0.57	0.14	0.31
3	25	51	72	128	19	295	0.31	0.56	0.14	0.31
4	13	56	68	106	19	262	0.31	0.56	0.14	0.3
5	18	44	67	112	18	259	0.31	0.57	0.13	0.32
6	17	47	72	116	19	271	0.31	0.56	0.14	0.32
7	19	44	61	114	18	256	0.32	0.56	0.14	0.32
8	21	43	61	117	19	261	0.33	0.56	0.13	0.34
9	19	49	64	110	21	263	0.31	0.56	0.13	0.3
10	26	52	61	118	19	276	0.31	0.57	0.14	0.31

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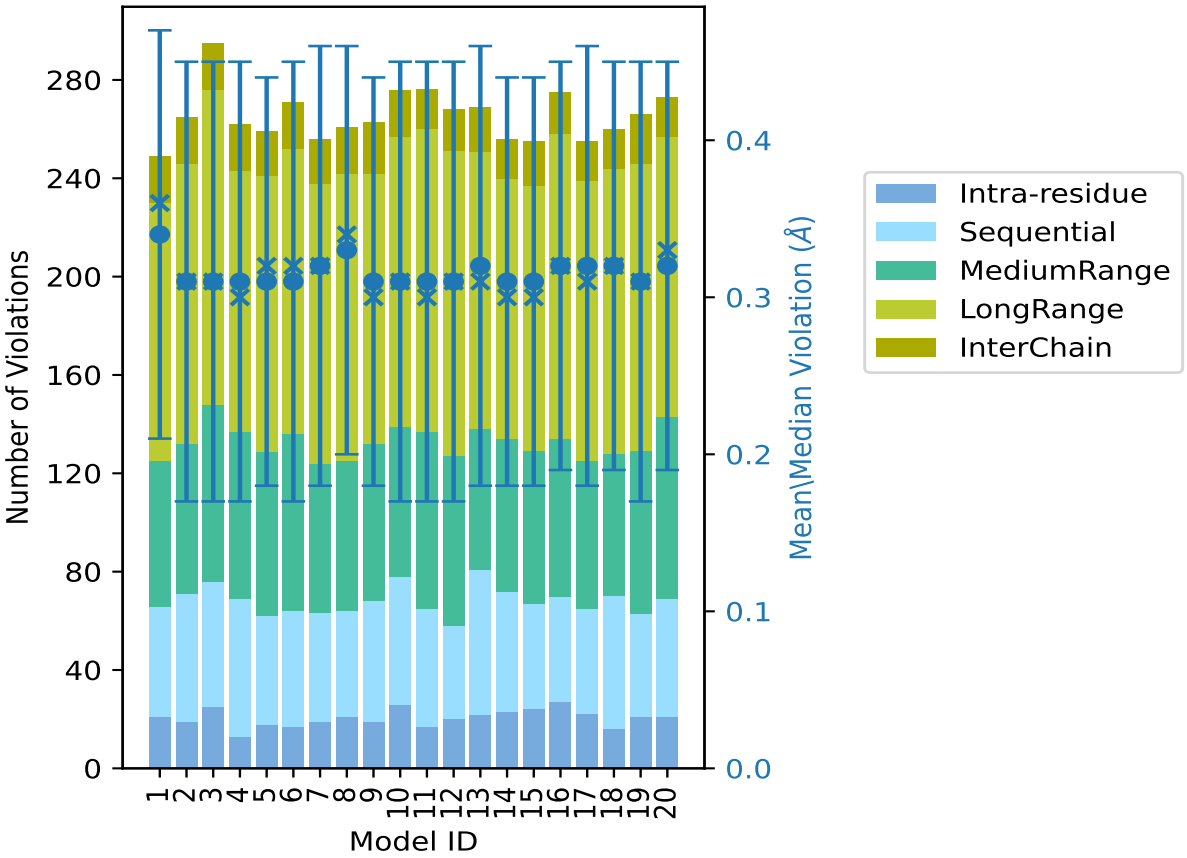
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	17	48	72	123	16	276	0.31	0.56	0.14	0.3
12	20	38	69	124	17	268	0.31	0.56	0.14	0.31
13	22	59	57	113	18	269	0.32	0.56	0.14	0.31
14	23	49	62	106	16	256	0.31	0.57	0.13	0.3
15	24	43	62	108	18	255	0.31	0.57	0.13	0.3
16	27	43	64	124	17	275	0.32	0.56	0.13	0.32
17	22	43	60	114	16	255	0.32	0.57	0.14	0.31
18	16	54	58	116	16	260	0.32	0.56	0.13	0.32
19	21	42	66	117	20	266	0.31	0.57	0.14	0.31
20	21	48	74	114	16	273	0.32	0.56	0.13	0.33

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

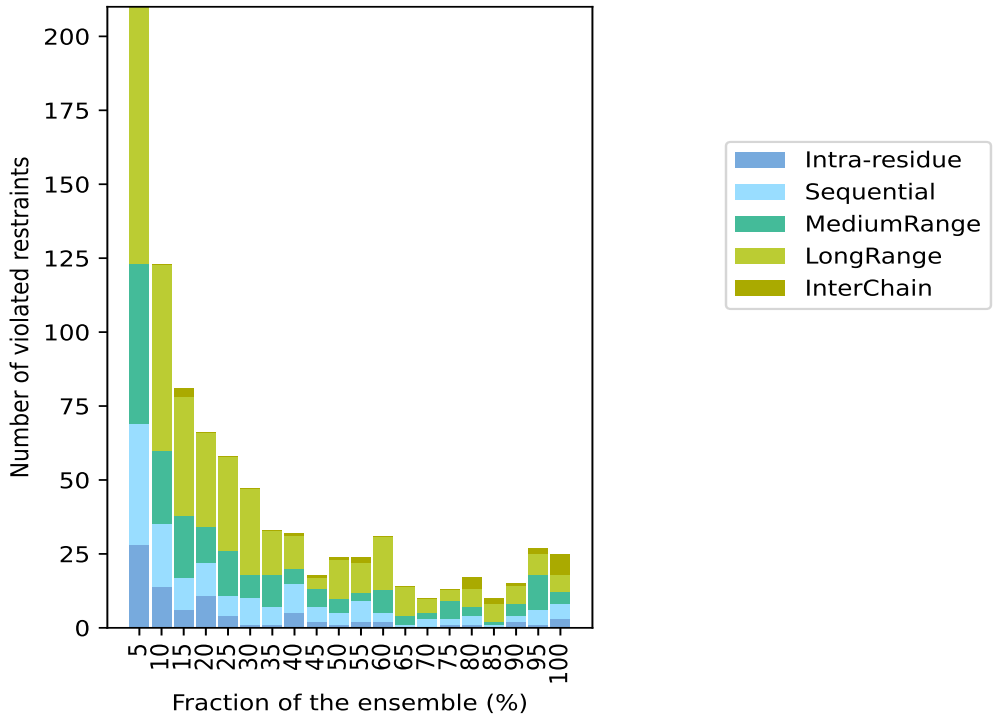
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2457(IR:710, SQ:702, MR:375, LR:659, IC:11) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
28	41	54	87	0	210	1	5.0
14	21	25	63	0	123	2	10.0
6	11	21	40	3	81	3	15.0
11	11	12	32	0	66	4	20.0
4	7	15	32	0	58	5	25.0
1	9	8	29	0	47	6	30.0
1	6	11	15	0	33	7	35.0
5	10	5	11	1	32	8	40.0
2	5	6	4	1	18	9	45.0
1	4	5	13	1	24	10	50.0
2	7	3	10	2	24	11	55.0
2	3	8	18	0	31	12	60.0
0	1	3	10	0	14	13	65.0
0	3	2	5	0	10	14	70.0
1	2	6	4	0	13	15	75.0
1	3	3	6	4	17	16	80.0
0	1	1	6	2	10	17	85.0
2	2	4	6	1	15	18	90.0
1	5	12	7	2	27	19	95.0
3	5	4	6	7	25	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

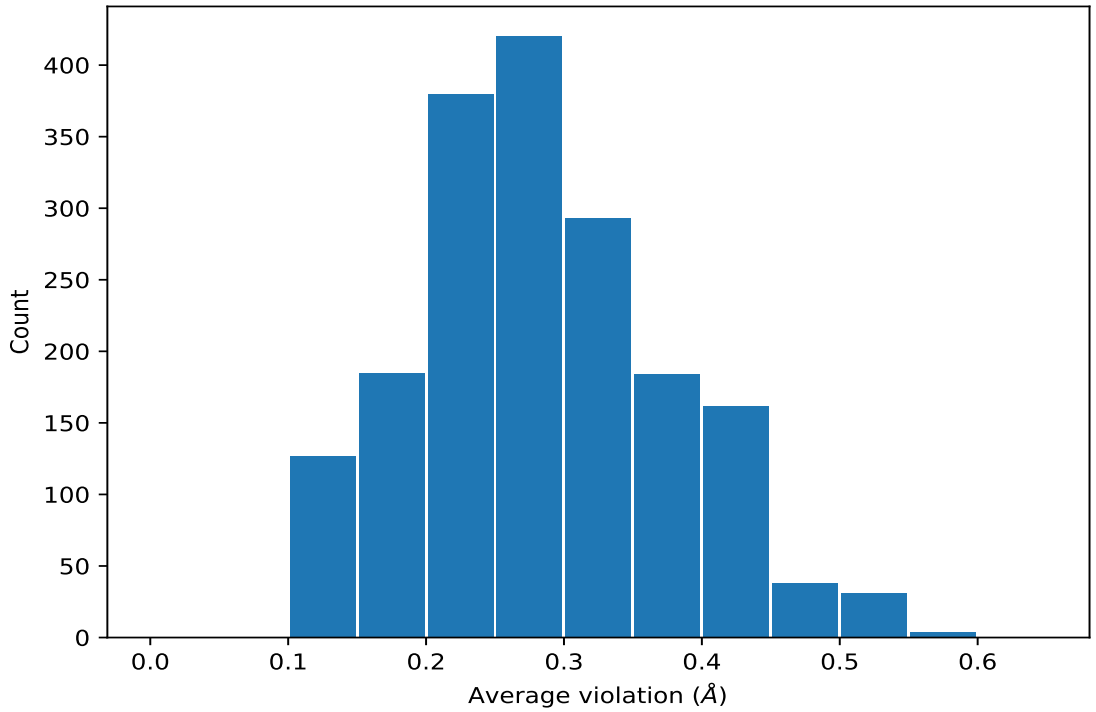
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	20	0.56	0.0	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	20	0.55	0.01	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	20	0.55	0.01	0.56
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	20	0.54	0.03	0.55
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	20	0.5	0.11	0.56
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	20	0.49	0.01	0.49
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	20	0.47	0.08	0.51
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	20	0.45	0.08	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	20	0.44	0.03	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	20	0.44	0.03	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	20	0.44	0.03	0.45
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	20	0.44	0.01	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	20	0.44	0.01	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	20	0.44	0.01	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	20	0.44	0.01	0.44
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	20	0.43	0.07	0.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	20	0.43	0.07	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	20	0.43	0.07	0.48
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	20	0.43	0.03	0.44
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	20	0.43	0.07	0.47
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	20	0.42	0.06	0.46
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	20	0.42	0.06	0.46
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	20	0.41	0.06	0.44
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	20	0.41	0.06	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	20	0.41	0.06	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	20	0.41	0.06	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	20	0.41	0.06	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	20	0.41	0.06	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	20	0.41	0.06	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	20	0.41	0.06	0.44
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	20	0.4	0.1	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	20	0.4	0.1	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	20	0.4	0.1	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	20	0.4	0.1	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	20	0.4	0.1	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	20	0.4	0.1	0.45
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	20	0.4	0.1	0.44
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	20	0.39	0.05	0.41
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	20	0.38	0.06	0.41
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	20	0.37	0.02	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	20	0.37	0.02	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	20	0.37	0.02	0.38
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	20	0.34	0.07	0.39
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	20	0.34	0.02	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	20	0.34	0.02	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	20	0.34	0.02	0.35
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	20	0.31	0.07	0.31
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	20	0.31	0.07	0.31
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	20	0.31	0.07	0.31
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	20	0.2	0.03	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	20	0.2	0.03	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	20	0.2	0.03	0.2
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	19	0.52	0.01	0.52
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	19	0.51	0.08	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	19	0.51	0.08	0.54
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	19	0.51	0.0	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	19	0.51	0.0	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	19	0.51	0.0	0.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	19	0.43	0.08	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	19	0.43	0.08	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	19	0.43	0.08	0.49
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	19	0.43	0.14	0.46
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	19	0.42	0.07	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	19	0.42	0.07	0.44
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	19	0.41	0.03	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	19	0.41	0.03	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	19	0.41	0.03	0.42
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	19	0.41	0.16	0.48
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	19	0.41	0.1	0.46
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	19	0.41	0.1	0.46
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	19	0.41	0.1	0.46
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	19	0.41	0.01	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	19	0.41	0.01	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	19	0.41	0.01	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	19	0.41	0.01	0.41
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	19	0.38	0.02	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	19	0.38	0.02	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	19	0.38	0.02	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	19	0.38	0.02	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	19	0.38	0.02	0.39
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	19	0.38	0.05	0.38
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	19	0.37	0.07	0.38
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	19	0.37	0.07	0.38
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	19	0.37	0.08	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	19	0.37	0.08	0.41
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	19	0.37	0.08	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	19	0.37	0.08	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	19	0.37	0.08	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	19	0.37	0.08	0.41
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	19	0.37	0.09	0.39
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	19	0.35	0.14	0.4
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	19	0.34	0.14	0.32
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	19	0.33	0.15	0.32
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	19	0.33	0.15	0.32
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	19	0.33	0.13	0.3
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	19	0.33	0.09	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	19	0.33	0.09	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	19	0.33	0.09	0.38
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	19	0.3	0.12	0.34
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	19	0.3	0.12	0.34
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	19	0.3	0.12	0.34
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	19	0.29	0.07	0.33
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	19	0.28	0.06	0.28
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	19	0.26	0.08	0.26
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	19	0.26	0.08	0.26
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	19	0.24	0.09	0.24
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	19	0.24	0.09	0.24
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	19	0.24	0.09	0.24
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	19	0.24	0.09	0.24
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	19	0.24	0.09	0.24
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	19	0.24	0.09	0.24
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	19	0.21	0.05	0.21
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	18	0.54	0.04	0.56
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	18	0.51	0.0	0.51
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	18	0.5	0.1	0.55
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	18	0.49	0.05	0.51
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	18	0.39	0.05	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	18	0.39	0.05	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	18	0.39	0.05	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	18	0.39	0.05	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	18	0.39	0.05	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	18	0.39	0.05	0.4
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	18	0.37	0.09	0.42
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	18	0.37	0.09	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	18	0.36	0.09	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	18	0.36	0.09	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	18	0.36	0.09	0.42
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	18	0.36	0.12	0.39
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	18	0.35	0.1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	18	0.35	0.1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	18	0.35	0.1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	18	0.35	0.1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	18	0.35	0.1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	18	0.35	0.1	0.38
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	18	0.33	0.11	0.34
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	18	0.33	0.07	0.37
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	18	0.32	0.1	0.33
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	18	0.32	0.1	0.33
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	18	0.32	0.1	0.33
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	18	0.31	0.07	0.33
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	18	0.31	0.07	0.33
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	18	0.31	0.07	0.33
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	18	0.3	0.1	0.33
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	18	0.3	0.1	0.33
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	18	0.3	0.1	0.33
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	18	0.3	0.1	0.33
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	18	0.3	0.1	0.33
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	18	0.3	0.1	0.33
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	18	0.26	0.1	0.24
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	17	0.54	0.02	0.55
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	17	0.44	0.08	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	17	0.44	0.08	0.47
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	17	0.43	0.05	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	17	0.43	0.05	0.46
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	17	0.38	0.12	0.36
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	17	0.38	0.12	0.36
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	17	0.34	0.12	0.3
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	17	0.34	0.12	0.3
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	17	0.32	0.13	0.35
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	17	0.32	0.11	0.32
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	17	0.32	0.11	0.32
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	17	0.3	0.07	0.32
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	17	0.27	0.12	0.24
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	17	0.27	0.12	0.24
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	17	0.21	0.06	0.23
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	17	0.21	0.06	0.23
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	17	0.21	0.06	0.23
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	16	0.49	0.12	0.55

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	16	0.49	0.1	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	16	0.49	0.14	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	16	0.49	0.14	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	16	0.49	0.14	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	16	0.49	0.14	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	16	0.49	0.14	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	16	0.49	0.14	0.55
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	16	0.46	0.08	0.49
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	16	0.45	0.14	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	16	0.45	0.14	0.55
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	16	0.45	0.01	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	16	0.45	0.01	0.45
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	16	0.43	0.07	0.46
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	16	0.42	0.05	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	16	0.42	0.05	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	16	0.42	0.05	0.43
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	16	0.41	0.13	0.43
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	16	0.37	0.14	0.37
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	16	0.37	0.14	0.46
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	16	0.35	0.17	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	16	0.35	0.17	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	16	0.35	0.17	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	16	0.35	0.17	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	16	0.35	0.17	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	16	0.35	0.17	0.47
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	16	0.33	0.02	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	16	0.33	0.02	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	16	0.33	0.02	0.34
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	16	0.27	0.09	0.28
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	16	0.27	0.12	0.22
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	16	0.27	0.12	0.22
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	16	0.17	0.02	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	16	0.17	0.02	0.16
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	16	0.17	0.05	0.15
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	16	0.17	0.05	0.15
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	16	0.17	0.05	0.15
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	15	0.51	0.07	0.54
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	15	0.42	0.13	0.47
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	15	0.42	0.13	0.47
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	15	0.4	0.06	0.44
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	15	0.39	0.08	0.43
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	15	0.39	0.16	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	15	0.39	0.16	0.42
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	15	0.34	0.13	0.36
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	15	0.32	0.13	0.34
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	15	0.26	0.1	0.26
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	15	0.26	0.05	0.24
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	15	0.25	0.11	0.25
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	15	0.25	0.11	0.25
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	15	0.25	0.11	0.25
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	15	0.24	0.1	0.25
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	15	0.24	0.1	0.25
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	15	0.19	0.05	0.18
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	15	0.19	0.05	0.18
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	15	0.19	0.05	0.18
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	15	0.18	0.07	0.17
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	14	0.36	0.14	0.43
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	14	0.36	0.14	0.43
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	14	0.36	0.1	0.38
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	14	0.35	0.1	0.42
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	14	0.35	0.1	0.42
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	14	0.35	0.1	0.42
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	14	0.35	0.06	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	14	0.35	0.06	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	14	0.35	0.06	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	14	0.35	0.06	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	14	0.35	0.06	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	14	0.35	0.06	0.39
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	14	0.34	0.12	0.32
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	14	0.33	0.15	0.38
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	14	0.3	0.1	0.3
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	14	0.25	0.09	0.25
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	14	0.25	0.09	0.25
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	14	0.25	0.09	0.25
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	14	0.25	0.09	0.25
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	14	0.25	0.09	0.25
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	14	0.25	0.09	0.25
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	14	0.21	0.04	0.21
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	14	0.2	0.09	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	14	0.2	0.09	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	14	0.2	0.09	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	14	0.2	0.09	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	14	0.2	0.09	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	14	0.2	0.09	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	13	0.45	0.17	0.56
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	13	0.44	0.09	0.48
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	13	0.44	0.09	0.48
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	13	0.44	0.09	0.48
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	13	0.41	0.13	0.4
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	13	0.39	0.08	0.39
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	13	0.39	0.08	0.39
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	13	0.38	0.13	0.4
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	13	0.37	0.16	0.41
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	13	0.36	0.15	0.42
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	13	0.35	0.07	0.38
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	13	0.3	0.12	0.34
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	13	0.3	0.12	0.34
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	13	0.3	0.1	0.26
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	13	0.3	0.1	0.26
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	13	0.3	0.1	0.26
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	13	0.29	0.06	0.29
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	13	0.29	0.06	0.29
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	13	0.29	0.06	0.29
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	13	0.28	0.09	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	13	0.28	0.09	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	13	0.28	0.09	0.26
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	13	0.24	0.07	0.25
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	13	0.24	0.07	0.25
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	13	0.23	0.08	0.22
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	13	0.23	0.08	0.22
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	13	0.23	0.08	0.22
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	12	0.5	0.09	0.54
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	12	0.5	0.09	0.54
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	12	0.5	0.09	0.54
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	12	0.46	0.08	0.48
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	12	0.44	0.16	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	12	0.44	0.16	0.55
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	12	0.43	0.05	0.46
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	12	0.43	0.05	0.46
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	12	0.42	0.1	0.45
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	12	0.38	0.14	0.4
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	12	0.38	0.14	0.4
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	12	0.38	0.14	0.4
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	12	0.38	0.1	0.43
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	12	0.36	0.11	0.38
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	12	0.36	0.07	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	12	0.36	0.14	0.33
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	12	0.36	0.14	0.33
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	12	0.35	0.07	0.38
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	12	0.35	0.07	0.38
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	12	0.35	0.07	0.38
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	12	0.35	0.07	0.38
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	12	0.35	0.07	0.38
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	12	0.35	0.07	0.38
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	12	0.34	0.09	0.38
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	12	0.34	0.09	0.38
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	12	0.33	0.16	0.29
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	12	0.33	0.07	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	12	0.33	0.07	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	12	0.33	0.07	0.37
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	12	0.32	0.12	0.32
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	12	0.32	0.13	0.3
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	12	0.32	0.15	0.31
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	12	0.32	0.15	0.31
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	12	0.31	0.03	0.3
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	12	0.3	0.11	0.35
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	12	0.3	0.11	0.35
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	12	0.28	0.11	0.32
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	12	0.28	0.11	0.32
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	12	0.28	0.11	0.32
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	12	0.28	0.08	0.3
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	12	0.27	0.11	0.28
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	12	0.27	0.09	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	12	0.27	0.09	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	12	0.27	0.09	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	12	0.27	0.09	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	12	0.27	0.09	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	12	0.27	0.09	0.24
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	12	0.26	0.09	0.31
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	12	0.26	0.09	0.31
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	12	0.26	0.09	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	12	0.26	0.09	0.31
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	12	0.26	0.09	0.31
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	12	0.26	0.09	0.31
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	12	0.26	0.06	0.26
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	12	0.26	0.06	0.27
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	12	0.26	0.06	0.27
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	12	0.26	0.06	0.27
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	12	0.26	0.06	0.27
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	12	0.26	0.06	0.27
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	12	0.26	0.06	0.27
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	12	0.25	0.07	0.26
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	12	0.23	0.09	0.2
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	12	0.22	0.08	0.2
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	12	0.22	0.08	0.2
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	12	0.22	0.08	0.2
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	12	0.22	0.08	0.2
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	12	0.22	0.08	0.2
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	12	0.22	0.08	0.2
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	12	0.22	0.07	0.25
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	12	0.2	0.06	0.2
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	11	0.56	0.0	0.56
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	11	0.5	0.0	0.5
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	11	0.5	0.0	0.5
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	11	0.46	0.09	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	11	0.46	0.09	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	11	0.46	0.09	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	11	0.46	0.09	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	11	0.46	0.09	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	11	0.46	0.09	0.49
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	11	0.42	0.13	0.44
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	11	0.42	0.13	0.44
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	11	0.42	0.13	0.44
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	11	0.42	0.13	0.44
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	11	0.42	0.13	0.44
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	11	0.42	0.13	0.44
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	11	0.4	0.11	0.45
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	11	0.39	0.08	0.42
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	11	0.38	0.17	0.39
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	11	0.35	0.14	0.43
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	11	0.33	0.0	0.33
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	11	0.33	0.15	0.34
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	11	0.33	0.15	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	11	0.33	0.15	0.34
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	11	0.32	0.14	0.3
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	11	0.32	0.14	0.3
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	11	0.32	0.14	0.3
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	11	0.31	0.11	0.38
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	11	0.31	0.11	0.38
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	11	0.31	0.11	0.38
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	11	0.31	0.13	0.29
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	11	0.3	0.13	0.23
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	11	0.3	0.13	0.23
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	11	0.3	0.13	0.23
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	11	0.3	0.13	0.23
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	11	0.3	0.13	0.23
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	11	0.3	0.13	0.23
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	11	0.29	0.16	0.21
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	11	0.29	0.16	0.21
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	11	0.29	0.1	0.27
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	11	0.29	0.1	0.27
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	11	0.29	0.1	0.27
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	11	0.26	0.09	0.28
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	11	0.26	0.08	0.28
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	11	0.25	0.1	0.21
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	11	0.24	0.11	0.25
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	11	0.24	0.11	0.25
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	11	0.24	0.11	0.25
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	11	0.24	0.11	0.25
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	11	0.24	0.11	0.25
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	11	0.24	0.11	0.25
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	11	0.23	0.08	0.21
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	11	0.21	0.06	0.21
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	11	0.2	0.08	0.16
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	11	0.17	0.05	0.17
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	11	0.17	0.05	0.17
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	10	0.44	0.16	0.54
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	10	0.44	0.16	0.54
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	10	0.42	0.1	0.47
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	10	0.42	0.1	0.47
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	10	0.42	0.1	0.47
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	10	0.41	0.17	0.48
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	10	0.41	0.17	0.48
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	10	0.41	0.17	0.48
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	10	0.39	0.1	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	10	0.39	0.1	0.38
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	10	0.39	0.1	0.46
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	10	0.34	0.11	0.37
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	10	0.34	0.11	0.37
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	10	0.33	0.11	0.32
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	10	0.33	0.11	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	10	0.33	0.11	0.38
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	10	0.33	0.14	0.36
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	10	0.33	0.14	0.36
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	10	0.33	0.14	0.36
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	10	0.33	0.14	0.36
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	10	0.33	0.14	0.36
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	10	0.33	0.14	0.36
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	10	0.32	0.16	0.31
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	10	0.32	0.08	0.36
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	10	0.32	0.08	0.36
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	10	0.31	0.15	0.24
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	10	0.31	0.15	0.24
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	10	0.31	0.15	0.24
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	10	0.3	0.13	0.29
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	10	0.3	0.1	0.35
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	10	0.3	0.1	0.35
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	10	0.3	0.1	0.35
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	10	0.3	0.1	0.35
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	10	0.3	0.1	0.35
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	10	0.3	0.1	0.35
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	10	0.28	0.09	0.32
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	10	0.28	0.09	0.32
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	10	0.28	0.09	0.32
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	10	0.28	0.1	0.3
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	10	0.28	0.08	0.3
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	10	0.25	0.1	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	10	0.25	0.1	0.24
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	10	0.25	0.1	0.24
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	10	0.25	0.1	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	10	0.25	0.1	0.3
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	10	0.25	0.09	0.25
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	10	0.25	0.09	0.25
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	10	0.25	0.09	0.25
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	10	0.22	0.07	0.22
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	10	0.17	0.03	0.17
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	10	0.16	0.06	0.14
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	10	0.14	0.01	0.13
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	9	0.44	0.0	0.44
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	9	0.37	0.03	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	9	0.37	0.03	0.38
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	9	0.35	0.08	0.38
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	9	0.3	0.09	0.27
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	9	0.3	0.13	0.33
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	9	0.3	0.13	0.33
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	9	0.3	0.13	0.33
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	9	0.29	0.16	0.25
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	9	0.28	0.1	0.28
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	9	0.28	0.1	0.28
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	9	0.27	0.09	0.28
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	9	0.27	0.09	0.28
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	9	0.26	0.1	0.29
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	9	0.26	0.1	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	9	0.26	0.1	0.29
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	9	0.26	0.1	0.29
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	9	0.26	0.1	0.29
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	9	0.26	0.1	0.29
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	9	0.25	0.07	0.24
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	9	0.25	0.07	0.24
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	9	0.24	0.1	0.21
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	9	0.24	0.1	0.21
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	9	0.24	0.1	0.21
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	9	0.24	0.11	0.22
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	9	0.21	0.07	0.2
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	9	0.21	0.07	0.2
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	9	0.21	0.07	0.19
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	9	0.2	0.05	0.21
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	9	0.2	0.05	0.21
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	9	0.2	0.05	0.21
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	9	0.18	0.05	0.16
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	9	0.18	0.05	0.16
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	9	0.16	0.06	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	9	0.15	0.04	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	9	0.15	0.04	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	9	0.15	0.04	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	9	0.15	0.04	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	9	0.15	0.04	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	9	0.15	0.04	0.13
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	8	0.49	0.07	0.52
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	8	0.49	0.07	0.52
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	8	0.38	0.11	0.42
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	8	0.38	0.15	0.42
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	8	0.36	0.07	0.38
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	8	0.34	0.04	0.34
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	8	0.34	0.0	0.34
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	8	0.34	0.0	0.34
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	8	0.34	0.0	0.34
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	8	0.33	0.09	0.34
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	8	0.32	0.12	0.34
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	8	0.32	0.12	0.34
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	8	0.32	0.12	0.34
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	8	0.31	0.09	0.3
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	8	0.3	0.07	0.28
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	8	0.3	0.07	0.28
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	8	0.3	0.07	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	8	0.3	0.07	0.28
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	8	0.3	0.07	0.28
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	8	0.3	0.07	0.28
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	8	0.28	0.11	0.26
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	8	0.28	0.11	0.26
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	8	0.28	0.15	0.26
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	8	0.28	0.15	0.26
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	8	0.27	0.09	0.26
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	8	0.27	0.09	0.26
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	8	0.27	0.09	0.26
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	8	0.27	0.09	0.26
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	8	0.27	0.09	0.26
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	8	0.27	0.09	0.26
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	8	0.25	0.09	0.28
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	8	0.25	0.09	0.25
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	8	0.24	0.08	0.22
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	8	0.24	0.08	0.22
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	8	0.24	0.07	0.24
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	8	0.23	0.1	0.21
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	8	0.23	0.1	0.21
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	8	0.22	0.09	0.22
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	8	0.22	0.1	0.21
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	8	0.22	0.07	0.23
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	8	0.22	0.07	0.23
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	8	0.22	0.07	0.23
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	8	0.22	0.07	0.24
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	8	0.22	0.07	0.24
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	8	0.21	0.06	0.22
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	8	0.21	0.09	0.22
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	8	0.21	0.09	0.22
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	8	0.21	0.02	0.21
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	8	0.21	0.06	0.19
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	8	0.21	0.06	0.19
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	8	0.19	0.05	0.19
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	8	0.18	0.03	0.2
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	8	0.17	0.04	0.16
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	8	0.17	0.05	0.16
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	8	0.15	0.04	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	8	0.15	0.04	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	8	0.15	0.04	0.12
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	8	0.11	0.01	0.11
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	7	0.45	0.15	0.55

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	7	0.45	0.15	0.55
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	7	0.4	0.09	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	7	0.4	0.09	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	7	0.4	0.09	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	7	0.4	0.09	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	7	0.4	0.09	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	7	0.4	0.09	0.46
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	7	0.39	0.01	0.39
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	7	0.39	0.01	0.39
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	7	0.36	0.1	0.41
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	7	0.36	0.14	0.36
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	7	0.36	0.14	0.36
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	7	0.35	0.07	0.34
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	7	0.35	0.07	0.34
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	7	0.35	0.07	0.34
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	7	0.35	0.07	0.34
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	7	0.35	0.07	0.34
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	7	0.35	0.07	0.34
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	7	0.35	0.0	0.35
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	7	0.35	0.0	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	7	0.35	0.0	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	7	0.35	0.0	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	7	0.35	0.0	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	7	0.35	0.0	0.35
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	7	0.33	0.06	0.36
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	7	0.33	0.06	0.36
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	7	0.33	0.06	0.36
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	7	0.31	0.13	0.3
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	7	0.3	0.05	0.31
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	7	0.3	0.05	0.31
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	7	0.3	0.05	0.31
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	7	0.3	0.05	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	7	0.3	0.05	0.31
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	7	0.3	0.05	0.31
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	7	0.29	0.09	0.34
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	7	0.29	0.09	0.34
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	7	0.29	0.09	0.34
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	7	0.29	0.09	0.34
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	7	0.29	0.09	0.34
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	7	0.29	0.09	0.34
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	7	0.29	0.07	0.3
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	7	0.29	0.07	0.3
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	7	0.28	0.01	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	7	0.28	0.01	0.29
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	7	0.28	0.11	0.27
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	7	0.28	0.11	0.27
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	7	0.28	0.11	0.22
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	7	0.28	0.11	0.22
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	7	0.28	0.11	0.22
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	7	0.27	0.11	0.22
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	7	0.27	0.11	0.22
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	7	0.27	0.08	0.28
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	7	0.27	0.08	0.28
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	7	0.26	0.15	0.2
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	7	0.26	0.09	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	7	0.26	0.09	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	7	0.26	0.09	0.25
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	7	0.26	0.1	0.26
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	7	0.26	0.11	0.2
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	7	0.26	0.11	0.2
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	7	0.26	0.11	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	7	0.26	0.11	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	7	0.26	0.11	0.24
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	7	0.24	0.07	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	7	0.24	0.07	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	7	0.24	0.07	0.23
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	7	0.24	0.07	0.21
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	7	0.24	0.13	0.22
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	7	0.2	0.06	0.2
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	7	0.2	0.06	0.2
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	7	0.2	0.06	0.2
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	7	0.2	0.06	0.2
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	7	0.2	0.06	0.2
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	7	0.2	0.06	0.2
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	7	0.2	0.06	0.18
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	7	0.2	0.06	0.18
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	7	0.2	0.06	0.18
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	7	0.19	0.07	0.17
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	7	0.19	0.07	0.17
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	7	0.19	0.07	0.17
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	7	0.19	0.07	0.17
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	7	0.19	0.07	0.17
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	7	0.19	0.07	0.17
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	7	0.18	0.04	0.18
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	7	0.18	0.04	0.18
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	7	0.17	0.05	0.17
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	7	0.17	0.05	0.17
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	7	0.17	0.05	0.17
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	7	0.17	0.04	0.18
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	7	0.17	0.04	0.18
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	7	0.17	0.04	0.18
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	7	0.16	0.02	0.16
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	7	0.13	0.02	0.13
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE1	6	0.43	0.13	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE2	6	0.43	0.13	0.5
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE1	6	0.41	0.07	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE2	6	0.41	0.07	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE1	6	0.41	0.07	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE2	6	0.41	0.07	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE1	6	0.41	0.07	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE2	6	0.41	0.07	0.44
(1,885)	1:161:A:ARG:HA	1:164:A:ARG:HE	6	0.39	0.12	0.44
(1,2620)	1:166:A:HIS:HB3	1:167:A:LYS:HB2	6	0.39	0.12	0.36
(1,1489)	1:95:A:HIS:HE1	1:99:A:GLN:HE22	6	0.37	0.12	0.39
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG11	6	0.36	0.1	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG12	6	0.36	0.1	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG13	6	0.36	0.1	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG21	6	0.36	0.1	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG22	6	0.36	0.1	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG23	6	0.36	0.1	0.4
(1,965)	1:43:A:GLN:HE22	1:50:A:THR:HB	6	0.36	0.15	0.31
(1,3008)	1:58:A:THR:HB	1:68:A:ARG:HE	6	0.36	0.08	0.4
(1,2663)	1:1:A:MET:HE1	1:43:A:GLN:HE22	6	0.34	0.06	0.37
(1,2663)	1:1:A:MET:HE2	1:43:A:GLN:HE22	6	0.34	0.06	0.37
(1,2663)	1:1:A:MET:HE3	1:43:A:GLN:HE22	6	0.34	0.06	0.37
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG2	6	0.33	0.01	0.33
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG3	6	0.33	0.01	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG2	6	0.33	0.01	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG3	6	0.33	0.01	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG2	6	0.33	0.01	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG3	6	0.33	0.01	0.33
(1,2627)	1:47:A:ASP:HB2	1:161:A:ARG:HE	6	0.33	0.13	0.36
(1,2627)	1:47:A:ASP:HB3	1:161:A:ARG:HE	6	0.33	0.13	0.36
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD11	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD12	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD13	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD21	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD22	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD23	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD11	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD12	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD13	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD21	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD22	6	0.32	0.11	0.33
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD23	6	0.32	0.11	0.33
(1,2535)	1:168:A:GLU:H	1:169:A:LYS:H	6	0.31	0.05	0.33

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1645)	1:128:A:LYS:HG2	1:129:A:GLN:HB2	6	0.3	0.1	0.33
(1,1645)	1:128:A:LYS:HG3	1:129:A:GLN:HB2	6	0.3	0.1	0.33
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE2	6	0.3	0.09	0.32
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE3	6	0.3	0.09	0.32
(1,2189)	1:4:A:TYR:HD1	1:52:A:LEU:H	6	0.3	0.12	0.32
(1,2189)	1:4:A:TYR:HD2	1:52:A:LEU:H	6	0.3	0.12	0.32
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG2	6	0.29	0.09	0.3
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG3	6	0.29	0.09	0.3
(1,957)	1:43:A:GLN:HG2	1:44:A:VAL:H	6	0.29	0.11	0.33
(1,957)	1:43:A:GLN:HG3	1:44:A:VAL:H	6	0.29	0.11	0.33
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD11	6	0.28	0.11	0.32
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD12	6	0.28	0.11	0.32
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD13	6	0.28	0.11	0.32
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD11	6	0.28	0.11	0.32
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD12	6	0.28	0.11	0.32
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD13	6	0.28	0.11	0.32
(1,3242)	1:3:A:GLU:HG2	1:4:A:TYR:HA	6	0.28	0.04	0.28
(1,3242)	1:3:A:GLU:HG3	1:4:A:TYR:HA	6	0.28	0.04	0.28
(1,2607)	1:21:A:ILE:HA	1:27:A:HIS:H	6	0.27	0.12	0.28
(1,1971)	1:6:A:LEU:HB2	1:78:A:PHE:HA	6	0.27	0.13	0.22
(1,1971)	1:6:A:LEU:HB3	1:78:A:PHE:HA	6	0.27	0.13	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD11	6	0.26	0.1	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD12	6	0.26	0.1	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD13	6	0.26	0.1	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD21	6	0.26	0.1	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD22	6	0.26	0.1	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD23	6	0.26	0.1	0.22
(1,2682)	1:25:A:GLN:HA	1:27:A:HIS:HE1	6	0.26	0.11	0.23
(1,2417)	1:4:A:TYR:HD1	1:163:A:ILE:HA	6	0.25	0.11	0.26
(1,2417)	1:4:A:TYR:HD2	1:163:A:ILE:HA	6	0.25	0.11	0.26
(1,1272)	1:9:A:VAL:HG11	1:96:A:TYR:H	6	0.24	0.09	0.26
(1,1272)	1:9:A:VAL:HG12	1:96:A:TYR:H	6	0.24	0.09	0.26
(1,1272)	1:9:A:VAL:HG13	1:96:A:TYR:H	6	0.24	0.09	0.26
(1,1272)	1:9:A:VAL:HG21	1:96:A:TYR:H	6	0.24	0.09	0.26
(1,1272)	1:9:A:VAL:HG22	1:96:A:TYR:H	6	0.24	0.09	0.26
(1,1272)	1:9:A:VAL:HG23	1:96:A:TYR:H	6	0.24	0.09	0.26
(1,2132)	1:45:A:VAL:HG11	1:51:A:CYS:H	6	0.24	0.09	0.2
(1,2132)	1:45:A:VAL:HG12	1:51:A:CYS:H	6	0.24	0.09	0.2
(1,2132)	1:45:A:VAL:HG13	1:51:A:CYS:H	6	0.24	0.09	0.2
(1,2132)	1:45:A:VAL:HG21	1:51:A:CYS:H	6	0.24	0.09	0.2
(1,2132)	1:45:A:VAL:HG22	1:51:A:CYS:H	6	0.24	0.09	0.2
(1,2132)	1:45:A:VAL:HG23	1:51:A:CYS:H	6	0.24	0.09	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2280)	1:144:A:THR:HA	1:151:A:GLY:HA2	6	0.24	0.08	0.2
(3,2)	1:17:A:SER:OG	2:201:A:GNP:O2B	6	0.24	0.1	0.2
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE1	6	0.24	0.13	0.2
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE2	6	0.24	0.13	0.2
(1,1774)	1:24:A:ILE:HD11	1:41:A:ARG:HA	6	0.24	0.11	0.21
(1,1774)	1:24:A:ILE:HD12	1:41:A:ARG:HA	6	0.24	0.11	0.21
(1,1774)	1:24:A:ILE:HD13	1:41:A:ARG:HA	6	0.24	0.11	0.21
(1,2690)	1:148:A:THR:H	1:150:A:GLN:HB2	6	0.23	0.1	0.22
(1,3063)	1:45:A:VAL:HB	1:48:A:GLY:H	6	0.22	0.11	0.2
(1,103)	1:16:A:LYS:HA	1:19:A:LEU:HB3	6	0.22	0.06	0.24
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD11	6	0.22	0.07	0.21
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD12	6	0.22	0.07	0.21
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD13	6	0.22	0.07	0.21
(1,2768)	1:145:A:SER:H	1:150:A:GLN:HG3	6	0.2	0.07	0.18
(1,2223)	1:114:A:VAL:HA	1:144:A:THR:H	6	0.19	0.06	0.18
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG12	6	0.19	0.07	0.21
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG13	6	0.19	0.07	0.21
(1,2267)	1:150:A:GLN:HG2	1:151:A:GLY:H	6	0.19	0.1	0.16
(1,3128)	1:1:A:MET:HA	1:51:A:CYS:HA	6	0.19	0.08	0.16
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB1	6	0.19	0.08	0.18
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB2	6	0.19	0.08	0.18
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB3	6	0.19	0.08	0.18
(1,1080)	1:1:A:MET:HG3	1:51:A:CYS:HA	6	0.16	0.09	0.13
(1,1685)	1:113:A:LEU:HD11	1:141:A:PHE:HA	6	0.16	0.03	0.17
(1,1685)	1:113:A:LEU:HD12	1:141:A:PHE:HA	6	0.16	0.03	0.17
(1,1685)	1:113:A:LEU:HD13	1:141:A:PHE:HA	6	0.16	0.03	0.17
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE1	6	0.16	0.06	0.12
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE2	6	0.16	0.06	0.12
(1,2067)	1:3:A:GLU:HA	1:4:A:TYR:HB2	6	0.15	0.04	0.15
(1,1823)	1:112:A:VAL:HA	1:162:A:GLU:HG3	6	0.15	0.04	0.15
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB1	6	0.15	0.05	0.14
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB2	6	0.15	0.05	0.14
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB3	6	0.15	0.05	0.14
(1,40)	1:106:A:SER:H	1:107:A:GLU:H	6	0.11	0.0	0.11
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD2	5	0.54	0.0	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD3	5	0.54	0.0	0.54
(1,861)	1:41:A:ARG:HG2	1:55:A:ILE:H	5	0.54	0.01	0.54
(1,861)	1:41:A:ARG:HG3	1:55:A:ILE:H	5	0.54	0.01	0.54
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE2	5	0.45	0.14	0.52
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE3	5	0.45	0.14	0.52
(1,1120)	1:12:A:GLY:H	1:61:A:GLN:HB3	5	0.44	0.14	0.54
(1,1831)	1:158:A:THR:HA	1:161:A:ARG:HE	5	0.44	0.05	0.47

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3249)	1:3:A:GLU:HG3	1:4:A:TYR:H	5	0.43	0.0	0.43
(1,982)	1:44:A:VAL:HG21	1:51:A:CYS:HB2	5	0.41	0.09	0.47
(1,982)	1:44:A:VAL:HG22	1:51:A:CYS:HB2	5	0.41	0.09	0.47
(1,982)	1:44:A:VAL:HG23	1:51:A:CYS:HB2	5	0.41	0.09	0.47
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD11	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD12	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD13	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD21	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD22	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD23	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD11	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD12	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD13	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD21	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD22	5	0.39	0.0	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD23	5	0.39	0.0	0.39
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE1	5	0.39	0.12	0.46
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE2	5	0.39	0.12	0.46
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE1	5	0.37	0.01	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE2	5	0.37	0.01	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE3	5	0.37	0.01	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE1	5	0.37	0.01	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE2	5	0.37	0.01	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE3	5	0.37	0.01	0.38
(1,1940)	1:120:A:LEU:HD11	1:121:A:PRO:HG3	5	0.36	0.1	0.35
(1,1940)	1:120:A:LEU:HD12	1:121:A:PRO:HG3	5	0.36	0.1	0.35
(1,1940)	1:120:A:LEU:HD13	1:121:A:PRO:HG3	5	0.36	0.1	0.35
(1,1940)	1:120:A:LEU:HD21	1:121:A:PRO:HG3	5	0.36	0.1	0.35
(1,1940)	1:120:A:LEU:HD22	1:121:A:PRO:HG3	5	0.36	0.1	0.35
(1,1940)	1:120:A:LEU:HD23	1:121:A:PRO:HG3	5	0.36	0.1	0.35
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG2	5	0.35	0.12	0.33
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG3	5	0.35	0.12	0.33
(1,2159)	1:140:A:PRO:HG3	1:162:A:GLU:HG2	5	0.34	0.09	0.4
(1,839)	1:4:A:TYR:HE1	1:52:A:LEU:H	5	0.33	0.1	0.33
(1,839)	1:4:A:TYR:HE2	1:52:A:LEU:H	5	0.33	0.1	0.33
(1,84)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	5	0.32	0.11	0.3
(1,3030)	1:32:A:TYR:HE1	1:34:A:PRO:HG3	5	0.31	0.08	0.35
(1,3030)	1:32:A:TYR:HE2	1:34:A:PRO:HG3	5	0.31	0.08	0.35
(1,2518)	1:164:A:ARG:H	1:165:A:LYS:HG2	5	0.3	0.13	0.23
(1,1661)	1:101:A:LYS:HD2	1:107:A:GLU:HA	5	0.3	0.11	0.35
(1,1661)	1:101:A:LYS:HD3	1:107:A:GLU:HA	5	0.3	0.11	0.35
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG11	5	0.28	0.04	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG12	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG13	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG21	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG22	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG23	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG11	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG12	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG13	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG21	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG22	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG23	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG11	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG12	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG13	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG21	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG22	5	0.28	0.04	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG23	5	0.28	0.04	0.29
(1,1891)	1:44:A:VAL:HB	1:51:A:CYS:H	5	0.28	0.1	0.26
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD2	5	0.28	0.09	0.33
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD3	5	0.28	0.09	0.33
(1,1714)	1:75:A:GLY:HA2	1:104:A:LYS:HD2	5	0.27	0.11	0.25
(1,952)	1:1:A:MET:HE1	1:43:A:GLN:HE21	5	0.27	0.11	0.27
(1,952)	1:1:A:MET:HE2	1:43:A:GLN:HE21	5	0.27	0.11	0.27
(1,952)	1:1:A:MET:HE3	1:43:A:GLN:HE21	5	0.27	0.11	0.27
(1,3116)	1:85:A:ASN:HB2	1:124:A:THR:H	5	0.27	0.11	0.25
(1,728)	1:65:A:SER:HA	1:66:A:ALA:H	5	0.26	0.04	0.25
(1,2398)	1:161:A:ARG:HA	1:165:A:LYS:H	5	0.25	0.14	0.22
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD1	5	0.25	0.04	0.25
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD2	5	0.25	0.04	0.25
(1,2762)	1:102:A:ARG:H	1:102:A:ARG:HE	5	0.25	0.09	0.21
(1,3133)	1:1:A:MET:HB2	1:2:A:THR:HB	5	0.24	0.11	0.19
(1,2501)	1:159:A:LEU:HD11	1:163:A:ILE:H	5	0.24	0.08	0.19
(1,2501)	1:159:A:LEU:HD12	1:163:A:ILE:H	5	0.24	0.08	0.19
(1,2501)	1:159:A:LEU:HD13	1:163:A:ILE:H	5	0.24	0.08	0.19
(1,2501)	1:159:A:LEU:HD21	1:163:A:ILE:H	5	0.24	0.08	0.19
(1,2501)	1:159:A:LEU:HD22	1:163:A:ILE:H	5	0.24	0.08	0.19
(1,2501)	1:159:A:LEU:HD23	1:163:A:ILE:H	5	0.24	0.08	0.19
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD1	5	0.24	0.07	0.22
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD2	5	0.24	0.07	0.22
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD1	5	0.24	0.07	0.22
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD2	5	0.24	0.07	0.22
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD1	5	0.24	0.07	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD2	5	0.24	0.07	0.22
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD11	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD12	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD13	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD11	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD12	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD13	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD11	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD12	5	0.24	0.06	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD13	5	0.24	0.06	0.23
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG11	5	0.24	0.06	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG12	5	0.24	0.06	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG13	5	0.24	0.06	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG21	5	0.24	0.06	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG22	5	0.24	0.06	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG23	5	0.24	0.06	0.24
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB2	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB3	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB2	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB3	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB2	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB3	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB2	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB3	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB2	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB3	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB2	5	0.22	0.08	0.21
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB3	5	0.22	0.08	0.21
(1,532)	1:166:A:HIS:HB2	1:168:A:GLU:H	5	0.22	0.05	0.19
(1,1752)	1:8:A:VAL:HG11	1:10:A:GLY:H	5	0.21	0.07	0.25
(1,1752)	1:8:A:VAL:HG12	1:10:A:GLY:H	5	0.21	0.07	0.25
(1,1752)	1:8:A:VAL:HG13	1:10:A:GLY:H	5	0.21	0.07	0.25
(1,1752)	1:8:A:VAL:HG21	1:10:A:GLY:H	5	0.21	0.07	0.25
(1,1752)	1:8:A:VAL:HG22	1:10:A:GLY:H	5	0.21	0.07	0.25
(1,1752)	1:8:A:VAL:HG23	1:10:A:GLY:H	5	0.21	0.07	0.25
(1,2328)	1:144:A:THR:HA	1:152:A:VAL:H	5	0.21	0.03	0.2
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG21	5	0.21	0.1	0.18
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG22	5	0.21	0.1	0.18
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG23	5	0.21	0.1	0.18
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG21	5	0.21	0.06	0.22
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG22	5	0.21	0.06	0.22
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG23	5	0.21	0.06	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB1	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB2	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB3	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB1	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB2	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB3	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB1	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB2	5	0.21	0.06	0.23
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB3	5	0.21	0.06	0.23
(1,2710)	1:102:A:ARG:HB3	1:102:A:ARG:HE	5	0.21	0.06	0.18
(1,2588)	1:153:A:ASP:HB2	1:155:A:ALA:H	5	0.21	0.07	0.17
(1,2588)	1:153:A:ASP:HB3	1:155:A:ALA:H	5	0.21	0.07	0.17
(1,377)	1:24:A:ILE:HD11	1:43:A:GLN:H	5	0.21	0.1	0.16
(1,377)	1:24:A:ILE:HD12	1:43:A:GLN:H	5	0.21	0.1	0.16
(1,377)	1:24:A:ILE:HD13	1:43:A:GLN:H	5	0.21	0.1	0.16
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB2	5	0.2	0.1	0.14
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB3	5	0.2	0.1	0.14
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB2	5	0.2	0.1	0.14
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB3	5	0.2	0.1	0.14
(1,2156)	1:111:A:MET:H	1:140:A:PRO:HD3	5	0.2	0.03	0.21
(1,3301)	1:120:A:LEU:HD11	1:122:A:SER:H	5	0.2	0.07	0.18
(1,3301)	1:120:A:LEU:HD12	1:122:A:SER:H	5	0.2	0.07	0.18
(1,3301)	1:120:A:LEU:HD13	1:122:A:SER:H	5	0.2	0.07	0.18
(1,3301)	1:120:A:LEU:HD21	1:122:A:SER:H	5	0.2	0.07	0.18
(1,3301)	1:120:A:LEU:HD22	1:122:A:SER:H	5	0.2	0.07	0.18
(1,3301)	1:120:A:LEU:HD23	1:122:A:SER:H	5	0.2	0.07	0.18
(1,319)	1:23:A:LEU:HB2	1:152:A:VAL:HB	5	0.19	0.06	0.19
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	5	0.19	0.09	0.18
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	5	0.19	0.09	0.18
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD1	5	0.18	0.07	0.18
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD2	5	0.18	0.07	0.18
(1,897)	1:79:A:LEU:HD11	1:157:A:TYR:H	5	0.17	0.08	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,897)	1:79:A:LEU:HD12	1:157:A:TYR:H	5	0.17	0.08	0.15
(1,897)	1:79:A:LEU:HD13	1:157:A:TYR:H	5	0.17	0.08	0.15
(1,897)	1:79:A:LEU:HD21	1:157:A:TYR:H	5	0.17	0.08	0.15
(1,897)	1:79:A:LEU:HD22	1:157:A:TYR:H	5	0.17	0.08	0.15
(1,897)	1:79:A:LEU:HD23	1:157:A:TYR:H	5	0.17	0.08	0.15
(1,962)	1:43:A:GLN:H	1:43:A:GLN:HG3	5	0.17	0.03	0.17
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG21	5	0.17	0.04	0.16
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG22	5	0.17	0.04	0.16
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG23	5	0.17	0.04	0.16
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG21	5	0.17	0.04	0.16
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG22	5	0.17	0.04	0.16
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG23	5	0.17	0.04	0.16
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD11	5	0.16	0.05	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD12	5	0.16	0.05	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD13	5	0.16	0.05	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD21	5	0.16	0.05	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD22	5	0.16	0.05	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD23	5	0.16	0.05	0.14
(1,2294)	1:112:A:VAL:HG11	1:159:A:LEU:H	5	0.16	0.04	0.17
(1,2294)	1:112:A:VAL:HG12	1:159:A:LEU:H	5	0.16	0.04	0.17
(1,2294)	1:112:A:VAL:HG13	1:159:A:LEU:H	5	0.16	0.04	0.17
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG21	5	0.15	0.03	0.15
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG22	5	0.15	0.03	0.15
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG23	5	0.15	0.03	0.15
(1,1115)	1:51:A:CYS:HB3	1:52:A:LEU:H	5	0.14	0.03	0.12
(1,478)	1:25:A:GLN:HB3	1:26:A:ASN:H	5	0.14	0.01	0.14
(1,2415)	1:77:A:GLY:HA3	1:163:A:ILE:HA	5	0.14	0.02	0.12
(1,3184)	1:132:A:ASP:HB2	1:135:A:ARG:HE	4	0.54	0.0	0.54
(1,3184)	1:132:A:ASP:HB3	1:135:A:ARG:HE	4	0.54	0.0	0.54
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB2	4	0.42	0.08	0.42
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB3	4	0.42	0.08	0.42
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB2	4	0.42	0.08	0.42
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB3	4	0.42	0.08	0.42
(1,631)	1:58:A:THR:HG21	1:68:A:ARG:H	4	0.41	0.13	0.49
(1,631)	1:58:A:THR:HG22	1:68:A:ARG:H	4	0.41	0.13	0.49
(1,631)	1:58:A:THR:HG23	1:68:A:ARG:H	4	0.41	0.13	0.49
(1,1382)	1:7:A:VAL:HG11	1:75:A:GLY:HA2	4	0.41	0.0	0.41
(1,1382)	1:7:A:VAL:HG12	1:75:A:GLY:HA2	4	0.41	0.0	0.41
(1,1382)	1:7:A:VAL:HG13	1:75:A:GLY:HA2	4	0.41	0.0	0.41
(1,1382)	1:7:A:VAL:HG21	1:75:A:GLY:HA2	4	0.41	0.0	0.41
(1,1382)	1:7:A:VAL:HG22	1:75:A:GLY:HA2	4	0.41	0.0	0.41
(1,1382)	1:7:A:VAL:HG23	1:75:A:GLY:HA2	4	0.41	0.0	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2150)	1:53:A:LEU:HD11	1:54:A:ASP:HA	4	0.4	0.13	0.47
(1,2150)	1:53:A:LEU:HD12	1:54:A:ASP:HA	4	0.4	0.13	0.47
(1,2150)	1:53:A:LEU:HD13	1:54:A:ASP:HA	4	0.4	0.13	0.47
(1,2150)	1:53:A:LEU:HD21	1:54:A:ASP:HA	4	0.4	0.13	0.47
(1,2150)	1:53:A:LEU:HD22	1:54:A:ASP:HA	4	0.4	0.13	0.47
(1,2150)	1:53:A:LEU:HD23	1:54:A:ASP:HA	4	0.4	0.13	0.47
(1,1412)	1:75:A:GLY:HA3	1:76:A:GLU:HG3	4	0.4	0.18	0.44
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE2	4	0.4	0.04	0.4
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE3	4	0.4	0.04	0.4
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD21	4	0.38	0.16	0.4
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD22	4	0.38	0.16	0.4
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD23	4	0.38	0.16	0.4
(1,1725)	1:104:A:LYS:HE3	1:109:A:VAL:HA	4	0.38	0.11	0.4
(1,1708)	1:142:A:ILE:HD11	1:143:A:GLU:HB3	4	0.36	0.07	0.36
(1,1708)	1:142:A:ILE:HD12	1:143:A:GLU:HB3	4	0.36	0.07	0.36
(1,1708)	1:142:A:ILE:HD13	1:143:A:GLU:HB3	4	0.36	0.07	0.36
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD1	4	0.36	0.12	0.4
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD2	4	0.36	0.12	0.4
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD1	4	0.36	0.12	0.4
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD2	4	0.36	0.12	0.4
(1,225)	1:6:A:LEU:H	1:6:A:LEU:HG	4	0.35	0.05	0.38
(1,1186)	1:56:A:LEU:HD11	1:71:A:TYR:HB3	4	0.35	0.11	0.42
(1,1186)	1:56:A:LEU:HD12	1:71:A:TYR:HB3	4	0.35	0.11	0.42
(1,1186)	1:56:A:LEU:HD13	1:71:A:TYR:HB3	4	0.35	0.11	0.42
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	4	0.35	0.08	0.36
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	4	0.35	0.08	0.36
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	4	0.35	0.08	0.36
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	4	0.35	0.08	0.36
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	4	0.35	0.08	0.36
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	4	0.35	0.08	0.36
(1,2254)	1:149:A:ARG:HB2	1:150:A:GLN:HE21	4	0.34	0.09	0.36
(1,2254)	1:149:A:ARG:HB3	1:150:A:GLN:HE21	4	0.34	0.09	0.36
(1,2730)	1:118:A:SER:H	1:147:A:LYS:H	4	0.34	0.12	0.38
(1,3331)	1:106:A:SER:HB2	1:109:A:VAL:H	4	0.34	0.09	0.32
(1,3331)	1:106:A:SER:HB3	1:109:A:VAL:H	4	0.34	0.09	0.32
(1,2733)	1:11:A:ALA:HB1	1:92:A:ASP:H	4	0.33	0.1	0.37
(1,2733)	1:11:A:ALA:HB2	1:92:A:ASP:H	4	0.33	0.1	0.37
(1,2733)	1:11:A:ALA:HB3	1:92:A:ASP:H	4	0.33	0.1	0.37
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG2	4	0.32	0.11	0.34
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG3	4	0.32	0.11	0.34
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG2	4	0.32	0.11	0.34
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG3	4	0.32	0.11	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG2	4	0.32	0.11	0.34
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG3	4	0.32	0.11	0.34
(1,3173)	1:1:A:MET:HG2	1:2:A:THR:H	4	0.31	0.12	0.36
(1,1849)	1:77:A:GLY:HA2	1:111:A:MET:HA	4	0.31	0.08	0.32
(1,2454)	1:162:A:GLU:HB2	1:165:A:LYS:HG2	4	0.3	0.11	0.29
(1,2454)	1:162:A:GLU:HB3	1:165:A:LYS:HG2	4	0.3	0.11	0.29
(1,1052)	1:128:A:LYS:H	1:131:A:GLN:HE22	4	0.3	0.15	0.24
(1,3144)	1:1:A:MET:HE1	1:52:A:LEU:H	4	0.29	0.11	0.33
(1,3144)	1:1:A:MET:HE2	1:52:A:LEU:H	4	0.29	0.11	0.33
(1,3144)	1:1:A:MET:HE3	1:52:A:LEU:H	4	0.29	0.11	0.33
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG11	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG12	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG13	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG21	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG22	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG23	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG11	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG12	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG13	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG21	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG22	4	0.29	0.07	0.29
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG23	4	0.29	0.07	0.29
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE1	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE2	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE1	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE2	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE1	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE2	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	4	0.29	0.05	0.29
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	4	0.29	0.05	0.29
(1,2908)	1:135:A:ARG:HD2	1:136:A:SER:H	4	0.29	0.09	0.3
(1,2908)	1:135:A:ARG:HD3	1:136:A:SER:H	4	0.29	0.09	0.3
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG2	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG3	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG2	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG3	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG2	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG3	4	0.29	0.1	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG2	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG3	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG2	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG3	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG2	4	0.29	0.1	0.34
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG3	4	0.29	0.1	0.34
(1,489)	1:160:A:VAL:HG11	1:164:A:ARG:HE	4	0.28	0.1	0.32
(1,489)	1:160:A:VAL:HG12	1:164:A:ARG:HE	4	0.28	0.1	0.32
(1,489)	1:160:A:VAL:HG13	1:164:A:ARG:HE	4	0.28	0.1	0.32
(1,489)	1:160:A:VAL:HG21	1:164:A:ARG:HE	4	0.28	0.1	0.32
(1,489)	1:160:A:VAL:HG22	1:164:A:ARG:HE	4	0.28	0.1	0.32
(1,489)	1:160:A:VAL:HG23	1:164:A:ARG:HE	4	0.28	0.1	0.32
(1,2564)	1:20:A:THR:HA	1:55:A:ILE:HG12	4	0.28	0.04	0.27
(1,1131)	1:1:A:MET:HE1	1:52:A:LEU:HB3	4	0.28	0.14	0.28
(1,1131)	1:1:A:MET:HE2	1:52:A:LEU:HB3	4	0.28	0.14	0.28
(1,1131)	1:1:A:MET:HE3	1:52:A:LEU:HB3	4	0.28	0.14	0.28
(1,2980)	1:132:A:ASP:H	1:132:A:ASP:HB3	4	0.28	0.06	0.31
(1,2056)	1:126:A:ASP:HB2	1:129:A:GLN:HG2	4	0.27	0.08	0.26
(1,2056)	1:126:A:ASP:HB3	1:129:A:GLN:HG2	4	0.27	0.08	0.26
(1,2785)	1:117:A:LYS:H	1:145:A:SER:H	4	0.24	0.08	0.26
(1,1730)	1:78:A:PHE:HZ	1:104:A:LYS:HE3	4	0.24	0.04	0.23
(1,2271)	1:144:A:THR:HA	1:150:A:GLN:HG2	4	0.24	0.08	0.22
(1,2302)	1:23:A:LEU:HD21	1:153:A:ASP:HA	4	0.24	0.06	0.22
(1,2302)	1:23:A:LEU:HD22	1:153:A:ASP:HA	4	0.24	0.06	0.22
(1,2302)	1:23:A:LEU:HD23	1:153:A:ASP:HA	4	0.24	0.06	0.22
(1,1251)	1:149:A:ARG:HB3	1:149:A:ARG:HE	4	0.24	0.08	0.23
(1,788)	1:8:A:VAL:HB	1:58:A:THR:H	4	0.23	0.17	0.14
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE1	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE2	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE3	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE1	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE2	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE3	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE1	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE2	4	0.23	0.06	0.23
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE3	4	0.23	0.06	0.23
(1,2630)	1:150:A:GLN:HG3	1:152:A:VAL:H	4	0.22	0.11	0.2
(1,2803)	1:116:A:ASN:HA	1:144:A:THR:H	4	0.22	0.1	0.18
(1,3156)	1:120:A:LEU:H	1:120:A:LEU:HG	4	0.21	0.05	0.2
(1,1033)	1:90:A:PHE:HB2	1:129:A:GLN:HE21	4	0.21	0.09	0.2
(1,1033)	1:90:A:PHE:HB3	1:129:A:GLN:HE21	4	0.21	0.09	0.2
(1,1294)	1:95:A:HIS:HD2	1:96:A:TYR:HA	4	0.21	0.07	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD1	4	0.21	0.08	0.18
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD2	4	0.21	0.08	0.18
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD1	4	0.21	0.1	0.18
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD2	4	0.21	0.1	0.18
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE1	4	0.2	0.05	0.22
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE2	4	0.2	0.05	0.22
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD1	4	0.2	0.07	0.2
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD2	4	0.2	0.07	0.2
(1,2559)	1:17:A:SER:HA	1:20:A:THR:HA	4	0.2	0.09	0.16
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB2	4	0.2	0.07	0.18
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB3	4	0.2	0.07	0.18
(1,2532)	1:19:A:LEU:HA	1:152:A:VAL:HA	4	0.19	0.06	0.22
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB2	4	0.19	0.09	0.16
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB3	4	0.19	0.09	0.16
(1,2818)	1:113:A:LEU:HB3	1:142:A:ILE:H	4	0.19	0.08	0.16
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD2	4	0.18	0.04	0.19
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD3	4	0.18	0.04	0.19
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE1	4	0.17	0.06	0.16
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE2	4	0.17	0.06	0.16
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE21	4	0.17	0.03	0.16
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE22	4	0.17	0.03	0.16
(1,955)	1:43:A:GLN:H	1:43:A:GLN:HE21	4	0.16	0.05	0.14
(1,1793)	1:130:A:ALA:HB1	1:131:A:GLN:HB2	4	0.15	0.02	0.16
(1,1793)	1:130:A:ALA:HB2	1:131:A:GLN:HB2	4	0.15	0.02	0.16
(1,1793)	1:130:A:ALA:HB3	1:131:A:GLN:HB2	4	0.15	0.02	0.16
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG21	4	0.15	0.01	0.15
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG22	4	0.15	0.01	0.15
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG23	4	0.15	0.01	0.15
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG21	4	0.15	0.02	0.15
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG22	4	0.15	0.02	0.15
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG23	4	0.15	0.02	0.15
(1,3302)	1:120:A:LEU:HD21	1:122:A:SER:H	4	0.15	0.07	0.12
(1,3302)	1:120:A:LEU:HD22	1:122:A:SER:H	4	0.15	0.07	0.12
(1,3302)	1:120:A:LEU:HD23	1:122:A:SER:H	4	0.15	0.07	0.12
(1,1281)	1:67:A:MET:HA	1:67:A:MET:HG3	4	0.14	0.01	0.15
(1,2735)	1:117:A:LYS:HA	1:146:A:ALA:H	4	0.14	0.04	0.12
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE1	4	0.13	0.01	0.14
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE2	4	0.13	0.01	0.14
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG2	4	0.12	0.02	0.12
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG3	4	0.12	0.02	0.12
(1,2100)	1:13:A:GLY:H	1:15:A:GLY:H	3	0.46	0.0	0.46
(1,1041)	1:23:A:LEU:HG	1:42:A:LYS:HD2	3	0.45	0.02	0.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2846)	1:140:A:PRO:HG2	1:141:A:PHE:H	3	0.43	0.03	0.44
(1,1375)	1:149:A:ARG:HB2	1:149:A:ARG:HE	3	0.42	0.01	0.43
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG11	3	0.42	0.01	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG12	3	0.42	0.01	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG13	3	0.42	0.01	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG21	3	0.42	0.01	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG22	3	0.42	0.01	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG23	3	0.42	0.01	0.42
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD11	3	0.4	0.08	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD12	3	0.4	0.08	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD13	3	0.4	0.08	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD21	3	0.4	0.08	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD22	3	0.4	0.08	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD23	3	0.4	0.08	0.46
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD11	3	0.39	0.0	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD12	3	0.39	0.0	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD13	3	0.39	0.0	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD11	3	0.39	0.0	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD12	3	0.39	0.0	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD13	3	0.39	0.0	0.39
(1,1130)	1:51:A:CYS:HB2	1:52:A:LEU:HB2	3	0.39	0.18	0.52
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB2	3	0.38	0.15	0.43
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB3	3	0.38	0.15	0.43
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG12	3	0.38	0.04	0.4
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG13	3	0.38	0.04	0.4
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG12	3	0.38	0.04	0.4
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG13	3	0.38	0.04	0.4
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD1	3	0.36	0.07	0.32
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD2	3	0.36	0.07	0.32
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG12	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG13	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG12	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG13	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG12	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG13	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG12	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG13	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG12	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG13	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG12	3	0.36	0.01	0.37
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG13	3	0.36	0.01	0.37
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE1	3	0.35	0.04	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE2	3	0.35	0.04	0.38
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE1	3	0.35	0.04	0.38
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE2	3	0.35	0.04	0.38
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE1	3	0.35	0.04	0.38
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE2	3	0.35	0.04	0.38
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	3	0.34	0.16	0.46
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	3	0.34	0.16	0.46
(1,2193)	1:143:A:GLU:HG3	1:144:A:THR:H	3	0.33	0.14	0.4
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE1	3	0.33	0.13	0.35
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE2	3	0.33	0.13	0.35
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG2	3	0.33	0.1	0.36
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG3	3	0.33	0.1	0.36
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD1	3	0.33	0.14	0.37
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD2	3	0.33	0.14	0.37
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD1	3	0.33	0.14	0.37
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD2	3	0.33	0.14	0.37
(1,2935)	1:73:A:ARG:H	1:73:A:ARG:HE	3	0.33	0.08	0.36
(1,1837)	1:77:A:GLY:HA3	1:111:A:MET:HA	3	0.32	0.02	0.32
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	3	0.32	0.07	0.3
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	3	0.32	0.07	0.3
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	3	0.32	0.07	0.3
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	3	0.32	0.07	0.3
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB1	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB2	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB3	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB1	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB2	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB3	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB1	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB2	3	0.32	0.09	0.33
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB3	3	0.32	0.09	0.33
(1,114)	1:164:A:ARG:HA	1:164:A:ARG:HE	3	0.31	0.13	0.24
(1,2574)	1:84:A:ILE:HD11	1:123:A:ARG:HE	3	0.31	0.11	0.39
(1,2574)	1:84:A:ILE:HD12	1:123:A:ARG:HE	3	0.31	0.11	0.39
(1,2574)	1:84:A:ILE:HD13	1:123:A:ARG:HE	3	0.31	0.11	0.39
(1,39)	1:64:A:TYR:HD1	1:65:A:SER:H	3	0.31	0.05	0.3
(1,39)	1:64:A:TYR:HD2	1:65:A:SER:H	3	0.31	0.05	0.3
(1,2562)	1:20:A:THR:HA	1:23:A:LEU:HG	3	0.3	0.11	0.36
(1,2764)	1:19:A:LEU:HG	1:146:A:ALA:H	3	0.3	0.13	0.25
(1,1632)	1:4:A:TYR:HD1	1:51:A:CYS:HB3	3	0.29	0.05	0.31
(1,1632)	1:4:A:TYR:HD2	1:51:A:CYS:HB3	3	0.29	0.05	0.31
(1,2050)	1:128:A:LYS:H	1:129:A:GLN:HG2	3	0.28	0.13	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1077)	1:4:A:TYR:HE1	1:51:A:CYS:HA	3	0.28	0.16	0.21
(1,1077)	1:4:A:TYR:HE2	1:51:A:CYS:HA	3	0.28	0.16	0.21
(1,824)	1:119:A:ASP:H	2:201:A:GNP:HN1	3	0.27	0.11	0.29
(1,947)	1:83:A:ALA:H	1:90:A:PHE:H	3	0.26	0.12	0.23
(1,1952)	1:123:A:ARG:HA	1:125:A:VAL:H	3	0.26	0.07	0.31
(1,2712)	1:11:A:ALA:HB1	1:89:A:SER:H	3	0.26	0.13	0.24
(1,2712)	1:11:A:ALA:HB2	1:89:A:SER:H	3	0.26	0.13	0.24
(1,2712)	1:11:A:ALA:HB3	1:89:A:SER:H	3	0.26	0.13	0.24
(1,1699)	1:72:A:MET:HG2	1:103:A:VAL:HB	3	0.26	0.1	0.24
(1,1699)	1:72:A:MET:HG3	1:103:A:VAL:HB	3	0.26	0.1	0.24
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD1	3	0.25	0.17	0.16
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD2	3	0.25	0.17	0.16
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG21	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG22	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG23	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG21	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG22	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG23	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG21	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG22	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG23	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG21	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG22	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG23	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG21	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG22	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG23	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG21	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG22	3	0.24	0.08	0.25
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG23	3	0.24	0.08	0.25
(1,258)	1:7:A:VAL:HG11	1:72:A:MET:HA	3	0.24	0.08	0.29
(1,258)	1:7:A:VAL:HG12	1:72:A:MET:HA	3	0.24	0.08	0.29
(1,258)	1:7:A:VAL:HG13	1:72:A:MET:HA	3	0.24	0.08	0.29
(1,815)	1:41:A:ARG:HD2	1:52:A:LEU:HB3	3	0.24	0.09	0.2
(1,815)	1:41:A:ARG:HD3	1:52:A:LEU:HB3	3	0.24	0.09	0.2
(1,2703)	1:22:A:GLN:HE21	1:148:A:THR:H	3	0.24	0.09	0.28
(1,2703)	1:22:A:GLN:HE22	1:148:A:THR:H	3	0.24	0.09	0.28
(1,164)	1:83:A:ALA:H	1:86:A:ASN:HB2	3	0.23	0.07	0.25
(1,1321)	1:56:A:LEU:HD11	1:71:A:TYR:HA	3	0.23	0.08	0.27
(1,1321)	1:56:A:LEU:HD12	1:71:A:TYR:HA	3	0.23	0.08	0.27
(1,1321)	1:56:A:LEU:HD13	1:71:A:TYR:HA	3	0.23	0.08	0.27
(1,1321)	1:56:A:LEU:HD21	1:71:A:TYR:HA	3	0.23	0.08	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1321)	1:56:A:LEU:HD22	1:71:A:TYR:HA	3	0.23	0.08	0.27
(1,1321)	1:56:A:LEU:HD23	1:71:A:TYR:HA	3	0.23	0.08	0.27
(1,3259)	1:113:A:LEU:H	1:141:A:PHE:HB3	3	0.22	0.05	0.25
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA2	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA3	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA2	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA3	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA2	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA3	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA2	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA3	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA2	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA3	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA2	3	0.22	0.06	0.21
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA3	3	0.22	0.06	0.21
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD2	3	0.22	0.07	0.22
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD3	3	0.22	0.07	0.22
(1,2683)	1:72:A:MET:H	1:75:A:GLY:H	3	0.21	0.07	0.2
(1,2897)	1:75:A:GLY:H	1:77:A:GLY:H	3	0.21	0.1	0.15
(1,1902)	1:116:A:ASN:HA	1:144:A:THR:HA	3	0.2	0.05	0.19
(1,2416)	1:110:A:PRO:HA	1:163:A:ILE:HA	3	0.2	0.07	0.25
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD11	3	0.2	0.06	0.22
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD12	3	0.2	0.06	0.22
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD13	3	0.2	0.06	0.22
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG2	3	0.19	0.07	0.19
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG3	3	0.19	0.07	0.19
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG2	3	0.19	0.07	0.19
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG3	3	0.19	0.07	0.19
(1,2190)	1:44:A:VAL:HG21	1:51:A:CYS:H	3	0.19	0.03	0.2
(1,2190)	1:44:A:VAL:HG22	1:51:A:CYS:H	3	0.19	0.03	0.2
(1,2190)	1:44:A:VAL:HG23	1:51:A:CYS:H	3	0.19	0.03	0.2
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	3	0.19	0.06	0.17
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD22	3	0.19	0.06	0.17
(1,2272)	1:144:A:THR:HA	1:150:A:GLN:HG3	3	0.19	0.02	0.2
(1,3005)	1:90:A:PHE:HE1	1:131:A:GLN:H	3	0.19	0.07	0.18
(1,3005)	1:90:A:PHE:HE2	1:131:A:GLN:H	3	0.19	0.07	0.18
(1,108)	1:166:A:HIS:HB3	1:167:A:LYS:H	3	0.18	0.07	0.15
(1,148)	1:28:A:PHE:HE1	2:201:A:GNP:H1'	3	0.18	0.06	0.16
(1,148)	1:28:A:PHE:HE2	2:201:A:GNP:H1'	3	0.18	0.06	0.16
(1,673)	1:35:A:SER:HA	1:36:A:ILE:H	3	0.18	0.06	0.15
(1,830)	1:146:A:ALA:HB1	2:201:A:GNP:HN1	3	0.17	0.02	0.18
(1,830)	1:146:A:ALA:HB2	2:201:A:GNP:HN1	3	0.17	0.02	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,830)	1:146:A:ALA:HB3	2:201:A:GNP:HN1	3	0.17	0.02	0.18
(1,1693)	1:72:A:MET:HB2	1:103:A:VAL:HA	3	0.17	0.03	0.17
(1,1693)	1:72:A:MET:HB3	1:103:A:VAL:HA	3	0.17	0.03	0.17
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG11	3	0.16	0.03	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG12	3	0.16	0.03	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG13	3	0.16	0.03	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG21	3	0.16	0.03	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG22	3	0.16	0.03	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG23	3	0.16	0.03	0.15
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE1	3	0.16	0.05	0.16
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE2	3	0.16	0.05	0.16
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE1	3	0.16	0.05	0.16
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE2	3	0.16	0.05	0.16
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE1	3	0.16	0.05	0.16
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE2	3	0.16	0.05	0.16
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD11	3	0.16	0.06	0.12
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD12	3	0.16	0.06	0.12
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD13	3	0.16	0.06	0.12
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE1	3	0.16	0.04	0.13
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE2	3	0.16	0.04	0.13
(1,323)	1:44:A:VAL:H	1:52:A:LEU:HA	3	0.16	0.02	0.16
(1,73)	1:102:A:ARG:H	1:104:A:LYS:H	3	0.16	0.03	0.17
(1,940)	1:26:A:ASN:H	1:26:A:ASN:HD22	3	0.16	0.04	0.15
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD21	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD22	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD23	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD21	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD22	3	0.16	0.03	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD23	3	0.16	0.03	0.17
(1,2869)	1:163:A:ILE:HG21	1:166:A:HIS:H	3	0.15	0.03	0.15
(1,2869)	1:163:A:ILE:HG22	1:166:A:HIS:H	3	0.15	0.03	0.15
(1,2869)	1:163:A:ILE:HG23	1:166:A:HIS:H	3	0.15	0.03	0.15
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG21	3	0.15	0.01	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG22	3	0.15	0.01	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG23	3	0.15	0.01	0.16
(1,1999)	1:132:A:ASP:HA	1:135:A:ARG:HE	3	0.15	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,289)	1:24:A:ILE:HD11	1:40:A:TYR:HB2	3	0.14	0.03	0.13
(1,289)	1:24:A:ILE:HD12	1:40:A:TYR:HB2	3	0.14	0.03	0.13
(1,289)	1:24:A:ILE:HD13	1:40:A:TYR:HB2	3	0.14	0.03	0.13
(1,1876)	1:114:A:VAL:HG11	1:144:A:THR:H	3	0.14	0.02	0.16
(1,1876)	1:114:A:VAL:HG12	1:144:A:THR:H	3	0.14	0.02	0.16
(1,1876)	1:114:A:VAL:HG13	1:144:A:THR:H	3	0.14	0.02	0.16
(1,1876)	1:114:A:VAL:HG21	1:144:A:THR:H	3	0.14	0.02	0.16
(1,1876)	1:114:A:VAL:HG22	1:144:A:THR:H	3	0.14	0.02	0.16
(1,1876)	1:114:A:VAL:HG23	1:144:A:THR:H	3	0.14	0.02	0.16
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD11	3	0.14	0.04	0.12
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD12	3	0.14	0.04	0.12
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD13	3	0.14	0.04	0.12
(1,482)	1:24:A:ILE:HG21	1:26:A:ASN:H	3	0.14	0.01	0.14
(1,482)	1:24:A:ILE:HG22	1:26:A:ASN:H	3	0.14	0.01	0.14
(1,482)	1:24:A:ILE:HG23	1:26:A:ASN:H	3	0.14	0.01	0.14
(1,1385)	1:84:A:ILE:HD11	1:123:A:ARG:HB3	3	0.13	0.03	0.12
(1,1385)	1:84:A:ILE:HD12	1:123:A:ARG:HB3	3	0.13	0.03	0.12
(1,1385)	1:84:A:ILE:HD13	1:123:A:ARG:HB3	3	0.13	0.03	0.12
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG11	3	0.13	0.02	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG12	3	0.13	0.02	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG13	3	0.13	0.02	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG21	3	0.13	0.02	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG22	3	0.13	0.02	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG23	3	0.13	0.02	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG11	3	0.13	0.02	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG12	3	0.13	0.02	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG13	3	0.13	0.02	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG21	3	0.13	0.02	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG22	3	0.13	0.02	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG23	3	0.13	0.02	0.14
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG21	3	0.12	0.0	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG22	3	0.12	0.0	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG23	3	0.12	0.0	0.12
(1,756)	1:64:A:TYR:H	1:65:A:SER:H	3	0.12	0.01	0.11
(1,3158)	1:1:A:MET:HA	1:1:A:MET:HG3	3	0.11	0.01	0.11
(1,1112)	1:50:A:THR:HA	1:51:A:CYS:HB3	2	0.52	0.0	0.52
(1,2089)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	2	0.5	0.0	0.5
(1,2089)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	2	0.5	0.0	0.5
(1,2089)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	2	0.5	0.0	0.5
(1,2089)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	2	0.5	0.0	0.5
(1,2089)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	2	0.5	0.0	0.5
(1,2089)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	2	0.5	0.0	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2287)	1:151:A:GLY:HA2	1:153:A:ASP:HB2	2	0.48	0.07	0.48
(1,2287)	1:151:A:GLY:HA2	1:153:A:ASP:HB3	2	0.48	0.07	0.48
(1,471)	1:22:A:GLN:HE21	1:28:A:PHE:HB3	2	0.46	0.0	0.46
(1,1652)	1:95:A:HIS:HA	1:99:A:GLN:HG2	2	0.45	0.12	0.45
(1,1652)	1:95:A:HIS:HA	1:99:A:GLN:HG3	2	0.45	0.12	0.45
(1,2534)	1:123:A:ARG:HB3	1:123:A:ARG:HE	2	0.42	0.01	0.42
(1,1210)	1:56:A:LEU:HD21	1:71:A:TYR:HB3	2	0.4	0.01	0.4
(1,1210)	1:56:A:LEU:HD22	1:71:A:TYR:HB3	2	0.4	0.01	0.4
(1,1210)	1:56:A:LEU:HD23	1:71:A:TYR:HB3	2	0.4	0.01	0.4
(1,2308)	1:153:A:ASP:HB2	1:154:A:ASP:HB2	2	0.4	0.05	0.4
(1,2308)	1:153:A:ASP:HB3	1:154:A:ASP:HB2	2	0.4	0.05	0.4
(1,2451)	1:2:A:THR:HB	1:51:A:CYS:HB3	2	0.4	0.05	0.4
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD11	2	0.39	0.05	0.39
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD12	2	0.39	0.05	0.39
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD13	2	0.39	0.05	0.39
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD21	2	0.39	0.05	0.39
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD22	2	0.39	0.05	0.39
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD23	2	0.39	0.05	0.39
(1,1284)	1:67:A:MET:HG2	1:71:A:TYR:HD1	2	0.38	0.02	0.38
(1,1284)	1:67:A:MET:HG2	1:71:A:TYR:HD2	2	0.38	0.02	0.38
(1,1284)	1:67:A:MET:HG3	1:71:A:TYR:HD1	2	0.38	0.02	0.38
(1,1284)	1:67:A:MET:HG3	1:71:A:TYR:HD2	2	0.38	0.02	0.38
(1,2835)	1:73:A:ARG:HB2	1:73:A:ARG:HE	2	0.38	0.02	0.38
(1,2835)	1:73:A:ARG:HB3	1:73:A:ARG:HE	2	0.38	0.02	0.38
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD11	2	0.38	0.07	0.38
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD12	2	0.38	0.07	0.38
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD13	2	0.38	0.07	0.38
(1,351)	1:62:A:GLU:H	1:62:A:GLU:HG2	2	0.38	0.0	0.38
(1,351)	1:62:A:GLU:H	1:62:A:GLU:HG3	2	0.38	0.0	0.38
(1,2463)	1:4:A:TYR:HE1	1:167:A:LYS:HB3	2	0.38	0.17	0.38
(1,2463)	1:4:A:TYR:HE2	1:167:A:LYS:HB3	2	0.38	0.17	0.38
(1,2886)	1:21:A:ILE:HG12	1:40:A:TYR:HE1	2	0.38	0.12	0.38
(1,2886)	1:21:A:ILE:HG12	1:40:A:TYR:HE2	2	0.38	0.12	0.38
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG21	2	0.38	0.03	0.38
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG22	2	0.38	0.03	0.38
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG23	2	0.38	0.03	0.38
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG21	2	0.38	0.03	0.38
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG22	2	0.38	0.03	0.38
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG23	2	0.38	0.03	0.38
(1,2668)	1:99:A:GLN:HA	1:102:A:ARG:HE	2	0.36	0.1	0.36
(1,1404)	1:5:A:LYS:H	1:76:A:GLU:HG3	2	0.36	0.01	0.36
(1,1243)	1:106:A:SER:HA	1:107:A:GLU:HG2	2	0.35	0.11	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1243)	1:106:A:SER:HA	1:107:A:GLU:HG3	2	0.35	0.11	0.35
(1,701)	1:36:A:ILE:HA	1:37:A:GLU:H	2	0.34	0.0	0.34
(1,221)	1:1:A:MET:HB3	1:50:A:THR:HB	2	0.34	0.1	0.34
(1,1132)	1:1:A:MET:HE1	1:52:A:LEU:HB2	2	0.34	0.05	0.34
(1,1132)	1:1:A:MET:HE2	1:52:A:LEU:HB2	2	0.34	0.05	0.34
(1,1132)	1:1:A:MET:HE3	1:52:A:LEU:HB2	2	0.34	0.05	0.34
(1,1175)	1:23:A:LEU:HD11	1:156:A:PHE:HB3	2	0.34	0.06	0.34
(1,1175)	1:23:A:LEU:HD12	1:156:A:PHE:HB3	2	0.34	0.06	0.34
(1,1175)	1:23:A:LEU:HD13	1:156:A:PHE:HB3	2	0.34	0.06	0.34
(1,1175)	1:23:A:LEU:HD21	1:156:A:PHE:HB3	2	0.34	0.06	0.34
(1,1175)	1:23:A:LEU:HD22	1:156:A:PHE:HB3	2	0.34	0.06	0.34
(1,1175)	1:23:A:LEU:HD23	1:156:A:PHE:HB3	2	0.34	0.06	0.34
(1,1365)	1:5:A:LYS:HB2	1:74:A:THR:HB	2	0.34	0.05	0.34
(1,1365)	1:5:A:LYS:HB3	1:74:A:THR:HB	2	0.34	0.05	0.34
(1,2547)	1:164:A:ARG:HB2	1:165:A:LYS:H	2	0.34	0.01	0.34
(1,2547)	1:164:A:ARG:HB3	1:165:A:LYS:H	2	0.34	0.01	0.34
(1,916)	1:22:A:GLN:HE21	1:27:A:HIS:HA	2	0.32	0.12	0.32
(1,916)	1:22:A:GLN:HE22	1:27:A:HIS:HA	2	0.32	0.12	0.32
(1,609)	1:45:A:VAL:HB	1:47:A:ASP:H	2	0.32	0.02	0.32
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG21	2	0.32	0.02	0.32
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG22	2	0.32	0.02	0.32
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG23	2	0.32	0.02	0.32
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG21	2	0.32	0.02	0.32
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG22	2	0.32	0.02	0.32
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG23	2	0.32	0.02	0.32
(1,523)	1:29:A:VAL:HG11	1:31:A:GLU:H	2	0.32	0.13	0.32
(1,523)	1:29:A:VAL:HG12	1:31:A:GLU:H	2	0.32	0.13	0.32
(1,523)	1:29:A:VAL:HG13	1:31:A:GLU:H	2	0.32	0.13	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD11	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD12	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD13	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD11	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD12	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD13	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD11	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD12	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD13	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD11	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD12	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD13	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD11	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD12	2	0.32	0.0	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD13	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD11	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD12	2	0.32	0.0	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD13	2	0.32	0.0	0.32
(1,735)	1:37:A:GLU:HA	1:37:A:GLU:HG2	2	0.32	0.01	0.32
(1,735)	1:37:A:GLU:HA	1:37:A:GLU:HG3	2	0.32	0.01	0.32
(1,750)	1:63:A:GLU:HG2	1:64:A:TYR:H	2	0.32	0.1	0.32
(1,750)	1:63:A:GLU:HG3	1:64:A:TYR:H	2	0.32	0.1	0.32
(1,1937)	1:8:A:VAL:HA	1:78:A:PHE:HA	2	0.32	0.16	0.32
(1,338)	1:24:A:ILE:HD11	1:42:A:LYS:H	2	0.31	0.01	0.31
(1,338)	1:24:A:ILE:HD12	1:42:A:LYS:H	2	0.31	0.01	0.31
(1,338)	1:24:A:ILE:HD13	1:42:A:LYS:H	2	0.31	0.01	0.31
(1,2625)	1:23:A:LEU:HD11	1:156:A:PHE:HB2	2	0.31	0.09	0.31
(1,2625)	1:23:A:LEU:HD12	1:156:A:PHE:HB2	2	0.31	0.09	0.31
(1,2625)	1:23:A:LEU:HD13	1:156:A:PHE:HB2	2	0.31	0.09	0.31
(1,1495)	1:99:A:GLN:HA	1:99:A:GLN:HE22	2	0.3	0.06	0.3
(1,1634)	1:22:A:GLN:HE21	1:149:A:ARG:HE	2	0.3	0.1	0.3
(1,1634)	1:22:A:GLN:HE22	1:149:A:ARG:HE	2	0.3	0.1	0.3
(1,61)	1:153:A:ASP:HB2	1:154:A:ASP:H	2	0.3	0.0	0.3
(1,61)	1:153:A:ASP:HB3	1:154:A:ASP:H	2	0.3	0.0	0.3
(1,1252)	1:63:A:GLU:HA	1:64:A:TYR:H	2	0.3	0.01	0.3
(1,1731)	1:100:A:ILE:HG21	1:104:A:LYS:HE2	2	0.3	0.16	0.3
(1,1731)	1:100:A:ILE:HG22	1:104:A:LYS:HE2	2	0.3	0.16	0.3
(1,1731)	1:100:A:ILE:HG23	1:104:A:LYS:HE2	2	0.3	0.16	0.3
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD11	2	0.3	0.01	0.3
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD12	2	0.3	0.01	0.3
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD13	2	0.3	0.01	0.3
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD21	2	0.3	0.01	0.3
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD22	2	0.3	0.01	0.3
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD23	2	0.3	0.01	0.3
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG21	2	0.29	0.01	0.29
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG22	2	0.29	0.01	0.29
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG23	2	0.29	0.01	0.29
(1,1194)	1:56:A:LEU:HD11	1:57:A:ASP:H	2	0.28	0.12	0.28
(1,1194)	1:56:A:LEU:HD12	1:57:A:ASP:H	2	0.28	0.12	0.28
(1,1194)	1:56:A:LEU:HD13	1:57:A:ASP:H	2	0.28	0.12	0.28
(1,1194)	1:56:A:LEU:HD21	1:57:A:ASP:H	2	0.28	0.12	0.28
(1,1194)	1:56:A:LEU:HD22	1:57:A:ASP:H	2	0.28	0.12	0.28
(1,1194)	1:56:A:LEU:HD23	1:57:A:ASP:H	2	0.28	0.12	0.28
(1,2606)	1:21:A:ILE:HA	1:40:A:TYR:HD1	2	0.28	0.16	0.28
(1,2606)	1:21:A:ILE:HA	1:40:A:TYR:HD2	2	0.28	0.16	0.28
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG21	2	0.28	0.13	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG22	2	0.28	0.13	0.28
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG23	2	0.28	0.13	0.28
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG21	2	0.28	0.13	0.28
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG22	2	0.28	0.13	0.28
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG23	2	0.28	0.13	0.28
(1,1117)	1:46:A:ILE:HD11	1:51:A:CYS:HB3	2	0.28	0.1	0.28
(1,1117)	1:46:A:ILE:HD12	1:51:A:CYS:HB3	2	0.28	0.1	0.28
(1,1117)	1:46:A:ILE:HD13	1:51:A:CYS:HB3	2	0.28	0.1	0.28
(1,491)	1:29:A:VAL:HA	1:31:A:GLU:H	2	0.27	0.15	0.27
(1,1880)	1:116:A:ASN:HA	1:144:A:THR:HB	2	0.27	0.04	0.27
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG11	2	0.27	0.05	0.27
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG12	2	0.27	0.05	0.27
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG13	2	0.27	0.05	0.27
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG21	2	0.27	0.04	0.27
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG22	2	0.27	0.04	0.27
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG23	2	0.27	0.04	0.27
(1,2487)	1:168:A:GLU:H	1:168:A:GLU:HG3	2	0.27	0.13	0.27
(1,447)	1:22:A:GLN:HE21	1:28:A:PHE:H	2	0.26	0.04	0.26
(1,447)	1:22:A:GLN:HE22	1:28:A:PHE:H	2	0.26	0.04	0.26
(1,991)	1:83:A:ALA:HB1	1:85:A:ASN:HD21	2	0.26	0.06	0.26
(1,991)	1:83:A:ALA:HB2	1:85:A:ASN:HD21	2	0.26	0.06	0.26
(1,991)	1:83:A:ALA:HB3	1:85:A:ASN:HD21	2	0.26	0.06	0.26
(1,1176)	1:23:A:LEU:HD11	1:156:A:PHE:HB3	2	0.26	0.08	0.26
(1,1176)	1:23:A:LEU:HD12	1:156:A:PHE:HB3	2	0.26	0.08	0.26
(1,1176)	1:23:A:LEU:HD13	1:156:A:PHE:HB3	2	0.26	0.08	0.26
(1,1846)	1:41:A:ARG:HD2	1:52:A:LEU:HB2	2	0.26	0.04	0.26
(1,1846)	1:41:A:ARG:HD3	1:52:A:LEU:HB2	2	0.26	0.04	0.26
(1,2250)	1:22:A:GLN:HE21	1:149:A:ARG:HB2	2	0.26	0.12	0.26
(1,2250)	1:22:A:GLN:HE21	1:149:A:ARG:HB3	2	0.26	0.12	0.26
(1,2250)	1:22:A:GLN:HE22	1:149:A:ARG:HB2	2	0.26	0.12	0.26
(1,2250)	1:22:A:GLN:HE22	1:149:A:ARG:HB3	2	0.26	0.12	0.26
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG11	2	0.26	0.1	0.26
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG12	2	0.26	0.1	0.26
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG13	2	0.26	0.1	0.26
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG21	2	0.26	0.1	0.26
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG22	2	0.26	0.1	0.26
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG23	2	0.26	0.1	0.26
(1,2521)	1:84:A:ILE:HB	1:123:A:ARG:HE	2	0.26	0.04	0.26
(1,840)	1:41:A:ARG:HD2	1:54:A:ASP:HB2	2	0.25	0.07	0.25
(1,840)	1:41:A:ARG:HD2	1:54:A:ASP:HB3	2	0.25	0.07	0.25
(1,840)	1:41:A:ARG:HD3	1:54:A:ASP:HB2	2	0.25	0.07	0.25
(1,840)	1:41:A:ARG:HD3	1:54:A:ASP:HB3	2	0.25	0.07	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1394)	1:75:A:GLY:HA3	1:77:A:GLY:H	2	0.25	0.15	0.25
(1,2069)	1:90:A:PHE:HD1	1:130:A:ALA:HA	2	0.25	0.03	0.25
(1,2069)	1:90:A:PHE:HD2	1:130:A:ALA:HA	2	0.25	0.03	0.25
(1,2824)	1:18:A:ALA:HB1	1:28:A:PHE:HD1	2	0.25	0.09	0.25
(1,2824)	1:18:A:ALA:HB1	1:28:A:PHE:HD2	2	0.25	0.09	0.25
(1,2824)	1:18:A:ALA:HB2	1:28:A:PHE:HD1	2	0.25	0.09	0.25
(1,2824)	1:18:A:ALA:HB2	1:28:A:PHE:HD2	2	0.25	0.09	0.25
(1,2824)	1:18:A:ALA:HB3	1:28:A:PHE:HD1	2	0.25	0.09	0.25
(1,2824)	1:18:A:ALA:HB3	1:28:A:PHE:HD2	2	0.25	0.09	0.25
(1,656)	1:36:A:ILE:HD11	1:37:A:GLU:HA	2	0.24	0.08	0.24
(1,656)	1:36:A:ILE:HD12	1:37:A:GLU:HA	2	0.24	0.08	0.24
(1,656)	1:36:A:ILE:HD13	1:37:A:GLU:HA	2	0.24	0.08	0.24
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG11	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG12	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG13	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG21	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG22	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG23	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG11	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG12	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG13	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG21	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG22	2	0.24	0.1	0.24
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG23	2	0.24	0.1	0.24
(1,1608)	1:9:A:VAL:HB	1:96:A:TYR:HB3	2	0.24	0.12	0.24
(1,1689)	1:102:A:ARG:H	1:102:A:ARG:HG2	2	0.24	0.02	0.24
(1,1689)	1:102:A:ARG:H	1:102:A:ARG:HG3	2	0.24	0.02	0.24
(1,623)	1:32:A:TYR:HE1	1:34:A:PRO:HA	2	0.24	0.04	0.24
(1,623)	1:32:A:TYR:HE2	1:34:A:PRO:HA	2	0.24	0.04	0.24
(1,1050)	1:90:A:PHE:HD1	1:129:A:GLN:HE22	2	0.24	0.04	0.24
(1,1050)	1:90:A:PHE:HD2	1:129:A:GLN:HE22	2	0.24	0.04	0.24
(1,1128)	1:3:A:GLU:HA	1:52:A:LEU:HB3	2	0.24	0.13	0.24
(1,1690)	1:102:A:ARG:H	1:102:A:ARG:HG3	2	0.24	0.05	0.24
(1,714)	1:36:A:ILE:HG12	1:37:A:GLU:H	2	0.23	0.11	0.23
(1,714)	1:36:A:ILE:HG13	1:37:A:GLU:H	2	0.23	0.11	0.23
(1,1684)	1:102:A:ARG:H	1:102:A:ARG:HD2	2	0.23	0.04	0.23
(1,1684)	1:102:A:ARG:H	1:102:A:ARG:HD3	2	0.23	0.04	0.23
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG21	2	0.23	0.06	0.23
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG22	2	0.23	0.06	0.23
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG23	2	0.23	0.06	0.23
(1,2536)	1:144:A:THR:HA	1:152:A:VAL:HA	2	0.23	0.12	0.23
(1,495)	1:29:A:VAL:HA	1:32:A:TYR:HD1	2	0.22	0.02	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,495)	1:29:A:VAL:HA	1:32:A:TYR:HD2	2	0.22	0.02	0.22
(1,2157)	1:15:A:GLY:H	1:17:A:SER:H	2	0.22	0.02	0.22
(1,2458)	1:165:A:LYS:HB2	1:166:A:HIS:HB2	2	0.22	0.0	0.22
(1,24)	1:106:A:SER:HB2	1:107:A:GLU:H	2	0.22	0.02	0.22
(1,1007)	1:90:A:PHE:HE1	1:129:A:GLN:HE21	2	0.22	0.01	0.22
(1,1007)	1:90:A:PHE:HE2	1:129:A:GLN:HE21	2	0.22	0.01	0.22
(1,2037)	1:129:A:GLN:HA	1:132:A:ASP:HB3	2	0.21	0.04	0.21
(1,2166)	1:131:A:GLN:HG3	1:141:A:PHE:HB3	2	0.21	0.04	0.21
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG21	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG22	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG23	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG21	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG22	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG23	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG21	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG22	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG23	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG21	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG22	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG23	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG21	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG22	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG23	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG21	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG22	2	0.21	0.09	0.21
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG23	2	0.21	0.09	0.21
(1,2080)	1:131:A:GLN:HA	1:141:A:PHE:HD1	2	0.2	0.03	0.2
(1,2080)	1:131:A:GLN:HA	1:141:A:PHE:HD2	2	0.2	0.03	0.2
(1,2380)	1:159:A:LEU:HD11	1:163:A:ILE:HA	2	0.2	0.06	0.2
(1,2380)	1:159:A:LEU:HD12	1:163:A:ILE:HA	2	0.2	0.06	0.2
(1,2380)	1:159:A:LEU:HD13	1:163:A:ILE:HA	2	0.2	0.06	0.2
(1,2380)	1:159:A:LEU:HD21	1:163:A:ILE:HA	2	0.2	0.06	0.2
(1,2380)	1:159:A:LEU:HD22	1:163:A:ILE:HA	2	0.2	0.06	0.2
(1,2380)	1:159:A:LEU:HD23	1:163:A:ILE:HA	2	0.2	0.06	0.2
(1,274)	1:1:A:MET:HG3	1:2:A:THR:H	2	0.2	0.02	0.2
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD11	2	0.2	0.03	0.2
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD12	2	0.2	0.03	0.2
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD13	2	0.2	0.03	0.2
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD21	2	0.2	0.03	0.2
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD22	2	0.2	0.03	0.2
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD23	2	0.2	0.03	0.2
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD11	2	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD12	2	0.2	0.01	0.2
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD13	2	0.2	0.01	0.2
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD11	2	0.2	0.01	0.2
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD12	2	0.2	0.01	0.2
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD13	2	0.2	0.01	0.2
(1,1044)	1:125:A:VAL:HG11	1:129:A:GLN:HE22	2	0.2	0.04	0.2
(1,1044)	1:125:A:VAL:HG12	1:129:A:GLN:HE22	2	0.2	0.04	0.2
(1,1044)	1:125:A:VAL:HG13	1:129:A:GLN:HE22	2	0.2	0.04	0.2
(1,2747)	1:118:A:SER:H	1:146:A:ALA:H	2	0.19	0.06	0.19
(1,2123)	1:154:A:ASP:HA	1:157:A:TYR:H	2	0.18	0.04	0.18
(1,2797)	1:143:A:GLU:HG2	1:144:A:THR:H	2	0.18	0.05	0.18
(1,2797)	1:143:A:GLU:HG3	1:144:A:THR:H	2	0.18	0.05	0.18
(1,337)	1:23:A:LEU:HD21	1:156:A:PHE:HB3	2	0.18	0.06	0.18
(1,337)	1:23:A:LEU:HD22	1:156:A:PHE:HB3	2	0.18	0.06	0.18
(1,337)	1:23:A:LEU:HD23	1:156:A:PHE:HB3	2	0.18	0.06	0.18
(1,1664)	1:113:A:LEU:HB3	1:141:A:PHE:HE1	2	0.18	0.02	0.18
(1,1664)	1:113:A:LEU:HB3	1:141:A:PHE:HE2	2	0.18	0.02	0.18
(1,2172)	1:114:A:VAL:HA	1:142:A:ILE:HB	2	0.18	0.0	0.18
(1,2407)	1:162:A:GLU:HA	1:164:A:ARG:H	2	0.18	0.01	0.18
(1,2512)	1:4:A:TYR:HE1	1:160:A:VAL:HA	2	0.18	0.02	0.18
(1,2512)	1:4:A:TYR:HE2	1:160:A:VAL:HA	2	0.18	0.02	0.18
(1,2306)	1:135:A:ARG:H	1:135:A:ARG:HE	2	0.18	0.04	0.18
(1,2837)	1:113:A:LEU:H	1:142:A:ILE:H	2	0.18	0.04	0.18
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD11	2	0.17	0.06	0.17
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD12	2	0.17	0.06	0.17
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD13	2	0.17	0.06	0.17
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD21	2	0.17	0.06	0.17
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD22	2	0.17	0.06	0.17
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD23	2	0.17	0.06	0.17
(1,1270)	1:65:A:SER:H	1:65:A:SER:HB3	2	0.17	0.06	0.17
(1,2461)	1:167:A:LYS:HB3	1:168:A:GLU:H	2	0.17	0.06	0.17
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG21	2	0.16	0.06	0.16
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG22	2	0.16	0.06	0.16
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG23	2	0.16	0.06	0.16
(1,2646)	1:150:A:GLN:HB3	1:151:A:GLY:H	2	0.16	0.06	0.16
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD11	2	0.16	0.01	0.16
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD12	2	0.16	0.01	0.16
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD13	2	0.16	0.01	0.16
(1,2312)	1:154:A:ASP:HA	1:157:A:TYR:HD1	2	0.16	0.04	0.16
(1,2312)	1:154:A:ASP:HA	1:157:A:TYR:HD2	2	0.16	0.04	0.16
(1,819)	1:142:A:ILE:HD11	1:154:A:ASP:H	2	0.16	0.05	0.16
(1,819)	1:142:A:ILE:HD12	1:154:A:ASP:H	2	0.16	0.05	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,819)	1:142:A:ILE:HD13	1:154:A:ASP:H	2	0.16	0.05	0.16
(1,1814)	1:100:A:ILE:HD11	1:111:A:MET:HG2	2	0.15	0.01	0.15
(1,1814)	1:100:A:ILE:HD12	1:111:A:MET:HG2	2	0.15	0.01	0.15
(1,1814)	1:100:A:ILE:HD13	1:111:A:MET:HG2	2	0.15	0.01	0.15
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB1	2	0.15	0.02	0.15
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB2	2	0.15	0.02	0.15
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB3	2	0.15	0.02	0.15
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB1	2	0.15	0.02	0.15
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB2	2	0.15	0.02	0.15
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB3	2	0.15	0.02	0.15
(1,2711)	1:11:A:ALA:HB1	1:12:A:GLY:H	2	0.15	0.0	0.15
(1,2711)	1:11:A:ALA:HB2	1:12:A:GLY:H	2	0.15	0.0	0.15
(1,2711)	1:11:A:ALA:HB3	1:12:A:GLY:H	2	0.15	0.0	0.15
(1,86)	1:15:A:GLY:HA2	1:116:A:ASN:HD22	2	0.15	0.02	0.15
(1,2652)	1:148:A:THR:HB	1:150:A:GLN:H	2	0.15	0.02	0.15
(1,789)	1:58:A:THR:H	1:58:A:THR:HG21	2	0.14	0.02	0.14
(1,789)	1:58:A:THR:H	1:58:A:THR:HG22	2	0.14	0.02	0.14
(1,789)	1:58:A:THR:H	1:58:A:THR:HG23	2	0.14	0.02	0.14
(1,2275)	1:150:A:GLN:HA	1:150:A:GLN:HG2	2	0.14	0.04	0.14
(1,2554)	1:100:A:ILE:HG21	1:111:A:MET:HG3	2	0.13	0.0	0.13
(1,2554)	1:100:A:ILE:HG22	1:111:A:MET:HG3	2	0.13	0.0	0.13
(1,2554)	1:100:A:ILE:HG23	1:111:A:MET:HG3	2	0.13	0.0	0.13
(1,2650)	1:72:A:MET:HE1	1:100:A:ILE:H	2	0.12	0.01	0.12
(1,2650)	1:72:A:MET:HE2	1:100:A:ILE:H	2	0.12	0.01	0.12
(1,2650)	1:72:A:MET:HE3	1:100:A:ILE:H	2	0.12	0.01	0.12
(1,2918)	1:133:A:LEU:HD11	1:136:A:SER:H	2	0.12	0.01	0.12
(1,2918)	1:133:A:LEU:HD12	1:136:A:SER:H	2	0.12	0.01	0.12
(1,2918)	1:133:A:LEU:HD13	1:136:A:SER:H	2	0.12	0.01	0.12
(1,2918)	1:133:A:LEU:HD21	1:136:A:SER:H	2	0.12	0.01	0.12
(1,2918)	1:133:A:LEU:HD22	1:136:A:SER:H	2	0.12	0.01	0.12
(1,2918)	1:133:A:LEU:HD23	1:136:A:SER:H	2	0.12	0.01	0.12
(1,2653)	1:75:A:GLY:H	1:78:A:PHE:HE1	2	0.12	0.02	0.12
(1,2653)	1:75:A:GLY:H	1:78:A:PHE:HE2	2	0.12	0.02	0.12
(1,498)	1:28:A:PHE:HD1	1:29:A:VAL:HA	2	0.12	0.01	0.12
(1,498)	1:28:A:PHE:HD2	1:29:A:VAL:HA	2	0.12	0.01	0.12
(1,2569)	1:156:A:PHE:H	1:156:A:PHE:HE1	2	0.12	0.02	0.12
(1,2569)	1:156:A:PHE:H	1:156:A:PHE:HE2	2	0.12	0.02	0.12
(1,2121)	1:134:A:ALA:HB1	1:139:A:ILE:HB	2	0.12	0.0	0.12
(1,2121)	1:134:A:ALA:HB2	1:139:A:ILE:HB	2	0.12	0.0	0.12
(1,2121)	1:134:A:ALA:HB3	1:139:A:ILE:HB	2	0.12	0.0	0.12
(1,2220)	1:147:A:LYS:HG2	1:148:A:THR:HA	2	0.12	0.0	0.12
(1,2220)	1:147:A:LYS:HG3	1:148:A:THR:HA	2	0.12	0.0	0.12

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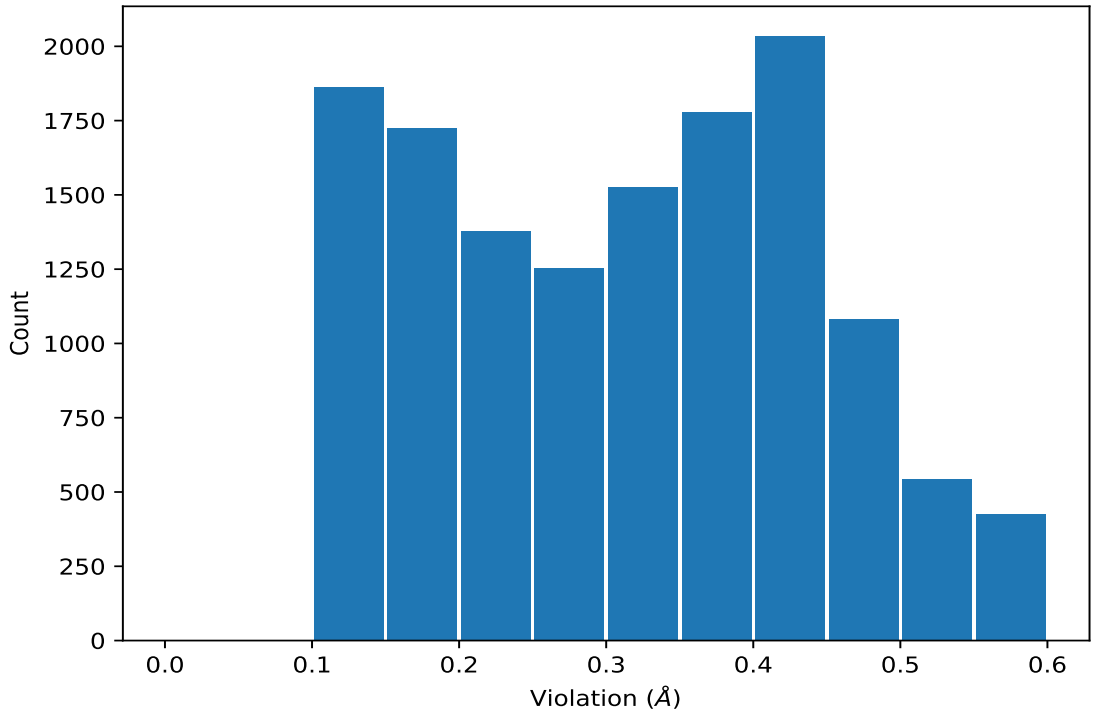
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,2)	3:202:A:MG:MG	2:201:A:GNP:O2B	2	0.11	0.0	0.11
(1,2986)	1:131:A:GLN:HB3	1:132:A:ASP:H	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	15	0.57
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	14	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	1	0.57
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	1	0.57
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	19	0.57
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	19	0.57
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	17	0.57
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	2	0.57
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	17	0.57
(1,1412)	1:75:A:GLY:HA3	1:76:A:GLU:HG3	5	0.57
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	2	0.57
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	10	0.57
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	15	0.57
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	1	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	3	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	4	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	5	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	6	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	7	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	10	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	12	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	14	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	17	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	19	0.56
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	5	0.56
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	1	0.56
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	19	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	2	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	2	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	3	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	3	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	5	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	5	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	7	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	7	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	8	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	8	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	9	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	9	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	11	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	11	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	12	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	12	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	13	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	15	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	15	0.56
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	18	0.56
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	18	0.56
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	9	0.56
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	9	0.56
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	7	0.56
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	7	0.56
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	20	0.56
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	20	0.56
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	4	0.56
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	7	0.56
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	8	0.56
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	11	0.56
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	13	0.56
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	14	0.56
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	1	0.56
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	3	0.56
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	7	0.56
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	10	0.56
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	12	0.56
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	13	0.56
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	14	0.56
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	19	0.56
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	19	0.56
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	4	0.56
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	5	0.56
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	9	0.56
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	11	0.56
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	12	0.56
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	19	0.56
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	20	0.56
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	12	0.56
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	12	0.56
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	12	0.56
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	13	0.56
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	13	0.56
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	13	0.56
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	14	0.56
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	14	0.56
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	14	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1652)	1:95:A:HIS:HA	1:99:A:GLN:HG2	10	0.56
(1,1652)	1:95:A:HIS:HA	1:99:A:GLN:HG3	10	0.56
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	6	0.56
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	7	0.56
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	13	0.56
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	15	0.56
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	16	0.56
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	18	0.56
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	7	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	1	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	4	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	5	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	6	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	7	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	8	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	9	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	11	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	12	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	13	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	14	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	17	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	18	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	19	0.56
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	20	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	10	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	10	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	11	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	11	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	14	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	14	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	18	0.56
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	18	0.56
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD21	13	0.56
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD22	13	0.56
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD23	13	0.56
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	11	0.56
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	11	0.56
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	11	0.56
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	11	0.56
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	11	0.56
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	11	0.56
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	14	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	14	0.56
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	14	0.56
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	14	0.56
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	14	0.56
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	14	0.56
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	16	0.56
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	16	0.56
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	16	0.56
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	16	0.56
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	16	0.56
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	16	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	6	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	6	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	6	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	17	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	17	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	17	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	18	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	18	0.56
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	18	0.56
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	7	0.56
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	7	0.56
(1,1120)	1:12:A:GLY:H	1:61:A:GLN:HB3	15	0.56
(1,1120)	1:12:A:GLY:H	1:61:A:GLN:HB3	16	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	4	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	7	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	10	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	11	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	12	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	13	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	17	0.56
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	18	0.56
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	14	0.56
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	15	0.56
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	16	0.56
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	16	0.56
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	17	0.56
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE2	1	0.56
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE3	1	0.56
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	8	0.55
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	20	0.55
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	6	0.55
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	8	0.55
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	14	0.55
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	19	0.55
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	20	0.55
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	10	0.55
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	10	0.55
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	15	0.55
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	15	0.55
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	19	0.55
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	19	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	1	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	2	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	4	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	7	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	8	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	9	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	11	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	12	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	13	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	14	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	15	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	17	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	18	0.55
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	20	0.55
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	9	0.55
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	1	0.55
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	17	0.55
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	5	0.55
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	8	0.55
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	9	0.55
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	10	0.55
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	11	0.55
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	12	0.55
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	14	0.55
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	7	0.55
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	7	0.55
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	4	0.55
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	4	0.55
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	10	0.55
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	10	0.55
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	16	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	16	0.55
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	17	0.55
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	17	0.55
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	20	0.55
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	20	0.55
(1,2819)	1:113:A:LEU:HG	1:142:A:ILE:H	7	0.55
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	4	0.55
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	4	0.55
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	6	0.55
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	6	0.55
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	13	0.55
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	13	0.55
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD2	14	0.55
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD3	14	0.55
(1,2463)	1:4:A:TYR:HE1	1:167:A:LYS:HB3	2	0.55
(1,2463)	1:4:A:TYR:HE2	1:167:A:LYS:HB3	2	0.55
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	6	0.55
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	6	0.55
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	13	0.55
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	13	0.55
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	15	0.55
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	15	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	1	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	2	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	5	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	6	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	8	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	9	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	10	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	11	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	13	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	17	0.55
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	18	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	1	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	3	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	4	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	5	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	6	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	9	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	10	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	12	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	15	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	16	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	17	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	19	0.55
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	20	0.55
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	9	0.55
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	20	0.55
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	3	0.55
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	8	0.55
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	19	0.55
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	5	0.55
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	6	0.55
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	9	0.55
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	15	0.55
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	19	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	5	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	5	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	6	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	6	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	9	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	9	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	12	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	12	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	18	0.55
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	18	0.55
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	2	0.55
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	7	0.55
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	7	0.55
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	7	0.55
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	11	0.55
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	11	0.55
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	11	0.55
(1,1624)	1:97:A:ARG:H	1:97:A:ARG:HD2	9	0.55
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	4	0.55
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	10	0.55
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	12	0.55
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	17	0.55
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	19	0.55
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	1	0.55
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	12	0.55
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	16	0.55
(1,1489)	1:95:A:HIS:HE1	1:99:A:GLN:HE22	16	0.55
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	3	0.55
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	9	0.55
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	9	0.55
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	11	0.55
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	14	0.55
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	3	0.55
(1,1320)	1:92:A:ASP:H	1:95:A:HIS:HD2	16	0.55
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	2	0.55
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	2	0.55
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	8	0.55
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	8	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	1	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	1	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	3	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	3	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	4	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	4	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	15	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	15	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	16	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	16	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	17	0.55
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	17	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	2	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	2	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	2	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	2	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	2	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	2	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	3	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	3	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	3	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	3	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	3	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	3	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	6	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	6	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	6	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	6	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	6	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	6	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	10	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	10	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	10	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	10	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	10	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	12	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	12	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	12	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	12	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	12	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	12	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	15	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	15	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	15	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	15	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	15	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	15	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	19	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	19	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	19	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	19	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	19	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	19	0.55
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	20	0.55
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	20	0.55
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	20	0.55
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	20	0.55
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	20	0.55
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	20	0.55
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	5	0.55
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	5	0.55
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	5	0.55
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	10	0.55
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	10	0.55
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	10	0.55
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	13	0.55
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	13	0.55
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	14	0.55
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	14	0.55
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	18	0.55
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	2	0.55
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	2	0.55
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	2	0.55
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	3	0.55
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	3	0.55
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	13	0.55
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	13	0.55
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	6	0.55
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	6	0.55
(1,1052)	1:128:A:LYS:H	1:131:A:GLN:HE22	5	0.55
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	1	0.55
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	2	0.55
(1,967)	1:43:A:GLN:HE22	1:50:A:THR:HA	6	0.55
(1,965)	1:43:A:GLN:HE22	1:50:A:THR:HB	1	0.55
(1,965)	1:43:A:GLN:HE22	1:50:A:THR:HB	17	0.55
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	1	0.55
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	19	0.55
(1,861)	1:41:A:ARG:HG2	1:55:A:ILE:H	8	0.55
(1,861)	1:41:A:ARG:HG3	1:55:A:ILE:H	8	0.55
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	1	0.55
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	1	0.55
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	18	0.55
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	18	0.55
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	3	0.55
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	6	0.55
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	8	0.55
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	10	0.55
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	13	0.55
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	16	0.55
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	13	0.55
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	15	0.55
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	12	0.55
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	13	0.55
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	16	0.55
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	4	0.55
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	9	0.55
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	5	0.55
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	10	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	4	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	4	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	4	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	7	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	7	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	7	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	17	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	17	0.55
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	17	0.55
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	3	0.54
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	11	0.54
(1,3184)	1:132:A:ASP:HB2	1:135:A:ARG:HE	2	0.54
(1,3184)	1:132:A:ASP:HB3	1:135:A:ARG:HE	2	0.54
(1,3184)	1:132:A:ASP:HB2	1:135:A:ARG:HE	3	0.54
(1,3184)	1:132:A:ASP:HB3	1:135:A:ARG:HE	3	0.54
(1,3184)	1:132:A:ASP:HB2	1:135:A:ARG:HE	13	0.54
(1,3184)	1:132:A:ASP:HB3	1:135:A:ARG:HE	13	0.54
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	3	0.54
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	19	0.54
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	4	0.54
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	4	0.54
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	7	0.54
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	7	0.54
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	15	0.54
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	15	0.54
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	17	0.54
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	17	0.54
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	18	0.54
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	18	0.54
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	20	0.54
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	20	0.54
(1,2716)	1:11:A:ALA:HB1	1:90:A:PHE:H	8	0.54
(1,2716)	1:11:A:ALA:HB2	1:90:A:PHE:H	8	0.54
(1,2716)	1:11:A:ALA:HB3	1:90:A:PHE:H	8	0.54
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	4	0.54
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	4	0.54
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	18	0.54
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	18	0.54
(1,2620)	1:166:A:HIS:HB3	1:167:A:LYS:HB2	10	0.54
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	10	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD2	4	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD3	4	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD2	8	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD3	8	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD2	11	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD3	11	0.54
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD2	12	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2464)	1:162:A:GLU:H	1:164:A:ARG:HD3	12	0.54
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	3	0.54
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	3	0.54
(1,2287)	1:151:A:GLY:HA2	1:153:A:ASP:HB2	6	0.54
(1,2287)	1:151:A:GLY:HA2	1:153:A:ASP:HB3	6	0.54
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	18	0.54
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	3	0.54
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	3	0.54
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	6	0.54
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	2	0.54
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	2	0.54
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	2	0.54
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	9	0.54
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	9	0.54
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	9	0.54
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	16	0.54
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	16	0.54
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	16	0.54
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	3	0.54
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	19	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	1	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	1	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	4	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	4	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	5	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	5	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	6	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	6	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	7	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	7	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	11	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	11	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	12	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	12	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	14	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	14	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	15	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	15	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	17	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	17	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	18	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	18	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	19	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	19	0.54
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	20	0.54
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	20	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	2	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	3	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	7	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	9	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	12	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	13	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	17	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	18	0.54
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	20	0.54
(1,1412)	1:75:A:GLY:HA3	1:76:A:GLU:HG3	16	0.54
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	8	0.54
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	6	0.54
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	6	0.54
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	9	0.54
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	9	0.54
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	13	0.54
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	13	0.54
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	15	0.54
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	15	0.54
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	13	0.54
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	13	0.54
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	13	0.54
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	13	0.54
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	13	0.54
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	13	0.54
(1,1120)	1:12:A:GLY:H	1:61:A:GLN:HB3	3	0.54
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	16	0.54
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	19	0.54
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	19	0.54
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	20	0.54
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	20	0.54
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB2	14	0.54
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB3	14	0.54
(1,861)	1:41:A:ARG:HG2	1:55:A:ILE:H	6	0.54
(1,861)	1:41:A:ARG:HG3	1:55:A:ILE:H	6	0.54
(1,861)	1:41:A:ARG:HG2	1:55:A:ILE:H	11	0.54
(1,861)	1:41:A:ARG:HG3	1:55:A:ILE:H	11	0.54
(1,861)	1:41:A:ARG:HG2	1:55:A:ILE:H	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	1:41:A:ARG:HG3	1:55:A:ILE:H	19	0.54
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	6	0.54
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	6	0.54
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	6	0.54
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	6	0.54
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	6	0.54
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	6	0.54
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	11	0.54
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	11	0.54
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	11	0.54
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	11	0.54
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	11	0.54
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	11	0.54
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	12	0.54
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	12	0.54
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	12	0.54
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	12	0.54
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	12	0.54
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	12	0.54
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	11	0.54
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	11	0.54
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	1	0.54
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE2	12	0.54
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE3	12	0.54
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	10	0.53
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	12	0.53
(1,3184)	1:132:A:ASP:HB2	1:135:A:ARG:HE	1	0.53
(1,3184)	1:132:A:ASP:HB3	1:135:A:ARG:HE	1	0.53
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	10	0.53
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	7	0.53
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	6	0.53
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	6	0.53
(1,2620)	1:166:A:HIS:HB3	1:167:A:LYS:HB2	11	0.53
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	16	0.53
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	16	0.53
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	1	0.53
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	8	0.53
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	8	0.53
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	16	0.53
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	1	0.53
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	8	0.53
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	11	0.53
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	4	0.53
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	4	0.53
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	7	0.53
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	7	0.53
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	17	0.53
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	17	0.53
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	18	0.53
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	18	0.53
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	18	0.53
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	18	0.53
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	18	0.53
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	18	0.53
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	19	0.53
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	8	0.53
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	4	0.53
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	13	0.53
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	13	0.53
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	19	0.53
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	19	0.53
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	13	0.53
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	1	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	2	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	4	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	6	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	7	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	9	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	13	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	16	0.52
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	2	0.52
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	7	0.52
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	8	0.52
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	17	0.52
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	13	0.52
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	14	0.52
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	3	0.52
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	5	0.52
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	10	0.52
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	13	0.52
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	15	0.52
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	19	0.52
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	6	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	6	0.52
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	6	0.52
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	11	0.52
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	1	0.52
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	17	0.52
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	11	0.52
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	3	0.52
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	4	0.52
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD21	12	0.52
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD22	12	0.52
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD23	12	0.52
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	16	0.52
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	16	0.52
(1,1130)	1:51:A:CYS:HB2	1:52:A:LEU:HB2	16	0.52
(1,1130)	1:51:A:CYS:HB2	1:52:A:LEU:HB2	18	0.52
(1,1112)	1:50:A:THR:HA	1:51:A:CYS:HB3	16	0.52
(1,1112)	1:50:A:THR:HA	1:51:A:CYS:HB3	18	0.52
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	13	0.52
(1,861)	1:41:A:ARG:HG2	1:55:A:ILE:H	17	0.52
(1,861)	1:41:A:ARG:HG3	1:55:A:ILE:H	17	0.52
(1,788)	1:8:A:VAL:HB	1:58:A:THR:H	16	0.52
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	16	0.52
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	16	0.52
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	8	0.52
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	8	0.52
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	10	0.52
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	11	0.52
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	7	0.52
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	7	0.52
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	7	0.52
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE2	8	0.52
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE3	8	0.52
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	3	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	8	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	11	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	14	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	15	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	17	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	18	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	19	0.51
(1,3318)	1:110:A:PRO:HG2	1:111:A:MET:H	20	0.51
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	5	0.51
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	18	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	2	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	6	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	7	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	8	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	9	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	11	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	14	0.51
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	20	0.51
(1,2888)	1:137:A:TYR:HE1	1:138:A:GLY:H	14	0.51
(1,2888)	1:137:A:TYR:HE2	1:138:A:GLY:H	14	0.51
(1,2756)	1:28:A:PHE:HE1	1:146:A:ALA:H	2	0.51
(1,2756)	1:28:A:PHE:HE2	1:146:A:ALA:H	2	0.51
(1,2627)	1:47:A:ASP:HB2	1:161:A:ARG:HE	13	0.51
(1,2627)	1:47:A:ASP:HB3	1:161:A:ARG:HE	13	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	1	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	4	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	5	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	7	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	8	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	10	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	11	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	14	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	15	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	16	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	17	0.51
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	18	0.51
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	16	0.51
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	20	0.51
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	15	0.51
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	15	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	1	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	3	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	5	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	6	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	7	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	10	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	11	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	15	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	17	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	18	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	19	0.51
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	20	0.51
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	9	0.51
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	9	0.51
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	9	0.51
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	6	0.51
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	6	0.51
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	14	0.51
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE1	17	0.51
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE2	17	0.51
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	5	0.51
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	5	0.51
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	19	0.51
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	19	0.51
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	16	0.51
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	6	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	4	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	4	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	4	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	5	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	5	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	5	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	6	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	6	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	6	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	7	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	7	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	7	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	8	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	8	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	8	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	9	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	9	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	9	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	10	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	10	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	10	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	11	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	11	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	11	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	12	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	12	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	13	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	13	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	13	0.51
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	18	0.51
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	18	0.51
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	18	0.51
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	12	0.51
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	17	0.51
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	17	0.51
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	17	0.51
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	4	0.51
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	18	0.5
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	18	0.5
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	18	0.5
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	18	0.5
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	3	0.5
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	15	0.5
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	16	0.5
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	19	0.5
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	7	0.5
(1,2886)	1:21:A:ILE:HG12	1:40:A:TYR:HE1	3	0.5
(1,2886)	1:21:A:ILE:HG12	1:40:A:TYR:HE2	3	0.5
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	5	0.5
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	5	0.5
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	5	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	1	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	1	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	1	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	7	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	7	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	7	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	20	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	20	0.5
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	20	0.5
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	1	0.5
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	1	0.5
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	2	0.5
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	2	0.5
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	3	0.5
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	3	0.5
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	7	0.5
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	12	0.5
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	12	0.5
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	16	0.5
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	16	0.5
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	17	0.5
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	17	0.5
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	20	0.5
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	20	0.5
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	2	0.5
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	3	0.5
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	6	0.5
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	13	0.5
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	19	0.5
(1,2331)	1:23:A:LEU:HG	1:156:A:PHE:HB3	20	0.5
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE1	7	0.5
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE2	7	0.5
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE1	8	0.5
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE2	8	0.5
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE1	13	0.5
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE2	13	0.5
(1,2089)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	4	0.5
(1,2089)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	4	0.5
(1,2089)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	4	0.5
(1,2089)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	4	0.5
(1,2089)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	4	0.5
(1,2089)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	4	0.5
(1,2089)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	15	0.5
(1,2089)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	15	0.5
(1,2089)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	15	0.5
(1,2089)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	15	0.5
(1,2089)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	15	0.5
(1,2089)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	15	0.5
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	17	0.5
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	17	0.5
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	17	0.5
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	18	0.5
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	2	0.5
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	2	0.5
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	2	0.5
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	8	0.5
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	12	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	14	0.5
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	16	0.5
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB2	2	0.5
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB3	2	0.5
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB2	2	0.5
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB3	2	0.5
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	5	0.5
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	5	0.5
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	5	0.5
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	19	0.5
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	19	0.5
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	19	0.5
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	20	0.5
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	20	0.5
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	20	0.5
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	9	0.5
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	9	0.5
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	9	0.5
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	9	0.5
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	9	0.5
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	9	0.5
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	20	0.5
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	20	0.5
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	20	0.5
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	20	0.5
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	20	0.5
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	20	0.5
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	2	0.5
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	3	0.5
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	3	0.5
(1,1077)	1:4:A:TYR:HE1	1:51:A:CYS:HA	17	0.5
(1,1077)	1:4:A:TYR:HE2	1:51:A:CYS:HA	17	0.5
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	15	0.5
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	3	0.5
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	3	0.5
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	1	0.5
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	3	0.5
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	5	0.5
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	10	0.5
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	11	0.5
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	13	0.5
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	19	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	4	0.5
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	4	0.5
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	4	0.5
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	4	0.5
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	4	0.5
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	4	0.5
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	17	0.5
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	17	0.5
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	17	0.5
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	17	0.5
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	17	0.5
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	17	0.5
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	20	0.5
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	20	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	4	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	4	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	4	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	4	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	4	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	4	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	6	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	6	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	6	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	6	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	6	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	6	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	7	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	7	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	7	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	7	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	7	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	7	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	12	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	12	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	12	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	12	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	12	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	12	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	15	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	15	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	15	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	15	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	15	0.5
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	15	0.5
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	4	0.5
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	1	0.5
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	19	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	1	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	1	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	1	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	2	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	2	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	2	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	3	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	3	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	3	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	15	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	15	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	15	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	16	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	16	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	16	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	17	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	17	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	17	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	19	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	19	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	19	0.5
(1,421)	1:21:A:ILE:HD11	1:25:A:GLN:HE22	20	0.5
(1,421)	1:21:A:ILE:HD12	1:25:A:GLN:HE22	20	0.5
(1,421)	1:21:A:ILE:HD13	1:25:A:GLN:HE22	20	0.5
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	1	0.5
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	12	0.5
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	12	0.5
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	12	0.5
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	3	0.5
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	3	0.5
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	3	0.5
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	5	0.5
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	6	0.5
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	8	0.5
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	15	0.5
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	17	0.5
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	18	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	19	0.5
(1,114)	1:164:A:ARG:HA	1:164:A:ARG:HE	15	0.5
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	1	0.49
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	1	0.49
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	6	0.49
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	6	0.49
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	17	0.49
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	9	0.49
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	12	0.49
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	17	0.49
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	4	0.49
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	10	0.49
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	10	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	5	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	5	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	5	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	8	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	8	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	8	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	10	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	10	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	10	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	11	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	11	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	11	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	12	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	12	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	12	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	16	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	16	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	16	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	17	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	17	0.49
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	17	0.49
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	12	0.49
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	12	0.49
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	9	0.49
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	9	0.49
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	13	0.49
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	13	0.49
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	14	0.49
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	14	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2636)	1:80:A:CYS:HB2	1:111:A:MET:HB3	18	0.49
(1,2636)	1:80:A:CYS:HB3	1:111:A:MET:HB3	18	0.49
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	3	0.49
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	13	0.49
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	13	0.49
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	7	0.49
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE1	12	0.49
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE2	12	0.49
(1,1725)	1:104:A:LYS:HE3	1:109:A:VAL:HA	8	0.49
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG2	10	0.49
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG3	10	0.49
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	10	0.49
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	10	0.49
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	10	0.49
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	11	0.49
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	11	0.49
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	11	0.49
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	5	0.49
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	7	0.49
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	11	0.49
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	12	0.49
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	15	0.49
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	19	0.49
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	4	0.49
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	4	0.49
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	4	0.49
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	8	0.49
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	8	0.49
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	8	0.49
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	15	0.49
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	15	0.49
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	15	0.49
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	2	0.49
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	2	0.49
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	10	0.49
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	10	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	1	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	1	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	1	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	1	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	1	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	3	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	3	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	3	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	3	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	3	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	3	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	5	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	5	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	5	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	5	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	5	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	5	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	6	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	6	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	6	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	6	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	6	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	6	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	14	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	14	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	14	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	14	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	14	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	14	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	16	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	16	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	16	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	16	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	16	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	16	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	19	0.49
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	19	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	19	0.49
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	19	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	19	0.49
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	19	0.49
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	11	0.49
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	19	0.49
(1,1049)	1:125:A:VAL:HA	1:129:A:GLN:HE22	20	0.49
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	13	0.49
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	9	0.49
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	15	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	15	0.49
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	15	0.49
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	10	0.49
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	10	0.49
(1,631)	1:58:A:THR:HG21	1:68:A:ARG:H	2	0.49
(1,631)	1:58:A:THR:HG22	1:68:A:ARG:H	2	0.49
(1,631)	1:58:A:THR:HG23	1:68:A:ARG:H	2	0.49
(1,631)	1:58:A:THR:HG21	1:68:A:ARG:H	15	0.49
(1,631)	1:58:A:THR:HG22	1:68:A:ARG:H	15	0.49
(1,631)	1:58:A:THR:HG23	1:68:A:ARG:H	15	0.49
(1,631)	1:58:A:THR:HG21	1:68:A:ARG:H	17	0.49
(1,631)	1:58:A:THR:HG22	1:68:A:ARG:H	17	0.49
(1,631)	1:58:A:THR:HG23	1:68:A:ARG:H	17	0.49
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	1	0.49
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	1	0.49
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	1	0.49
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	1	0.49
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	1	0.49
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	1	0.49
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	12	0.49
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	17	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	1	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	2	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	3	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	7	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	9	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	10	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	11	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	16	0.49
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	20	0.49
(1,3331)	1:106:A:SER:HB2	1:109:A:VAL:H	17	0.48
(1,3331)	1:106:A:SER:HB3	1:109:A:VAL:H	17	0.48
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	17	0.48
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	20	0.48
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	20	0.48
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	20	0.48
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	7	0.48
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	17	0.48
(1,2682)	1:25:A:GLN:HA	1:27:A:HIS:HE1	14	0.48
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	20	0.48
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	20	0.48
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	13	0.48
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	19	0.48
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	20	0.48
(1,2062)	1:128:A:LYS:H	1:129:A:GLN:HG3	20	0.48
(1,1940)	1:120:A:LEU:HD11	1:121:A:PRO:HG3	18	0.48
(1,1940)	1:120:A:LEU:HD12	1:121:A:PRO:HG3	18	0.48
(1,1940)	1:120:A:LEU:HD13	1:121:A:PRO:HG3	18	0.48
(1,1940)	1:120:A:LEU:HD21	1:121:A:PRO:HG3	18	0.48
(1,1940)	1:120:A:LEU:HD22	1:121:A:PRO:HG3	18	0.48
(1,1940)	1:120:A:LEU:HD23	1:121:A:PRO:HG3	18	0.48
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	12	0.48
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	1	0.48
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	4	0.48
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	6	0.48
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	19	0.48
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	7	0.48
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	7	0.48
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	3	0.48
(1,1725)	1:104:A:LYS:HE3	1:109:A:VAL:HA	16	0.48
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	9	0.48
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	9	0.48
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	9	0.48
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE1	1	0.48
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE2	1	0.48
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG2	12	0.48
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG3	12	0.48
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	11	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	2	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	2	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	2	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	3	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	3	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	3	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	8	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	8	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	8	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	9	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	9	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	9	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	10	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	10	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	14	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	14	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	14	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	15	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	15	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	15	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	16	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	16	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	16	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	17	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	17	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	17	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	19	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	19	0.48
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	19	0.48
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB2	11	0.48
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB3	11	0.48
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB2	11	0.48
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB3	11	0.48
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	11	0.48
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	14	0.48
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	1	0.48
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	2	0.48
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	6	0.48
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	8	0.48
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	1	0.48
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	2	0.48
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	5	0.48
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	6	0.48
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	16	0.48
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	17	0.48
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	10	0.48
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	10	0.48
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	10	0.48
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	17	0.48
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	17	0.48
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	17	0.48
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	18	0.48
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	18	0.48
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	18	0.48
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	13	0.48
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	13	0.48
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	13	0.48
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	13	0.48
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	13	0.48
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	1	0.48
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	3	0.48
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	2	0.48
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	14	0.48
(1,1041)	1:23:A:LEU:HG	1:42:A:LYS:HD2	12	0.48
(1,982)	1:44:A:VAL:HG21	1:51:A:CYS:HB2	8	0.48
(1,982)	1:44:A:VAL:HG22	1:51:A:CYS:HB2	8	0.48
(1,982)	1:44:A:VAL:HG23	1:51:A:CYS:HB2	8	0.48
(1,982)	1:44:A:VAL:HG21	1:51:A:CYS:HB2	20	0.48
(1,982)	1:44:A:VAL:HG22	1:51:A:CYS:HB2	20	0.48
(1,982)	1:44:A:VAL:HG23	1:51:A:CYS:HB2	20	0.48
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	3	0.48
(1,837)	1:46:A:ILE:HG21	1:161:A:ARG:HD2	4	0.48
(1,837)	1:46:A:ILE:HG21	1:161:A:ARG:HD3	4	0.48
(1,837)	1:46:A:ILE:HG22	1:161:A:ARG:HD2	4	0.48
(1,837)	1:46:A:ILE:HG22	1:161:A:ARG:HD3	4	0.48
(1,837)	1:46:A:ILE:HG23	1:161:A:ARG:HD2	4	0.48
(1,837)	1:46:A:ILE:HG23	1:161:A:ARG:HD3	4	0.48
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	3	0.48
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	18	0.48
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD1	7	0.48
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD2	7	0.48
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	8	0.48
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	8	0.48
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	8	0.48
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	8	0.48
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	8	0.48
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	8	0.48
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	3	0.48
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	7	0.48
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	1	0.48
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	3	0.48
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	3	0.48
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	6	0.48
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	6	0.48
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	16	0.48
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	16	0.48
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	13	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	3	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	3	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	3	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	3	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	3	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	3	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	7	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	7	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	7	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	7	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	7	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	7	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	9	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	9	0.48
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	9	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	9	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	9	0.48
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	9	0.48
(1,84)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	4	0.48
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	4	0.47
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	4	0.47
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	4	0.47
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	4	0.47
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	4	0.47
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	5	0.47
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	5	0.47
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	5	0.47
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	7	0.47
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	7	0.47
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	7	0.47
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	9	0.47
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	9	0.47
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	9	0.47
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	13	0.47
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	13	0.47
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	13	0.47
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	18	0.47
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	18	0.47
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	18	0.47
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	18	0.47
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	20	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	13	0.47
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	16	0.47
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	2	0.47
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	2	0.47
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	1	0.47
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	1	0.47
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	1	0.47
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	18	0.47
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	18	0.47
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	18	0.47
(1,2846)	1:140:A:PRO:HG2	1:141:A:PHE:H	20	0.47
(1,2764)	1:19:A:LEU:HG	1:146:A:ALA:H	20	0.47
(1,2763)	1:59:A:ALA:HB1	1:61:A:GLN:HE21	7	0.47
(1,2763)	1:59:A:ALA:HB1	1:61:A:GLN:HE22	7	0.47
(1,2763)	1:59:A:ALA:HB2	1:61:A:GLN:HE21	7	0.47
(1,2763)	1:59:A:ALA:HB2	1:61:A:GLN:HE22	7	0.47
(1,2763)	1:59:A:ALA:HB3	1:61:A:GLN:HE21	7	0.47
(1,2763)	1:59:A:ALA:HB3	1:61:A:GLN:HE22	7	0.47
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	14	0.47
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	14	0.47
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	14	0.47
(1,2668)	1:99:A:GLN:HA	1:102:A:ARG:HE	12	0.47
(1,2618)	1:110:A:PRO:HG3	1:166:A:HIS:HB3	16	0.47
(1,2605)	1:21:A:ILE:HA	1:25:A:GLN:HG2	14	0.47
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	4	0.47
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	4	0.47
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	10	0.47
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	10	0.47
(1,2518)	1:164:A:ARG:H	1:165:A:LYS:HG2	11	0.47
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	10	0.47
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	6	0.47
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	6	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	2	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	5	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	7	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	9	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	10	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	11	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	12	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	15	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	16	0.47
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	4	0.47
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	4	0.47
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	7	0.47
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	7	0.47
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	10	0.47
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	10	0.47
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	11	0.47
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	11	0.47
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	13	0.47
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	13	0.47
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	17	0.47
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	17	0.47
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	10	0.47
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	4	0.47
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	6	0.47
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	8	0.47
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	9	0.47
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	10	0.47
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	13	0.47
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	20	0.47
(1,2150)	1:53:A:LEU:HD11	1:54:A:ASP:HA	4	0.47
(1,2150)	1:53:A:LEU:HD12	1:54:A:ASP:HA	4	0.47
(1,2150)	1:53:A:LEU:HD13	1:54:A:ASP:HA	4	0.47
(1,2150)	1:53:A:LEU:HD21	1:54:A:ASP:HA	4	0.47
(1,2150)	1:53:A:LEU:HD22	1:54:A:ASP:HA	4	0.47
(1,2150)	1:53:A:LEU:HD23	1:54:A:ASP:HA	4	0.47
(1,2150)	1:53:A:LEU:HD11	1:54:A:ASP:HA	12	0.47
(1,2150)	1:53:A:LEU:HD12	1:54:A:ASP:HA	12	0.47
(1,2150)	1:53:A:LEU:HD13	1:54:A:ASP:HA	12	0.47
(1,2150)	1:53:A:LEU:HD21	1:54:A:ASP:HA	12	0.47
(1,2150)	1:53:A:LEU:HD22	1:54:A:ASP:HA	12	0.47
(1,2150)	1:53:A:LEU:HD23	1:54:A:ASP:HA	12	0.47
(1,2150)	1:53:A:LEU:HD11	1:54:A:ASP:HA	15	0.47
(1,2150)	1:53:A:LEU:HD12	1:54:A:ASP:HA	15	0.47
(1,2150)	1:53:A:LEU:HD13	1:54:A:ASP:HA	15	0.47
(1,2150)	1:53:A:LEU:HD21	1:54:A:ASP:HA	15	0.47
(1,2150)	1:53:A:LEU:HD22	1:54:A:ASP:HA	15	0.47
(1,2150)	1:53:A:LEU:HD23	1:54:A:ASP:HA	15	0.47
(1,2100)	1:13:A:GLY:H	1:15:A:GLY:H	4	0.47
(1,1937)	1:8:A:VAL:HA	1:78:A:PHE:HA	2	0.47
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	10	0.47
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD11	7	0.47
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD12	7	0.47
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD13	7	0.47
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD21	7	0.47
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD22	7	0.47
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD23	7	0.47
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD11	7	0.47
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD12	7	0.47
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD13	7	0.47
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD21	7	0.47
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD22	7	0.47
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD23	7	0.47
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	3	0.47
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	3	0.47
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	18	0.47
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	18	0.47
(1,1891)	1:44:A:VAL:HB	1:51:A:CYS:H	20	0.47
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	13	0.47
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	14	0.47
(1,1831)	1:158:A:THR:HA	1:161:A:ARG:HE	2	0.47
(1,1831)	1:158:A:THR:HA	1:161:A:ARG:HE	11	0.47
(1,1831)	1:158:A:THR:HA	1:161:A:ARG:HE	15	0.47
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	2	0.47
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	2	0.47
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	3	0.47
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	3	0.47
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	17	0.47
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	17	0.47
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	18	0.47
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	18	0.47
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	20	0.47
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	20	0.47
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	4	0.47
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	4	0.47
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	19	0.47
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	19	0.47
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	19	0.47
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	19	0.47
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	5	0.47
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	10	0.47
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	10	0.47
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	20	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	20	0.47
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	20	0.47
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	13	0.47
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD1	3	0.47
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD2	3	0.47
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD1	3	0.47
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD2	3	0.47
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	5	0.47
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	5	0.47
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	5	0.47
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	12	0.47
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	12	0.47
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	8	0.47
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	8	0.47
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	8	0.47
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	10	0.47
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	10	0.47
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	10	0.47
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	11	0.47
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	11	0.47
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	11	0.47
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	15	0.47
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	15	0.47
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	15	0.47
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	17	0.47
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	17	0.47
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	17	0.47
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	20	0.47
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	20	0.47
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	20	0.47
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	5	0.47
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	5	0.47
(1,982)	1:44:A:VAL:HG21	1:51:A:CYS:HB2	2	0.47
(1,982)	1:44:A:VAL:HG22	1:51:A:CYS:HB2	2	0.47
(1,982)	1:44:A:VAL:HG23	1:51:A:CYS:HB2	2	0.47
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	7	0.47
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	10	0.47
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	12	0.47
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	12	0.47
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	12	0.47
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	2	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	5	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	5	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	5	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	5	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	5	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	9	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	9	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	9	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	9	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	9	0.47
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	9	0.47
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD1	2	0.47
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD2	2	0.47
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD1	2	0.47
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD2	2	0.47
(1,471)	1:22:A:GLN:HE21	1:28:A:PHE:HB3	5	0.47
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	19	0.47
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	6	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	2	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	6	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	7	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	10	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	11	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	14	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	16	0.47
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	17	0.47
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	2	0.47
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	2	0.47
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	18	0.47
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	17	0.47
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	17	0.47
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	17	0.47
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	17	0.47
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	17	0.47
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	17	0.47
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	19	0.47
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	19	0.47
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	19	0.47
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	19	0.47
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	19	0.47
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	19	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	2	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	2	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	2	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	2	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	2	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	4	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	4	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	4	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	4	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	4	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	4	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	6	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	6	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	6	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	6	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	6	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	6	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	10	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	10	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	10	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	10	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	10	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	10	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	17	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	17	0.47
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	17	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	17	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	17	0.47
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	17	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	1	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	1	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	5	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	5	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	7	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	7	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	8	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	8	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	9	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	9	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	10	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	10	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	12	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	13	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	13	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	17	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	17	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	18	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	18	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	19	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	19	0.47
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	20	0.47
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	20	0.47
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	2	0.47
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	2	0.47
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	2	0.47
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	2	0.47
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	2	0.47
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	2	0.47
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	11	0.46
(1,3116)	1:85:A:ASN:HB2	1:124:A:THR:H	7	0.46
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	2	0.46
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	8	0.46
(1,2798)	1:143:A:GLU:HG2	1:144:A:THR:H	6	0.46
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	13	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	1	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	1	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	1	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	1	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	1	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	1	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	3	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	3	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	3	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	3	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	3	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	3	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	10	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	10	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	10	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	10	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	10	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	10	0.46
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	13	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	13	0.46
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	13	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	13	0.46
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	13	0.46
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	4	0.46
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	4	0.46
(1,2607)	1:21:A:ILE:HA	1:27:A:HIS:H	11	0.46
(1,2518)	1:164:A:ARG:H	1:165:A:LYS:HG2	16	0.46
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	1	0.46
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	1	0.46
(1,2454)	1:162:A:GLU:HB2	1:165:A:LYS:HG2	11	0.46
(1,2454)	1:162:A:GLU:HB3	1:165:A:LYS:HG2	11	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	14	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	14	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	14	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	14	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	14	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	14	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	15	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	15	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	15	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	15	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	15	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	15	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	16	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	16	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	16	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	16	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	16	0.46
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	16	0.46
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	19	0.46
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	19	0.46
(1,2193)	1:143:A:GLU:HG3	1:144:A:THR:H	1	0.46
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	12	0.46
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	5	0.46
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	5	0.46
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	5	0.46
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	20	0.46
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	20	0.46
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	20	0.46
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	2	0.46
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	11	0.46
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	12	0.46
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	15	0.46
(1,2100)	1:13:A:GLY:H	1:15:A:GLY:H	11	0.46
(1,2100)	1:13:A:GLY:H	1:15:A:GLY:H	20	0.46
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	8	0.46
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	8	0.46
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	10	0.46
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	10	0.46
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	16	0.46
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	16	0.46
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	8	0.46
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	6	0.46
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	6	0.46
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	16	0.46
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	16	0.46
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	18	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	1	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	1	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	4	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	4	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	5	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	5	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	8	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	8	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	9	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	9	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	12	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	12	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	13	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	13	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	14	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	14	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	19	0.46
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	19	0.46
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	15	0.46
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	16	0.46
(1,1831)	1:158:A:THR:HA	1:161:A:ARG:HE	3	0.46
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	12	0.46
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	12	0.46
(1,1731)	1:100:A:ILE:HG21	1:104:A:LYS:HE2	19	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1731)	1:100:A:ILE:HG22	1:104:A:LYS:HE2	19	0.46
(1,1731)	1:100:A:ILE:HG23	1:104:A:LYS:HE2	19	0.46
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE1	1	0.46
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE2	1	0.46
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE1	7	0.46
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE2	7	0.46
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE1	8	0.46
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE2	8	0.46
(1,1489)	1:95:A:HIS:HE1	1:99:A:GLN:HE22	17	0.46
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	14	0.46
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	14	0.46
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	14	0.46
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD1	8	0.46
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD2	8	0.46
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD1	8	0.46
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD2	8	0.46
(1,1243)	1:106:A:SER:HA	1:107:A:GLU:HG2	1	0.46
(1,1243)	1:106:A:SER:HA	1:107:A:GLU:HG3	1	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD11	2	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD12	2	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD13	2	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD21	2	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD22	2	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD23	2	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD11	14	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD12	14	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD13	14	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD21	14	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD22	14	0.46
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD23	14	0.46
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	2	0.46
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	2	0.46
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	2	0.46
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	6	0.46
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	6	0.46
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	6	0.46
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	7	0.46
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	7	0.46
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	7	0.46
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	9	0.46
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	9	0.46
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	19	0.46
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	19	0.46
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	19	0.46
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	6	0.46
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	9	0.46
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	9	0.46
(1,1041)	1:23:A:LEU:HG	1:42:A:LYS:HD2	9	0.46
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	1	0.46
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	10	0.46
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	18	0.46
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	19	0.46
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	20	0.46
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD1	1	0.46
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD2	1	0.46
(1,885)	1:161:A:ARG:HA	1:164:A:ARG:HE	19	0.46
(1,839)	1:4:A:TYR:HE1	1:52:A:LEU:H	3	0.46
(1,839)	1:4:A:TYR:HE2	1:52:A:LEU:H	3	0.46
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	4	0.46
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	8	0.46
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	5	0.46
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	20	0.46
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	15	0.46
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	18	0.46
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	18	0.46
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	18	0.46
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	18	0.46
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	18	0.46
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	18	0.46
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	18	0.46
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	20	0.46
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	20	0.46
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	20	0.46
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	20	0.46
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	20	0.46
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	20	0.46
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	2	0.46
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	2	0.46
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	13	0.46
(1,471)	1:22:A:GLN:HE21	1:28:A:PHE:HB3	11	0.46
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	12	0.46
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	12	0.46
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	12	0.46
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	18	0.46
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	5	0.46
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	5	0.46
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	8	0.46
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	8	0.46
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	9	0.46
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	9	0.46
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	14	0.46
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	14	0.46
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	19	0.46
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	19	0.46
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	20	0.46
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	20	0.46
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	6	0.46
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	11	0.46
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	16	0.46
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	19	0.46
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	11	0.46
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	20	0.46
(1,192)	1:15:A:GLY:HA2	2:201:A:GNP:H1'	14	0.46
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	13	0.46
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	13	0.46
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	13	0.46
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	13	0.46
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	13	0.46
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	13	0.46
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	14	0.46
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	14	0.46
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	14	0.46
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	14	0.46
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	14	0.46
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	14	0.46
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	20	0.46
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	20	0.46
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	20	0.46
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	20	0.46
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	20	0.46
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	20	0.46
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	11	0.46
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	11	0.46
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	11	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	2	0.46
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	2	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	8	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	8	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	8	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	8	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	8	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	8	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	18	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	18	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	18	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	18	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	18	0.46
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	18	0.46
(1,3179)	1:1:A:MET:HG3	1:51:A:CYS:H	16	0.45
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	5	0.45
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	5	0.45
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	5	0.45
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	6	0.45
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	6	0.45
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	6	0.45
(1,3133)	1:1:A:MET:HB2	1:2:A:THR:HB	16	0.45
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	20	0.45
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	7	0.45
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	10	0.45
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	16	0.45
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	20	0.45
(1,3063)	1:45:A:VAL:HB	1:48:A:GLY:H	20	0.45
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	12	0.45
(1,2730)	1:118:A:SER:H	1:147:A:LYS:H	6	0.45
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	16	0.45
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	1	0.45
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	4	0.45
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	17	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	4	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	4	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	4	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	4	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	4	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	4	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	5	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	5	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	5	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	5	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	5	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	6	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	6	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	6	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	6	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	6	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	6	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	7	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	7	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	7	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	7	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	7	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	7	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	8	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	8	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	8	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	8	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	8	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	8	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	10	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	10	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	10	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	10	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	10	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	10	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	11	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	11	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	11	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	11	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	11	0.45
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	11	0.45
(1,2308)	1:153:A:ASP:HB2	1:154:A:ASP:HB2	16	0.45
(1,2308)	1:153:A:ASP:HB3	1:154:A:ASP:HB2	16	0.45
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	4	0.45
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	4	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	2	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	2	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	2	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	7	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	7	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	8	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	8	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	8	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	9	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	9	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	9	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	11	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	11	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	11	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	12	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	12	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	12	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	14	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	14	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	14	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	15	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	15	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	15	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	17	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	17	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	17	0.45
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	19	0.45
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	19	0.45
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	19	0.45
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	1	0.45
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE1	2	0.45
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE2	2	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	1	0.45
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	1	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	2	0.45
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	2	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	5	0.45
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	5	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	8	0.45
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	8	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	9	0.45
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	9	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	11	0.45
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	11	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	14	0.45
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	15	0.45
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	15	0.45
(1,1971)	1:6:A:LEU:HB2	1:78:A:PHE:HA	5	0.45
(1,1971)	1:6:A:LEU:HB3	1:78:A:PHE:HA	5	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	1	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	1	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	2	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	2	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	6	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	6	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	7	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	7	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	12	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	12	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	13	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	13	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	14	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	14	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	15	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	15	0.45
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	20	0.45
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	20	0.45
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	11	0.45
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	11	0.45
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	10	0.45
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	5	0.45
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	11	0.45
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	11	0.45
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	13	0.45
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	13	0.45
(1,1714)	1:75:A:GLY:HA2	1:104:A:LYS:HD2	8	0.45
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	4	0.45
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	3	0.45
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	13	0.45
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	15	0.45
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	19	0.45
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	20	0.45
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	18	0.45
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	9	0.45
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	9	0.45
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE1	13	0.45
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE2	13	0.45
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE1	13	0.45
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE2	13	0.45
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE1	13	0.45
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE2	13	0.45
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	18	0.45
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	18	0.45
(1,1131)	1:1:A:MET:HE1	1:52:A:LEU:HB3	10	0.45
(1,1131)	1:1:A:MET:HE2	1:52:A:LEU:HB3	10	0.45
(1,1131)	1:1:A:MET:HE3	1:52:A:LEU:HB3	10	0.45
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	14	0.45
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	18	0.45
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	18	0.45
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	18	0.45
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	5	0.45
(1,916)	1:22:A:GLN:HE21	1:27:A:HIS:HA	5	0.45
(1,916)	1:22:A:GLN:HE22	1:27:A:HIS:HA	5	0.45
(1,885)	1:161:A:ARG:HA	1:164:A:ARG:HE	1	0.45
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	20	0.45
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	7	0.45
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	6	0.45
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	14	0.45
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	14	0.45
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	14	0.45
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	14	0.45
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	14	0.45
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	14	0.45
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	17	0.45
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	17	0.45
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	17	0.45
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	17	0.45
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	17	0.45
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	17	0.45
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	4	0.45
(1,523)	1:29:A:VAL:HG11	1:31:A:GLU:H	2	0.45
(1,523)	1:29:A:VAL:HG12	1:31:A:GLU:H	2	0.45
(1,523)	1:29:A:VAL:HG13	1:31:A:GLU:H	2	0.45
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	15	0.45
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	2	0.45
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	14	0.45
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	11	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	11	0.45
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	1	0.45
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	1	0.45
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	4	0.45
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	4	0.45
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	10	0.45
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	10	0.45
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	4	0.45
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	15	0.45
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	3	0.45
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	4	0.45
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	5	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	13	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	13	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	13	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	13	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	13	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	13	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	16	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	16	0.45
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	16	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	16	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	16	0.45
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	16	0.45
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD11	5	0.45
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD12	5	0.45
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD13	5	0.45
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	1	0.45
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	1	0.45
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	1	0.45
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	13	0.45
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	13	0.45
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	13	0.45
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	11	0.45
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	11	0.45
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	2	0.44
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	2	0.44
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	16	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	4	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	4	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	4	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	8	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	8	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	9	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	9	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	9	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	11	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	11	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	11	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	13	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	13	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	13	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	17	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	17	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	17	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	20	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	20	0.44
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	20	0.44
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	10	0.44
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	10	0.44
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	10	0.44
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	5	0.44
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	13	0.44
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	14	0.44
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	17	0.44
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	19	0.44
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	8	0.44
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	6	0.44
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	6	0.44
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	6	0.44
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	8	0.44
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	8	0.44
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	8	0.44
(1,2846)	1:140:A:PRO:HG2	1:141:A:PHE:H	15	0.44
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	8	0.44
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	8	0.44
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	1	0.44
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	2	0.44
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	3	0.44
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	15	0.44
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	19	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	1	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	3	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	4	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	5	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	6	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	7	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	10	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	11	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	12	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	15	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	17	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	18	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	19	0.44
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	20	0.44
(1,2620)	1:166:A:HIS:HB3	1:167:A:LYS:HB2	13	0.44
(1,2606)	1:21:A:ILE:HA	1:40:A:TYR:HD1	3	0.44
(1,2606)	1:21:A:ILE:HA	1:40:A:TYR:HD2	3	0.44
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	17	0.44
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	17	0.44
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	17	0.44
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	17	0.44
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	17	0.44
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	17	0.44
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	19	0.44
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	19	0.44
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	19	0.44
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	19	0.44
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	19	0.44
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	19	0.44
(1,2451)	1:2:A:THR:HB	1:51:A:CYS:HB3	8	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	3	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	3	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	3	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	3	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	3	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	3	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	18	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	18	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	18	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	18	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	18	0.44
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	18	0.44
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	4	0.44
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	13	0.44
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	13	0.44
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	3	0.44
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	3	0.44
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE2	20	0.44
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE3	20	0.44
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	1	0.44
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	1	0.44
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	19	0.44
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	19	0.44
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	1	0.44
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	1	0.44
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	1	0.44
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	3	0.44
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	3	0.44
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	3	0.44
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	6	0.44
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	6	0.44
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	6	0.44
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	10	0.44
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	10	0.44
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	10	0.44
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	13	0.44
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	13	0.44
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	13	0.44
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	16	0.44
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	16	0.44
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	16	0.44
(1,2050)	1:128:A:LYS:H	1:129:A:GLN:HG2	13	0.44
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	4	0.44
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	4	0.44
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	6	0.44
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	6	0.44
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	10	0.44
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	10	0.44
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	12	0.44
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	12	0.44
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	16	0.44
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	16	0.44
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	17	0.44
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:6:A:LEU:HB2	1:78:A:PHE:HA	13	0.44
(1,1971)	1:6:A:LEU:HB3	1:78:A:PHE:HA	13	0.44
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	3	0.44
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	3	0.44
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	4	0.44
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	4	0.44
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	5	0.44
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	5	0.44
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	10	0.44
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	10	0.44
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	15	0.44
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	15	0.44
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	10	0.44
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	10	0.44
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	10	0.44
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	9	0.44
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	9	0.44
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	8	0.44
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	1	0.44
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	2	0.44
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	2	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	1	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	1	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	1	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	1	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	1	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	1	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	1	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	1	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	1	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	1	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	1	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	1	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	12	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	12	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	12	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	12	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	12	0.44
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	12	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	12	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	12	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	12	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	12	0.44
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	12	0.44
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	2	0.44
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	17	0.44
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	8	0.44
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	8	0.44
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	8	0.44
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	1	0.44
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	1	0.44
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	6	0.44
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	10	0.44
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	1	0.44
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	1	0.44
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	1	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE1	2	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE2	2	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE1	2	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE2	2	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE1	2	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE2	2	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE1	12	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE2	12	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE1	12	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE2	12	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE1	12	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE2	12	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE1	14	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE2	14	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE1	14	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE2	14	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE1	14	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE2	14	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE1	16	0.44
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE2	16	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE1	16	0.44
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE2	16	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE1	16	0.44
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE2	16	0.44
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	15	0.44
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	15	0.44
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	15	0.44
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	15	0.44
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	15	0.44
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	4	0.44
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	4	0.44
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	8	0.44
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	10	0.44
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	17	0.44
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	18	0.44
(1,885)	1:161:A:ARG:HA	1:164:A:ARG:HE	6	0.44
(1,885)	1:161:A:ARG:HA	1:164:A:ARG:HE	16	0.44
(1,885)	1:161:A:ARG:HA	1:164:A:ARG:HE	20	0.44
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD11	7	0.44
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD12	7	0.44
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD13	7	0.44
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD21	7	0.44
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD22	7	0.44
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD23	7	0.44
(1,839)	1:4:A:TYR:HE1	1:52:A:LEU:H	17	0.44
(1,839)	1:4:A:TYR:HE2	1:52:A:LEU:H	17	0.44
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	6	0.44
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	12	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	1	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	2	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	4	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	5	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	8	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	9	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	10	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	14	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	15	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	18	0.44
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	20	0.44
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	3	0.44
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	3	0.44
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	16	0.44
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	16	0.44
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	16	0.44
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	20	0.44
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	20	0.44
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	20	0.44
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	20	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	20	0.44
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	20	0.44
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	5	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	6	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	6	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	10	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	10	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	12	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	12	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	13	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	13	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	20	0.44
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	20	0.44
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	5	0.44
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	1	0.44
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	1	0.44
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	1	0.44
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	9	0.44
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	9	0.44
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	9	0.44
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	13	0.44
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	13	0.44
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	13	0.44
(1,221)	1:1:A:MET:HB3	1:50:A:THR:HB	1	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	1	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	1	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	1	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	1	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	1	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	1	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	1	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	1	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	1	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	1	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	1	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	1	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	1	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	1	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	1	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	1	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	1	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	2	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	2	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	2	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	2	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	2	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	2	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	2	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	2	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	2	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	2	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	2	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	2	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	2	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	2	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	2	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	2	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	2	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	2	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	3	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	3	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	3	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	3	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	3	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	3	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	3	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	3	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	3	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	3	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	3	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	3	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	3	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	3	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	3	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	3	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	3	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	3	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	4	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	4	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	4	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	4	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	4	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	4	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	4	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	4	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	4	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	4	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	4	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	4	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	4	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	4	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	4	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	4	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	4	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	6	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	6	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	6	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	6	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	6	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	6	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	6	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	6	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	6	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	6	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	6	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	6	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	6	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	6	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	6	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	6	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	6	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	6	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	7	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	7	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	7	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	7	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	7	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	7	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	7	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	7	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	7	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	7	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	7	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	7	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	7	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	7	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	7	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	7	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	7	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	8	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	8	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	8	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	8	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	8	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	8	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	8	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	8	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	8	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	8	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	8	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	8	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	8	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	8	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	8	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	8	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	8	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	8	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	10	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	10	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	10	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	10	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	10	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	10	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	10	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	10	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	10	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	10	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	10	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	10	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	10	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	10	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	10	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	10	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	10	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	11	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	11	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	11	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	11	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	11	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	11	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	11	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	11	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	11	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	11	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	11	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	11	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	11	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	11	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	11	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	11	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	11	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	11	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	13	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	13	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	13	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	13	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	13	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	13	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	13	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	13	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	13	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	13	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	13	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	13	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	13	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	13	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	13	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	13	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	13	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	13	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	15	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	15	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	15	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	15	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	15	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	15	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	15	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	15	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	15	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	15	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	15	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	15	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	15	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	15	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	15	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	15	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	15	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	16	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	16	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	16	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	16	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	16	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	16	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	16	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	16	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	16	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	16	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	16	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	16	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	16	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	16	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	16	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	16	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	16	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	16	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	17	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	17	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	17	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	17	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	17	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	17	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	17	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	17	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	17	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	17	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	17	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	17	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	17	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	17	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	17	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	17	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	17	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	18	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	18	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	18	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	18	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	18	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	18	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	18	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	18	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	18	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	18	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	18	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	18	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	18	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	18	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	18	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	18	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	18	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	18	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	19	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	19	0.44
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	19	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	19	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	19	0.44
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	19	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	19	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	19	0.44
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	19	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	19	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	19	0.44
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	19	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	19	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	19	0.44
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	19	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	19	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	19	0.44
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	19	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	10	0.44
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	10	0.44
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	15	0.44
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	15	0.44
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	18	0.44
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	18	0.44
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	18	0.44
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	12	0.44
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	12	0.44
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	12	0.44
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	12	0.44
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	12	0.44
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	12	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	2	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	2	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	2	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	9	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	9	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	9	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	10	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	10	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	10	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	15	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	15	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	15	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	16	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	16	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	16	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	17	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	17	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	17	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	18	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	18	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	18	0.44
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	20	0.44
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	20	0.44
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	20	0.44
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	17	0.44
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	17	0.44
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	17	0.44
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	17	0.44
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	17	0.44
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE2	11	0.44
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE3	11	0.44
(1,3249)	1:3:A:GLU:HG3	1:4:A:TYR:H	8	0.43
(1,3249)	1:3:A:GLU:HG3	1:4:A:TYR:H	11	0.43
(1,3249)	1:3:A:GLU:HG3	1:4:A:TYR:H	20	0.43
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	13	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	2	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	2	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	2	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	3	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	3	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	3	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	7	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	7	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	7	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	14	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	14	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	14	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	15	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	15	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	15	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	18	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	18	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	18	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	19	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	19	0.43
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	19	0.43
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	9	0.43
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	5	0.43
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	19	0.43
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	3	0.43
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	3	0.43
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	16	0.43
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	6	0.43
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	9	0.43
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	12	0.43
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	14	0.43
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	20	0.43
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	9	0.43
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	9	0.43
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2712)	1:11:A:ALA:HB1	1:89:A:SER:H	8	0.43
(1,2712)	1:11:A:ALA:HB2	1:89:A:SER:H	8	0.43
(1,2712)	1:11:A:ALA:HB3	1:89:A:SER:H	8	0.43
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	12	0.43
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	12	0.43
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	12	0.43
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	12	0.43
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	12	0.43
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	12	0.43
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	8	0.43
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	8	0.43
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	8	0.43
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	9	0.43
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	9	0.43
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	9	0.43
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	5	0.43
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	6	0.43
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	8	0.43
(1,2626)	1:165:A:LYS:HB2	1:166:A:HIS:HD2	20	0.43
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	8	0.43
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	13	0.43
(1,2398)	1:161:A:ARG:HA	1:165:A:LYS:H	16	0.43
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	20	0.43
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	20	0.43
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	20	0.43
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	20	0.43
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	20	0.43
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	20	0.43
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	14	0.43
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	14	0.43
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE2	10	0.43
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE3	10	0.43
(1,2254)	1:149:A:ARG:HB2	1:150:A:GLN:HE21	5	0.43
(1,2254)	1:149:A:ARG:HB3	1:150:A:GLN:HE21	5	0.43
(1,2254)	1:149:A:ARG:HB2	1:150:A:GLN:HE21	19	0.43
(1,2254)	1:149:A:ARG:HB3	1:150:A:GLN:HE21	19	0.43
(1,2212)	1:78:A:PHE:HZ	1:100:A:ILE:HB	2	0.43
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	18	0.43
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	18	0.43
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	18	0.43
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	18	0.43
(1,1940)	1:120:A:LEU:HD11	1:121:A:PRO:HG3	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1940)	1:120:A:LEU:HD12	1:121:A:PRO:HG3	20	0.43
(1,1940)	1:120:A:LEU:HD13	1:121:A:PRO:HG3	20	0.43
(1,1940)	1:120:A:LEU:HD21	1:121:A:PRO:HG3	20	0.43
(1,1940)	1:120:A:LEU:HD22	1:121:A:PRO:HG3	20	0.43
(1,1940)	1:120:A:LEU:HD23	1:121:A:PRO:HG3	20	0.43
(1,1939)	1:10:A:GLY:H	1:12:A:GLY:H	18	0.43
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	17	0.43
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	3	0.43
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	3	0.43
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	15	0.43
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	15	0.43
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	18	0.43
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	18	0.43
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	18	0.43
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	18	0.43
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	19	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	3	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	4	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	8	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	10	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	11	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	12	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	14	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	15	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	16	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	19	0.43
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	20	0.43
(1,1708)	1:142:A:ILE:HD11	1:143:A:GLU:HB3	1	0.43
(1,1708)	1:142:A:ILE:HD12	1:143:A:GLU:HB3	1	0.43
(1,1708)	1:142:A:ILE:HD13	1:143:A:GLU:HB3	1	0.43
(1,1708)	1:142:A:ILE:HD11	1:143:A:GLU:HB3	18	0.43
(1,1708)	1:142:A:ILE:HD12	1:143:A:GLU:HB3	18	0.43
(1,1708)	1:142:A:ILE:HD13	1:143:A:GLU:HB3	18	0.43
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG2	10	0.43
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG3	10	0.43
(1,1645)	1:128:A:LYS:HG2	1:129:A:GLN:HB2	9	0.43
(1,1645)	1:128:A:LYS:HG3	1:129:A:GLN:HB2	9	0.43
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	13	0.43
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	13	0.43
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	15	0.43
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE1	14	0.43
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE2	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	10	0.43
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	2	0.43
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	10	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	1	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	1	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	1	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	4	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	4	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	4	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	7	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	7	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	7	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	11	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	11	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	11	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	13	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	13	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	13	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	15	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	15	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	15	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	17	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	17	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	17	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	20	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	20	0.43
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	20	0.43
(1,1375)	1:149:A:ARG:HB2	1:149:A:ARG:HE	4	0.43
(1,1375)	1:149:A:ARG:HB2	1:149:A:ARG:HE	17	0.43
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	1	0.43
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	3	0.43
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	8	0.43
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	9	0.43
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	14	0.43
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	15	0.43
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	14	0.43
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	14	0.43
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG2	13	0.43
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG3	13	0.43
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG2	13	0.43
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG3	13	0.43
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG2	13	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG3	13	0.43
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	4	0.43
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	4	0.43
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	4	0.43
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	1	0.43
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	20	0.43
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	6	0.43
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	6	0.43
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	6	0.43
(1,1155)	1:91:A:GLU:HA	1:94:A:HIS:HD2	3	0.43
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	15	0.43
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	3	0.43
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	7	0.43
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	20	0.43
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	2	0.43
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	7	0.43
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	16	0.43
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	17	0.43
(1,947)	1:83:A:ALA:H	1:90:A:PHE:H	7	0.43
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	5	0.43
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	5	0.43
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	8	0.43
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	8	0.43
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	10	0.43
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	10	0.43
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB2	3	0.43
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB3	3	0.43
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	15	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	3	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	7	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	11	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	12	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	13	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	16	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	17	0.43
(1,823)	1:118:A:SER:H	2:201:A:GNP:HN1	19	0.43
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	5	0.43
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	5	0.43
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	8	0.43
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	8	0.43
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	15	0.43
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	2	0.43
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	2	0.43
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	2	0.43
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	3	0.43
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	3	0.43
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	3	0.43
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	6	0.43
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	6	0.43
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	6	0.43
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	7	0.43
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	7	0.43
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	7	0.43
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	16	0.43
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	16	0.43
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	16	0.43
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	3	0.43
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG11	11	0.43
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG12	11	0.43
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG13	11	0.43
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG21	11	0.43
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG22	11	0.43
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG23	11	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	3	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	3	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	3	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	8	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	8	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	8	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	15	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	15	0.43
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	15	0.43
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	20	0.43
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	12	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	5	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	5	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	5	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	5	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	5	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	5	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	5	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	5	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	5	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	5	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	5	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	5	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	5	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	5	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	5	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	5	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	5	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	14	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	14	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	14	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	14	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	14	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	14	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	14	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	14	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	14	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	14	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	14	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	14	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	14	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	14	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	14	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	14	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	14	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	14	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	20	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	20	0.43
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	20	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	20	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	20	0.43
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	20	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	20	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	20	0.43
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	20	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	20	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	20	0.43
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	20	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	20	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	20	0.43
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	20	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	20	0.43
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	20	0.43
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	1	0.43
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	1	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	3	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	3	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	3	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	4	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	4	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	4	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	5	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	5	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	5	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	6	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	6	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	6	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	7	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	7	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	7	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	8	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	8	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	8	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	12	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	12	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	12	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	14	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	14	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	14	0.43
(1,152)	1:29:A:VAL:HG11	2:201:A:GNP:H8	19	0.43
(1,152)	1:29:A:VAL:HG12	2:201:A:GNP:H8	19	0.43
(1,152)	1:29:A:VAL:HG13	2:201:A:GNP:H8	19	0.43
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	4	0.43
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	4	0.43
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	6	0.43
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	6	0.43
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	6	0.43
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	6	0.43
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	6	0.43
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	6	0.43
(3,2)	1:17:A:SER:OG	2:201:A:GNP:O2B	9	0.42
(1,3249)	1:3:A:GLU:HG3	1:4:A:TYR:H	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3249)	1:3:A:GLU:HG3	1:4:A:TYR:H	13	0.42
(1,3223)	1:3:A:GLU:HG2	1:4:A:TYR:H	14	0.42
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	20	0.42
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	14	0.42
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	18	0.42
(1,3125)	1:58:A:THR:HG21	1:68:A:ARG:HE	1	0.42
(1,3125)	1:58:A:THR:HG22	1:68:A:ARG:HE	1	0.42
(1,3125)	1:58:A:THR:HG23	1:68:A:ARG:HE	1	0.42
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	1	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	1	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	1	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	1	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	2	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	2	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	2	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	3	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	3	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	3	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	4	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	4	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	4	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	5	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	5	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	5	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	6	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	6	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	6	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	7	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	7	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	7	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	8	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	8	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	8	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	10	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	10	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	10	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	11	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	11	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	11	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	12	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	12	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	12	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	13	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	13	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	13	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	15	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	15	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	15	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	16	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	16	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	16	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	17	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	17	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	17	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	18	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	18	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	18	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	19	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	19	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	19	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	20	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	20	0.42
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	20	0.42
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	1	0.42
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	1	0.42
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	5	0.42
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	11	0.42
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	20	0.42
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	4	0.42
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	5	0.42
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	16	0.42
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	18	0.42
(1,2733)	1:11:A:ALA:HB1	1:92:A:ASP:H	8	0.42
(1,2733)	1:11:A:ALA:HB2	1:92:A:ASP:H	8	0.42
(1,2733)	1:11:A:ALA:HB3	1:92:A:ASP:H	8	0.42
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	1	0.42
(1,2627)	1:47:A:ASP:HB2	1:161:A:ARG:HE	7	0.42
(1,2627)	1:47:A:ASP:HB3	1:161:A:ARG:HE	7	0.42
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	1	0.42
(1,2534)	1:123:A:ARG:HB3	1:123:A:ARG:HE	3	0.42
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	8	0.42
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	8	0.42
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	10	0.42
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	7	0.42
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	1	0.42
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	1	0.42
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	3	0.42
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	3	0.42
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	1	0.42
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	14	0.42
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	8	0.42
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	8	0.42
(1,2189)	1:4:A:TYR:HD1	1:52:A:LEU:H	3	0.42
(1,2189)	1:4:A:TYR:HD2	1:52:A:LEU:H	3	0.42
(1,2189)	1:4:A:TYR:HD1	1:52:A:LEU:H	17	0.42
(1,2189)	1:4:A:TYR:HD2	1:52:A:LEU:H	17	0.42
(1,2189)	1:4:A:TYR:HD1	1:52:A:LEU:H	20	0.42
(1,2189)	1:4:A:TYR:HD2	1:52:A:LEU:H	20	0.42
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB1	19	0.42
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB2	19	0.42
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB3	19	0.42
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB1	19	0.42
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB2	19	0.42
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB3	19	0.42
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB1	19	0.42
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB2	19	0.42
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB3	19	0.42
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	10	0.42
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	10	0.42
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	10	0.42
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	10	0.42
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	12	0.42
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	12	0.42
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	16	0.42
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	16	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	6	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	6	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	6	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	6	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	6	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	6	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	8	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	8	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	8	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	8	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	8	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	11	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	11	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	11	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	11	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	11	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	11	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	12	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	12	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	12	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	12	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	12	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	12	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	13	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	13	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	13	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	13	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	13	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	13	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	16	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	16	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	16	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	16	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	16	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	16	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	17	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	17	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	17	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	17	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	17	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	17	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	18	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	18	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	18	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	18	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	18	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	18	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	19	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	19	0.42
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	19	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	19	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	19	0.42
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	19	0.42
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	1	0.42
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	1	0.42
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	1	0.42
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	1	0.42
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	12	0.42
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	12	0.42
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	12	0.42
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	13	0.42
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	13	0.42
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	13	0.42
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE2	11	0.42
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE3	11	0.42
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	5	0.42
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	6	0.42
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	20	0.42
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	8	0.42
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	7	0.42
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	7	0.42
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	18	0.42
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG2	12	0.42
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG3	12	0.42
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	2	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	2	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	2	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	2	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	10	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	10	0.42
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	10	0.42
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	12	0.42
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	12	0.42
(1,1277)	1:67:A:MET:HG3	1:68:A:ARG:H	6	0.42
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	13	0.42
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	13	0.42
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	13	0.42
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	18	0.42
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	18	0.42
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	18	0.42
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	3	0.42
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	18	0.42
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	4	0.42
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	4	0.42
(1,1186)	1:56:A:LEU:HD11	1:71:A:TYR:HB3	12	0.42
(1,1186)	1:56:A:LEU:HD12	1:71:A:TYR:HB3	12	0.42
(1,1186)	1:56:A:LEU:HD13	1:71:A:TYR:HB3	12	0.42
(1,1186)	1:56:A:LEU:HD11	1:71:A:TYR:HB3	13	0.42
(1,1186)	1:56:A:LEU:HD12	1:71:A:TYR:HB3	13	0.42
(1,1186)	1:56:A:LEU:HD13	1:71:A:TYR:HB3	13	0.42
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	20	0.42
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	20	0.42
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	9	0.42
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	9	0.42
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	3	0.42
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	3	0.42
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	3	0.42
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	20	0.42
(1,1041)	1:23:A:LEU:HG	1:42:A:LYS:HD2	1	0.42
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	3	0.42
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	3	0.42
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	3	0.42
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	4	0.42
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	4	0.42
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	4	0.42
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	11	0.42
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	11	0.42
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	11	0.42
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	15	0.42
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	15	0.42
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	15	0.42
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	18	0.42
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	18	0.42
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	18	0.42
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	19	0.42
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	19	0.42
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	19	0.42
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	20	0.42
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	20	0.42
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	20	0.42
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	20	0.42
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	20	0.42
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	20	0.42
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	18	0.42
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	3	0.42
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	6	0.42
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	7	0.42
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	9	0.42
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	12	0.42
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	16	0.42
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	17	0.42
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	20	0.42
(1,750)	1:63:A:GLU:HG2	1:64:A:TYR:H	14	0.42
(1,750)	1:63:A:GLU:HG3	1:64:A:TYR:H	14	0.42
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	7	0.42
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	7	0.42
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	7	0.42
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	7	0.42
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	7	0.42
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	7	0.42
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	19	0.42
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	19	0.42
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	19	0.42
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	19	0.42
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	19	0.42
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	19	0.42
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	9	0.42
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	19	0.42
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	14	0.42
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	14	0.42
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	7	0.42
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	7	0.42
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	1	0.42
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	1	0.42
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	1	0.42
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	4	0.42
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	4	0.42
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	4	0.42
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	8	0.42
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	8	0.42
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	8	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG11	12	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG12	12	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG13	12	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG21	12	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG22	12	0.42
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG23	12	0.42
(1,527)	1:21:A:ILE:HD11	1:25:A:GLN:HG2	14	0.42
(1,527)	1:21:A:ILE:HD11	1:25:A:GLN:HG3	14	0.42
(1,527)	1:21:A:ILE:HD12	1:25:A:GLN:HG2	14	0.42
(1,527)	1:21:A:ILE:HD12	1:25:A:GLN:HG3	14	0.42
(1,527)	1:21:A:ILE:HD13	1:25:A:GLN:HG2	14	0.42
(1,527)	1:21:A:ILE:HD13	1:25:A:GLN:HG3	14	0.42
(1,491)	1:29:A:VAL:HA	1:31:A:GLU:H	9	0.42
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	9	0.42
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	9	0.42
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	9	0.42
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	9	0.42
(1,287)	1:60:A:GLY:HA2	1:63:A:GLU:H	15	0.42
(1,287)	1:60:A:GLY:HA3	1:63:A:GLU:H	15	0.42
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	3	0.42
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	1	0.42
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	1	0.42
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	1	0.42
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD11	9	0.42
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD12	9	0.42
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD13	9	0.42
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD21	9	0.42
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD22	9	0.42
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD23	9	0.42
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	7	0.42
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	7	0.42
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	14	0.42
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	2	0.42
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	2	0.42
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	2	0.42
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	2	0.42
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	2	0.42
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	2	0.42
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	13	0.42
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	13	0.42
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	13	0.42
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	13	0.42
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	13	0.42
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	13	0.42
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	16	0.41
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	10	0.41
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	10	0.41
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	10	0.41
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	5	0.41
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	16	0.41
(1,3173)	1:1:A:MET:HG2	1:2:A:THR:H	1	0.41
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	11	0.41
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	20	0.41
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	18	0.41
(1,3008)	1:58:A:THR:HB	1:68:A:ARG:HE	6	0.41
(1,3008)	1:58:A:THR:HB	1:68:A:ARG:HE	7	0.41
(1,3008)	1:58:A:THR:HB	1:68:A:ARG:HE	12	0.41
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	2	0.41
(1,2935)	1:73:A:ARG:H	1:73:A:ARG:HE	13	0.41
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	7	0.41
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	19	0.41
(1,2835)	1:73:A:ARG:HB2	1:73:A:ARG:HE	14	0.41
(1,2835)	1:73:A:ARG:HB3	1:73:A:ARG:HE	14	0.41
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	20	0.41
(1,2730)	1:118:A:SER:H	1:147:A:LYS:H	9	0.41
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	8	0.41
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	8	0.41
(1,2543)	1:123:A:ARG:HB2	1:123:A:ARG:HE	16	0.41
(1,2534)	1:123:A:ARG:HB3	1:123:A:ARG:HE	2	0.41
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	19	0.41
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	18	0.41
(1,2398)	1:161:A:ARG:HA	1:165:A:LYS:H	4	0.41
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	6	0.41
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	6	0.41
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	8	0.41
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	8	0.41
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	9	0.41
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	9	0.41
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	14	0.41
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	14	0.41
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	8	0.41
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	9	0.41
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	9	0.41
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	2	0.41
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	2	0.41
(1,2287)	1:151:A:GLY:HA2	1:153:A:ASP:HB2	16	0.41
(1,2287)	1:151:A:GLY:HA2	1:153:A:ASP:HB3	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	5	0.41
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	5	0.41
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	15	0.41
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	15	0.41
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	12	0.41
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	12	0.41
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	12	0.41
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	13	0.41
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	13	0.41
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	13	0.41
(1,2159)	1:140:A:PRO:HG3	1:162:A:GLU:HG2	15	0.41
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	19	0.41
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	19	0.41
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	19	0.41
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	5	0.41
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	5	0.41
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	5	0.41
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	5	0.41
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	5	0.41
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	5	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	1	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	1	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	1	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	1	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	2	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	2	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	2	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	2	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	5	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	5	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	5	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	5	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	6	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	6	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	6	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	6	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	7	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	7	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	7	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	7	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	8	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	8	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	8	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	11	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	11	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	11	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	11	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	13	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	13	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	13	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	13	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	14	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	14	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	14	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	14	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	16	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	16	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	16	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	16	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	17	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	17	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	17	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	17	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	18	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	18	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	18	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	18	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	19	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	19	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	19	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	19	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	20	0.41
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	20	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	20	0.41
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	20	0.41
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	19	0.41
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	19	0.41
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	15	0.41
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	15	0.41
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	15	0.41
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	15	0.41
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	15	0.41
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	15	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG21	7	0.41
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG22	7	0.41
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG23	7	0.41
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG21	7	0.41
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG22	7	0.41
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG23	7	0.41
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	20	0.41
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	20	0.41
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	20	0.41
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	20	0.41
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD11	6	0.41
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD12	6	0.41
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD13	6	0.41
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD21	6	0.41
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD22	6	0.41
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD23	6	0.41
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD11	6	0.41
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD12	6	0.41
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD13	6	0.41
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD21	6	0.41
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD22	6	0.41
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD23	6	0.41
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	7	0.41
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	7	0.41
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	2	0.41
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	2	0.41
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	2	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	2	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	2	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	2	0.41
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	5	0.41
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	5	0.41
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	5	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	5	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	5	0.41
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	5	0.41
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	18	0.41
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG12	7	0.41
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG13	7	0.41
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG12	7	0.41
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG13	7	0.41
(1,1774)	1:24:A:ILE:HD11	1:41:A:ARG:HA	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:24:A:ILE:HD12	1:41:A:ARG:HA	18	0.41
(1,1774)	1:24:A:ILE:HD13	1:41:A:ARG:HA	18	0.41
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	2	0.41
(1,1727)	1:78:A:PHE:HE1	1:104:A:LYS:HE3	8	0.41
(1,1727)	1:78:A:PHE:HE2	1:104:A:LYS:HE3	8	0.41
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	4	0.41
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	4	0.41
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	4	0.41
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	5	0.41
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	20	0.41
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	8	0.41
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	3	0.41
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	3	0.41
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	3	0.41
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	3	0.41
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	3	0.41
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	3	0.41
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	9	0.41
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	9	0.41
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	9	0.41
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	9	0.41
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	9	0.41
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	9	0.41
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	12	0.41
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	12	0.41
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	12	0.41
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	12	0.41
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	12	0.41
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	12	0.41
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	15	0.41
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	15	0.41
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	15	0.41
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	15	0.41
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	15	0.41
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	15	0.41
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	3	0.41
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	19	0.41
(1,1382)	1:7:A:VAL:HG11	1:75:A:GLY:HA2	5	0.41
(1,1382)	1:7:A:VAL:HG12	1:75:A:GLY:HA2	5	0.41
(1,1382)	1:7:A:VAL:HG13	1:75:A:GLY:HA2	5	0.41
(1,1382)	1:7:A:VAL:HG21	1:75:A:GLY:HA2	5	0.41
(1,1382)	1:7:A:VAL:HG22	1:75:A:GLY:HA2	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:7:A:VAL:HG23	1:75:A:GLY:HA2	5	0.41
(1,1382)	1:7:A:VAL:HG11	1:75:A:GLY:HA2	8	0.41
(1,1382)	1:7:A:VAL:HG12	1:75:A:GLY:HA2	8	0.41
(1,1382)	1:7:A:VAL:HG13	1:75:A:GLY:HA2	8	0.41
(1,1382)	1:7:A:VAL:HG21	1:75:A:GLY:HA2	8	0.41
(1,1382)	1:7:A:VAL:HG22	1:75:A:GLY:HA2	8	0.41
(1,1382)	1:7:A:VAL:HG23	1:75:A:GLY:HA2	8	0.41
(1,1382)	1:7:A:VAL:HG11	1:75:A:GLY:HA2	19	0.41
(1,1382)	1:7:A:VAL:HG12	1:75:A:GLY:HA2	19	0.41
(1,1382)	1:7:A:VAL:HG13	1:75:A:GLY:HA2	19	0.41
(1,1382)	1:7:A:VAL:HG21	1:75:A:GLY:HA2	19	0.41
(1,1382)	1:7:A:VAL:HG22	1:75:A:GLY:HA2	19	0.41
(1,1382)	1:7:A:VAL:HG23	1:75:A:GLY:HA2	19	0.41
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	18	0.41
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	18	0.41
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	18	0.41
(1,1375)	1:149:A:ARG:HB2	1:149:A:ARG:HE	1	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG11	3	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG12	3	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG13	3	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG21	3	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG22	3	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG23	3	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG11	5	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG12	5	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG13	5	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG21	5	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG22	5	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG23	5	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG11	16	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG12	16	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG13	16	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG21	16	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG22	16	0.41
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG23	16	0.41
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	5	0.41
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	13	0.41
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	20	0.41
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	20	0.41
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	20	0.41
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	16	0.41
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	1	0.41
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	1	0.41
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	1	0.41
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	1	0.41
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	1	0.41
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	1	0.41
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	1	0.41
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	1	0.41
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	1	0.41
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	15	0.41
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	15	0.41
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	15	0.41
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	15	0.41
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	15	0.41
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	15	0.41
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	15	0.41
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	15	0.41
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	15	0.41
(1,1210)	1:56:A:LEU:HD21	1:71:A:TYR:HB3	8	0.41
(1,1210)	1:56:A:LEU:HD22	1:71:A:TYR:HB3	8	0.41
(1,1210)	1:56:A:LEU:HD23	1:71:A:TYR:HB3	8	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	6	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	6	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	6	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	9	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	9	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	9	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	18	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	18	0.41
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	18	0.41
(1,1194)	1:56:A:LEU:HD11	1:57:A:ASP:H	11	0.41
(1,1194)	1:56:A:LEU:HD12	1:57:A:ASP:H	11	0.41
(1,1194)	1:56:A:LEU:HD13	1:57:A:ASP:H	11	0.41
(1,1194)	1:56:A:LEU:HD21	1:57:A:ASP:H	11	0.41
(1,1194)	1:56:A:LEU:HD22	1:57:A:ASP:H	11	0.41
(1,1194)	1:56:A:LEU:HD23	1:57:A:ASP:H	11	0.41
(1,1186)	1:56:A:LEU:HD11	1:71:A:TYR:HB3	2	0.41
(1,1186)	1:56:A:LEU:HD12	1:71:A:TYR:HB3	2	0.41
(1,1186)	1:56:A:LEU:HD13	1:71:A:TYR:HB3	2	0.41
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	12	0.41
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	12	0.41
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	12	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	6	0.41
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	14	0.41
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	14	0.41
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	4	0.41
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	4	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	1	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	2	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	4	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	8	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	10	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	14	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	18	0.41
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	19	0.41
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	1	0.41
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	1	0.41
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	1	0.41
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	1	0.41
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	1	0.41
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	1	0.41
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	17	0.41
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	17	0.41
(1,559)	1:31:A:GLU:HG2	1:32:A:TYR:H	13	0.41
(1,559)	1:31:A:GLU:HG3	1:32:A:TYR:H	13	0.41
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG11	1	0.41
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG12	1	0.41
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG13	1	0.41
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG21	1	0.41
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG22	1	0.41
(1,551)	1:107:A:GLU:HA	1:109:A:VAL:HG23	1	0.41
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	11	0.41
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	17	0.41
(1,377)	1:24:A:ILE:HD11	1:43:A:GLN:H	3	0.41
(1,377)	1:24:A:ILE:HD12	1:43:A:GLN:H	3	0.41
(1,377)	1:24:A:ILE:HD13	1:43:A:GLN:H	3	0.41
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	16	0.41
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	16	0.41
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	16	0.41
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	19	0.41
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	19	0.41
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	19	0.41
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	16	0.41
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	3	0.41
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	3	0.41
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	3	0.41
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	3	0.41
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	3	0.41
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	18	0.4
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	10	0.4
(1,3173)	1:1:A:MET:HG2	1:2:A:THR:H	12	0.4
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	8	0.4
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	2	0.4
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	6	0.4
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	11	0.4
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	6	0.4
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	20	0.4
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	6	0.4
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	6	0.4
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	6	0.4
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	15	0.4
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	15	0.4
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	15	0.4
(1,2733)	1:11:A:ALA:HB1	1:92:A:ASP:H	7	0.4
(1,2733)	1:11:A:ALA:HB2	1:92:A:ASP:H	7	0.4
(1,2733)	1:11:A:ALA:HB3	1:92:A:ASP:H	7	0.4
(1,2690)	1:148:A:THR:H	1:150:A:GLN:HB2	5	0.4
(1,2625)	1:23:A:LEU:HD11	1:156:A:PHE:HB2	9	0.4
(1,2625)	1:23:A:LEU:HD12	1:156:A:PHE:HB2	9	0.4
(1,2625)	1:23:A:LEU:HD13	1:156:A:PHE:HB2	9	0.4
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	14	0.4
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	16	0.4
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	16	0.4
(1,2487)	1:168:A:GLU:H	1:168:A:GLU:HG3	19	0.4
(1,2417)	1:4:A:TYR:HD1	1:163:A:ILE:HA	5	0.4
(1,2417)	1:4:A:TYR:HD2	1:163:A:ILE:HA	5	0.4
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	6	0.4
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	6	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	4	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	4	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	4	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	4	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	4	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	4	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	6	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	6	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	6	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	6	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	6	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	8	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	8	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	8	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	8	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	8	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	8	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	12	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	12	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	12	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	12	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	12	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	12	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	13	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	13	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	13	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	13	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	13	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	13	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	15	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	15	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	15	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	15	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	15	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	15	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	17	0.4
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	17	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	17	0.4
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	17	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	17	0.4
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	17	0.4
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	6	0.4
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	18	0.4
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	18	0.4
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	19	0.4
(1,2267)	1:150:A:GLN:HG2	1:151:A:GLY:H	3	0.4
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	16	0.4
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	16	0.4
(1,2193)	1:143:A:GLU:HG3	1:144:A:THR:H	9	0.4
(1,2159)	1:140:A:PRO:HG3	1:162:A:GLU:HG2	12	0.4
(1,2159)	1:140:A:PRO:HG3	1:162:A:GLU:HG2	20	0.4
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	11	0.4
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	11	0.4
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	11	0.4
(1,2056)	1:126:A:ASP:HB2	1:129:A:GLN:HG2	13	0.4
(1,2056)	1:126:A:ASP:HB3	1:129:A:GLN:HG2	13	0.4
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	12	0.4
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	12	0.4
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	12	0.4
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	12	0.4
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	15	0.4
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	15	0.4
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	15	0.4
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	15	0.4
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	18	0.4
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	18	0.4
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	14	0.4
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	18	0.4
(1,1965)	1:123:A:ARG:HD2	1:124:A:THR:HA	17	0.4
(1,1965)	1:123:A:ARG:HD3	1:124:A:THR:HA	17	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD11	5	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD12	5	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD13	5	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD21	5	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD22	5	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD23	5	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD11	5	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD12	5	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD13	5	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD21	5	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD22	5	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD23	5	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD11	10	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD12	10	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD13	10	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD21	10	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD22	10	0.4
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD23	10	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD11	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD12	10	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD13	10	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD21	10	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD22	10	0.4
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD23	10	0.4
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD11	4	0.4
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD12	4	0.4
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD13	4	0.4
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD21	4	0.4
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD22	4	0.4
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD23	4	0.4
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD11	4	0.4
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD12	4	0.4
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD13	4	0.4
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD21	4	0.4
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD22	4	0.4
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD23	4	0.4
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	1	0.4
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	1	0.4
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	1	0.4
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	1	0.4
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	1	0.4
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	1	0.4
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	4	0.4
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	4	0.4
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	4	0.4
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	4	0.4
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	4	0.4
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	4	0.4
(1,1849)	1:77:A:GLY:HA2	1:111:A:MET:HA	1	0.4
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	20	0.4
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG12	8	0.4
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG13	8	0.4
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG12	8	0.4
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG13	8	0.4
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	13	0.4
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	13	0.4
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	13	0.4
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	16	0.4
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	16	0.4
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	16	0.4
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	1:101:A:LYS:HD2	1:107:A:GLU:HA	1	0.4
(1,1661)	1:101:A:LYS:HD3	1:107:A:GLU:HA	1	0.4
(1,1634)	1:22:A:GLN:HE21	1:149:A:ARG:HE	13	0.4
(1,1634)	1:22:A:GLN:HE22	1:149:A:ARG:HE	13	0.4
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	16	0.4
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD11	11	0.4
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD12	11	0.4
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD13	11	0.4
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD11	11	0.4
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD12	11	0.4
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD13	11	0.4
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	17	0.4
(1,1489)	1:95:A:HIS:HE1	1:99:A:GLN:HE22	10	0.4
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD11	8	0.4
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD12	8	0.4
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD13	8	0.4
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD11	8	0.4
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD12	8	0.4
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD13	8	0.4
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	20	0.4
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	20	0.4
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	20	0.4
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	20	0.4
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	20	0.4
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	20	0.4
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	20	0.4
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	20	0.4
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	20	0.4
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	20	0.4
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	20	0.4
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	20	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	1	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	1	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	1	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	1	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	1	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	1	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	2	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	2	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	2	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	2	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	2	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	4	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	4	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	4	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	4	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	4	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	4	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	5	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	5	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	5	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	5	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	5	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	5	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	8	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	8	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	8	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	8	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	8	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	8	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	10	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	10	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	10	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	10	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	10	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	10	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	13	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	13	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	13	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	13	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	13	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	13	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	14	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	14	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	14	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	14	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	14	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	14	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	17	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	17	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	17	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	17	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	17	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	17	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	18	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	18	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	18	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	18	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	18	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	18	0.4
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	19	0.4
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	19	0.4
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	19	0.4
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	19	0.4
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	19	0.4
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	19	0.4
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	1	0.4
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	1	0.4
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	1	0.4
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	1	0.4
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	1	0.4
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	1	0.4
(1,1394)	1:75:A:GLY:HA3	1:77:A:GLY:H	5	0.4
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	13	0.4
(1,1382)	1:7:A:VAL:HG11	1:75:A:GLY:HA2	11	0.4
(1,1382)	1:7:A:VAL:HG12	1:75:A:GLY:HA2	11	0.4
(1,1382)	1:7:A:VAL:HG13	1:75:A:GLY:HA2	11	0.4
(1,1382)	1:7:A:VAL:HG21	1:75:A:GLY:HA2	11	0.4
(1,1382)	1:7:A:VAL:HG22	1:75:A:GLY:HA2	11	0.4
(1,1382)	1:7:A:VAL:HG23	1:75:A:GLY:HA2	11	0.4
(1,1335)	1:73:A:ARG:HD2	1:103:A:VAL:HG11	2	0.4
(1,1335)	1:73:A:ARG:HD2	1:103:A:VAL:HG12	2	0.4
(1,1335)	1:73:A:ARG:HD2	1:103:A:VAL:HG13	2	0.4
(1,1335)	1:73:A:ARG:HD2	1:103:A:VAL:HG21	2	0.4
(1,1335)	1:73:A:ARG:HD2	1:103:A:VAL:HG22	2	0.4
(1,1335)	1:73:A:ARG:HD2	1:103:A:VAL:HG23	2	0.4
(1,1335)	1:73:A:ARG:HD3	1:103:A:VAL:HG11	2	0.4
(1,1335)	1:73:A:ARG:HD3	1:103:A:VAL:HG12	2	0.4
(1,1335)	1:73:A:ARG:HD3	1:103:A:VAL:HG13	2	0.4
(1,1335)	1:73:A:ARG:HD3	1:103:A:VAL:HG21	2	0.4
(1,1335)	1:73:A:ARG:HD3	1:103:A:VAL:HG22	2	0.4
(1,1335)	1:73:A:ARG:HD3	1:103:A:VAL:HG23	2	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG11	4	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG12	4	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG13	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG21	4	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG22	4	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG23	4	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG11	8	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG12	8	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG13	8	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG21	8	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG22	8	0.4
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG23	8	0.4
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	7	0.4
(1,1284)	1:67:A:MET:HG2	1:71:A:TYR:HD1	15	0.4
(1,1284)	1:67:A:MET:HG2	1:71:A:TYR:HD2	15	0.4
(1,1284)	1:67:A:MET:HG3	1:71:A:TYR:HD1	15	0.4
(1,1284)	1:67:A:MET:HG3	1:71:A:TYR:HD2	15	0.4
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG2	1	0.4
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG3	1	0.4
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG2	1	0.4
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG3	1	0.4
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG2	1	0.4
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG3	1	0.4
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	13	0.4
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	13	0.4
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	13	0.4
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	13	0.4
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	13	0.4
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	13	0.4
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	13	0.4
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	13	0.4
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	13	0.4
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	18	0.4
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	18	0.4
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	18	0.4
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	18	0.4
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	18	0.4
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	18	0.4
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	18	0.4
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	18	0.4
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	18	0.4
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	7	0.4
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	3	0.4
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	3	0.4
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	4	0.4
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	4	0.4
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	4	0.4
(1,1175)	1:23:A:LEU:HD11	1:156:A:PHE:HB3	9	0.4
(1,1175)	1:23:A:LEU:HD12	1:156:A:PHE:HB3	9	0.4
(1,1175)	1:23:A:LEU:HD13	1:156:A:PHE:HB3	9	0.4
(1,1175)	1:23:A:LEU:HD21	1:156:A:PHE:HB3	9	0.4
(1,1175)	1:23:A:LEU:HD22	1:156:A:PHE:HB3	9	0.4
(1,1175)	1:23:A:LEU:HD23	1:156:A:PHE:HB3	9	0.4
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	18	0.4
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	18	0.4
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	18	0.4
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	18	0.4
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	18	0.4
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	18	0.4
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	8	0.4
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	9	0.4
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	20	0.4
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	20	0.4
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	20	0.4
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG21	1	0.4
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG22	1	0.4
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG23	1	0.4
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG21	1	0.4
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG22	1	0.4
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG23	1	0.4
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	2	0.4
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	2	0.4
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	3	0.4
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	3	0.4
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	3	0.4
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	3	0.4
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	3	0.4
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	3	0.4
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	3	0.4
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	3	0.4
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	3	0.4
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	3	0.4
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	3	0.4
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	3	0.4
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	15	0.4
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	15	0.4
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	15	0.4
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	15	0.4
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	15	0.4
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	15	0.4
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	15	0.4
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	15	0.4
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	15	0.4
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	15	0.4
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	15	0.4
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	5	0.4
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	19	0.4
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	4	0.4
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	4	0.4
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	10	0.4
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	8	0.4
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	20	0.4
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	5	0.4
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	5	0.4
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	5	0.4
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	5	0.4
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	2	0.4
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	2	0.4
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	2	0.4
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	2	0.4
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	2	0.4
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	2	0.4
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	20	0.4
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	20	0.4
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	15	0.4
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	15	0.4
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	7	0.4
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	14	0.4
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	18	0.4
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	18	0.4
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	18	0.4
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	18	0.4
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	18	0.4
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	18	0.4
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	19	0.4
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	19	0.4
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	19	0.4
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	19	0.4
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	19	0.4
(1,84)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	8	0.4
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	7	0.4
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	7	0.4
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	7	0.4
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	7	0.4
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	7	0.4
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	7	0.4
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	14	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	3	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	3	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	3	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	3	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	3	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	3	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	10	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	10	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	10	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	10	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	10	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	10	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	12	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	12	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	12	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	12	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	12	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	12	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	13	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	13	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	13	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	13	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	13	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	13	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	16	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	16	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	16	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	16	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	16	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	16	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	18	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	18	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	18	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	18	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	18	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	18	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	19	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	19	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	19	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	19	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	19	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	19	0.39
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	20	0.39
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	20	0.39
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	20	0.39
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	20	0.39
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	20	0.39
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	20	0.39
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	14	0.39
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	16	0.39
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	16	0.39
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	16	0.39
(1,3144)	1:1:A:MET:HE1	1:52:A:LEU:H	6	0.39
(1,3144)	1:1:A:MET:HE2	1:52:A:LEU:H	6	0.39
(1,3144)	1:1:A:MET:HE3	1:52:A:LEU:H	6	0.39
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	4	0.39
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	18	0.39
(1,2985)	1:129:A:GLN:HA	1:132:A:ASP:HB2	20	0.39
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	12	0.39
(1,2846)	1:140:A:PRO:HG2	1:141:A:PHE:H	17	0.39
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	1	0.39
(1,2762)	1:102:A:ARG:H	1:102:A:ARG:HE	16	0.39
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	15	0.39
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	15	0.39
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	15	0.39
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	19	0.39
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	19	0.39
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	19	0.39
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	9	0.39
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	8	0.39
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	8	0.39
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	8	0.39
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	8	0.39
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	8	0.39
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	17	0.39
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	17	0.39
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	20	0.39
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	20	0.39
(1,2630)	1:150:A:GLN:HG3	1:152:A:VAL:H	3	0.39
(1,2627)	1:47:A:ASP:HB2	1:161:A:ARG:HE	16	0.39
(1,2627)	1:47:A:ASP:HB3	1:161:A:ARG:HE	16	0.39
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	11	0.39
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	16	0.39
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	20	0.39
(1,2574)	1:84:A:ILE:HD11	1:123:A:ARG:HE	9	0.39
(1,2574)	1:84:A:ILE:HD12	1:123:A:ARG:HE	9	0.39
(1,2574)	1:84:A:ILE:HD13	1:123:A:ARG:HE	9	0.39
(1,2574)	1:84:A:ILE:HD11	1:123:A:ARG:HE	16	0.39
(1,2574)	1:84:A:ILE:HD12	1:123:A:ARG:HE	16	0.39
(1,2574)	1:84:A:ILE:HD13	1:123:A:ARG:HE	16	0.39
(1,2562)	1:20:A:THR:HA	1:23:A:LEU:HG	2	0.39
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	9	0.39
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	9	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	2	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	2	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	3	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	3	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	4	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	4	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	5	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	5	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	6	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	6	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	8	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	8	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	9	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	9	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	10	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	10	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	11	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	11	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	12	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	12	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	13	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	14	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	14	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	15	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	15	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	17	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	17	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	18	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	18	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	20	0.39
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	20	0.39
(1,2472)	1:128:A:LYS:H	1:128:A:LYS:HE2	8	0.39
(1,2472)	1:128:A:LYS:H	1:128:A:LYS:HE3	8	0.39
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	3	0.39
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	3	0.39
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	5	0.39
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	8	0.39
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	12	0.39
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	17	0.39
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	4	0.39
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	4	0.39
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	8	0.39
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	8	0.39
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	8	0.39
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	10	0.39
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	10	0.39
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	10	0.39
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	16	0.39
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	16	0.39
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	16	0.39
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	15	0.39
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	15	0.39
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	18	0.39
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	18	0.39
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	18	0.39
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG11	7	0.39
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG12	7	0.39
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG13	7	0.39
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG21	7	0.39
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG22	7	0.39
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG23	7	0.39
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG11	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG12	7	0.39
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG13	7	0.39
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG21	7	0.39
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG22	7	0.39
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG23	7	0.39
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	5	0.39
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	13	0.39
(1,2132)	1:45:A:VAL:HG11	1:51:A:CYS:H	1	0.39
(1,2132)	1:45:A:VAL:HG12	1:51:A:CYS:H	1	0.39
(1,2132)	1:45:A:VAL:HG13	1:51:A:CYS:H	1	0.39
(1,2132)	1:45:A:VAL:HG21	1:51:A:CYS:H	1	0.39
(1,2132)	1:45:A:VAL:HG22	1:51:A:CYS:H	1	0.39
(1,2132)	1:45:A:VAL:HG23	1:51:A:CYS:H	1	0.39
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	3	0.39
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	3	0.39
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	3	0.39
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	3	0.39
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	13	0.39
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	13	0.39
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	3	0.39
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	3	0.39
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	3	0.39
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	3	0.39
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	3	0.39
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	3	0.39
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	3	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD11	9	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD12	9	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD13	9	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD21	9	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD22	9	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD23	9	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD11	9	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD12	9	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD13	9	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD21	9	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD22	9	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD23	9	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD11	13	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD12	13	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD13	13	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD21	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD22	13	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD23	13	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD11	13	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD12	13	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD13	13	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD21	13	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD22	13	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD23	13	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD11	17	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD12	17	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD13	17	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD21	17	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD22	17	0.39
(1,1927)	1:85:A:ASN:HD21	1:120:A:LEU:HD23	17	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD11	17	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD12	17	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD13	17	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD21	17	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD22	17	0.39
(1,1927)	1:85:A:ASN:HD22	1:120:A:LEU:HD23	17	0.39
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	20	0.39
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	20	0.39
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	1	0.39
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	9	0.39
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	9	0.39
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	9	0.39
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	9	0.39
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	9	0.39
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	9	0.39
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	16	0.39
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	16	0.39
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	16	0.39
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	16	0.39
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	16	0.39
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	16	0.39
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	20	0.39
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	20	0.39
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	20	0.39
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	20	0.39
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	20	0.39
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	20	0.39
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	6	0.39
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	20	0.39
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	20	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	1	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	1	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	1	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	2	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	2	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	2	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	3	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	3	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	3	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	4	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	4	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	4	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	7	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	7	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	7	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	8	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	8	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	8	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	9	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	9	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	9	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	10	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	10	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	10	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	11	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	11	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	11	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	12	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	12	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	12	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	14	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	14	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	14	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	17	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	17	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	17	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	18	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	18	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	18	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	20	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	20	0.39
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	20	0.39
(1,1699)	1:72:A:MET:HG2	1:103:A:VAL:HB	1	0.39
(1,1699)	1:72:A:MET:HG3	1:103:A:VAL:HB	1	0.39
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	7	0.39
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	20	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD11	7	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD12	7	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD13	7	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD11	7	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD12	7	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD13	7	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD11	15	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD12	15	0.39
(1,1482)	1:162:A:GLU:HB2	1:163:A:ILE:HD13	15	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD11	15	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD12	15	0.39
(1,1482)	1:162:A:GLU:HB3	1:163:A:ILE:HD13	15	0.39
(1,1426)	1:8:A:VAL:HG11	1:79:A:LEU:HB2	2	0.39
(1,1426)	1:8:A:VAL:HG11	1:79:A:LEU:HB3	2	0.39
(1,1426)	1:8:A:VAL:HG12	1:79:A:LEU:HB2	2	0.39
(1,1426)	1:8:A:VAL:HG12	1:79:A:LEU:HB3	2	0.39
(1,1426)	1:8:A:VAL:HG13	1:79:A:LEU:HB2	2	0.39
(1,1426)	1:8:A:VAL:HG13	1:79:A:LEU:HB3	2	0.39
(1,1426)	1:8:A:VAL:HG21	1:79:A:LEU:HB2	2	0.39
(1,1426)	1:8:A:VAL:HG21	1:79:A:LEU:HB3	2	0.39
(1,1426)	1:8:A:VAL:HG22	1:79:A:LEU:HB2	2	0.39
(1,1426)	1:8:A:VAL:HG22	1:79:A:LEU:HB3	2	0.39
(1,1426)	1:8:A:VAL:HG23	1:79:A:LEU:HB2	2	0.39
(1,1426)	1:8:A:VAL:HG23	1:79:A:LEU:HB3	2	0.39
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	3	0.39
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	3	0.39
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	15	0.39
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	15	0.39
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	12	0.39
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	12	0.39
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	12	0.39
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	12	0.39
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	12	0.39
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	12	0.39
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	14	0.39
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	14	0.39
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	14	0.39
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	14	0.39
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	14	0.39
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	17	0.39
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	17	0.39
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	17	0.39
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	17	0.39
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	17	0.39
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	17	0.39
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	10	0.39
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	14	0.39
(1,1347)	1:73:A:ARG:HA	1:73:A:ARG:HD2	15	0.39
(1,1347)	1:73:A:ARG:HA	1:73:A:ARG:HD3	15	0.39
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	4	0.39
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	9	0.39
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	9	0.39
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	7	0.39
(1,1210)	1:56:A:LEU:HD21	1:71:A:TYR:HB3	5	0.39
(1,1210)	1:56:A:LEU:HD22	1:71:A:TYR:HB3	5	0.39
(1,1210)	1:56:A:LEU:HD23	1:71:A:TYR:HB3	5	0.39
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	11	0.39
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	11	0.39
(1,1132)	1:1:A:MET:HE1	1:52:A:LEU:HB2	10	0.39
(1,1132)	1:1:A:MET:HE2	1:52:A:LEU:HB2	10	0.39
(1,1132)	1:1:A:MET:HE3	1:52:A:LEU:HB2	10	0.39
(1,1131)	1:1:A:MET:HE1	1:52:A:LEU:HB3	5	0.39
(1,1131)	1:1:A:MET:HE2	1:52:A:LEU:HB3	5	0.39
(1,1131)	1:1:A:MET:HE3	1:52:A:LEU:HB3	5	0.39
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	13	0.39
(1,1051)	1:126:A:ASP:H	1:129:A:GLN:HE22	20	0.39
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	4	0.39
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	7	0.39
(1,957)	1:43:A:GLN:HG2	1:44:A:VAL:H	6	0.39
(1,957)	1:43:A:GLN:HG3	1:44:A:VAL:H	6	0.39
(1,957)	1:43:A:GLN:HG2	1:44:A:VAL:H	7	0.39
(1,957)	1:43:A:GLN:HG3	1:44:A:VAL:H	7	0.39
(1,957)	1:43:A:GLN:HG2	1:44:A:VAL:H	10	0.39
(1,957)	1:43:A:GLN:HG3	1:44:A:VAL:H	10	0.39
(1,952)	1:1:A:MET:HE1	1:43:A:GLN:HE21	5	0.39
(1,952)	1:1:A:MET:HE2	1:43:A:GLN:HE21	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,952)	1:1:A:MET:HE3	1:43:A:GLN:HE21	5	0.39
(1,952)	1:1:A:MET:HE1	1:43:A:GLN:HE21	17	0.39
(1,952)	1:1:A:MET:HE2	1:43:A:GLN:HE21	17	0.39
(1,952)	1:1:A:MET:HE3	1:43:A:GLN:HE21	17	0.39
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	3	0.39
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	13	0.39
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	13	0.39
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	13	0.39
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	13	0.39
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	13	0.39
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	13	0.39
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	13	0.39
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	13	0.39
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	13	0.39
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	13	0.39
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	13	0.39
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	13	0.39
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	14	0.39
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	14	0.39
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	14	0.39
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	14	0.39
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	14	0.39
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	14	0.39
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	14	0.39
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	14	0.39
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	14	0.39
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	14	0.39
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	14	0.39
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	14	0.39
(1,824)	1:119:A:ASP:H	2:201:A:GNP:HN1	8	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	1	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	2	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	3	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	4	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	7	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	10	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	11	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	13	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	16	0.39
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	18	0.39
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	12	0.39
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	3	0.39
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	17	0.39
(1,489)	1:160:A:VAL:HG11	1:164:A:ARG:HE	6	0.39
(1,489)	1:160:A:VAL:HG12	1:164:A:ARG:HE	6	0.39
(1,489)	1:160:A:VAL:HG13	1:164:A:ARG:HE	6	0.39
(1,489)	1:160:A:VAL:HG21	1:164:A:ARG:HE	6	0.39
(1,489)	1:160:A:VAL:HG22	1:164:A:ARG:HE	6	0.39
(1,489)	1:160:A:VAL:HG23	1:164:A:ARG:HE	6	0.39
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	18	0.39
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	19	0.39
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	19	0.39
(1,225)	1:6:A:LEU:H	1:6:A:LEU:HG	12	0.39
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	4	0.39
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	4	0.39
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	4	0.39
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	4	0.39
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	4	0.39
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	4	0.39
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	7	0.39
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	7	0.39
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	6	0.39
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	7	0.39
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	13	0.39
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	13	0.39
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	13	0.39
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	13	0.39
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	13	0.39
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	13	0.39
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	16	0.39
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	16	0.39
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	16	0.39
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	16	0.39
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	16	0.39
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	16	0.39
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	11	0.39
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	13	0.38
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	11	0.38
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	11	0.38
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG21	2	0.38
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG22	2	0.38
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG23	2	0.38
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	12	0.38
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	12	0.38
(1,3144)	1:1:A:MET:HE1	1:52:A:LEU:H	10	0.38
(1,3144)	1:1:A:MET:HE2	1:52:A:LEU:H	10	0.38
(1,3144)	1:1:A:MET:HE3	1:52:A:LEU:H	10	0.38
(1,3008)	1:58:A:THR:HB	1:68:A:ARG:HE	14	0.38
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	3	0.38
(1,2908)	1:135:A:ARG:HD2	1:136:A:SER:H	16	0.38
(1,2908)	1:135:A:ARG:HD3	1:136:A:SER:H	16	0.38
(1,2899)	1:28:A:PHE:HE1	1:147:A:LYS:HD3	16	0.38
(1,2899)	1:28:A:PHE:HE2	1:147:A:LYS:HD3	16	0.38
(1,2816)	1:66:A:ALA:HB1	1:69:A:ASP:HB2	9	0.38
(1,2816)	1:66:A:ALA:HB1	1:69:A:ASP:HB3	9	0.38
(1,2816)	1:66:A:ALA:HB2	1:69:A:ASP:HB2	9	0.38
(1,2816)	1:66:A:ALA:HB2	1:69:A:ASP:HB3	9	0.38
(1,2816)	1:66:A:ALA:HB3	1:69:A:ASP:HB2	9	0.38
(1,2816)	1:66:A:ALA:HB3	1:69:A:ASP:HB3	9	0.38
(1,2803)	1:116:A:ASN:HA	1:144:A:THR:H	10	0.38
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	4	0.38
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	4	0.38
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	4	0.38
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	18	0.38
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	18	0.38
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	18	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE1	1	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE2	1	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE3	1	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE1	1	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE2	1	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE3	1	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE1	6	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE2	6	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE3	6	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE1	6	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE2	6	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE3	6	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE1	15	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE2	15	0.38
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE3	15	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE1	15	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE2	15	0.38
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE3	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	13	0.38
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	13	0.38
(1,2663)	1:1:A:MET:HE1	1:43:A:GLN:HE22	19	0.38
(1,2663)	1:1:A:MET:HE2	1:43:A:GLN:HE22	19	0.38
(1,2663)	1:1:A:MET:HE3	1:43:A:GLN:HE22	19	0.38
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	4	0.38
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	4	0.38
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	4	0.38
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	19	0.38
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	19	0.38
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	3	0.38
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	3	0.38
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	10	0.38
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	12	0.38
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	12	0.38
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	19	0.38
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	19	0.38
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	18	0.38
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	18	0.38
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	18	0.38
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	18	0.38
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	18	0.38
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	18	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	1	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	1	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	1	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	2	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	2	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	2	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	3	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	3	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	3	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	4	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	4	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	4	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	6	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	6	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	6	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	7	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	7	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	7	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	9	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	9	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	11	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	11	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	11	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	14	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	14	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	14	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	19	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	19	0.38
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	19	0.38
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	1	0.38
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	10	0.38
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	14	0.38
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	20	0.38
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	10	0.38
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	10	0.38
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	17	0.38
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	17	0.38
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	17	0.38
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	17	0.38
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	17	0.38
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	17	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	1	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	1	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	1	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	5	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	5	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	5	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	7	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	7	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	7	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	11	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	11	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	11	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	12	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	12	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	12	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	13	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	13	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	13	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	15	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	15	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	17	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	17	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	17	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	18	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	18	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	18	0.38
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	20	0.38
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	20	0.38
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	20	0.38
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	5	0.38
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	5	0.38
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	10	0.38
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	10	0.38
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	9	0.38
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	9	0.38
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	20	0.38
(1,2280)	1:144:A:THR:HA	1:151:A:GLY:HA2	8	0.38
(1,2250)	1:22:A:GLN:HE21	1:149:A:ARG:HB2	13	0.38
(1,2250)	1:22:A:GLN:HE21	1:149:A:ARG:HB3	13	0.38
(1,2250)	1:22:A:GLN:HE22	1:149:A:ARG:HB2	13	0.38
(1,2250)	1:22:A:GLN:HE22	1:149:A:ARG:HB3	13	0.38
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	18	0.38
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	18	0.38
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	6	0.38
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	11	0.38
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	10	0.38
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	11	0.38
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	11	0.38
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	11	0.38
(1,1849)	1:77:A:GLY:HA2	1:111:A:MET:HA	6	0.38
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	19	0.38
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	11	0.38
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	3	0.38
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	3	0.38
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	3	0.38
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	3	0.38
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	3	0.38
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	3	0.38
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	11	0.38
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	11	0.38
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	11	0.38
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	11	0.38
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	11	0.38
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	12	0.38
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	12	0.38
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	12	0.38
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	12	0.38
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	12	0.38
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	12	0.38
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	14	0.38
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	14	0.38
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	14	0.38
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	14	0.38
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	14	0.38
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	14	0.38
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	17	0.38
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	17	0.38
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	17	0.38
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	17	0.38
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	17	0.38
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	17	0.38
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	18	0.38
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	18	0.38
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	18	0.38
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	18	0.38
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	18	0.38
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	18	0.38
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	10	0.38
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	5	0.38
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	5	0.38
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	5	0.38
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	6	0.38
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	6	0.38
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	6	0.38
(1,1661)	1:101:A:LYS:HD2	1:107:A:GLU:HA	5	0.38
(1,1661)	1:101:A:LYS:HD3	1:107:A:GLU:HA	5	0.38
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	10	0.38
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	2	0.38
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	11	0.38
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	9	0.38
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	14	0.38
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	14	0.38
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	14	0.38
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	14	0.38
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	14	0.38
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	14	0.38
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	17	0.38
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	17	0.38
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	17	0.38
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	17	0.38
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	17	0.38
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	17	0.38
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	19	0.38
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	19	0.38
(1,1489)	1:95:A:HIS:HE1	1:99:A:GLN:HE22	18	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	4	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	4	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	4	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	4	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	4	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	4	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	4	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	4	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	4	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	4	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	4	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	4	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	8	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	8	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	8	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	8	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	8	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	8	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	8	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	8	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	8	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	8	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	8	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	8	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	14	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	14	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	14	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	14	0.38
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	14	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	14	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	14	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	14	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	14	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	14	0.38
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	14	0.38
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	9	0.38
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE1	3	0.38
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE2	3	0.38
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE1	3	0.38
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE2	3	0.38
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE1	3	0.38
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE2	3	0.38
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE1	16	0.38
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE2	16	0.38
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE1	16	0.38
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE2	16	0.38
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE1	16	0.38
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE2	16	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	6	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	6	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	9	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	9	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	10	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	10	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	18	0.38
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	18	0.38
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	10	0.38
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	10	0.38
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	10	0.38
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	10	0.38
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	10	0.38
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	10	0.38
(1,1365)	1:5:A:LYS:HB2	1:74:A:THR:HB	8	0.38
(1,1365)	1:5:A:LYS:HB3	1:74:A:THR:HB	8	0.38
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	3	0.38
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	3	0.38
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	11	0.38
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	11	0.38
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	3	0.38
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	3	0.38
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	3	0.38
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	3	0.38
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	3	0.38
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	3	0.38
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	3	0.38
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	3	0.38
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	3	0.38
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	5	0.38
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	5	0.38
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	5	0.38
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	4	0.38
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	4	0.38
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	2	0.38
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	13	0.38
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	18	0.38
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	18	0.38
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	6	0.38
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	6	0.38
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	14	0.38
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	14	0.38
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	10	0.38
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	2	0.38
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	2	0.38
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	2	0.38
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	2	0.38
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	2	0.38
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	2	0.38
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	2	0.38
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	2	0.38
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	2	0.38
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	2	0.38
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	2	0.38
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	2	0.38
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	19	0.38
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	19	0.38
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	19	0.38
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	19	0.38
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	19	0.38
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	19	0.38
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	19	0.38
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	19	0.38
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	19	0.38
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	19	0.38
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	19	0.38
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE2	20	0.38
(1,934)	1:23:A:LEU:HD11	1:42:A:LYS:HE3	20	0.38
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE2	20	0.38
(1,934)	1:23:A:LEU:HD12	1:42:A:LYS:HE3	20	0.38
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE2	20	0.38
(1,934)	1:23:A:LEU:HD13	1:42:A:LYS:HE3	20	0.38
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE2	20	0.38
(1,934)	1:23:A:LEU:HD21	1:42:A:LYS:HE3	20	0.38
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE2	20	0.38
(1,934)	1:23:A:LEU:HD22	1:42:A:LYS:HE3	20	0.38
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE2	20	0.38
(1,934)	1:23:A:LEU:HD23	1:42:A:LYS:HE3	20	0.38
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	2	0.38
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	11	0.38
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	2	0.38
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	2	0.38
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	14	0.38
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	14	0.38
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	14	0.38
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	14	0.38
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	14	0.38
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	3	0.38
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	3	0.38
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	3	0.38
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	3	0.38
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	3	0.38
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	3	0.38
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	18	0.38
(1,351)	1:62:A:GLU:H	1:62:A:GLU:HG2	9	0.38
(1,351)	1:62:A:GLU:H	1:62:A:GLU:HG3	9	0.38
(1,351)	1:62:A:GLU:H	1:62:A:GLU:HG2	17	0.38
(1,351)	1:62:A:GLU:H	1:62:A:GLU:HG3	17	0.38
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	13	0.38
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	13	0.38
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	13	0.38
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	4	0.38
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	6	0.38
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	6	0.38
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	9	0.38
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	9	0.38
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	16	0.38
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	16	0.38
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	8	0.38
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	8	0.38
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	8	0.38
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	3	0.38
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	3	0.38
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	3	0.38
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	3	0.38
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	3	0.38
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	3	0.38
(1,225)	1:6:A:LEU:H	1:6:A:LEU:HG	6	0.38
(1,225)	1:6:A:LEU:H	1:6:A:LEU:HG	7	0.38
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD11	11	0.38
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD12	11	0.38
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD13	11	0.38
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD21	11	0.38
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD22	11	0.38
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD23	11	0.38
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	8	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	1	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	16	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	16	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	16	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	16	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	16	0.38
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	16	0.38
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	19	0.38
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	19	0.38
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	19	0.38
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	19	0.38
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	19	0.38
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	2	0.38
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	7	0.38
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	9	0.38
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	10	0.38
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	13	0.38
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	14	0.38
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	20	0.38
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	11	0.37
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	11	0.37
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	11	0.37
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	11	0.37
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	11	0.37
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	11	0.37
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	5	0.37
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	5	0.37
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	12	0.37
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	12	0.37
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	13	0.37
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	13	0.37
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	13	0.37
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	7	0.37
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	7	0.37
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	7	0.37
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	7	0.37
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	7	0.37
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	7	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	1	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	1	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	1	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	2	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	2	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	2	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	4	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	4	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	4	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	6	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	6	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	6	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	8	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	8	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	15	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	15	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	15	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	19	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	19	0.37
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	19	0.37
(1,2663)	1:1:A:MET:HE1	1:43:A:GLN:HE22	3	0.37
(1,2663)	1:1:A:MET:HE2	1:43:A:GLN:HE22	3	0.37
(1,2663)	1:1:A:MET:HE3	1:43:A:GLN:HE22	3	0.37
(1,2663)	1:1:A:MET:HE1	1:43:A:GLN:HE22	14	0.37
(1,2663)	1:1:A:MET:HE2	1:43:A:GLN:HE22	14	0.37
(1,2663)	1:1:A:MET:HE3	1:43:A:GLN:HE22	14	0.37
(1,2663)	1:1:A:MET:HE1	1:43:A:GLN:HE22	17	0.37
(1,2663)	1:1:A:MET:HE2	1:43:A:GLN:HE22	17	0.37
(1,2663)	1:1:A:MET:HE3	1:43:A:GLN:HE22	17	0.37
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	16	0.37
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	16	0.37
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	16	0.37
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG12	7	0.37
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG13	7	0.37
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG12	7	0.37
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG13	7	0.37
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG12	7	0.37
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG13	7	0.37
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG12	7	0.37
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG13	7	0.37
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG12	7	0.37
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG13	7	0.37
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG12	7	0.37
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG13	7	0.37
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG12	8	0.37
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG13	8	0.37
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG12	8	0.37
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG13	8	0.37
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG12	8	0.37
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG13	8	0.37
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG12	8	0.37
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG13	8	0.37
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG12	8	0.37
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG13	8	0.37
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG12	8	0.37
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG13	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2501)	1:159:A:LEU:HD11	1:163:A:ILE:H	7	0.37
(1,2501)	1:159:A:LEU:HD12	1:163:A:ILE:H	7	0.37
(1,2501)	1:159:A:LEU:HD13	1:163:A:ILE:H	7	0.37
(1,2501)	1:159:A:LEU:HD21	1:163:A:ILE:H	7	0.37
(1,2501)	1:159:A:LEU:HD22	1:163:A:ILE:H	7	0.37
(1,2501)	1:159:A:LEU:HD23	1:163:A:ILE:H	7	0.37
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD2	12	0.37
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD3	12	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	5	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	5	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	5	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	8	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	8	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	8	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	10	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	10	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	10	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	15	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	15	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	15	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	16	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	16	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	16	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	18	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	18	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	18	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	20	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	20	0.37
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	20	0.37
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	9	0.37
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	9	0.37
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	9	0.37
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	9	0.37
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	9	0.37
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	9	0.37
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	9	0.37
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	9	0.37
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	9	0.37
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	15	0.37
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	20	0.37
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	8	0.37
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	8	0.37
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	9	0.37
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	9	0.37
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	9	0.37
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE2	2	0.37
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE3	2	0.37
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	9	0.37
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	15	0.37
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	16	0.37
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	4	0.37
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	14	0.37
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	14	0.37
(1,1794)	1:111:A:MET:HB2	1:111:A:MET:HE1	10	0.37
(1,1794)	1:111:A:MET:HB2	1:111:A:MET:HE2	10	0.37
(1,1794)	1:111:A:MET:HB2	1:111:A:MET:HE3	10	0.37
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	5	0.37
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	5	0.37
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	5	0.37
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	17	0.37
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	17	0.37
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	17	0.37
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE2	19	0.37
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE3	19	0.37
(1,1608)	1:9:A:VAL:HB	1:96:A:TYR:HB3	13	0.37
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	18	0.37
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	16	0.37
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	16	0.37
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	10	0.37
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	10	0.37
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	10	0.37
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	10	0.37
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	10	0.37
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	10	0.37
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	18	0.37
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	18	0.37
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	18	0.37
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	18	0.37
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	18	0.37
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	18	0.37
(1,1495)	1:99:A:GLN:HA	1:99:A:GLN:HE22	3	0.37
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	6	0.37
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	6	0.37
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	6	0.37
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	6	0.37
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	6	0.37
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	6	0.37
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	6	0.37
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	6	0.37
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	6	0.37
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	6	0.37
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	6	0.37
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	5	0.37
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	5	0.37
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	1	0.37
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	5	0.37
(1,1404)	1:5:A:LYS:H	1:76:A:GLU:HG3	11	0.37
(1,1284)	1:67:A:MET:HG2	1:71:A:TYR:HD1	6	0.37
(1,1284)	1:67:A:MET:HG2	1:71:A:TYR:HD2	6	0.37
(1,1284)	1:67:A:MET:HG3	1:71:A:TYR:HD1	6	0.37
(1,1284)	1:67:A:MET:HG3	1:71:A:TYR:HD2	6	0.37
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	2	0.37
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	2	0.37
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	2	0.37
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	2	0.37
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	2	0.37
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	2	0.37
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	2	0.37
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	2	0.37
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	2	0.37
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	8	0.37
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	8	0.37
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	8	0.37
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	8	0.37
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	8	0.37
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	8	0.37
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	2	0.37
(1,1128)	1:3:A:GLU:HA	1:52:A:LEU:HB3	3	0.37
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	6	0.37
(1,1117)	1:46:A:ILE:HD11	1:51:A:CYS:HB3	1	0.37
(1,1117)	1:46:A:ILE:HD12	1:51:A:CYS:HB3	1	0.37
(1,1117)	1:46:A:ILE:HD13	1:51:A:CYS:HB3	1	0.37
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	20	0.37
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	18	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	5	0.37
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	5	0.37
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	5	0.37
(1,1080)	1:1:A:MET:HG3	1:51:A:CYS:HA	16	0.37
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	10	0.37
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	10	0.37
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	10	0.37
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB2	19	0.37
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB3	19	0.37
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB2	19	0.37
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB3	19	0.37
(1,965)	1:43:A:GLN:HE22	1:50:A:THR:HB	19	0.37
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	11	0.37
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	11	0.37
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	1	0.37
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	1	0.37
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	7	0.37
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	5	0.37
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	8	0.37
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	8	0.37
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	8	0.37
(1,726)	1:84:A:ILE:HD11	1:123:A:ARG:HG3	1	0.37
(1,726)	1:84:A:ILE:HD12	1:123:A:ARG:HG3	1	0.37
(1,726)	1:84:A:ILE:HD13	1:123:A:ARG:HG3	1	0.37
(1,602)	1:14:A:VAL:H	1:16:A:LYS:H	9	0.37
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	19	0.37
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	20	0.37
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD1	4	0.37
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD2	4	0.37
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD1	4	0.37
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD2	4	0.37
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	16	0.37
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	16	0.37
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	16	0.37
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	16	0.37
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	16	0.37
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	16	0.37
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	10	0.37
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	13	0.37
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	13	0.37
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	3	0.37
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	2	0.37
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	15	0.37
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	15	0.37
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	9	0.37
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	9	0.37
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	9	0.37
(1,39)	1:64:A:TYR:HD1	1:65:A:SER:H	9	0.37
(1,39)	1:64:A:TYR:HD2	1:65:A:SER:H	9	0.37
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	6	0.37
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	18	0.37
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	3	0.36
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	18	0.36
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	16	0.36
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	16	0.36
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	14	0.36
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	14	0.36
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	14	0.36
(1,3030)	1:32:A:TYR:HE1	1:34:A:PRO:HG3	3	0.36
(1,3030)	1:32:A:TYR:HE2	1:34:A:PRO:HG3	3	0.36
(1,3030)	1:32:A:TYR:HE1	1:34:A:PRO:HG3	10	0.36
(1,3030)	1:32:A:TYR:HE2	1:34:A:PRO:HG3	10	0.36
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	16	0.36
(1,2935)	1:73:A:ARG:H	1:73:A:ARG:HE	9	0.36
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	17	0.36
(1,2835)	1:73:A:ARG:HB2	1:73:A:ARG:HE	13	0.36
(1,2835)	1:73:A:ARG:HB3	1:73:A:ARG:HE	13	0.36
(1,2809)	1:157:A:TYR:HA	1:160:A:VAL:HG11	6	0.36
(1,2809)	1:157:A:TYR:HA	1:160:A:VAL:HG12	6	0.36
(1,2809)	1:157:A:TYR:HA	1:160:A:VAL:HG13	6	0.36
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	12	0.36
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	12	0.36
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	12	0.36
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	17	0.36
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE1	4	0.36
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE2	4	0.36
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE3	4	0.36
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE1	4	0.36
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE2	4	0.36
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE3	4	0.36
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE1	19	0.36
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE2	19	0.36
(1,2679)	1:78:A:PHE:HD1	1:111:A:MET:HE3	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE1	19	0.36
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE2	19	0.36
(1,2679)	1:78:A:PHE:HD2	1:111:A:MET:HE3	19	0.36
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	11	0.36
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	11	0.36
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	11	0.36
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	3	0.36
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	3	0.36
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	17	0.36
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	17	0.36
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	16	0.36
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	18	0.36
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	18	0.36
(1,2562)	1:20:A:THR:HA	1:23:A:LEU:HG	16	0.36
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	3	0.36
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	3	0.36
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	3	0.36
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	15	0.36
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	15	0.36
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	15	0.36
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	16	0.36
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	16	0.36
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	16	0.36
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	19	0.36
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	19	0.36
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	19	0.36
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	5	0.36
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	5	0.36
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	16	0.36
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD2	4	0.36
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD3	4	0.36
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	10	0.36
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	10	0.36
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	10	0.36
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	10	0.36
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	10	0.36
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	10	0.36
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	17	0.36
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	17	0.36
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	7	0.36
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	7	0.36
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	15	0.36
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	15	0.36
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	15	0.36
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	4	0.36
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	2	0.36
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	2	0.36
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	11	0.36
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	11	0.36
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	12	0.36
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	12	0.36
(1,2271)	1:144:A:THR:HA	1:150:A:GLN:HG2	1	0.36
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	1	0.36
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	10	0.36
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	17	0.36
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD1	9	0.36
(1,2039)	1:156:A:PHE:HD1	1:157:A:TYR:HD2	9	0.36
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD1	9	0.36
(1,2039)	1:156:A:PHE:HD2	1:157:A:TYR:HD2	9	0.36
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	4	0.36
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	4	0.36
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	4	0.36
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	8	0.36
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	8	0.36
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	8	0.36
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	9	0.36
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	9	0.36
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	9	0.36
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	12	0.36
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	12	0.36
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	12	0.36
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	4	0.36
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	7	0.36
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	7	0.36
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	9	0.36
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	9	0.36
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	9	0.36
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	9	0.36
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	9	0.36
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	9	0.36
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	12	0.36
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	5	0.36
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	2	0.36
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	2	0.36
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	2	0.36
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	2	0.36
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	2	0.36
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	8	0.36
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	16	0.36
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	16	0.36
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG11	11	0.36
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG12	11	0.36
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG13	11	0.36
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG21	11	0.36
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG22	11	0.36
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG23	11	0.36
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	15	0.36
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	15	0.36
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	15	0.36
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	7	0.36
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	7	0.36
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG2	16	0.36
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG3	16	0.36
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	12	0.36
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	4	0.36
(1,1415)	1:77:A:GLY:HA2	1:111:A:MET:HG3	6	0.36
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	1	0.36
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	12	0.36
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	20	0.36
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	5	0.36
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	5	0.36
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	8	0.36
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	8	0.36
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	8	0.36
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	8	0.36
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	8	0.36
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	8	0.36
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	8	0.36
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	8	0.36
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	8	0.36
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	8	0.36
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	8	0.36
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	8	0.36
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	8	0.36
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	8	0.36
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	8	0.36
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	8	0.36
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	8	0.36
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	10	0.36
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	10	0.36
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	10	0.36
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	10	0.36
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	10	0.36
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	10	0.36
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	10	0.36
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	10	0.36
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	10	0.36
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	10	0.36
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	10	0.36
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	10	0.36
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	10	0.36
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	10	0.36
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	10	0.36
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	10	0.36
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	10	0.36
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	10	0.36
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	2	0.36
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	2	0.36
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	2	0.36
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	15	0.36
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	17	0.36
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	8	0.36
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	8	0.36
(1,969)	1:12:A:GLY:H	1:61:A:GLN:HE21	3	0.36
(1,969)	1:12:A:GLY:H	1:61:A:GLN:HE22	3	0.36
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	2	0.36
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	16	0.36
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	16	0.36
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	11	0.36
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	20	0.36
(1,815)	1:41:A:ARG:HD2	1:52:A:LEU:HB3	3	0.36
(1,815)	1:41:A:ARG:HD3	1:52:A:LEU:HB3	3	0.36
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	3	0.36
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	3	0.36
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB2	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB3	5	0.36
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB2	5	0.36
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB3	5	0.36
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB2	5	0.36
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB3	5	0.36
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB2	5	0.36
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB3	5	0.36
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB2	5	0.36
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB3	5	0.36
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB2	5	0.36
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB3	5	0.36
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	14	0.36
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	9	0.36
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	6	0.36
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	20	0.36
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	20	0.36
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	20	0.36
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	6	0.36
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	6	0.36
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	6	0.36
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	5	0.36
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	5	0.36
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	5	0.36
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	5	0.36
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	5	0.36
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	5	0.36
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	11	0.36
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	11	0.36
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	8	0.36
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	8	0.36
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	8	0.36
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	8	0.36
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	8	0.36
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	8	0.36
(1,156)	1:86:A:ASN:H	1:125:A:VAL:HG11	16	0.36
(1,156)	1:86:A:ASN:H	1:125:A:VAL:HG12	16	0.36
(1,156)	1:86:A:ASN:H	1:125:A:VAL:HG13	16	0.36
(1,156)	1:86:A:ASN:H	1:125:A:VAL:HG21	16	0.36
(1,156)	1:86:A:ASN:H	1:125:A:VAL:HG22	16	0.36
(1,156)	1:86:A:ASN:H	1:125:A:VAL:HG23	16	0.36
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	17	0.36
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	17	0.36
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	17	0.36
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	17	0.36
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	17	0.36
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	3	0.36
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	3	0.36
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	3	0.36
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	5	0.36
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	5	0.36
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	5	0.36
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	14	0.36
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	14	0.36
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	14	0.36
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	17	0.36
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	17	0.36
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	17	0.36
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	5	0.36
(1,3331)	1:106:A:SER:HB2	1:109:A:VAL:H	5	0.35
(1,3331)	1:106:A:SER:HB3	1:109:A:VAL:H	5	0.35
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG2	9	0.35
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG3	9	0.35
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG2	9	0.35
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG3	9	0.35
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG2	9	0.35
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG3	9	0.35
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG2	9	0.35
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG3	9	0.35
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG2	9	0.35
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG3	9	0.35
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG2	9	0.35
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG3	9	0.35
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG2	12	0.35
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG3	12	0.35
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG2	12	0.35
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG3	12	0.35
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG2	12	0.35
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG3	12	0.35
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG2	12	0.35
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG3	12	0.35
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG2	12	0.35
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG3	12	0.35
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG2	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG3	12	0.35
(1,3230)	1:3:A:GLU:HG2	1:52:A:LEU:HB3	3	0.35
(1,3230)	1:3:A:GLU:HG3	1:52:A:LEU:HB3	3	0.35
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	15	0.35
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	15	0.35
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	15	0.35
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	15	0.35
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	15	0.35
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	15	0.35
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB2	15	0.35
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB3	15	0.35
(1,3030)	1:32:A:TYR:HE1	1:34:A:PRO:HG3	16	0.35
(1,3030)	1:32:A:TYR:HE2	1:34:A:PRO:HG3	16	0.35
(1,3030)	1:32:A:TYR:HE1	1:34:A:PRO:HG3	19	0.35
(1,3030)	1:32:A:TYR:HE2	1:34:A:PRO:HG3	19	0.35
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	13	0.35
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD1	5	0.35
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD2	5	0.35
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	15	0.35
(1,2908)	1:135:A:ARG:HD2	1:136:A:SER:H	8	0.35
(1,2908)	1:135:A:ARG:HD3	1:136:A:SER:H	8	0.35
(1,2897)	1:75:A:GLY:H	1:77:A:GLY:H	9	0.35
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	1	0.35
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	1	0.35
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	1	0.35
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	13	0.35
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	13	0.35
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	13	0.35
(1,2730)	1:118:A:SER:H	1:147:A:LYS:H	1	0.35
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	2	0.35
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	15	0.35
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	15	0.35
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	18	0.35
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	18	0.35
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG12	15	0.35
(1,2622)	1:160:A:VAL:HG11	1:163:A:ILE:HG13	15	0.35
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG12	15	0.35
(1,2622)	1:160:A:VAL:HG12	1:163:A:ILE:HG13	15	0.35
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG12	15	0.35
(1,2622)	1:160:A:VAL:HG13	1:163:A:ILE:HG13	15	0.35
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG12	15	0.35
(1,2622)	1:160:A:VAL:HG21	1:163:A:ILE:HG13	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG12	15	0.35
(1,2622)	1:160:A:VAL:HG22	1:163:A:ILE:HG13	15	0.35
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG12	15	0.35
(1,2622)	1:160:A:VAL:HG23	1:163:A:ILE:HG13	15	0.35
(1,2564)	1:20:A:THR:HA	1:55:A:ILE:HG12	19	0.35
(1,2559)	1:17:A:SER:HA	1:20:A:THR:HA	6	0.35
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	9	0.35
(1,2547)	1:164:A:ARG:HB2	1:165:A:LYS:H	2	0.35
(1,2547)	1:164:A:ARG:HB3	1:165:A:LYS:H	2	0.35
(1,2536)	1:144:A:THR:HA	1:152:A:VAL:HA	17	0.35
(1,2535)	1:168:A:GLU:H	1:169:A:LYS:H	2	0.35
(1,2451)	1:2:A:THR:HB	1:51:A:CYS:HB3	6	0.35
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	1	0.35
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	1	0.35
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	1	0.35
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	1	0.35
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	1	0.35
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	1	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	1	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	1	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	1	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	2	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	2	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	2	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	4	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	4	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	4	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	6	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	6	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	6	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	8	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	8	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	8	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	9	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	9	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	9	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	10	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	10	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	10	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	11	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	11	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	12	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	12	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	12	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	13	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	13	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	13	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	17	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	17	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	17	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	19	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	19	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	19	0.35
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	20	0.35
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	20	0.35
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	20	0.35
(1,2308)	1:153:A:ASP:HB2	1:154:A:ASP:HB2	6	0.35
(1,2308)	1:153:A:ASP:HB3	1:154:A:ASP:HB2	6	0.35
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	15	0.35
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	15	0.35
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	5	0.35
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	8	0.35
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	11	0.35
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	14	0.35
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	20	0.35
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	17	0.35
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	7	0.35
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	7	0.35
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	7	0.35
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	7	0.35
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	7	0.35
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	7	0.35
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE1	11	0.35
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE2	11	0.35
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE1	11	0.35
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE2	11	0.35
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE1	11	0.35
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE2	11	0.35
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	11	0.35
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	11	0.35
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	11	0.35
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	11	0.35
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	11	0.35
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	1	0.35
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	1	0.35
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	1	0.35
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	5	0.35
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	5	0.35
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	5	0.35
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	5	0.35
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	5	0.35
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	5	0.35
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	5	0.35
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	5	0.35
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	5	0.35
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	5	0.35
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	5	0.35
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	5	0.35
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	5	0.35
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	5	0.35
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	5	0.35
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	5	0.35
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	5	0.35
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	5	0.35
(1,1940)	1:120:A:LEU:HD11	1:121:A:PRO:HG3	14	0.35
(1,1940)	1:120:A:LEU:HD12	1:121:A:PRO:HG3	14	0.35
(1,1940)	1:120:A:LEU:HD13	1:121:A:PRO:HG3	14	0.35
(1,1940)	1:120:A:LEU:HD21	1:121:A:PRO:HG3	14	0.35
(1,1940)	1:120:A:LEU:HD22	1:121:A:PRO:HG3	14	0.35
(1,1940)	1:120:A:LEU:HD23	1:121:A:PRO:HG3	14	0.35
(1,1904)	1:12:A:GLY:H	1:61:A:GLN:H	20	0.35
(1,1837)	1:77:A:GLY:HA3	1:111:A:MET:HA	19	0.35
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	3	0.35
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	3	0.35
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	3	0.35
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	7	0.35
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	13	0.35
(1,1661)	1:101:A:LYS:HD2	1:107:A:GLU:HA	16	0.35
(1,1661)	1:101:A:LYS:HD3	1:107:A:GLU:HA	16	0.35
(1,1645)	1:128:A:LYS:HG2	1:129:A:GLN:HB2	17	0.35
(1,1645)	1:128:A:LYS:HG3	1:129:A:GLN:HB2	17	0.35
(1,1645)	1:128:A:LYS:HG2	1:129:A:GLN:HB2	20	0.35
(1,1645)	1:128:A:LYS:HG3	1:129:A:GLN:HB2	20	0.35
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	10	0.35
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG21	11	0.35
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG22	11	0.35
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG23	11	0.35
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG21	11	0.35
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG22	11	0.35
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG23	11	0.35
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	15	0.35
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE1	10	0.35
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE2	10	0.35
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	5	0.35
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD11	16	0.35
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD12	16	0.35
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD13	16	0.35
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD11	16	0.35
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD12	16	0.35
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD13	16	0.35
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD11	19	0.35
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD12	19	0.35
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD13	19	0.35
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD11	19	0.35
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD12	19	0.35
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD13	19	0.35
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	2	0.35
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	2	0.35
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	2	0.35
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG2	6	0.35
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG3	6	0.35
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	11	0.35
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	11	0.35
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	11	0.35
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	11	0.35
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	11	0.35
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	11	0.35
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	6	0.35
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	6	0.35
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	6	0.35
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	8	0.35
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	8	0.35
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	8	0.35
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	10	0.35
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	10	0.35
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	12	0.35
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	12	0.35
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	12	0.35
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	18	0.35
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	9	0.35
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG11	5	0.35
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG12	5	0.35
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG13	5	0.35
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG21	5	0.35
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG22	5	0.35
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG23	5	0.35
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG11	5	0.35
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG12	5	0.35
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG13	5	0.35
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG21	5	0.35
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG22	5	0.35
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG23	5	0.35
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	5	0.35
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	5	0.35
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB2	6	0.35
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB3	6	0.35
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB2	6	0.35
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB3	6	0.35
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	8	0.35
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	8	0.35
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	5	0.35
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	4	0.35
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	20	0.35
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	20	0.35
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	20	0.35
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	20	0.35
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	20	0.35
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	20	0.35
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	20	0.35
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	20	0.35
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	20	0.35
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	20	0.35
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	20	0.35
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	20	0.35
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	20	0.35
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	20	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	15	0.35
(1,1120)	1:12:A:GLY:H	1:61:A:GLN:HB3	20	0.35
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	14	0.35
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	16	0.35
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	16	0.35
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	16	0.35
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	9	0.35
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG21	2	0.35
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG22	2	0.35
(1,972)	1:43:A:GLN:HG2	1:50:A:THR:HG23	2	0.35
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG21	2	0.35
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG22	2	0.35
(1,972)	1:43:A:GLN:HG3	1:50:A:THR:HG23	2	0.35
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	1	0.35
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	9	0.35
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	9	0.35
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	14	0.35
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	3	0.35
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	3	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	3	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	3	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	3	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	3	0.35
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	6	0.35
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	6	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	6	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	6	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	6	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	6	0.35
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	12	0.35
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	12	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	12	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	12	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	12	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	12	0.35
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	14	0.35
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	14	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	14	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	14	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	14	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	14	0.35
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	15	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	15	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	15	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	15	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	15	0.35
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	16	0.35
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	16	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	16	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	16	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	16	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	16	0.35
(1,876)	1:45:A:VAL:HG11	1:49:A:GLU:H	19	0.35
(1,876)	1:45:A:VAL:HG12	1:49:A:GLU:H	19	0.35
(1,876)	1:45:A:VAL:HG13	1:49:A:GLU:H	19	0.35
(1,876)	1:45:A:VAL:HG21	1:49:A:GLU:H	19	0.35
(1,876)	1:45:A:VAL:HG22	1:49:A:GLU:H	19	0.35
(1,876)	1:45:A:VAL:HG23	1:49:A:GLU:H	19	0.35
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	13	0.35
(1,773)	1:39:A:SER:HA	1:56:A:LEU:HA	7	0.35
(1,701)	1:36:A:ILE:HA	1:37:A:GLU:H	12	0.35
(1,688)	1:36:A:ILE:HA	1:37:A:GLU:HG2	12	0.35
(1,688)	1:36:A:ILE:HA	1:37:A:GLU:HG3	12	0.35
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD11	14	0.35
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD12	14	0.35
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD13	14	0.35
(1,609)	1:45:A:VAL:HB	1:47:A:ASP:H	20	0.35
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	16	0.35
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	15	0.35
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	15	0.35
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	15	0.35
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	15	0.35
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	15	0.35
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	15	0.35
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	2	0.35
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	2	0.35
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	2	0.35
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	12	0.35
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	12	0.35
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	10	0.35
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	19	0.35
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	19	0.35
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	19	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	19	0.35
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	19	0.35
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	19	0.35
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	1	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	4	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	4	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	4	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	4	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	4	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	4	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	7	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	7	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	7	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	7	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	7	0.35
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	7	0.35
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	20	0.35
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	20	0.35
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	20	0.35
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	20	0.35
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	20	0.35
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	20	0.35
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	10	0.35
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	10	0.35
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	10	0.35
(1,3334)	1:80:A:CYS:HA	1:93:A:ILE:HD11	5	0.34
(1,3334)	1:80:A:CYS:HA	1:93:A:ILE:HD12	5	0.34
(1,3334)	1:80:A:CYS:HA	1:93:A:ILE:HD13	5	0.34
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	17	0.34
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	19	0.34
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	11	0.34
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	11	0.34
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	11	0.34
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	11	0.34
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	11	0.34
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	6	0.34
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	6	0.34
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	6	0.34
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	6	0.34
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	6	0.34
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	6	0.34
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	3	0.34
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	4	0.34
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	4	0.34
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	4	0.34
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	5	0.34
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	20	0.34
(1,3128)	1:1:A:MET:HA	1:51:A:CYS:HA	14	0.34
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	8	0.34
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	8	0.34
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	6	0.34
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	6	0.34
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	6	0.34
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	6	0.34
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	6	0.34
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	6	0.34
(1,2824)	1:18:A:ALA:HB1	1:28:A:PHE:HD1	5	0.34
(1,2824)	1:18:A:ALA:HB1	1:28:A:PHE:HD2	5	0.34
(1,2824)	1:18:A:ALA:HB2	1:28:A:PHE:HD1	5	0.34
(1,2824)	1:18:A:ALA:HB2	1:28:A:PHE:HD2	5	0.34
(1,2824)	1:18:A:ALA:HB3	1:28:A:PHE:HD1	5	0.34
(1,2824)	1:18:A:ALA:HB3	1:28:A:PHE:HD2	5	0.34
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	14	0.34
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	14	0.34
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	14	0.34
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	16	0.34
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	16	0.34
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	16	0.34
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	18	0.34
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	18	0.34
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	18	0.34
(1,2733)	1:11:A:ALA:HB1	1:92:A:ASP:H	5	0.34
(1,2733)	1:11:A:ALA:HB2	1:92:A:ASP:H	5	0.34
(1,2733)	1:11:A:ALA:HB3	1:92:A:ASP:H	5	0.34
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	11	0.34
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	11	0.34
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	11	0.34
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	11	0.34
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	11	0.34
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	11	0.34
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD11	19	0.34
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD12	19	0.34
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD13	19	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD11	19	0.34
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD12	19	0.34
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD13	19	0.34
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD11	19	0.34
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD12	19	0.34
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD13	19	0.34
(1,2627)	1:47:A:ASP:HB2	1:161:A:ARG:HE	4	0.34
(1,2627)	1:47:A:ASP:HB3	1:161:A:ARG:HE	4	0.34
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB1	11	0.34
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB2	11	0.34
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB3	11	0.34
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	6	0.34
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	15	0.34
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	15	0.34
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	15	0.34
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	19	0.34
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	19	0.34
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	19	0.34
(1,2535)	1:168:A:GLU:H	1:169:A:LYS:H	4	0.34
(1,2535)	1:168:A:GLU:H	1:169:A:LYS:H	18	0.34
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	18	0.34
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	18	0.34
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	10	0.34
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	10	0.34
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	10	0.34
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	10	0.34
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	10	0.34
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	10	0.34
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE1	12	0.34
(1,2489)	1:58:A:THR:HB	1:71:A:TYR:HE2	12	0.34
(1,2417)	1:4:A:TYR:HD1	1:163:A:ILE:HA	8	0.34
(1,2417)	1:4:A:TYR:HD2	1:163:A:ILE:HA	8	0.34
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	2	0.34
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	2	0.34
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	2	0.34
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	2	0.34
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	2	0.34
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	2	0.34
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE2	19	0.34
(1,2256)	1:165:A:LYS:HB2	1:165:A:LYS:HE3	19	0.34
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	19	0.34
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	4	0.34
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	6	0.34
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	19	0.34
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	13	0.34
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	13	0.34
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	13	0.34
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	5	0.34
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	15	0.34
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	8	0.34
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	8	0.34
(1,1831)	1:158:A:THR:HA	1:161:A:ARG:HE	9	0.34
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	3	0.34
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	14	0.34
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	2	0.34
(1,1774)	1:24:A:ILE:HD11	1:41:A:ARG:HA	14	0.34
(1,1774)	1:24:A:ILE:HD12	1:41:A:ARG:HA	14	0.34
(1,1774)	1:24:A:ILE:HD13	1:41:A:ARG:HA	14	0.34
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	14	0.34
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	14	0.34
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	14	0.34
(1,1632)	1:4:A:TYR:HD1	1:51:A:CYS:HB3	20	0.34
(1,1632)	1:4:A:TYR:HD2	1:51:A:CYS:HB3	20	0.34
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	16	0.34
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	16	0.34
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	16	0.34
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	6	0.34
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	6	0.34
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	6	0.34
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	6	0.34
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	6	0.34
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	6	0.34
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	19	0.34
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	19	0.34
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	19	0.34
(1,1412)	1:75:A:GLY:HA3	1:76:A:GLU:HG3	4	0.34
(1,1404)	1:5:A:LYS:H	1:76:A:GLU:HG3	8	0.34
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	13	0.34
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	13	0.34
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	13	0.34
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	14	0.34
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	14	0.34
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	19	0.34
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD1	18	0.34
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD2	18	0.34
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	12	0.34
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	12	0.34
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD1	19	0.34
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD2	19	0.34
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD1	19	0.34
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD2	19	0.34
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	11	0.34
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	11	0.34
(1,1272)	1:9:A:VAL:HG11	1:96:A:TYR:H	4	0.34
(1,1272)	1:9:A:VAL:HG12	1:96:A:TYR:H	4	0.34
(1,1272)	1:9:A:VAL:HG13	1:96:A:TYR:H	4	0.34
(1,1272)	1:9:A:VAL:HG21	1:96:A:TYR:H	4	0.34
(1,1272)	1:9:A:VAL:HG22	1:96:A:TYR:H	4	0.34
(1,1272)	1:9:A:VAL:HG23	1:96:A:TYR:H	4	0.34
(1,1272)	1:9:A:VAL:HG11	1:96:A:TYR:H	7	0.34
(1,1272)	1:9:A:VAL:HG12	1:96:A:TYR:H	7	0.34
(1,1272)	1:9:A:VAL:HG13	1:96:A:TYR:H	7	0.34
(1,1272)	1:9:A:VAL:HG21	1:96:A:TYR:H	7	0.34
(1,1272)	1:9:A:VAL:HG22	1:96:A:TYR:H	7	0.34
(1,1272)	1:9:A:VAL:HG23	1:96:A:TYR:H	7	0.34
(1,1251)	1:149:A:ARG:HB3	1:149:A:ARG:HE	1	0.34
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	17	0.34
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	20	0.34
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	20	0.34
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	20	0.34
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	20	0.34
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	20	0.34
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	20	0.34
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	20	0.34
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	20	0.34
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	20	0.34
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	20	0.34
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	20	0.34
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	20	0.34
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	20	0.34
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	20	0.34
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	20	0.34
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	20	0.34
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	20	0.34
(1,1176)	1:23:A:LEU:HD11	1:156:A:PHE:HB3	9	0.34
(1,1176)	1:23:A:LEU:HD12	1:156:A:PHE:HB3	9	0.34
(1,1176)	1:23:A:LEU:HD13	1:156:A:PHE:HB3	9	0.34
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	16	0.34
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	7	0.34
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	12	0.34
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	10	0.34
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	10	0.34
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	12	0.34
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	12	0.34
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	13	0.34
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	13	0.34
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	13	0.34
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG2	7	0.34
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG3	7	0.34
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG2	7	0.34
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG3	7	0.34
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG2	7	0.34
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG3	7	0.34
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG2	16	0.34
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG3	16	0.34
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG2	16	0.34
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG3	16	0.34
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG2	16	0.34
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG3	16	0.34
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	9	0.34
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	9	0.34
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	9	0.34
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	9	0.34
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	9	0.34
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	9	0.34
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD11	8	0.34
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD12	8	0.34
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD13	8	0.34
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD21	8	0.34
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD22	8	0.34
(1,873)	1:42:A:LYS:HA	1:52:A:LEU:HD23	8	0.34
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	2	0.34
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	2	0.34
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	2	0.34
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	14	0.34
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	14	0.34
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	16	0.34
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	16	0.34
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	16	0.34
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	17	0.34
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	17	0.34
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	17	0.34
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	18	0.34
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	18	0.34
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	18	0.34
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	20	0.34
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	20	0.34
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	20	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	1	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	1	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	1	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	2	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	2	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	2	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	3	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	3	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	3	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	4	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	4	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	4	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	5	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	5	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	5	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	6	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	6	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	6	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	7	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	7	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	7	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	8	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	8	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	8	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	9	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	9	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	9	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	10	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	10	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	11	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	11	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	11	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	13	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	13	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	13	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	15	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	15	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	15	0.34
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	19	0.34
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	19	0.34
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	19	0.34
(1,714)	1:36:A:ILE:HG12	1:37:A:GLU:H	19	0.34
(1,714)	1:36:A:ILE:HG13	1:37:A:GLU:H	19	0.34
(1,701)	1:36:A:ILE:HA	1:37:A:GLU:H	18	0.34
(1,593)	1:12:A:GLY:HA2	1:14:A:VAL:H	20	0.34
(1,593)	1:12:A:GLY:HA3	1:14:A:VAL:H	20	0.34
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	15	0.34
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	6	0.34
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	6	0.34
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	6	0.34
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	6	0.34
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	6	0.34
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	6	0.34
(1,420)	1:21:A:ILE:HG21	1:25:A:GLN:HG2	14	0.34
(1,420)	1:21:A:ILE:HG22	1:25:A:GLN:HG2	14	0.34
(1,420)	1:21:A:ILE:HG23	1:25:A:GLN:HG2	14	0.34
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	1	0.34
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	8	0.34
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	8	0.34
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	18	0.34
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	18	0.34
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	18	0.34
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	20	0.34
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	20	0.34
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	20	0.34
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	8	0.34
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	8	0.34
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	8	0.34
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	8	0.34
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	8	0.34
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	1	0.34
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	17	0.34
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	17	0.34
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	18	0.34
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	18	0.34
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	18	0.34
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	18	0.34
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	18	0.34
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	18	0.34
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	19	0.34
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	19	0.34
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	19	0.34
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	3	0.34
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	11	0.33
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG2	8	0.33
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG3	8	0.33
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG2	8	0.33
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG3	8	0.33
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG2	8	0.33
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG3	8	0.33
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG2	8	0.33
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG3	8	0.33
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG2	8	0.33
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG3	8	0.33
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG2	8	0.33
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG3	8	0.33
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	20	0.33
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	20	0.33
(1,3242)	1:3:A:GLU:HG2	1:4:A:TYR:HA	5	0.33
(1,3242)	1:3:A:GLU:HG3	1:4:A:TYR:HA	5	0.33
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	11	0.33
(1,3173)	1:1:A:MET:HG2	1:2:A:THR:H	7	0.33
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	7	0.33
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	7	0.33
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	7	0.33
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	4	0.33
(1,3064)	1:46:A:ILE:HG21	1:161:A:ARG:HE	4	0.33
(1,3064)	1:46:A:ILE:HG22	1:161:A:ARG:HE	4	0.33
(1,3064)	1:46:A:ILE:HG23	1:161:A:ARG:HE	4	0.33
(1,3008)	1:58:A:THR:HB	1:68:A:ARG:HE	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2980)	1:132:A:ASP:H	1:132:A:ASP:HB3	11	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	11	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	11	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	11	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	11	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	11	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	11	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	14	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	14	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	14	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	14	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	14	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	14	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	16	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	16	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	16	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	16	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	16	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	16	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	17	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	17	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	17	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	17	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	17	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	17	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	18	0.33
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	18	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	18	0.33
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	18	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	18	0.33
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	18	0.33
(1,2762)	1:102:A:ARG:H	1:102:A:ARG:HE	12	0.33
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	7	0.33
(1,2673)	1:111:A:MET:HG3	1:111:A:MET:HE1	5	0.33
(1,2673)	1:111:A:MET:HG3	1:111:A:MET:HE2	5	0.33
(1,2673)	1:111:A:MET:HG3	1:111:A:MET:HE3	5	0.33
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	14	0.33
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	14	0.33
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	14	0.33
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	14	0.33
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	14	0.33
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	10	0.33
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	10	0.33
(1,2623)	1:25:A:GLN:HB2	1:27:A:HIS:HE1	9	0.33
(1,2607)	1:21:A:ILE:HA	1:27:A:HIS:H	10	0.33
(1,2607)	1:21:A:ILE:HA	1:27:A:HIS:H	20	0.33
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	4	0.33
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	4	0.33
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	3	0.33
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	3	0.33
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	3	0.33
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	8	0.33
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	8	0.33
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	8	0.33
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	3	0.33
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	7	0.33
(1,2454)	1:162:A:GLU:HB2	1:165:A:LYS:HG2	18	0.33
(1,2454)	1:162:A:GLU:HB3	1:165:A:LYS:HG2	18	0.33
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	10	0.33
(1,2417)	1:4:A:TYR:HD1	1:163:A:ILE:HA	20	0.33
(1,2417)	1:4:A:TYR:HD2	1:163:A:ILE:HA	20	0.33
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	13	0.33
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	13	0.33
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD2	14	0.33
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD3	14	0.33
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	1	0.33
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	1	0.33
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	1	0.33
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	1	0.33
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	1	0.33
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	1	0.33
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	9	0.33
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	9	0.33
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	9	0.33
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	9	0.33
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	9	0.33
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	9	0.33
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	17	0.33
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	17	0.33
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	17	0.33
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	19	0.33
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	19	0.33
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	19	0.33
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	19	0.33
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	19	0.33
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	18	0.33
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	18	0.33
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	18	0.33
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	7	0.33
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	7	0.33
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	16	0.33
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	16	0.33
(1,2302)	1:23:A:LEU:HD21	1:153:A:ASP:HA	3	0.33
(1,2302)	1:23:A:LEU:HD22	1:153:A:ASP:HA	3	0.33
(1,2302)	1:23:A:LEU:HD23	1:153:A:ASP:HA	3	0.33
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	20	0.33
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	7	0.33
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB1	13	0.33
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB2	13	0.33
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB3	13	0.33
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB1	13	0.33
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB2	13	0.33
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB3	13	0.33
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB1	13	0.33
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB2	13	0.33
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB3	13	0.33
(1,1940)	1:120:A:LEU:HD11	1:121:A:PRO:HG3	17	0.33
(1,1940)	1:120:A:LEU:HD12	1:121:A:PRO:HG3	17	0.33
(1,1940)	1:120:A:LEU:HD13	1:121:A:PRO:HG3	17	0.33
(1,1940)	1:120:A:LEU:HD21	1:121:A:PRO:HG3	17	0.33
(1,1940)	1:120:A:LEU:HD22	1:121:A:PRO:HG3	17	0.33
(1,1940)	1:120:A:LEU:HD23	1:121:A:PRO:HG3	17	0.33
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	3	0.33
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	3	0.33
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	3	0.33
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	3	0.33
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	3	0.33
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	3	0.33
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	2	0.33
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	7	0.33
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	13	0.33
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	20	0.33
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	20	0.33
(1,1725)	1:104:A:LYS:HE3	1:109:A:VAL:HA	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE2	20	0.33
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE3	20	0.33
(1,1652)	1:95:A:HIS:HA	1:99:A:GLN:HG2	16	0.33
(1,1652)	1:95:A:HIS:HA	1:99:A:GLN:HG3	16	0.33
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	14	0.33
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG2	9	0.33
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG3	9	0.33
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	16	0.33
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	16	0.33
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	20	0.33
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	20	0.33
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	20	0.33
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	20	0.33
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	20	0.33
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	20	0.33
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	12	0.33
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	12	0.33
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG21	11	0.33
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG22	11	0.33
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG23	11	0.33
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG21	11	0.33
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG22	11	0.33
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG23	11	0.33
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG21	11	0.33
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG22	11	0.33
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG23	11	0.33
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG21	11	0.33
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG22	11	0.33
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG23	11	0.33
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG21	11	0.33
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG22	11	0.33
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG23	11	0.33
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG21	11	0.33
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG22	11	0.33
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG23	11	0.33
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	17	0.33
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB2	14	0.33
(1,1264)	1:63:A:GLU:HG2	1:64:A:TYR:HB3	14	0.33
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB2	14	0.33
(1,1264)	1:63:A:GLU:HG3	1:64:A:TYR:HB3	14	0.33
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	6	0.33
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	10	0.33
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	10	0.33
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	10	0.33
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	10	0.33
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	10	0.33
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	10	0.33
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	10	0.33
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	10	0.33
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	18	0.33
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	5	0.33
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	5	0.33
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	5	0.33
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	5	0.33
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	5	0.33
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	5	0.33
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	5	0.33
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	5	0.33
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	5	0.33
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	5	0.33
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	5	0.33
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	5	0.33
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	5	0.33
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	5	0.33
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	5	0.33
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	5	0.33
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	5	0.33
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	5	0.33
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	11	0.33
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	17	0.33
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	17	0.33
(1,1033)	1:90:A:PHE:HB2	1:129:A:GLN:HE21	19	0.33
(1,1033)	1:90:A:PHE:HB3	1:129:A:GLN:HE21	19	0.33
(1,982)	1:44:A:VAL:HG21	1:51:A:CYS:HB2	19	0.33
(1,982)	1:44:A:VAL:HG22	1:51:A:CYS:HB2	19	0.33
(1,982)	1:44:A:VAL:HG23	1:51:A:CYS:HB2	19	0.33
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG2	2	0.33
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG3	2	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG2	2	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG3	2	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG2	2	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG3	2	0.33
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG2	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG3	6	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG2	6	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG3	6	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG2	6	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG3	6	0.33
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG2	10	0.33
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG3	10	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG2	10	0.33
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG3	10	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG2	10	0.33
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG3	10	0.33
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	16	0.33
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	16	0.33
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	16	0.33
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	16	0.33
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	16	0.33
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	16	0.33
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	16	0.33
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	16	0.33
(1,897)	1:79:A:LEU:HD11	1:157:A:TYR:H	20	0.33
(1,897)	1:79:A:LEU:HD12	1:157:A:TYR:H	20	0.33
(1,897)	1:79:A:LEU:HD13	1:157:A:TYR:H	20	0.33
(1,897)	1:79:A:LEU:HD21	1:157:A:TYR:H	20	0.33
(1,897)	1:79:A:LEU:HD22	1:157:A:TYR:H	20	0.33
(1,897)	1:79:A:LEU:HD23	1:157:A:TYR:H	20	0.33
(1,845)	1:41:A:ARG:HA	1:41:A:ARG:HD3	7	0.33
(1,839)	1:4:A:TYR:HE1	1:52:A:LEU:H	12	0.33
(1,839)	1:4:A:TYR:HE2	1:52:A:LEU:H	12	0.33
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	12	0.33
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	12	0.33
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	12	0.33
(1,828)	1:120:A:LEU:HD21	2:201:A:GNP:HN1	15	0.33
(1,828)	1:120:A:LEU:HD22	2:201:A:GNP:HN1	15	0.33
(1,828)	1:120:A:LEU:HD23	2:201:A:GNP:HN1	15	0.33
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	15	0.33
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	7	0.33
(1,656)	1:36:A:ILE:HD11	1:37:A:GLU:HA	7	0.33
(1,656)	1:36:A:ILE:HD12	1:37:A:GLU:HA	7	0.33
(1,656)	1:36:A:ILE:HD13	1:37:A:GLU:HA	7	0.33
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	2	0.33
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	2	0.33
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	14	0.33
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	17	0.33
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	17	0.33
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	17	0.33
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	17	0.33
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	17	0.33
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	17	0.33
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	18	0.33
(1,489)	1:160:A:VAL:HG11	1:164:A:ARG:HE	3	0.33
(1,489)	1:160:A:VAL:HG12	1:164:A:ARG:HE	3	0.33
(1,489)	1:160:A:VAL:HG13	1:164:A:ARG:HE	3	0.33
(1,489)	1:160:A:VAL:HG21	1:164:A:ARG:HE	3	0.33
(1,489)	1:160:A:VAL:HG22	1:164:A:ARG:HE	3	0.33
(1,489)	1:160:A:VAL:HG23	1:164:A:ARG:HE	3	0.33
(1,368)	1:24:A:ILE:HA	1:42:A:LYS:HE2	4	0.33
(1,368)	1:24:A:ILE:HA	1:42:A:LYS:HE3	4	0.33
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	7	0.33
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	6	0.33
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	6	0.33
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	6	0.33
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	8	0.33
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	8	0.33
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	8	0.33
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	18	0.33
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	18	0.33
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	18	0.33
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	11	0.33
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	11	0.33
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	11	0.33
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	11	0.33
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	11	0.33
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	11	0.33
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	2	0.33
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	2	0.33
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	2	0.33
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	2	0.33
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	2	0.33
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	2	0.33
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	7	0.33
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	7	0.33
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	7	0.33
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	13	0.33
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	13	0.33
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	16	0.33
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	16	0.33
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	16	0.33
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	3	0.33
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	3	0.33
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	4	0.33
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	5	0.33
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	9	0.33
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	10	0.33
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	14	0.33
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	17	0.33
(1,19)	1:31:A:GLU:HA	1:32:A:TYR:HD1	2	0.33
(1,19)	1:31:A:GLU:HA	1:32:A:TYR:HD2	2	0.33
(3,2)	1:17:A:SER:OG	2:201:A:GNP:O2B	5	0.32
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	1	0.32
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	16	0.32
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	9	0.32
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	18	0.32
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	18	0.32
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	12	0.32
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	14	0.32
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD1	5	0.32
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD2	5	0.32
(1,3242)	1:3:A:GLU:HG2	1:4:A:TYR:HA	20	0.32
(1,3242)	1:3:A:GLU:HG3	1:4:A:TYR:HA	20	0.32
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	9	0.32
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	14	0.32
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	16	0.32
(1,2785)	1:117:A:LYS:H	1:145:A:SER:H	10	0.32
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	2	0.32
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	2	0.32
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	2	0.32
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	19	0.32
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	19	0.32
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	19	0.32
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	2	0.32
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	2	0.32
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	2	0.32
(1,2703)	1:22:A:GLN:HE21	1:148:A:THR:H	18	0.32
(1,2703)	1:22:A:GLN:HE22	1:148:A:THR:H	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD1	3	0.32
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD2	3	0.32
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD1	3	0.32
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD2	3	0.32
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD1	3	0.32
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD2	3	0.32
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD1	10	0.32
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD2	10	0.32
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD1	10	0.32
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD2	10	0.32
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD1	10	0.32
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD2	10	0.32
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	14	0.32
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	14	0.32
(1,2547)	1:164:A:ARG:HB2	1:165:A:LYS:H	6	0.32
(1,2547)	1:164:A:ARG:HB3	1:165:A:LYS:H	6	0.32
(1,2535)	1:168:A:GLU:H	1:169:A:LYS:H	16	0.32
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	3	0.32
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	3	0.32
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	3	0.32
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	3	0.32
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	3	0.32
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	3	0.32
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	13	0.32
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	18	0.32
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	20	0.32
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	20	0.32
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	2	0.32
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	2	0.32
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	13	0.32
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	13	0.32
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	13	0.32
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	19	0.32
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	14	0.32
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	14	0.32
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	14	0.32
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	11	0.32
(1,2280)	1:144:A:THR:HA	1:151:A:GLY:HA2	16	0.32
(1,2195)	1:118:A:SER:HB2	1:143:A:GLU:HG2	6	0.32
(1,2195)	1:118:A:SER:HB2	1:143:A:GLU:HG3	6	0.32
(1,2195)	1:118:A:SER:HB3	1:143:A:GLU:HG2	6	0.32
(1,2195)	1:118:A:SER:HB3	1:143:A:GLU:HG3	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	13	0.32
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	3	0.32
(1,2132)	1:45:A:VAL:HG11	1:51:A:CYS:H	10	0.32
(1,2132)	1:45:A:VAL:HG12	1:51:A:CYS:H	10	0.32
(1,2132)	1:45:A:VAL:HG13	1:51:A:CYS:H	10	0.32
(1,2132)	1:45:A:VAL:HG21	1:51:A:CYS:H	10	0.32
(1,2132)	1:45:A:VAL:HG22	1:51:A:CYS:H	10	0.32
(1,2132)	1:45:A:VAL:HG23	1:51:A:CYS:H	10	0.32
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	18	0.32
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	20	0.32
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE1	20	0.32
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE2	20	0.32
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE1	20	0.32
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE2	20	0.32
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE1	20	0.32
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE2	20	0.32
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	20	0.32
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	20	0.32
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	20	0.32
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	20	0.32
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	20	0.32
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	20	0.32
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	6	0.32
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	6	0.32
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	6	0.32
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	6	0.32
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	6	0.32
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	6	0.32
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	6	0.32
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	6	0.32
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	6	0.32
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	6	0.32
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	6	0.32
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	6	0.32
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	6	0.32
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	6	0.32
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	6	0.32
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	6	0.32
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	6	0.32
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	6	0.32
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	20	0.32
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	20	0.32
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	20	0.32
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	20	0.32
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	20	0.32
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG11	12	0.32
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG12	12	0.32
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG13	12	0.32
(1,1837)	1:77:A:GLY:HA3	1:111:A:MET:HA	1	0.32
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG12	15	0.32
(1,1829)	1:4:A:TYR:HD1	1:163:A:ILE:HG13	15	0.32
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG12	15	0.32
(1,1829)	1:4:A:TYR:HD2	1:163:A:ILE:HG13	15	0.32
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	9	0.32
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	12	0.32
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	9	0.32
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	12	0.32
(1,1714)	1:75:A:GLY:HA2	1:104:A:LYS:HD2	4	0.32
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE2	1	0.32
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE3	1	0.32
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	6	0.32
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	9	0.32
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	1	0.32
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	1	0.32
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	1	0.32
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	1	0.32
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	1	0.32
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	1	0.32
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG11	14	0.32
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG12	14	0.32
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG13	14	0.32
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG21	14	0.32
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG22	14	0.32
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG23	14	0.32
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG11	14	0.32
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG12	14	0.32
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG13	14	0.32
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG21	14	0.32
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG22	14	0.32
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG23	14	0.32
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG11	14	0.32
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG12	14	0.32
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG13	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG21	14	0.32
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG22	14	0.32
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG23	14	0.32
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	9	0.32
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	9	0.32
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	9	0.32
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	9	0.32
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	9	0.32
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	9	0.32
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	11	0.32
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	6	0.32
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	6	0.32
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	6	0.32
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	7	0.32
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	3	0.32
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	13	0.32
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	16	0.32
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	3	0.32
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	10	0.32
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	1	0.32
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	1	0.32
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	1	0.32
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	6	0.32
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	6	0.32
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	6	0.32
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	3	0.32
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	3	0.32
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	3	0.32
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	3	0.32
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	3	0.32
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	3	0.32
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	12	0.32
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	12	0.32
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	12	0.32
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	12	0.32
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	12	0.32
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	12	0.32
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	15	0.32
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	15	0.32
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	15	0.32
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	15	0.32
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	15	0.32
(1,991)	1:83:A:ALA:HB1	1:85:A:ASN:HD21	9	0.32
(1,991)	1:83:A:ALA:HB2	1:85:A:ASN:HD21	9	0.32
(1,991)	1:83:A:ALA:HB3	1:85:A:ASN:HD21	9	0.32
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG2	1	0.32
(1,970)	1:1:A:MET:HE1	1:43:A:GLN:HG3	1	0.32
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG2	1	0.32
(1,970)	1:1:A:MET:HE2	1:43:A:GLN:HG3	1	0.32
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG2	1	0.32
(1,970)	1:1:A:MET:HE3	1:43:A:GLN:HG3	1	0.32
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	8	0.32
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	8	0.32
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	8	0.32
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	8	0.32
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	8	0.32
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	8	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD11	9	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD12	9	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD13	9	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD11	9	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD12	9	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD13	9	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD11	9	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD12	9	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD13	9	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD11	9	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD12	9	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD13	9	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD11	9	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD12	9	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD13	9	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD11	9	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD12	9	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD13	9	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD11	12	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD12	12	0.32
(1,927)	1:23:A:LEU:HD11	1:55:A:ILE:HD13	12	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD11	12	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD12	12	0.32
(1,927)	1:23:A:LEU:HD12	1:55:A:ILE:HD13	12	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD11	12	0.32
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD12	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:23:A:LEU:HD13	1:55:A:ILE:HD13	12	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD11	12	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD12	12	0.32
(1,927)	1:23:A:LEU:HD21	1:55:A:ILE:HD13	12	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD11	12	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD12	12	0.32
(1,927)	1:23:A:LEU:HD22	1:55:A:ILE:HD13	12	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD11	12	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD12	12	0.32
(1,927)	1:23:A:LEU:HD23	1:55:A:ILE:HD13	12	0.32
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD1	5	0.32
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD2	5	0.32
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	18	0.32
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	18	0.32
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	20	0.32
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	20	0.32
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	6	0.32
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	17	0.32
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	18	0.32
(1,840)	1:41:A:ARG:HD2	1:54:A:ASP:HB2	7	0.32
(1,840)	1:41:A:ARG:HD2	1:54:A:ASP:HB3	7	0.32
(1,840)	1:41:A:ARG:HD3	1:54:A:ASP:HB2	7	0.32
(1,840)	1:41:A:ARG:HD3	1:54:A:ASP:HB3	7	0.32
(1,735)	1:37:A:GLU:HA	1:37:A:GLU:HG2	10	0.32
(1,735)	1:37:A:GLU:HA	1:37:A:GLU:HG3	10	0.32
(1,728)	1:65:A:SER:HA	1:66:A:ALA:H	12	0.32
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	20	0.32
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	1	0.32
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	1	0.32
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	16	0.32
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	5	0.32
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	4	0.32
(1,338)	1:24:A:ILE:HD11	1:42:A:LYS:H	12	0.32
(1,338)	1:24:A:ILE:HD12	1:42:A:LYS:H	12	0.32
(1,338)	1:24:A:ILE:HD13	1:42:A:LYS:H	12	0.32
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	16	0.32
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	16	0.32
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	16	0.32
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	9	0.32
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	9	0.32
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	15	0.32
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	1	0.32
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	1	0.32
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	1	0.32
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	1	0.32
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	1	0.32
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	5	0.32
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	9	0.32
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	14	0.32
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	14	0.32
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	14	0.32
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	14	0.32
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	14	0.32
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	14	0.32
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	1	0.32
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	1	0.32
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	1	0.32
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	6	0.32
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	6	0.32
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	6	0.32
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	12	0.32
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	12	0.32
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	12	0.32
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	2	0.32
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	6	0.32
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	13	0.32
(1,30)	1:105:A:ASP:HA	1:106:A:SER:H	18	0.32
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	4	0.31
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	13	0.31
(1,3301)	1:120:A:LEU:HD11	1:122:A:SER:H	1	0.31
(1,3301)	1:120:A:LEU:HD12	1:122:A:SER:H	1	0.31
(1,3301)	1:120:A:LEU:HD13	1:122:A:SER:H	1	0.31
(1,3301)	1:120:A:LEU:HD21	1:122:A:SER:H	1	0.31
(1,3301)	1:120:A:LEU:HD22	1:122:A:SER:H	1	0.31
(1,3301)	1:120:A:LEU:HD23	1:122:A:SER:H	1	0.31
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	7	0.31
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	7	0.31
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	12	0.31
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB2	15	0.31
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB3	15	0.31
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	12	0.31
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	13	0.31
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	17	0.31
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	17	0.31
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	15	0.31
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	3	0.31
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	3	0.31
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	2	0.31
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	2	0.31
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	2	0.31
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	2	0.31
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	2	0.31
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	2	0.31
(1,2980)	1:132:A:ASP:H	1:132:A:ASP:HB3	8	0.31
(1,2980)	1:132:A:ASP:H	1:132:A:ASP:HB3	17	0.31
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	9	0.31
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	11	0.31
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	15	0.31
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	10	0.31
(1,2818)	1:113:A:LEU:HB3	1:142:A:ILE:H	18	0.31
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	5	0.31
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	5	0.31
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	5	0.31
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	2	0.31
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	2	0.31
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	18	0.31
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	10	0.31
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	10	0.31
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	10	0.31
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	20	0.31
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG21	12	0.31
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG22	12	0.31
(1,2358)	1:112:A:VAL:HB	1:158:A:THR:HG23	12	0.31
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	7	0.31
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	5	0.31
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	5	0.31
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	5	0.31
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	5	0.31
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	5	0.31
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	16	0.31
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	18	0.31
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	18	0.31
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	18	0.31
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	1	0.31
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	1	0.31
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	6	0.31
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	7	0.31
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG21	20	0.31
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG22	20	0.31
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG23	20	0.31
(1,2159)	1:140:A:PRO:HG3	1:162:A:GLU:HG2	17	0.31
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	12	0.31
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	12	0.31
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	12	0.31
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	13	0.31
(1,1952)	1:123:A:ARG:HA	1:125:A:VAL:H	9	0.31
(1,1952)	1:123:A:ARG:HA	1:125:A:VAL:H	11	0.31
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	4	0.31
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	4	0.31
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	4	0.31
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	4	0.31
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	4	0.31
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	4	0.31
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	13	0.31
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	13	0.31
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	13	0.31
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	13	0.31
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	13	0.31
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	13	0.31
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	14	0.31
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	14	0.31
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	14	0.31
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	14	0.31
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	14	0.31
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	14	0.31
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	18	0.31
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	18	0.31
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	2	0.31
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	2	0.31
(1,1880)	1:116:A:ASN:HA	1:144:A:THR:HB	1	0.31
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	10	0.31
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	10	0.31
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	10	0.31
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	10	0.31
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	10	0.31
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	10	0.31
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	13	0.31
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	19	0.31
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	15	0.31
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	15	0.31
(1,1801)	1:78:A:PHE:HD1	1:111:A:MET:HG2	13	0.31
(1,1801)	1:78:A:PHE:HD2	1:111:A:MET:HG2	13	0.31
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD11	2	0.31
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD12	2	0.31
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD13	2	0.31
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD21	2	0.31
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD22	2	0.31
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD23	2	0.31
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	2	0.31
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	2	0.31
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	16	0.31
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	16	0.31
(1,1645)	1:128:A:LYS:HG2	1:129:A:GLN:HB2	18	0.31
(1,1645)	1:128:A:LYS:HG3	1:129:A:GLN:HB2	18	0.31
(1,1632)	1:4:A:TYR:HD1	1:51:A:CYS:HB3	17	0.31
(1,1632)	1:4:A:TYR:HD2	1:51:A:CYS:HB3	17	0.31
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	4	0.31
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	8	0.31
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	8	0.31
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	8	0.31
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	19	0.31
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	19	0.31
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	3	0.31
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	3	0.31
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	3	0.31
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	3	0.31
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	3	0.31
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	3	0.31
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG11	8	0.31
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG12	8	0.31
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG13	8	0.31
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG21	8	0.31
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG22	8	0.31
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG23	8	0.31
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG11	8	0.31
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG12	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG13	8	0.31
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG21	8	0.31
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG22	8	0.31
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG23	8	0.31
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG11	8	0.31
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG12	8	0.31
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG13	8	0.31
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG21	8	0.31
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG22	8	0.31
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG23	8	0.31
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG11	14	0.31
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG12	14	0.31
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG13	14	0.31
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG21	14	0.31
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG22	14	0.31
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG23	14	0.31
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD1	9	0.31
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD2	9	0.31
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG2	3	0.31
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG3	3	0.31
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	3	0.31
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	3	0.31
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	3	0.31
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE1	19	0.31
(1,1418)	1:11:A:ALA:HA	1:96:A:TYR:HE2	19	0.31
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	20	0.31
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	20	0.31
(1,1294)	1:95:A:HIS:HD2	1:96:A:TYR:HA	10	0.31
(1,1252)	1:63:A:GLU:HA	1:64:A:TYR:H	1	0.31
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	4	0.31
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	4	0.31
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	4	0.31
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	4	0.31
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	4	0.31
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	4	0.31
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	12	0.31
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	6	0.31
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	6	0.31
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	6	0.31
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	6	0.31
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	6	0.31
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	14	0.31
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	14	0.31
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	14	0.31
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	14	0.31
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	14	0.31
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	14	0.31
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	19	0.31
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	19	0.31
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	19	0.31
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	19	0.31
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	19	0.31
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	19	0.31
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	3	0.31
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	3	0.31
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD1	11	0.31
(1,907)	1:22:A:GLN:HE21	1:28:A:PHE:HD2	11	0.31
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	5	0.31
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	16	0.31
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	16	0.31
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	16	0.31
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	6	0.31
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	14	0.31
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	10	0.31
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	10	0.31
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	10	0.31
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	20	0.31
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	20	0.31
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	20	0.31
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	4	0.31
(1,735)	1:37:A:GLU:HA	1:37:A:GLU:HG2	19	0.31
(1,735)	1:37:A:GLU:HA	1:37:A:GLU:HG3	19	0.31
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	15	0.31
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	15	0.31
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	15	0.31
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	15	0.31
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	15	0.31
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	15	0.31
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	7	0.31
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	7	0.31
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	17	0.31
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	17	0.31
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	2	0.31
(1,532)	1:166:A:HIS:HB2	1:168:A:GLU:H	5	0.31
(1,447)	1:22:A:GLN:HE21	1:28:A:PHE:H	5	0.31
(1,447)	1:22:A:GLN:HE22	1:28:A:PHE:H	5	0.31
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	2	0.31
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	2	0.31
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	2	0.31
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	3	0.31
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	3	0.31
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	3	0.31
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	4	0.31
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	4	0.31
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	4	0.31
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	4	0.31
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	4	0.31
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	4	0.31
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD11	11	0.31
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD12	11	0.31
(1,167)	1:80:A:CYS:H	1:93:A:ILE:HD13	11	0.31
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	12	0.31
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	11	0.31
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	11	0.31
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	11	0.31
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	18	0.31
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	18	0.31
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	18	0.31
(1,3331)	1:106:A:SER:HB2	1:109:A:VAL:H	2	0.3
(1,3331)	1:106:A:SER:HB3	1:109:A:VAL:H	2	0.3
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	2	0.3
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	18	0.3
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	2	0.3
(1,3156)	1:120:A:LEU:H	1:120:A:LEU:HG	14	0.3
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	17	0.3
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	17	0.3
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	17	0.3
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	3	0.3
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	6	0.3
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	12	0.3
(1,2981)	1:59:A:ALA:H	1:68:A:ARG:HE	4	0.3
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	13	0.3
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	13	0.3
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	17	0.3
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	17	0.3
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	17	0.3
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	7	0.3
(1,2768)	1:145:A:SER:H	1:150:A:GLN:HG3	1	0.3
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	7	0.3
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	7	0.3
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	7	0.3
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	8	0.3
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	8	0.3
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	8	0.3
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	20	0.3
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	20	0.3
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	20	0.3
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	6	0.3
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	6	0.3
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	6	0.3
(1,2728)	1:11:A:ALA:HB1	1:14:A:VAL:HG11	20	0.3
(1,2728)	1:11:A:ALA:HB1	1:14:A:VAL:HG12	20	0.3
(1,2728)	1:11:A:ALA:HB1	1:14:A:VAL:HG13	20	0.3
(1,2728)	1:11:A:ALA:HB1	1:14:A:VAL:HG21	20	0.3
(1,2728)	1:11:A:ALA:HB1	1:14:A:VAL:HG22	20	0.3
(1,2728)	1:11:A:ALA:HB1	1:14:A:VAL:HG23	20	0.3
(1,2728)	1:11:A:ALA:HB2	1:14:A:VAL:HG11	20	0.3
(1,2728)	1:11:A:ALA:HB2	1:14:A:VAL:HG12	20	0.3
(1,2728)	1:11:A:ALA:HB2	1:14:A:VAL:HG13	20	0.3
(1,2728)	1:11:A:ALA:HB2	1:14:A:VAL:HG21	20	0.3
(1,2728)	1:11:A:ALA:HB2	1:14:A:VAL:HG22	20	0.3
(1,2728)	1:11:A:ALA:HB2	1:14:A:VAL:HG23	20	0.3
(1,2728)	1:11:A:ALA:HB3	1:14:A:VAL:HG11	20	0.3
(1,2728)	1:11:A:ALA:HB3	1:14:A:VAL:HG12	20	0.3
(1,2728)	1:11:A:ALA:HB3	1:14:A:VAL:HG13	20	0.3
(1,2728)	1:11:A:ALA:HB3	1:14:A:VAL:HG21	20	0.3
(1,2728)	1:11:A:ALA:HB3	1:14:A:VAL:HG22	20	0.3
(1,2728)	1:11:A:ALA:HB3	1:14:A:VAL:HG23	20	0.3
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB1	4	0.3
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB2	4	0.3
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB3	4	0.3
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB1	4	0.3
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB2	4	0.3
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB3	4	0.3
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB1	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB2	4	0.3
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB3	4	0.3
(1,2683)	1:72:A:MET:H	1:75:A:GLY:H	8	0.3
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	5	0.3
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	5	0.3
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	5	0.3
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	5	0.3
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	5	0.3
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	5	0.3
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	5	0.3
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	5	0.3
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	5	0.3
(1,2663)	1:1:A:MET:HE1	1:43:A:GLN:HE22	5	0.3
(1,2663)	1:1:A:MET:HE2	1:43:A:GLN:HE22	5	0.3
(1,2663)	1:1:A:MET:HE3	1:43:A:GLN:HE22	5	0.3
(1,2588)	1:153:A:ASP:HB2	1:155:A:ALA:H	6	0.3
(1,2588)	1:153:A:ASP:HB3	1:155:A:ALA:H	6	0.3
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	20	0.3
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	20	0.3
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	20	0.3
(1,2521)	1:84:A:ILE:HB	1:123:A:ARG:HE	9	0.3
(1,2501)	1:159:A:LEU:HD11	1:163:A:ILE:H	2	0.3
(1,2501)	1:159:A:LEU:HD12	1:163:A:ILE:H	2	0.3
(1,2501)	1:159:A:LEU:HD13	1:163:A:ILE:H	2	0.3
(1,2501)	1:159:A:LEU:HD21	1:163:A:ILE:H	2	0.3
(1,2501)	1:159:A:LEU:HD22	1:163:A:ILE:H	2	0.3
(1,2501)	1:159:A:LEU:HD23	1:163:A:ILE:H	2	0.3
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	13	0.3
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	13	0.3
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	13	0.3
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	13	0.3
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	13	0.3
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	13	0.3
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	2	0.3
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	5	0.3
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	3	0.3
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	3	0.3
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	3	0.3
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	10	0.3
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG21	2	0.3
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG22	2	0.3
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG23	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	18	0.3
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG11	8	0.3
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG12	8	0.3
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG13	8	0.3
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG21	8	0.3
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG22	8	0.3
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG23	8	0.3
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG11	8	0.3
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG12	8	0.3
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG13	8	0.3
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG21	8	0.3
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG22	8	0.3
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG23	8	0.3
(1,2176)	1:148:A:THR:HG21	2:201:A:GNP:HN1	4	0.3
(1,2176)	1:148:A:THR:HG22	2:201:A:GNP:HN1	4	0.3
(1,2176)	1:148:A:THR:HG23	2:201:A:GNP:HN1	4	0.3
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	10	0.3
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	2	0.3
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	3	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	7	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	7	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	7	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	7	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	7	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	7	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	13	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	13	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	13	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	13	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	13	0.3
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	13	0.3
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	15	0.3
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	10	0.3
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	10	0.3
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	10	0.3
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	10	0.3
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	10	0.3
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	10	0.3
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	16	0.3
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	16	0.3
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	16	0.3
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	16	0.3
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	16	0.3
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	3	0.3
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	3	0.3
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	3	0.3
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	3	0.3
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	10	0.3
(1,1903)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	10	0.3
(1,1846)	1:41:A:ARG:HD2	1:52:A:LEU:HB2	3	0.3
(1,1846)	1:41:A:ARG:HD3	1:52:A:LEU:HB2	3	0.3
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	11	0.3
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	14	0.3
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	17	0.3
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	14	0.3
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	14	0.3
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	10	0.3
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG21	6	0.3
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG22	6	0.3
(1,1766)	1:104:A:LYS:HE3	1:109:A:VAL:HG23	6	0.3
(1,1730)	1:78:A:PHE:HZ	1:104:A:LYS:HE3	6	0.3
(1,1708)	1:142:A:ILE:HD11	1:143:A:GLU:HB3	6	0.3
(1,1708)	1:142:A:ILE:HD12	1:143:A:GLU:HB3	6	0.3
(1,1708)	1:142:A:ILE:HD13	1:143:A:GLU:HB3	6	0.3
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	15	0.3
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	15	0.3
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	15	0.3
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	12	0.3
(1,1590)	1:93:A:ILE:HB	1:94:A:HIS:HB3	17	0.3
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG21	5	0.3
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG22	5	0.3
(1,1580)	1:80:A:CYS:HB2	1:93:A:ILE:HG23	5	0.3
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG21	5	0.3
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG22	5	0.3
(1,1580)	1:80:A:CYS:HB3	1:93:A:ILE:HG23	5	0.3
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	13	0.3
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	13	0.3
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	15	0.3
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	15	0.3
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD11	20	0.3
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD12	20	0.3
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD13	20	0.3
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD11	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD12	20	0.3
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD13	20	0.3
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	15	0.3
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	15	0.3
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	9	0.3
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	9	0.3
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	9	0.3
(1,1386)	1:95:A:HIS:HE1	1:99:A:GLN:HE21	18	0.3
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD2	2	0.3
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD3	2	0.3
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	4	0.3
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	4	0.3
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	4	0.3
(1,1321)	1:56:A:LEU:HD11	1:71:A:TYR:HA	11	0.3
(1,1321)	1:56:A:LEU:HD12	1:71:A:TYR:HA	11	0.3
(1,1321)	1:56:A:LEU:HD13	1:71:A:TYR:HA	11	0.3
(1,1321)	1:56:A:LEU:HD21	1:71:A:TYR:HA	11	0.3
(1,1321)	1:56:A:LEU:HD22	1:71:A:TYR:HA	11	0.3
(1,1321)	1:56:A:LEU:HD23	1:71:A:TYR:HA	11	0.3
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	13	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	6	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	6	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	6	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	6	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	6	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	6	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	6	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	6	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	6	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	6	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	6	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	6	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	6	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	6	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	6	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	6	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	6	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	6	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	11	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	11	0.3
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	11	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	11	0.3
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	11	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	11	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	11	0.3
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	11	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	11	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	11	0.3
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	11	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	11	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	11	0.3
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	11	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	11	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	11	0.3
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	11	0.3
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	11	0.3
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	11	0.3
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	11	0.3
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	13	0.3
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	17	0.3
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	16	0.3
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	16	0.3
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	11	0.3
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	6	0.3
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG21	1	0.3
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG22	1	0.3
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG23	1	0.3
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG21	1	0.3
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG22	1	0.3
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG23	1	0.3
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG21	1	0.3
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG22	1	0.3
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG23	1	0.3
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG21	1	0.3
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG22	1	0.3
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG23	1	0.3
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG21	1	0.3
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG22	1	0.3
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG23	1	0.3
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG21	1	0.3
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG22	1	0.3
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG23	1	0.3
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	4	0.3
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	7	0.3
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	7	0.3
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	15	0.3
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	15	0.3
(1,609)	1:45:A:VAL:HB	1:47:A:ASP:H	11	0.3
(1,510)	1:24:A:ILE:H	1:25:A:GLN:HE21	14	0.3
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	11	0.3
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	11	0.3
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	11	0.3
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	8	0.3
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	8	0.3
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	9	0.3
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	9	0.3
(1,489)	1:160:A:VAL:HG11	1:164:A:ARG:HE	20	0.3
(1,489)	1:160:A:VAL:HG12	1:164:A:ARG:HE	20	0.3
(1,489)	1:160:A:VAL:HG13	1:164:A:ARG:HE	20	0.3
(1,489)	1:160:A:VAL:HG21	1:164:A:ARG:HE	20	0.3
(1,489)	1:160:A:VAL:HG22	1:164:A:ARG:HE	20	0.3
(1,489)	1:160:A:VAL:HG23	1:164:A:ARG:HE	20	0.3
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	7	0.3
(1,338)	1:24:A:ILE:HD11	1:42:A:LYS:H	3	0.3
(1,338)	1:24:A:ILE:HD12	1:42:A:LYS:H	3	0.3
(1,338)	1:24:A:ILE:HD13	1:42:A:LYS:H	3	0.3
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	8	0.3
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	8	0.3
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	13	0.3
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	13	0.3
(1,164)	1:83:A:ALA:H	1:86:A:ASN:HB2	3	0.3
(1,103)	1:16:A:LYS:HA	1:19:A:LEU:HB3	4	0.3
(1,84)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	17	0.3
(1,61)	1:153:A:ASP:HB2	1:154:A:ASP:H	6	0.3
(1,61)	1:153:A:ASP:HB3	1:154:A:ASP:H	6	0.3
(1,61)	1:153:A:ASP:HB2	1:154:A:ASP:H	16	0.3
(1,61)	1:153:A:ASP:HB3	1:154:A:ASP:H	16	0.3
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	8	0.3
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	8	0.3
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	8	0.3
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	5	0.3
(1,39)	1:64:A:TYR:HD1	1:65:A:SER:H	18	0.3
(1,39)	1:64:A:TYR:HD2	1:65:A:SER:H	18	0.3
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	3	0.29
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	19	0.29
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	2	0.29
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	2	0.29
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	2	0.29
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	17	0.29
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	16	0.29
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	18	0.29
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	3	0.29
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD11	9	0.29
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD12	9	0.29
(1,3024)	1:130:A:ALA:HA	1:133:A:LEU:HD13	9	0.29
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	15	0.29
(1,2768)	1:145:A:SER:H	1:150:A:GLN:HG3	3	0.29
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	4	0.29
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	4	0.29
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	4	0.29
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	17	0.29
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	17	0.29
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	17	0.29
(1,2710)	1:102:A:ARG:HB3	1:102:A:ARG:HE	4	0.29
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	8	0.29
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	8	0.29
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	8	0.29
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	8	0.29
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	8	0.29
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	8	0.29
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE1	8	0.29
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE2	8	0.29
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE3	8	0.29
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE1	8	0.29
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE2	8	0.29
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE3	8	0.29
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE1	8	0.29
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE2	8	0.29
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE3	8	0.29
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE1	19	0.29
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE2	19	0.29
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE3	19	0.29
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE1	19	0.29
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE2	19	0.29
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE3	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE1	19	0.29
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE2	19	0.29
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE3	19	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	4	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	4	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	4	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	4	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	4	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	4	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	4	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	4	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	4	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	8	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	8	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	8	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	8	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	8	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	8	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	8	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	8	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	8	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	19	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	19	0.29
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	19	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	19	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	19	0.29
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	19	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	19	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	19	0.29
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	19	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	5	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	5	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	7	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	7	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	10	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	10	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB2	13	0.29
(1,2642)	1:123:A:ARG:HE	1:126:A:ASP:HB3	13	0.29
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	20	0.29
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	20	0.29
(1,2620)	1:166:A:HIS:HB3	1:167:A:LYS:HB2	9	0.29
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG12	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG13	10	0.29
(1,2588)	1:153:A:ASP:HB2	1:155:A:ALA:H	16	0.29
(1,2588)	1:153:A:ASP:HB3	1:155:A:ALA:H	16	0.29
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	2	0.29
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	2	0.29
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	2	0.29
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	14	0.29
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	14	0.29
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG21	19	0.29
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG22	19	0.29
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG23	19	0.29
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	1	0.29
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	17	0.29
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	17	0.29
(1,2254)	1:149:A:ARG:HB2	1:150:A:GLN:HE21	14	0.29
(1,2254)	1:149:A:ARG:HB3	1:150:A:GLN:HE21	14	0.29
(1,2223)	1:114:A:VAL:HA	1:144:A:THR:H	18	0.29
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	14	0.29
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	14	0.29
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	9	0.29
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	20	0.29
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	20	0.29
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	9	0.29
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	9	0.29
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	9	0.29
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	9	0.29
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	9	0.29
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	9	0.29
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	9	0.29
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	9	0.29
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	9	0.29
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	9	0.29
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	9	0.29
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	9	0.29
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	9	0.29
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	9	0.29
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	9	0.29
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	9	0.29
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	9	0.29
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	9	0.29
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	9	0.29
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG21	16	0.29
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG22	16	0.29
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG23	16	0.29
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	15	0.29
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	8	0.29
(1,1837)	1:77:A:GLY:HA3	1:111:A:MET:HA	6	0.29
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	10	0.29
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	16	0.29
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	6	0.29
(1,1752)	1:8:A:VAL:HG11	1:10:A:GLY:H	18	0.29
(1,1752)	1:8:A:VAL:HG12	1:10:A:GLY:H	18	0.29
(1,1752)	1:8:A:VAL:HG13	1:10:A:GLY:H	18	0.29
(1,1752)	1:8:A:VAL:HG21	1:10:A:GLY:H	18	0.29
(1,1752)	1:8:A:VAL:HG22	1:10:A:GLY:H	18	0.29
(1,1752)	1:8:A:VAL:HG23	1:10:A:GLY:H	18	0.29
(1,1708)	1:142:A:ILE:HD11	1:143:A:GLU:HB3	9	0.29
(1,1708)	1:142:A:ILE:HD12	1:143:A:GLU:HB3	9	0.29
(1,1708)	1:142:A:ILE:HD13	1:143:A:GLU:HB3	9	0.29
(1,1690)	1:102:A:ARG:H	1:102:A:ARG:HG3	10	0.29
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD1	13	0.29
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD2	13	0.29
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	5	0.29
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	5	0.29
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	5	0.29
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	5	0.29
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	5	0.29
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	5	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG11	6	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG12	6	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG13	6	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG21	6	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG22	6	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG23	6	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG11	6	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG12	6	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG13	6	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG21	6	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG22	6	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG23	6	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG11	6	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG12	6	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG13	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG21	6	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG22	6	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG23	6	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG11	9	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG12	9	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG13	9	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG21	9	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG22	9	0.29
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG23	9	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG11	9	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG12	9	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG13	9	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG21	9	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG22	9	0.29
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG23	9	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG11	9	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG12	9	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG13	9	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG21	9	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG22	9	0.29
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG23	9	0.29
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG11	9	0.29
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG12	9	0.29
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG13	9	0.29
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG21	9	0.29
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG22	9	0.29
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG23	9	0.29
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	9	0.29
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	9	0.29
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE1	10	0.29
(1,1423)	1:72:A:MET:HE1	1:96:A:TYR:HE2	10	0.29
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE1	10	0.29
(1,1423)	1:72:A:MET:HE2	1:96:A:TYR:HE2	10	0.29
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE1	10	0.29
(1,1423)	1:72:A:MET:HE3	1:96:A:TYR:HE2	10	0.29
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	4	0.29
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	4	0.29
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	4	0.29
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	7	0.29
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	16	0.29
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	16	0.29
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1365)	1:5:A:LYS:HB2	1:74:A:THR:HB	11	0.29
(1,1365)	1:5:A:LYS:HB3	1:74:A:THR:HB	11	0.29
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	6	0.29
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	6	0.29
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	10	0.29
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	10	0.29
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	10	0.29
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	2	0.29
(1,1272)	1:9:A:VAL:HG11	1:96:A:TYR:H	16	0.29
(1,1272)	1:9:A:VAL:HG12	1:96:A:TYR:H	16	0.29
(1,1272)	1:9:A:VAL:HG13	1:96:A:TYR:H	16	0.29
(1,1272)	1:9:A:VAL:HG21	1:96:A:TYR:H	16	0.29
(1,1272)	1:9:A:VAL:HG22	1:96:A:TYR:H	16	0.29
(1,1272)	1:9:A:VAL:HG23	1:96:A:TYR:H	16	0.29
(1,1252)	1:63:A:GLU:HA	1:64:A:TYR:H	8	0.29
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	2	0.29
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	20	0.29
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	14	0.29
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	12	0.29
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	12	0.29
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	19	0.29
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	19	0.29
(1,1014)	1:45:A:VAL:HG11	1:50:A:THR:HB	5	0.29
(1,1014)	1:45:A:VAL:HG12	1:50:A:THR:HB	5	0.29
(1,1014)	1:45:A:VAL:HG13	1:50:A:THR:HB	5	0.29
(1,1014)	1:45:A:VAL:HG21	1:50:A:THR:HB	5	0.29
(1,1014)	1:45:A:VAL:HG22	1:50:A:THR:HB	5	0.29
(1,1014)	1:45:A:VAL:HG23	1:50:A:THR:HB	5	0.29
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA2	14	0.29
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA3	14	0.29
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA2	14	0.29
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA3	14	0.29
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA2	14	0.29
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA3	14	0.29
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA2	14	0.29
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA3	14	0.29
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA2	14	0.29
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA3	14	0.29
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA2	14	0.29
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA3	14	0.29
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	15	0.29
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	15	0.29
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	15	0.29
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	15	0.29
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	15	0.29
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	10	0.29
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	13	0.29
(1,824)	1:119:A:ASP:H	2:201:A:GNP:HN1	4	0.29
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	15	0.29
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	9	0.29
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	9	0.29
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	15	0.29
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	15	0.29
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	15	0.29
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	1	0.29
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	1	0.29
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	14	0.29
(1,258)	1:7:A:VAL:HG11	1:72:A:MET:HA	9	0.29
(1,258)	1:7:A:VAL:HG12	1:72:A:MET:HA	9	0.29
(1,258)	1:7:A:VAL:HG13	1:72:A:MET:HA	9	0.29
(1,258)	1:7:A:VAL:HG11	1:72:A:MET:HA	11	0.29
(1,258)	1:7:A:VAL:HG12	1:72:A:MET:HA	11	0.29
(1,258)	1:7:A:VAL:HG13	1:72:A:MET:HA	11	0.29
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	2	0.29
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	2	0.29
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	2	0.29
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	2	0.29
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	2	0.29
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	2	0.29
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	9	0.29
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	9	0.29
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	9	0.29
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	9	0.29
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	9	0.29
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	9	0.29
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	2	0.29
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	2	0.29
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	2	0.29
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	17	0.29
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	11	0.29
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	11	0.29
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	11	0.29
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	11	0.29
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	11	0.29
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	4	0.29
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	4	0.29
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	4	0.29
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	4	0.29
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	4	0.29
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	4	0.29
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	15	0.28
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	13	0.28
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	17	0.28
(1,3242)	1:3:A:GLU:HG2	1:4:A:TYR:HA	14	0.28
(1,3242)	1:3:A:GLU:HG3	1:4:A:TYR:HA	14	0.28
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	14	0.28
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	8	0.28
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	18	0.28
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	18	0.28
(1,3144)	1:1:A:MET:HE1	1:52:A:LEU:H	5	0.28
(1,3144)	1:1:A:MET:HE2	1:52:A:LEU:H	5	0.28
(1,3144)	1:1:A:MET:HE3	1:52:A:LEU:H	5	0.28
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	2	0.28
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	17	0.28
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG2	16	0.28
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG3	16	0.28
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG2	16	0.28
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG3	16	0.28
(1,3116)	1:85:A:ASN:HB2	1:124:A:THR:H	8	0.28
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	6	0.28
(1,3005)	1:90:A:PHE:HE1	1:131:A:GLN:H	10	0.28
(1,3005)	1:90:A:PHE:HE2	1:131:A:GLN:H	10	0.28
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	3	0.28
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	9	0.28
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	9	0.28
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	9	0.28
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	9	0.28
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	9	0.28
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	9	0.28
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	15	0.28
(1,2703)	1:22:A:GLN:HE21	1:148:A:THR:H	4	0.28
(1,2703)	1:22:A:GLN:HE22	1:148:A:THR:H	4	0.28
(1,2693)	1:148:A:THR:H	1:149:A:ARG:HA	4	0.28
(1,2690)	1:148:A:THR:H	1:150:A:GLN:HB2	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2682)	1:25:A:GLN:HA	1:27:A:HIS:HE1	19	0.28
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	13	0.28
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	13	0.28
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	13	0.28
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	14	0.28
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	14	0.28
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	14	0.28
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	6	0.28
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	6	0.28
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	6	0.28
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	6	0.28
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	6	0.28
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	6	0.28
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	6	0.28
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	6	0.28
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	6	0.28
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	15	0.28
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	15	0.28
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	15	0.28
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	15	0.28
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	15	0.28
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	15	0.28
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	15	0.28
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	15	0.28
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	15	0.28
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	2	0.28
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	2	0.28
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	10	0.28
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	10	0.28
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	2	0.28
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE1	7	0.28
(1,2506)	1:2:A:THR:HB	1:4:A:TYR:HE2	7	0.28
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	8	0.28
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	20	0.28
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	15	0.28
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	15	0.28
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	12	0.28
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	12	0.28
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	12	0.28
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	12	0.28
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	12	0.28
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	14	0.28
(1,2324)	1:144:A:THR:HG21	1:155:A:ALA:HA	16	0.28
(1,2324)	1:144:A:THR:HG22	1:155:A:ALA:HA	16	0.28
(1,2324)	1:144:A:THR:HG23	1:155:A:ALA:HA	16	0.28
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	17	0.28
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	17	0.28
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	17	0.28
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	3	0.28
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	4	0.28
(1,2221)	1:147:A:LYS:HG3	1:148:A:THR:HA	6	0.28
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG11	1	0.28
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG12	1	0.28
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG13	1	0.28
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG21	1	0.28
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG22	1	0.28
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG23	1	0.28
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG11	1	0.28
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG12	1	0.28
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG13	1	0.28
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG21	1	0.28
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG22	1	0.28
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG23	1	0.28
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	2	0.28
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	1	0.28
(1,2163)	1:110:A:PRO:HD2	1:166:A:HIS:HE1	19	0.28
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	7	0.28
(1,2069)	1:90:A:PHE:HD1	1:130:A:ALA:HA	10	0.28
(1,2069)	1:90:A:PHE:HD2	1:130:A:ALA:HA	10	0.28
(1,2050)	1:128:A:LYS:H	1:129:A:GLN:HG2	19	0.28
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	7	0.28
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	7	0.28
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	17	0.28
(1,1975)	1:19:A:LEU:HA	1:156:A:PHE:HZ	9	0.28
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	20	0.28
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	15	0.28
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	18	0.28
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	20	0.28
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	15	0.28
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD11	14	0.28
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD12	14	0.28
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD13	14	0.28
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD21	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD22	14	0.28
(1,1790)	1:110:A:PRO:HG3	1:159:A:LEU:HD23	14	0.28
(1,1774)	1:24:A:ILE:HD11	1:41:A:ARG:HA	12	0.28
(1,1774)	1:24:A:ILE:HD12	1:41:A:ARG:HA	12	0.28
(1,1774)	1:24:A:ILE:HD13	1:41:A:ARG:HA	12	0.28
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	17	0.28
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	17	0.28
(1,1696)	1:113:A:LEU:HG	1:141:A:PHE:HA	7	0.28
(1,1661)	1:101:A:LYS:HD2	1:107:A:GLU:HA	18	0.28
(1,1661)	1:101:A:LYS:HD3	1:107:A:GLU:HA	18	0.28
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	11	0.28
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	18	0.28
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	18	0.28
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG2	19	0.28
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG3	19	0.28
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	17	0.28
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	15	0.28
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	15	0.28
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	19	0.28
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	19	0.28
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	12	0.28
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	12	0.28
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG2	3	0.28
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG3	3	0.28
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG2	3	0.28
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG3	3	0.28
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG2	3	0.28
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG3	3	0.28
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	7	0.28
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	7	0.28
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	7	0.28
(1,1251)	1:149:A:ARG:HB3	1:149:A:ARG:HE	14	0.28
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	7	0.28
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD21	14	0.28
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD22	14	0.28
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD23	14	0.28
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD11	16	0.28
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD12	16	0.28
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD13	16	0.28
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD21	16	0.28
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD22	16	0.28
(1,1197)	1:39:A:SER:H	1:56:A:LEU:HD23	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	8	0.28
(1,1132)	1:1:A:MET:HE1	1:52:A:LEU:HB2	16	0.28
(1,1132)	1:1:A:MET:HE2	1:52:A:LEU:HB2	16	0.28
(1,1132)	1:1:A:MET:HE3	1:52:A:LEU:HB2	16	0.28
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	20	0.28
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	9	0.28
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	17	0.28
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	1	0.28
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	13	0.28
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	13	0.28
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	10	0.28
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	20	0.28
(1,982)	1:44:A:VAL:HG21	1:51:A:CYS:HB2	9	0.28
(1,982)	1:44:A:VAL:HG22	1:51:A:CYS:HB2	9	0.28
(1,982)	1:44:A:VAL:HG23	1:51:A:CYS:HB2	9	0.28
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	2	0.28
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	17	0.28
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	17	0.28
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	17	0.28
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	20	0.28
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	20	0.28
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	8	0.28
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	8	0.28
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	19	0.28
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	19	0.28
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	13	0.28
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	13	0.28
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	13	0.28
(1,728)	1:65:A:SER:HA	1:66:A:ALA:H	6	0.28
(1,623)	1:32:A:TYR:HE1	1:34:A:PRO:HA	1	0.28
(1,623)	1:32:A:TYR:HE2	1:34:A:PRO:HA	1	0.28
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	10	0.28
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	10	0.28
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	10	0.28
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	7	0.28
(1,319)	1:23:A:LEU:HB2	1:152:A:VAL:HB	1	0.28
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE1	19	0.28
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE2	19	0.28
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	17	0.28
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	5	0.28
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	5	0.28
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	5	0.28
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	5	0.28
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	5	0.28
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	19	0.28
(1,108)	1:166:A:HIS:HB3	1:167:A:LYS:H	11	0.28
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	15	0.28
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	15	0.28
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	15	0.28
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	11	0.27
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	18	0.27
(1,3302)	1:120:A:LEU:HD21	1:122:A:SER:H	1	0.27
(1,3302)	1:120:A:LEU:HD22	1:122:A:SER:H	1	0.27
(1,3302)	1:120:A:LEU:HD23	1:122:A:SER:H	1	0.27
(1,3259)	1:113:A:LEU:H	1:141:A:PHE:HB3	13	0.27
(1,3242)	1:3:A:GLU:HG2	1:4:A:TYR:HA	13	0.27
(1,3242)	1:3:A:GLU:HG3	1:4:A:TYR:HA	13	0.27
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	2	0.27
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	2	0.27
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	2	0.27
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	2	0.27
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	2	0.27
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	2	0.27
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	1	0.27
(1,3194)	1:84:A:ILE:HA	1:125:A:VAL:HG11	4	0.27
(1,3194)	1:84:A:ILE:HA	1:125:A:VAL:HG12	4	0.27
(1,3194)	1:84:A:ILE:HA	1:125:A:VAL:HG13	4	0.27
(1,3194)	1:84:A:ILE:HA	1:125:A:VAL:HG21	4	0.27
(1,3194)	1:84:A:ILE:HA	1:125:A:VAL:HG22	4	0.27
(1,3194)	1:84:A:ILE:HA	1:125:A:VAL:HG23	4	0.27
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	4	0.27
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	1	0.27
(1,3068)	1:123:A:ARG:HE	1:127:A:THR:H	9	0.27
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	12	0.27
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	3	0.27
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	16	0.27
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	16	0.27
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	16	0.27
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	16	0.27
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	16	0.27
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	16	0.27
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	4	0.27
(1,2898)	1:28:A:PHE:HE1	1:147:A:LYS:HD2	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2898)	1:28:A:PHE:HE1	1:147:A:LYS:HD3	16	0.27
(1,2898)	1:28:A:PHE:HE2	1:147:A:LYS:HD2	16	0.27
(1,2898)	1:28:A:PHE:HE2	1:147:A:LYS:HD3	16	0.27
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	5	0.27
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	5	0.27
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	5	0.27
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	5	0.27
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	5	0.27
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	5	0.27
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	9	0.27
(1,2785)	1:117:A:LYS:H	1:145:A:SER:H	11	0.27
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	13	0.27
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	13	0.27
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	13	0.27
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	16	0.27
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	6	0.27
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	6	0.27
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	6	0.27
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	6	0.27
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	6	0.27
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	6	0.27
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	16	0.27
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	16	0.27
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	16	0.27
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	7	0.27
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	7	0.27
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	7	0.27
(1,2620)	1:166:A:HIS:HB3	1:167:A:LYS:HB2	7	0.27
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	8	0.27
(1,2589)	1:153:A:ASP:HB2	1:155:A:ALA:H	20	0.27
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	7	0.27
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	7	0.27
(1,2564)	1:20:A:THR:HA	1:55:A:ILE:HG12	3	0.27
(1,2564)	1:20:A:THR:HA	1:55:A:ILE:HG12	14	0.27
(1,2535)	1:168:A:GLU:H	1:169:A:LYS:H	15	0.27
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	8	0.27
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	8	0.27
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	8	0.27
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	15	0.27
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	15	0.27
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	15	0.27
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	14	0.27
(1,2380)	1:159:A:LEU:HD11	1:163:A:ILE:HA	7	0.27
(1,2380)	1:159:A:LEU:HD12	1:163:A:ILE:HA	7	0.27
(1,2380)	1:159:A:LEU:HD13	1:163:A:ILE:HA	7	0.27
(1,2380)	1:159:A:LEU:HD21	1:163:A:ILE:HA	7	0.27
(1,2380)	1:159:A:LEU:HD22	1:163:A:ILE:HA	7	0.27
(1,2380)	1:159:A:LEU:HD23	1:163:A:ILE:HA	7	0.27
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD11	13	0.27
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD12	13	0.27
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD13	13	0.27
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD21	13	0.27
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD22	13	0.27
(1,2330)	1:156:A:PHE:HB3	1:159:A:LEU:HD23	13	0.27
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	13	0.27
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG21	15	0.27
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG22	15	0.27
(1,2232)	1:118:A:SER:H	1:148:A:THR:HG23	15	0.27
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	8	0.27
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	8	0.27
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	8	0.27
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	12	0.27
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	3	0.27
(1,2056)	1:126:A:ASP:HB2	1:129:A:GLN:HG2	4	0.27
(1,2056)	1:126:A:ASP:HB3	1:129:A:GLN:HG2	4	0.27
(1,2038)	1:90:A:PHE:HE1	1:129:A:GLN:HA	3	0.27
(1,2038)	1:90:A:PHE:HE2	1:129:A:GLN:HA	3	0.27
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	15	0.27
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	15	0.27
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	8	0.27
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	8	0.27
(1,1902)	1:116:A:ASN:HA	1:144:A:THR:HA	10	0.27
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	6	0.27
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	3	0.27
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	13	0.27
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	17	0.27
(1,1815)	1:100:A:ILE:HG21	1:111:A:MET:HG2	20	0.27
(1,1815)	1:100:A:ILE:HG22	1:111:A:MET:HG2	20	0.27
(1,1815)	1:100:A:ILE:HG23	1:111:A:MET:HG2	20	0.27
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	10	0.27
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	10	0.27
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	2	0.27
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	12	0.27
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	12	0.27
(1,1684)	1:102:A:ARG:H	1:102:A:ARG:HD2	10	0.27
(1,1684)	1:102:A:ARG:H	1:102:A:ARG:HD3	10	0.27
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	2	0.27
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	20	0.27
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	4	0.27
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	4	0.27
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	12	0.27
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	17	0.27
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	17	0.27
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	17	0.27
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	18	0.27
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	13	0.27
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	13	0.27
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	3	0.27
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	3	0.27
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	3	0.27
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	14	0.27
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	14	0.27
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	14	0.27
(1,1321)	1:56:A:LEU:HD11	1:71:A:TYR:HA	2	0.27
(1,1321)	1:56:A:LEU:HD12	1:71:A:TYR:HA	2	0.27
(1,1321)	1:56:A:LEU:HD13	1:71:A:TYR:HA	2	0.27
(1,1321)	1:56:A:LEU:HD21	1:71:A:TYR:HA	2	0.27
(1,1321)	1:56:A:LEU:HD22	1:71:A:TYR:HA	2	0.27
(1,1321)	1:56:A:LEU:HD23	1:71:A:TYR:HA	2	0.27
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD11	12	0.27
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD12	12	0.27
(1,1266)	1:138:A:GLY:HA2	1:139:A:ILE:HD13	12	0.27
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	15	0.27
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	13	0.27
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	8	0.27
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	8	0.27
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	8	0.27
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	8	0.27
(1,1175)	1:23:A:LEU:HD11	1:156:A:PHE:HB3	12	0.27
(1,1175)	1:23:A:LEU:HD12	1:156:A:PHE:HB3	12	0.27
(1,1175)	1:23:A:LEU:HD13	1:156:A:PHE:HB3	12	0.27
(1,1175)	1:23:A:LEU:HD21	1:156:A:PHE:HB3	12	0.27
(1,1175)	1:23:A:LEU:HD22	1:156:A:PHE:HB3	12	0.27
(1,1175)	1:23:A:LEU:HD23	1:156:A:PHE:HB3	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	1	0.27
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	1	0.27
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	7	0.27
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	9	0.27
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	4	0.27
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	8	0.27
(1,1058)	1:127:A:THR:HG21	1:131:A:GLN:HE22	11	0.27
(1,1058)	1:127:A:THR:HG22	1:131:A:GLN:HE22	11	0.27
(1,1058)	1:127:A:THR:HG23	1:131:A:GLN:HE22	11	0.27
(1,1052)	1:128:A:LYS:H	1:131:A:GLN:HE22	13	0.27
(1,1050)	1:90:A:PHE:HD1	1:129:A:GLN:HE22	19	0.27
(1,1050)	1:90:A:PHE:HD2	1:129:A:GLN:HE22	19	0.27
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	8	0.27
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	8	0.27
(1,1048)	1:90:A:PHE:HB2	1:129:A:GLN:HE22	15	0.27
(1,1048)	1:90:A:PHE:HB3	1:129:A:GLN:HE22	15	0.27
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	2	0.27
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	2	0.27
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	2	0.27
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	7	0.27
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	7	0.27
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	7	0.27
(1,957)	1:43:A:GLN:HG2	1:44:A:VAL:H	2	0.27
(1,957)	1:43:A:GLN:HG3	1:44:A:VAL:H	2	0.27
(1,952)	1:1:A:MET:HE1	1:43:A:GLN:HE21	3	0.27
(1,952)	1:1:A:MET:HE2	1:43:A:GLN:HE21	3	0.27
(1,952)	1:1:A:MET:HE3	1:43:A:GLN:HE21	3	0.27
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	5	0.27
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	18	0.27
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	11	0.27
(1,827)	1:120:A:LEU:HD11	2:201:A:GNP:HN1	12	0.27
(1,827)	1:120:A:LEU:HD12	2:201:A:GNP:HN1	12	0.27
(1,827)	1:120:A:LEU:HD13	2:201:A:GNP:HN1	12	0.27
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	8	0.27
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	9	0.27
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	14	0.27
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	14	0.27
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	6	0.27
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	13	0.27
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	18	0.27
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	18	0.27
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	19	0.27
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	18	0.27
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	18	0.27
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	4	0.27
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	17	0.27
(1,379)	1:112:A:VAL:HB	1:139:A:ILE:HB	15	0.27
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	11	0.27
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	11	0.27
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	16	0.27
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	16	0.27
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	16	0.27
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	16	0.27
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	16	0.27
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	16	0.27
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	16	0.27
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	19	0.27
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	19	0.27
(1,204)	1:32:A:TYR:HD1	2:201:A:GNP:H1'	18	0.27
(1,204)	1:32:A:TYR:HD2	2:201:A:GNP:H1'	18	0.27
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	19	0.27
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	15	0.27
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	15	0.27
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	15	0.27
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	15	0.27
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	15	0.27
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	15	0.27
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	6	0.27
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD22	6	0.27
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	18	0.27
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	18	0.27
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	18	0.27
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	18	0.27
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	18	0.27
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	18	0.27
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	17	0.27
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	19	0.27
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	7	0.26
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	8	0.26
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	15	0.26
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	8	0.26
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	8	0.26
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	16	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	20	0.26
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	6	0.26
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	5	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	13	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	13	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	13	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	20	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	20	0.26
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	20	0.26
(1,3128)	1:1:A:MET:HA	1:51:A:CYS:HA	10	0.26
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD11	10	0.26
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD12	10	0.26
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD13	10	0.26
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD21	10	0.26
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD22	10	0.26
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD23	10	0.26
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	17	0.26
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	9	0.26
(1,2908)	1:135:A:ARG:HD2	1:136:A:SER:H	9	0.26
(1,2908)	1:135:A:ARG:HD3	1:136:A:SER:H	9	0.26
(1,2886)	1:21:A:ILE:HG12	1:40:A:TYR:HE1	19	0.26
(1,2886)	1:21:A:ILE:HG12	1:40:A:TYR:HE2	19	0.26
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	10	0.26
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	11	0.26
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	3	0.26
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	3	0.26
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	3	0.26
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	5	0.26
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	5	0.26
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	5	0.26
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB1	9	0.26
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB2	9	0.26
(1,2748)	1:15:A:GLY:HA3	1:146:A:ALA:HB3	9	0.26
(1,2710)	1:102:A:ARG:HB3	1:102:A:ARG:HE	14	0.26
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE1	1	0.26
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE2	1	0.26
(1,2675)	1:100:A:ILE:HG21	1:111:A:MET:HE3	1	0.26
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE1	1	0.26
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE2	1	0.26
(1,2675)	1:100:A:ILE:HG22	1:111:A:MET:HE3	1	0.26
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE1	1	0.26
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE2	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2675)	1:100:A:ILE:HG23	1:111:A:MET:HE3	1	0.26
(1,2668)	1:99:A:GLN:HA	1:102:A:ARG:HE	19	0.26
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	18	0.26
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	18	0.26
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	18	0.26
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	15	0.26
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	17	0.26
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	17	0.26
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	17	0.26
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	5	0.26
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	5	0.26
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	5	0.26
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	5	0.26
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	5	0.26
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	5	0.26
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	5	0.26
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	10	0.26
(1,2328)	1:144:A:THR:HA	1:152:A:VAL:H	17	0.26
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	14	0.26
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	14	0.26
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	14	0.26
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	8	0.26
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	8	0.26
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	7	0.26
(1,2271)	1:144:A:THR:HA	1:150:A:GLN:HG2	6	0.26
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	4	0.26
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	4	0.26
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	4	0.26
(1,2223)	1:114:A:VAL:HA	1:144:A:THR:H	8	0.26
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	7	0.26
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	17	0.26
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	10	0.26
(1,1971)	1:6:A:LEU:HB2	1:78:A:PHE:HA	11	0.26
(1,1971)	1:6:A:LEU:HB3	1:78:A:PHE:HA	11	0.26
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD11	19	0.26
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD12	19	0.26
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD13	19	0.26
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD21	19	0.26
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD22	19	0.26
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD23	19	0.26
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD11	19	0.26
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD12	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD13	19	0.26
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD21	19	0.26
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD22	19	0.26
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD23	19	0.26
(1,1891)	1:44:A:VAL:HB	1:51:A:CYS:H	8	0.26
(1,1891)	1:44:A:VAL:HB	1:51:A:CYS:H	9	0.26
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	13	0.26
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	16	0.26
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	11	0.26
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	11	0.26
(1,1805)	1:111:A:MET:H	1:111:A:MET:HG3	3	0.26
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	11	0.26
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	11	0.26
(1,1689)	1:102:A:ARG:H	1:102:A:ARG:HG2	16	0.26
(1,1689)	1:102:A:ARG:H	1:102:A:ARG:HG3	16	0.26
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	19	0.26
(1,1614)	1:127:A:THR:HG21	1:141:A:PHE:HD1	12	0.26
(1,1614)	1:127:A:THR:HG21	1:141:A:PHE:HD2	12	0.26
(1,1614)	1:127:A:THR:HG22	1:141:A:PHE:HD1	12	0.26
(1,1614)	1:127:A:THR:HG22	1:141:A:PHE:HD2	12	0.26
(1,1614)	1:127:A:THR:HG23	1:141:A:PHE:HD1	12	0.26
(1,1614)	1:127:A:THR:HG23	1:141:A:PHE:HD2	12	0.26
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	16	0.26
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	6	0.26
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	6	0.26
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	12	0.26
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	12	0.26
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	6	0.26
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	6	0.26
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	6	0.26
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	6	0.26
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	6	0.26
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	6	0.26
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD1	18	0.26
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD2	18	0.26
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	9	0.26
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	9	0.26
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	9	0.26
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE1	4	0.26
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE2	4	0.26
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	6	0.26
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	9	0.26
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE1	15	0.26
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE2	15	0.26
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	10	0.26
(1,1104)	1:80:A:CYS:H	1:111:A:MET:HB3	18	0.26
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	6	0.26
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	6	0.26
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	3	0.26
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	9	0.26
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	12	0.26
(1,1059)	1:131:A:GLN:HA	1:131:A:GLN:HE22	13	0.26
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	17	0.26
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	18	0.26
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB2	12	0.26
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB3	12	0.26
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB2	12	0.26
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB3	12	0.26
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	9	0.26
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	5	0.26
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	5	0.26
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	17	0.26
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	17	0.26
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	15	0.26
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	10	0.26
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	19	0.26
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	19	0.26
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	19	0.26
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	14	0.26
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	14	0.26
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	14	0.26
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	14	0.26
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	14	0.26
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	14	0.26
(1,673)	1:35:A:SER:HA	1:36:A:ILE:H	9	0.26
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	18	0.26
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	19	0.26
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	19	0.26
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	19	0.26
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	19	0.26
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	19	0.26
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	19	0.26
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	16	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	16	0.26
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	18	0.26
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	18	0.26
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	18	0.26
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	18	0.26
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	18	0.26
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	18	0.26
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	2	0.26
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	18	0.26
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	16	0.26
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	16	0.26
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	16	0.26
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	18	0.26
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	18	0.26
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	19	0.26
(1,225)	1:6:A:LEU:H	1:6:A:LEU:HG	10	0.26
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	19	0.26
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	19	0.26
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	19	0.26
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	19	0.26
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	19	0.26
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	19	0.26
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	4	0.26
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	4	0.26
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	2	0.26
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	12	0.26
(1,148)	1:28:A:PHE:HE1	2:201:A:GNP:H1'	19	0.26
(1,148)	1:28:A:PHE:HE2	2:201:A:GNP:H1'	19	0.26
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	12	0.26
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	12	0.26
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	12	0.26
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	13	0.26
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	13	0.26
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	13	0.26
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	4	0.26
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	12	0.25
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG21	15	0.25
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG22	15	0.25
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG23	15	0.25
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG21	15	0.25
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG22	15	0.25
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG23	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	10	0.25
(1,3259)	1:113:A:LEU:H	1:141:A:PHE:HB3	6	0.25
(1,3242)	1:3:A:GLU:HG2	1:4:A:TYR:HA	11	0.25
(1,3242)	1:3:A:GLU:HG3	1:4:A:TYR:HA	11	0.25
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	11	0.25
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	6	0.25
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD11	16	0.25
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD12	16	0.25
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD13	16	0.25
(1,3116)	1:85:A:ASN:HB2	1:124:A:THR:H	3	0.25
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	7	0.25
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	7	0.25
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	8	0.25
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	8	0.25
(1,3102)	1:123:A:ARG:HG2	1:125:A:VAL:H	16	0.25
(1,3102)	1:123:A:ARG:HG3	1:125:A:VAL:H	16	0.25
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	4	0.25
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	13	0.25
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	14	0.25
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	8	0.25
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	11	0.25
(1,2785)	1:117:A:LYS:H	1:145:A:SER:H	15	0.25
(1,2764)	1:19:A:LEU:HG	1:146:A:ALA:H	12	0.25
(1,2747)	1:118:A:SER:H	1:146:A:ALA:H	9	0.25
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	4	0.25
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	18	0.25
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	3	0.25
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	3	0.25
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	3	0.25
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	3	0.25
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	3	0.25
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	3	0.25
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	6	0.25
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	6	0.25
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	6	0.25
(1,2630)	1:150:A:GLN:HG3	1:152:A:VAL:H	11	0.25
(1,2620)	1:166:A:HIS:HB3	1:167:A:LYS:HB2	12	0.25
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG12	11	0.25
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG13	11	0.25
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	9	0.25
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	9	0.25
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	4	0.25
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	17	0.25
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	10	0.25
(1,2454)	1:162:A:GLU:HB2	1:165:A:LYS:HG2	2	0.25
(1,2454)	1:162:A:GLU:HB3	1:165:A:LYS:HG2	2	0.25
(1,2416)	1:110:A:PRO:HA	1:163:A:ILE:HA	9	0.25
(1,2416)	1:110:A:PRO:HA	1:163:A:ILE:HA	13	0.25
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	2	0.25
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	2	0.25
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	2	0.25
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	2	0.25
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	2	0.25
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	2	0.25
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	16	0.25
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	16	0.25
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	16	0.25
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	16	0.25
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	16	0.25
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	16	0.25
(1,2341)	1:81:A:VAL:HA	1:113:A:LEU:HD11	7	0.25
(1,2341)	1:81:A:VAL:HA	1:113:A:LEU:HD12	7	0.25
(1,2341)	1:81:A:VAL:HA	1:113:A:LEU:HD13	7	0.25
(1,2341)	1:81:A:VAL:HA	1:113:A:LEU:HD21	7	0.25
(1,2341)	1:81:A:VAL:HA	1:113:A:LEU:HD22	7	0.25
(1,2341)	1:81:A:VAL:HA	1:113:A:LEU:HD23	7	0.25
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	16	0.25
(1,2302)	1:23:A:LEU:HD21	1:153:A:ASP:HA	1	0.25
(1,2302)	1:23:A:LEU:HD22	1:153:A:ASP:HA	1	0.25
(1,2302)	1:23:A:LEU:HD23	1:153:A:ASP:HA	1	0.25
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	10	0.25
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	10	0.25
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	10	0.25
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	15	0.25
(1,2166)	1:131:A:GLN:HG3	1:141:A:PHE:HB3	6	0.25
(1,2157)	1:15:A:GLY:H	1:17:A:SER:H	3	0.25
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	9	0.25
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	9	0.25
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	9	0.25
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	9	0.25
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	9	0.25
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	9	0.25
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE1	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE2	6	0.25
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE1	6	0.25
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE2	6	0.25
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE1	6	0.25
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE2	6	0.25
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	6	0.25
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	6	0.25
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	6	0.25
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	6	0.25
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	6	0.25
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	6	0.25
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE1	16	0.25
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE2	16	0.25
(1,2037)	1:129:A:GLN:HA	1:132:A:ASP:HB3	11	0.25
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	13	0.25
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	13	0.25
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	2	0.25
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	2	0.25
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	15	0.25
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	15	0.25
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	15	0.25
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	15	0.25
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	15	0.25
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	15	0.25
(1,1849)	1:77:A:GLY:HA2	1:111:A:MET:HA	19	0.25
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	7	0.25
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	7	0.25
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	7	0.25
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	7	0.25
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	7	0.25
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	7	0.25
(1,1804)	1:111:A:MET:HG3	1:112:A:VAL:H	8	0.25
(1,1752)	1:8:A:VAL:HG11	1:10:A:GLY:H	8	0.25
(1,1752)	1:8:A:VAL:HG12	1:10:A:GLY:H	8	0.25
(1,1752)	1:8:A:VAL:HG13	1:10:A:GLY:H	8	0.25
(1,1752)	1:8:A:VAL:HG21	1:10:A:GLY:H	8	0.25
(1,1752)	1:8:A:VAL:HG22	1:10:A:GLY:H	8	0.25
(1,1752)	1:8:A:VAL:HG23	1:10:A:GLY:H	8	0.25
(1,1752)	1:8:A:VAL:HG11	1:10:A:GLY:H	9	0.25
(1,1752)	1:8:A:VAL:HG12	1:10:A:GLY:H	9	0.25
(1,1752)	1:8:A:VAL:HG13	1:10:A:GLY:H	9	0.25
(1,1752)	1:8:A:VAL:HG21	1:10:A:GLY:H	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1752)	1:8:A:VAL:HG22	1:10:A:GLY:H	9	0.25
(1,1752)	1:8:A:VAL:HG23	1:10:A:GLY:H	9	0.25
(1,1730)	1:78:A:PHE:HZ	1:104:A:LYS:HE3	11	0.25
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	19	0.25
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	19	0.25
(1,1714)	1:75:A:GLY:HA2	1:104:A:LYS:HD2	15	0.25
(1,1649)	1:99:A:GLN:H	1:99:A:GLN:HG2	16	0.25
(1,1649)	1:99:A:GLN:H	1:99:A:GLN:HG3	16	0.25
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD11	10	0.25
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD12	10	0.25
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD13	10	0.25
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	20	0.25
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	20	0.25
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	20	0.25
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	20	0.25
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	20	0.25
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	20	0.25
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG2	4	0.25
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG3	4	0.25
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD1	16	0.25
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD2	16	0.25
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	12	0.25
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	12	0.25
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	12	0.25
(1,1489)	1:95:A:HIS:HE1	1:99:A:GLN:HE22	7	0.25
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	15	0.25
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	15	0.25
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	15	0.25
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	15	0.25
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	15	0.25
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	15	0.25
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	15	0.25
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	15	0.25
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	15	0.25
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	15	0.25
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	15	0.25
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	15	0.25
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	5	0.25
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	5	0.25
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	5	0.25
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	5	0.25
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	5	0.25
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	8	0.25
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	14	0.25
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	14	0.25
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	14	0.25
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG21	8	0.25
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG22	8	0.25
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG23	8	0.25
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG21	8	0.25
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG22	8	0.25
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG23	8	0.25
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG21	8	0.25
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG22	8	0.25
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG23	8	0.25
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG21	8	0.25
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG22	8	0.25
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG23	8	0.25
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG21	8	0.25
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG22	8	0.25
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG23	8	0.25
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG21	8	0.25
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG22	8	0.25
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG23	8	0.25
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	16	0.25
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	16	0.25
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	16	0.25
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	18	0.25
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	18	0.25
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	18	0.25
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	16	0.25
(1,1325)	1:95:A:HIS:H	1:95:A:HIS:HD2	19	0.25
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	19	0.25
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	19	0.25
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	19	0.25
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	19	0.25
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE1	11	0.25
(1,1192)	1:56:A:LEU:HD11	1:71:A:TYR:HE2	11	0.25
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE1	11	0.25
(1,1192)	1:56:A:LEU:HD12	1:71:A:TYR:HE2	11	0.25
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE1	11	0.25
(1,1192)	1:56:A:LEU:HD13	1:71:A:TYR:HE2	11	0.25
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	14	0.25
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	14	0.25
(1,965)	1:43:A:GLN:HE22	1:50:A:THR:HB	4	0.25
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	8	0.25
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	8	0.25
(1,955)	1:43:A:GLN:H	1:43:A:GLN:HE21	11	0.25
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	10	0.25
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	10	0.25
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	9	0.25
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	9	0.25
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	10	0.25
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	10	0.25
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	8	0.25
(1,839)	1:4:A:TYR:HE1	1:52:A:LEU:H	7	0.25
(1,839)	1:4:A:TYR:HE2	1:52:A:LEU:H	7	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	3	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	3	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	3	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	18	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	18	0.25
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	18	0.25
(1,728)	1:65:A:SER:HA	1:66:A:ALA:H	1	0.25
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	1	0.25
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	10	0.25
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB2	4	0.25
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB3	4	0.25
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB2	4	0.25
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB3	4	0.25
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB2	4	0.25
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB3	4	0.25
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB2	4	0.25
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB3	4	0.25
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB2	4	0.25
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB3	4	0.25
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB2	4	0.25
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB3	4	0.25
(1,495)	1:29:A:VAL:HA	1:32:A:TYR:HD1	18	0.25
(1,495)	1:29:A:VAL:HA	1:32:A:TYR:HD2	18	0.25
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	10	0.25
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	17	0.25
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	7	0.25
(1,354)	1:42:A:LYS:H	1:54:A:ASP:HA	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	17	0.25
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	17	0.25
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	17	0.25
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	15	0.25
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	15	0.25
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	15	0.25
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	16	0.25
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	16	0.25
(1,164)	1:83:A:ALA:H	1:86:A:ASN:HB2	16	0.25
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	3	0.25
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	3	0.25
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	3	0.25
(1,103)	1:16:A:LYS:HA	1:19:A:LEU:HB3	13	0.25
(1,84)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	12	0.25
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	6	0.25
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	6	0.25
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	6	0.25
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	6	0.25
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	6	0.25
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	6	0.25
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	9	0.25
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	9	0.25
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	9	0.25
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	9	0.25
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	9	0.25
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	9	0.25
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	15	0.25
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	15	0.25
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	15	0.25
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	15	0.25
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	15	0.25
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	15	0.25
(1,39)	1:64:A:TYR:HD1	1:65:A:SER:H	6	0.25
(1,39)	1:64:A:TYR:HD2	1:65:A:SER:H	6	0.25
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	9	0.24
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	10	0.24
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	8	0.24
(1,3301)	1:120:A:LEU:HD11	1:122:A:SER:H	3	0.24
(1,3301)	1:120:A:LEU:HD12	1:122:A:SER:H	3	0.24
(1,3301)	1:120:A:LEU:HD13	1:122:A:SER:H	3	0.24
(1,3301)	1:120:A:LEU:HD21	1:122:A:SER:H	3	0.24
(1,3301)	1:120:A:LEU:HD22	1:122:A:SER:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3301)	1:120:A:LEU:HD23	1:122:A:SER:H	3	0.24
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	13	0.24
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG21	10	0.24
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG22	10	0.24
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG23	10	0.24
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	1	0.24
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	14	0.24
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	16	0.24
(1,3063)	1:45:A:VAL:HB	1:48:A:GLY:H	11	0.24
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD1	6	0.24
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD2	6	0.24
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	18	0.24
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	20	0.24
(1,2825)	1:18:A:ALA:HB1	1:28:A:PHE:HE1	5	0.24
(1,2825)	1:18:A:ALA:HB1	1:28:A:PHE:HE2	5	0.24
(1,2825)	1:18:A:ALA:HB2	1:28:A:PHE:HE1	5	0.24
(1,2825)	1:18:A:ALA:HB2	1:28:A:PHE:HE2	5	0.24
(1,2825)	1:18:A:ALA:HB3	1:28:A:PHE:HE1	5	0.24
(1,2825)	1:18:A:ALA:HB3	1:28:A:PHE:HE2	5	0.24
(1,2797)	1:143:A:GLU:HG2	1:144:A:THR:H	6	0.24
(1,2797)	1:143:A:GLU:HG3	1:144:A:THR:H	6	0.24
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	2	0.24
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	7	0.24
(1,2712)	1:11:A:ALA:HB1	1:89:A:SER:H	16	0.24
(1,2712)	1:11:A:ALA:HB2	1:89:A:SER:H	16	0.24
(1,2712)	1:11:A:ALA:HB3	1:89:A:SER:H	16	0.24
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	5	0.24
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB1	12	0.24
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB2	12	0.24
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB3	12	0.24
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB1	12	0.24
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB2	12	0.24
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB3	12	0.24
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB1	12	0.24
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB2	12	0.24
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB3	12	0.24
(1,2682)	1:25:A:GLN:HA	1:27:A:HIS:HE1	4	0.24
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD11	13	0.24
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD12	13	0.24
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD13	13	0.24
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD11	13	0.24
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD12	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD13	13	0.24
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD11	13	0.24
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD12	13	0.24
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD13	13	0.24
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	14	0.24
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	14	0.24
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG12	17	0.24
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG13	17	0.24
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	12	0.24
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	5	0.24
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	5	0.24
(1,2564)	1:20:A:THR:HA	1:55:A:ILE:HG12	16	0.24
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	16	0.24
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	16	0.24
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	16	0.24
(1,2532)	1:19:A:LEU:HA	1:152:A:VAL:HA	1	0.24
(1,2493)	1:14:A:VAL:HG11	1:81:A:VAL:HB	11	0.24
(1,2493)	1:14:A:VAL:HG12	1:81:A:VAL:HB	11	0.24
(1,2493)	1:14:A:VAL:HG13	1:81:A:VAL:HB	11	0.24
(1,2493)	1:14:A:VAL:HG21	1:81:A:VAL:HB	11	0.24
(1,2493)	1:14:A:VAL:HG22	1:81:A:VAL:HB	11	0.24
(1,2493)	1:14:A:VAL:HG23	1:81:A:VAL:HB	11	0.24
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	1	0.24
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	3	0.24
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	10	0.24
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	10	0.24
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	12	0.24
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	12	0.24
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	2	0.24
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	14	0.24
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	16	0.24
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	12	0.24
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	12	0.24
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	12	0.24
(1,2056)	1:126:A:ASP:HB2	1:129:A:GLN:HG2	6	0.24
(1,2056)	1:126:A:ASP:HB3	1:129:A:GLN:HG2	6	0.24
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	19	0.24
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	19	0.24
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	19	0.24
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	19	0.24
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	19	0.24
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD1	12	0.24
(1,1929)	1:153:A:ASP:HB2	1:157:A:TYR:HD2	12	0.24
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	12	0.24
(1,1929)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	12	0.24
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	12	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	13	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	13	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	13	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	16	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	16	0.24
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	16	0.24
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	20	0.24
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	20	0.24
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	20	0.24
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	20	0.24
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	20	0.24
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	20	0.24
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	1	0.24
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	1	0.24
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	7	0.24
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	7	0.24
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	7	0.24
(1,1699)	1:72:A:MET:HG2	1:103:A:VAL:HB	7	0.24
(1,1699)	1:72:A:MET:HG3	1:103:A:VAL:HB	7	0.24
(1,1687)	1:102:A:ARG:H	1:102:A:ARG:HG2	16	0.24
(1,1645)	1:128:A:LYS:HG2	1:129:A:GLN:HB2	3	0.24
(1,1645)	1:128:A:LYS:HG3	1:129:A:GLN:HB2	3	0.24
(1,1642)	1:98:A:GLU:HG2	1:99:A:GLN:HA	10	0.24
(1,1642)	1:98:A:GLU:HG3	1:99:A:GLN:HA	10	0.24
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	7	0.24
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	14	0.24
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	11	0.24
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	4	0.24
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	4	0.24
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	4	0.24
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	4	0.24
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	4	0.24
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	4	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG11	5	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG12	5	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG13	5	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG21	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG22	5	0.24
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG23	5	0.24
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	8	0.24
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	8	0.24
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG2	13	0.24
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG3	13	0.24
(1,1495)	1:99:A:GLN:HA	1:99:A:GLN:HE22	9	0.24
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	3	0.24
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	11	0.24
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	7	0.24
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	7	0.24
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	7	0.24
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	15	0.24
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	15	0.24
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	15	0.24
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	4	0.24
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	20	0.24
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	20	0.24
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	20	0.24
(1,1294)	1:95:A:HIS:HD2	1:96:A:TYR:HA	18	0.24
(1,1272)	1:9:A:VAL:HG11	1:96:A:TYR:H	11	0.24
(1,1272)	1:9:A:VAL:HG12	1:96:A:TYR:H	11	0.24
(1,1272)	1:9:A:VAL:HG13	1:96:A:TYR:H	11	0.24
(1,1272)	1:9:A:VAL:HG21	1:96:A:TYR:H	11	0.24
(1,1272)	1:9:A:VAL:HG22	1:96:A:TYR:H	11	0.24
(1,1272)	1:9:A:VAL:HG23	1:96:A:TYR:H	11	0.24
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	20	0.24
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	20	0.24
(1,1243)	1:106:A:SER:HA	1:107:A:GLU:HG2	2	0.24
(1,1243)	1:106:A:SER:HA	1:107:A:GLU:HG3	2	0.24
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	17	0.24
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE1	2	0.24
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE2	2	0.24
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	15	0.24
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	15	0.24
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	15	0.24
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	11	0.24
(1,1145)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	11	0.24
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	11	0.24
(1,1145)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	11	0.24
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	11	0.24
(1,1145)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	5	0.24
(1,1044)	1:125:A:VAL:HG11	1:129:A:GLN:HE22	9	0.24
(1,1044)	1:125:A:VAL:HG12	1:129:A:GLN:HE22	9	0.24
(1,1044)	1:125:A:VAL:HG13	1:129:A:GLN:HE22	9	0.24
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	5	0.24
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	5	0.24
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	5	0.24
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	11	0.24
(1,1033)	1:90:A:PHE:HB2	1:129:A:GLN:HE21	12	0.24
(1,1033)	1:90:A:PHE:HB3	1:129:A:GLN:HE21	12	0.24
(1,962)	1:43:A:GLN:H	1:43:A:GLN:HG3	8	0.24
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	9	0.24
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	11	0.24
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	20	0.24
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	9	0.24
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	9	0.24
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	7	0.24
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	7	0.24
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	7	0.24
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	20	0.24
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	20	0.24
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	20	0.24
(1,728)	1:65:A:SER:HA	1:66:A:ALA:H	4	0.24
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	16	0.24
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	16	0.24
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD11	1	0.24
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD12	1	0.24
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD13	1	0.24
(1,532)	1:166:A:HIS:HB2	1:168:A:GLU:H	8	0.24
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	14	0.24
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	14	0.24
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	14	0.24
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	8	0.24
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	19	0.24
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	19	0.24
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	19	0.24
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	19	0.24
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	19	0.24
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	19	0.24
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	17	0.24
(1,337)	1:23:A:LEU:HD21	1:156:A:PHE:HB3	9	0.24
(1,337)	1:23:A:LEU:HD22	1:156:A:PHE:HB3	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:23:A:LEU:HD23	1:156:A:PHE:HB3	9	0.24
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	20	0.24
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	20	0.24
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	20	0.24
(1,114)	1:164:A:ARG:HA	1:164:A:ARG:HE	7	0.24
(1,103)	1:16:A:LYS:HA	1:19:A:LEU:HB3	3	0.24
(1,103)	1:16:A:LYS:HA	1:19:A:LEU:HB3	20	0.24
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	10	0.24
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	10	0.24
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	10	0.24
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	10	0.24
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	10	0.24
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	10	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	8	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	8	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	8	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	8	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	8	0.24
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	8	0.24
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	3	0.24
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	3	0.24
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	3	0.24
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	3	0.24
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	3	0.24
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	3	0.24
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	17	0.24
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	12	0.24
(1,3331)	1:106:A:SER:HB2	1:109:A:VAL:H	3	0.23
(1,3331)	1:106:A:SER:HB3	1:109:A:VAL:H	3	0.23
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	2	0.23
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	3	0.23
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	7	0.23
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD11	2	0.23
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD12	2	0.23
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD13	2	0.23
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD21	2	0.23
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD22	2	0.23
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD23	2	0.23
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	8	0.23
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	8	0.23
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	8	0.23
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	9	0.23
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	9	0.23
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG21	1	0.23
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG22	1	0.23
(1,3152)	1:1:A:MET:HG3	1:50:A:THR:HG23	1	0.23
(1,3133)	1:1:A:MET:HB2	1:2:A:THR:HB	8	0.23
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	8	0.23
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	19	0.23
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	15	0.23
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	15	0.23
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	1	0.23
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	15	0.23
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	11	0.23
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	16	0.23
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	4	0.23
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	12	0.23
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	9	0.23
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	9	0.23
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	9	0.23
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	4	0.23
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB1	6	0.23
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB2	6	0.23
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB3	6	0.23
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB1	6	0.23
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB2	6	0.23
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB3	6	0.23
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB1	6	0.23
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB2	6	0.23
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB3	6	0.23
(1,2690)	1:148:A:THR:H	1:150:A:GLN:HB2	20	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD11	3	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD12	3	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD13	3	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD11	3	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD12	3	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD13	3	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD11	3	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD12	3	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD13	3	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD11	17	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD12	17	0.23
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD13	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD11	17	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD12	17	0.23
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD13	17	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD11	17	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD12	17	0.23
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD13	17	0.23
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	2	0.23
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	2	0.23
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	2	0.23
(1,2532)	1:19:A:LEU:HA	1:152:A:VAL:HA	10	0.23
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	5	0.23
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	5	0.23
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	5	0.23
(1,2518)	1:164:A:ARG:H	1:165:A:LYS:HG2	18	0.23
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB1	4	0.23
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB2	4	0.23
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB3	4	0.23
(1,2467)	1:165:A:LYS:HA	1:165:A:LYS:HD2	11	0.23
(1,2467)	1:165:A:LYS:HA	1:165:A:LYS:HD3	11	0.23
(1,2461)	1:167:A:LYS:HB3	1:168:A:GLU:H	20	0.23
(1,2438)	1:164:A:ARG:HA	1:164:A:ARG:HD2	6	0.23
(1,2438)	1:164:A:ARG:HA	1:164:A:ARG:HD3	6	0.23
(1,2328)	1:144:A:THR:HA	1:152:A:VAL:H	7	0.23
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	9	0.23
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	3	0.23
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	5	0.23
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	19	0.23
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	13	0.23
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	13	0.23
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	13	0.23
(1,2189)	1:4:A:TYR:HD1	1:52:A:LEU:H	6	0.23
(1,2189)	1:4:A:TYR:HD2	1:52:A:LEU:H	6	0.23
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	8	0.23
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	17	0.23
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG21	17	0.23
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG22	17	0.23
(1,2161)	1:140:A:PRO:HG3	1:158:A:THR:HG23	17	0.23
(1,2156)	1:111:A:MET:H	1:140:A:PRO:HD3	6	0.23
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	8	0.23
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	8	0.23
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	8	0.23
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE1	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:53:A:LEU:HD11	1:157:A:TYR:HE2	17	0.23
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE1	17	0.23
(1,2088)	1:53:A:LEU:HD12	1:157:A:TYR:HE2	17	0.23
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE1	17	0.23
(1,2088)	1:53:A:LEU:HD13	1:157:A:TYR:HE2	17	0.23
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE1	17	0.23
(1,2088)	1:53:A:LEU:HD21	1:157:A:TYR:HE2	17	0.23
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE1	17	0.23
(1,2088)	1:53:A:LEU:HD22	1:157:A:TYR:HE2	17	0.23
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE1	17	0.23
(1,2088)	1:53:A:LEU:HD23	1:157:A:TYR:HE2	17	0.23
(1,2080)	1:131:A:GLN:HA	1:141:A:PHE:HD1	17	0.23
(1,2080)	1:131:A:GLN:HA	1:141:A:PHE:HD2	17	0.23
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE1	2	0.23
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE2	2	0.23
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	12	0.23
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	12	0.23
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	12	0.23
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	12	0.23
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	12	0.23
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	12	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	14	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	14	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	14	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	14	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	14	0.23
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	14	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	14	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	14	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	14	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	14	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	14	0.23
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	14	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	14	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	14	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	14	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	14	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	14	0.23
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	14	0.23
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG21	6	0.23
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG22	6	0.23
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG23	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1880)	1:116:A:ASN:HA	1:144:A:THR:HB	4	0.23
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	7	0.23
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	7	0.23
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	7	0.23
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	17	0.23
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	2	0.23
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	5	0.23
(1,1810)	1:111:A:MET:HG2	1:139:A:ILE:HG12	10	0.23
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG21	13	0.23
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG22	13	0.23
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG23	13	0.23
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	18	0.23
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	18	0.23
(1,1725)	1:104:A:LYS:HE3	1:109:A:VAL:HA	4	0.23
(1,1689)	1:102:A:ARG:H	1:102:A:ARG:HG2	10	0.23
(1,1689)	1:102:A:ARG:H	1:102:A:ARG:HG3	10	0.23
(1,1523)	1:87:A:THR:HG21	1:125:A:VAL:HG21	8	0.23
(1,1523)	1:87:A:THR:HG21	1:125:A:VAL:HG22	8	0.23
(1,1523)	1:87:A:THR:HG21	1:125:A:VAL:HG23	8	0.23
(1,1523)	1:87:A:THR:HG22	1:125:A:VAL:HG21	8	0.23
(1,1523)	1:87:A:THR:HG22	1:125:A:VAL:HG22	8	0.23
(1,1523)	1:87:A:THR:HG22	1:125:A:VAL:HG23	8	0.23
(1,1523)	1:87:A:THR:HG23	1:125:A:VAL:HG21	8	0.23
(1,1523)	1:87:A:THR:HG23	1:125:A:VAL:HG22	8	0.23
(1,1523)	1:87:A:THR:HG23	1:125:A:VAL:HG23	8	0.23
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	19	0.23
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	19	0.23
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	19	0.23
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	19	0.23
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	19	0.23
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	19	0.23
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	19	0.23
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	19	0.23
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	19	0.23
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	12	0.23
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	12	0.23
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	12	0.23
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	19	0.23
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	19	0.23
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	19	0.23
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	15	0.23
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	15	0.23
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	17	0.23
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	17	0.23
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	17	0.23
(1,1270)	1:65:A:SER:H	1:65:A:SER:HB3	9	0.23
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	11	0.23
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	11	0.23
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	5	0.23
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	5	0.23
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	14	0.23
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	14	0.23
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	1	0.23
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	1	0.23
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	1	0.23
(1,947)	1:83:A:ALA:H	1:90:A:PHE:H	12	0.23
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	6	0.23
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	6	0.23
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	14	0.23
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	14	0.23
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	12	0.23
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	2	0.23
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	17	0.23
(1,779)	1:39:A:SER:HA	1:56:A:LEU:HG	14	0.23
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD11	14	0.23
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD12	14	0.23
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD13	14	0.23
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD21	14	0.23
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD22	14	0.23
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD23	14	0.23
(1,661)	1:6:A:LEU:HA	1:76:A:GLU:H	5	0.23
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	6	0.23
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	6	0.23
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	6	0.23
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	6	0.23
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	6	0.23
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	6	0.23
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	4	0.23
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	4	0.23
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD11	10	0.23
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD12	10	0.23
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD13	10	0.23
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	16	0.23
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	19	0.23
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	19	0.23
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	10	0.23
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	17	0.23
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	17	0.23
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	17	0.23
(1,429)	1:61:A:GLN:HG2	1:62:A:GLU:HA	7	0.23
(1,429)	1:61:A:GLN:HG3	1:62:A:GLU:HA	7	0.23
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	14	0.23
(1,319)	1:23:A:LEU:HB2	1:152:A:VAL:HB	15	0.23
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	5	0.23
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	5	0.23
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	5	0.23
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	9	0.23
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	9	0.23
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	9	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	7	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	7	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	7	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	9	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	9	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	9	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	14	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	14	0.23
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	14	0.23
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	16	0.23
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	16	0.23
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	16	0.23
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	16	0.23
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	16	0.23
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	16	0.23
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE1	13	0.23
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE2	13	0.23
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE1	13	0.23
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE2	13	0.23
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE1	13	0.23
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE2	13	0.23
(1,221)	1:1:A:MET:HB3	1:50:A:THR:HB	14	0.23
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD11	15	0.23
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD12	15	0.23
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD13	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD21	15	0.23
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD22	15	0.23
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD23	15	0.23
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	6	0.23
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	6	0.23
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	7	0.23
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	7	0.23
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	7	0.23
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	7	0.23
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	7	0.23
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	7	0.23
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	19	0.23
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	19	0.23
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	19	0.23
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	8	0.23
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	3	0.23
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	3	0.23
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	3	0.23
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	3	0.23
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	3	0.23
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	3	0.23
(1,24)	1:106:A:SER:HB2	1:107:A:GLU:H	5	0.23
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	14	0.22
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	14	0.22
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	14	0.22
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	14	0.22
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	14	0.22
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	14	0.22
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	17	0.22
(1,3163)	1:1:A:MET:HG2	1:52:A:LEU:HB2	7	0.22
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD11	2	0.22
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD12	2	0.22
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD13	2	0.22
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	20	0.22
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	20	0.22
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	20	0.22
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	3	0.22
(1,3116)	1:85:A:ASN:HB2	1:124:A:THR:H	15	0.22
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	6	0.22
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	6	0.22
(1,3108)	1:123:A:ARG:HE	1:125:A:VAL:H	13	0.22
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	13	0.22
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	19	0.22
(1,2837)	1:113:A:LEU:H	1:142:A:ILE:H	18	0.22
(1,2803)	1:116:A:ASN:HA	1:144:A:THR:H	16	0.22
(1,2682)	1:25:A:GLN:HA	1:27:A:HIS:HE1	12	0.22
(1,2663)	1:1:A:MET:HE1	1:43:A:GLN:HE22	4	0.22
(1,2663)	1:1:A:MET:HE2	1:43:A:GLN:HE22	4	0.22
(1,2663)	1:1:A:MET:HE3	1:43:A:GLN:HE22	4	0.22
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD1	16	0.22
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD2	16	0.22
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD1	16	0.22
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD2	16	0.22
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD1	16	0.22
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD2	16	0.22
(1,2646)	1:150:A:GLN:HB3	1:151:A:GLY:H	5	0.22
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE1	9	0.22
(1,2643)	1:67:A:MET:HE1	1:71:A:TYR:HE2	9	0.22
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE1	9	0.22
(1,2643)	1:67:A:MET:HE2	1:71:A:TYR:HE2	9	0.22
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE1	9	0.22
(1,2643)	1:67:A:MET:HE3	1:71:A:TYR:HE2	9	0.22
(1,2625)	1:23:A:LEU:HD11	1:156:A:PHE:HB2	12	0.22
(1,2625)	1:23:A:LEU:HD12	1:156:A:PHE:HB2	12	0.22
(1,2625)	1:23:A:LEU:HD13	1:156:A:PHE:HB2	12	0.22
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB1	7	0.22
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB2	7	0.22
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB3	7	0.22
(1,2607)	1:21:A:ILE:HA	1:27:A:HIS:H	17	0.22
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	7	0.22
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	7	0.22
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	7	0.22
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	13	0.22
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	13	0.22
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	13	0.22
(1,2535)	1:168:A:GLU:H	1:169:A:LYS:H	11	0.22
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	9	0.22
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	9	0.22
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	9	0.22
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	19	0.22
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	19	0.22
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	19	0.22
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2458)	1:165:A:LYS:HB2	1:166:A:HIS:HB2	4	0.22
(1,2458)	1:165:A:LYS:HB2	1:166:A:HIS:HB2	18	0.22
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	8	0.22
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	8	0.22
(1,2398)	1:161:A:ARG:HA	1:165:A:LYS:H	17	0.22
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	5	0.22
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	5	0.22
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	1	0.22
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	3	0.22
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	7	0.22
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	15	0.22
(1,2306)	1:135:A:ARG:H	1:135:A:ARG:HE	13	0.22
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	4	0.22
(1,2289)	1:151:A:GLY:HA2	1:155:A:ALA:HB1	4	0.22
(1,2289)	1:151:A:GLY:HA2	1:155:A:ALA:HB2	4	0.22
(1,2289)	1:151:A:GLY:HA2	1:155:A:ALA:HB3	4	0.22
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	3	0.22
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	3	0.22
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	3	0.22
(1,2190)	1:44:A:VAL:HG21	1:51:A:CYS:H	15	0.22
(1,2190)	1:44:A:VAL:HG22	1:51:A:CYS:H	15	0.22
(1,2190)	1:44:A:VAL:HG23	1:51:A:CYS:H	15	0.22
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	14	0.22
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	9	0.22
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	12	0.22
(1,2156)	1:111:A:MET:H	1:140:A:PRO:HD3	11	0.22
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	1	0.22
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	1	0.22
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	1	0.22
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	1	0.22
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	1	0.22
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	1	0.22
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	19	0.22
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	19	0.22
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	19	0.22
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	19	0.22
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	19	0.22
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	19	0.22
(1,2132)	1:45:A:VAL:HG11	1:51:A:CYS:H	7	0.22
(1,2132)	1:45:A:VAL:HG12	1:51:A:CYS:H	7	0.22
(1,2132)	1:45:A:VAL:HG13	1:51:A:CYS:H	7	0.22
(1,2132)	1:45:A:VAL:HG21	1:51:A:CYS:H	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:45:A:VAL:HG22	1:51:A:CYS:H	7	0.22
(1,2132)	1:45:A:VAL:HG23	1:51:A:CYS:H	7	0.22
(1,2123)	1:154:A:ASP:HA	1:157:A:TYR:H	11	0.22
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	19	0.22
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	19	0.22
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	19	0.22
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	19	0.22
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	19	0.22
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	19	0.22
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	6	0.22
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE1	15	0.22
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE2	15	0.22
(1,2069)	1:90:A:PHE:HD1	1:130:A:ALA:HA	20	0.22
(1,2069)	1:90:A:PHE:HD2	1:130:A:ALA:HA	20	0.22
(1,2067)	1:3:A:GLU:HA	1:4:A:TYR:HB2	16	0.22
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	11	0.22
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	11	0.22
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	11	0.22
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	3	0.22
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	3	0.22
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD11	1	0.22
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD12	1	0.22
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD13	1	0.22
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD21	1	0.22
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD22	1	0.22
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD23	1	0.22
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD11	1	0.22
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD12	1	0.22
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD13	1	0.22
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD21	1	0.22
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD22	1	0.22
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD23	1	0.22
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	12	0.22
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	12	0.22
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG21	12	0.22
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG22	12	0.22
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG23	12	0.22
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	13	0.22
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	13	0.22
(1,1891)	1:44:A:VAL:HB	1:51:A:CYS:H	15	0.22
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG11	10	0.22
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG12	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1889)	1:90:A:PHE:HB3	1:125:A:VAL:HG13	10	0.22
(1,1849)	1:77:A:GLY:HA2	1:111:A:MET:HA	4	0.22
(1,1846)	1:41:A:ARG:HD2	1:52:A:LEU:HB2	7	0.22
(1,1846)	1:41:A:ARG:HD3	1:52:A:LEU:HB2	7	0.22
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	8	0.22
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	18	0.22
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	17	0.22
(1,1714)	1:75:A:GLY:HA2	1:104:A:LYS:HD2	3	0.22
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	20	0.22
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	20	0.22
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	20	0.22
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD1	18	0.22
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD2	18	0.22
(1,1632)	1:4:A:TYR:HD1	1:51:A:CYS:HB3	6	0.22
(1,1632)	1:4:A:TYR:HD2	1:51:A:CYS:HB3	6	0.22
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	1	0.22
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	17	0.22
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	17	0.22
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	7	0.22
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	7	0.22
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	7	0.22
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	7	0.22
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	7	0.22
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	7	0.22
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD1	10	0.22
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD2	10	0.22
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	7	0.22
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	7	0.22
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	7	0.22
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	6	0.22
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	6	0.22
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	6	0.22
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	6	0.22
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	6	0.22
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	6	0.22
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	2	0.22
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	2	0.22
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	2	0.22
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	14	0.22
(1,1370)	1:95:A:HIS:HE1	1:99:A:GLN:HG2	10	0.22
(1,1370)	1:95:A:HIS:HE1	1:99:A:GLN:HG3	10	0.22
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD2	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD3	5	0.22
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	7	0.22
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	7	0.22
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	1	0.22
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	1	0.22
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	1	0.22
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	3	0.22
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE21	14	0.22
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE22	14	0.22
(1,1173)	1:93:A:ILE:HB	1:94:A:HIS:HD2	3	0.22
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	20	0.22
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	8	0.22
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	14	0.22
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	14	0.22
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	14	0.22
(1,1052)	1:128:A:LYS:H	1:131:A:GLN:HE22	4	0.22
(1,1007)	1:90:A:PHE:HE1	1:129:A:GLN:HE21	12	0.22
(1,1007)	1:90:A:PHE:HE2	1:129:A:GLN:HE21	12	0.22
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	17	0.22
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	17	0.22
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	3	0.22
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	3	0.22
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	3	0.22
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	17	0.22
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	17	0.22
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	17	0.22
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	13	0.22
(1,814)	1:1:A:MET:HB2	1:52:A:LEU:H	14	0.22
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	19	0.22
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	1	0.22
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	13	0.22
(1,447)	1:22:A:GLN:HE21	1:28:A:PHE:H	11	0.22
(1,447)	1:22:A:GLN:HE22	1:28:A:PHE:H	11	0.22
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	12	0.22
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	5	0.22
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	5	0.22
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	5	0.22
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	2	0.22
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	2	0.22
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	18	0.22
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE1	20	0.22
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE2	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	13	0.22
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	13	0.22
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	13	0.22
(1,274)	1:1:A:MET:HG3	1:2:A:THR:H	1	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	2	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	2	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	2	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	12	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	12	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	12	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	17	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	17	0.22
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	17	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD11	8	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD12	8	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD13	8	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD21	8	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD22	8	0.22
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD23	8	0.22
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	17	0.22
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	17	0.22
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	17	0.22
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	17	0.22
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	17	0.22
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	17	0.22
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	16	0.22
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	16	0.22
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	16	0.22
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	12	0.22
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	12	0.22
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	12	0.22
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	12	0.22
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	12	0.22
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	12	0.22
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	2	0.22
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	2	0.22
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	2	0.22
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	14	0.22
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	1	0.22
(3,2)	1:17:A:SER:OG	2:201:A:GNP:O2B	4	0.21
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	12	0.21
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3242)	1:3:A:GLU:HG2	1:4:A:TYR:HA	8	0.21
(1,3242)	1:3:A:GLU:HG3	1:4:A:TYR:HA	8	0.21
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	15	0.21
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	19	0.21
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	3	0.21
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	8	0.21
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	4	0.21
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	12	0.21
(1,3063)	1:45:A:VAL:HB	1:48:A:GLY:H	1	0.21
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	19	0.21
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	19	0.21
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	8	0.21
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	15	0.21
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	20	0.21
(1,2935)	1:73:A:ARG:H	1:73:A:ARG:HE	15	0.21
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	14	0.21
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	14	0.21
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	14	0.21
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	5	0.21
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	14	0.21
(1,2762)	1:102:A:ARG:H	1:102:A:ARG:HE	19	0.21
(1,2735)	1:117:A:LYS:HA	1:146:A:ALA:H	1	0.21
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	14	0.21
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	15	0.21
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	20	0.21
(1,2690)	1:148:A:THR:H	1:150:A:GLN:HB2	6	0.21
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB1	17	0.21
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB2	17	0.21
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB3	17	0.21
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	3	0.21
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	3	0.21
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	3	0.21
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	4	0.21
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	19	0.21
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	14	0.21
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	14	0.21
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	14	0.21
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	17	0.21
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	17	0.21
(1,2521)	1:84:A:ILE:HB	1:123:A:ARG:HE	11	0.21
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD2	15	0.21
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD3	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2463)	1:4:A:TYR:HE1	1:167:A:LYS:HB3	6	0.21
(1,2463)	1:4:A:TYR:HE2	1:167:A:LYS:HB3	6	0.21
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	13	0.21
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	14	0.21
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	15	0.21
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	7	0.21
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	7	0.21
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	7	0.21
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	7	0.21
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	7	0.21
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	7	0.21
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	4	0.21
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	18	0.21
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	19	0.21
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	19	0.21
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	19	0.21
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	19	0.21
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	8	0.21
(1,2291)	1:144:A:THR:HG21	1:151:A:GLY:HA2	16	0.21
(1,2291)	1:144:A:THR:HG22	1:151:A:GLY:HA2	16	0.21
(1,2291)	1:144:A:THR:HG23	1:151:A:GLY:HA2	16	0.21
(1,2280)	1:144:A:THR:HA	1:151:A:GLY:HA2	10	0.21
(1,2254)	1:149:A:ARG:HB2	1:150:A:GLN:HE21	12	0.21
(1,2254)	1:149:A:ARG:HB3	1:150:A:GLN:HE21	12	0.21
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	18	0.21
(1,2156)	1:111:A:MET:H	1:140:A:PRO:HD3	10	0.21
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	14	0.21
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	14	0.21
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	14	0.21
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	10	0.21
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	10	0.21
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	10	0.21
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	10	0.21
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	10	0.21
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	10	0.21
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	7	0.21
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	13	0.21
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	6	0.21
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	6	0.21
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	6	0.21
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	6	0.21
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	6	0.21
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	10	0.21
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	10	0.21
(1,1823)	1:112:A:VAL:HA	1:162:A:GLU:HG3	2	0.21
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	8	0.21
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	8	0.21
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	10	0.21
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	10	0.21
(1,1763)	1:10:A:GLY:H	1:96:A:TYR:HD1	4	0.21
(1,1763)	1:10:A:GLY:H	1:96:A:TYR:HD2	4	0.21
(1,1730)	1:78:A:PHE:HZ	1:104:A:LYS:HE3	18	0.21
(1,1634)	1:22:A:GLN:HE21	1:149:A:ARG:HE	1	0.21
(1,1634)	1:22:A:GLN:HE22	1:149:A:ARG:HE	1	0.21
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	4	0.21
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG11	5	0.21
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG12	5	0.21
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG13	5	0.21
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG21	5	0.21
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG22	5	0.21
(1,1522)	1:87:A:THR:HG21	1:125:A:VAL:HG23	5	0.21
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG11	5	0.21
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG12	5	0.21
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG13	5	0.21
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG21	5	0.21
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG22	5	0.21
(1,1522)	1:87:A:THR:HG22	1:125:A:VAL:HG23	5	0.21
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG11	5	0.21
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG12	5	0.21
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG13	5	0.21
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG21	5	0.21
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG22	5	0.21
(1,1522)	1:87:A:THR:HG23	1:125:A:VAL:HG23	5	0.21
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD1	7	0.21
(1,1515)	1:87:A:THR:HA	1:90:A:PHE:HD2	7	0.21
(1,1439)	1:125:A:VAL:HG11	1:129:A:GLN:HG2	16	0.21
(1,1439)	1:125:A:VAL:HG12	1:129:A:GLN:HG2	16	0.21
(1,1439)	1:125:A:VAL:HG13	1:129:A:GLN:HG2	16	0.21
(1,1439)	1:125:A:VAL:HG21	1:129:A:GLN:HG2	16	0.21
(1,1439)	1:125:A:VAL:HG22	1:129:A:GLN:HG2	16	0.21
(1,1439)	1:125:A:VAL:HG23	1:129:A:GLN:HG2	16	0.21
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	6	0.21
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	6	0.21
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	6	0.21
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	6	0.21
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	6	0.21
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	3	0.21
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	3	0.21
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	3	0.21
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	14	0.21
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	12	0.21
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	17	0.21
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	17	0.21
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	17	0.21
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	17	0.21
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	17	0.21
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	17	0.21
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	17	0.21
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	17	0.21
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	17	0.21
(1,1239)	1:94:A:HIS:HE1	1:97:A:ARG:HD2	19	0.21
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	10	0.21
(1,1190)	1:94:A:HIS:H	1:94:A:HIS:HD2	3	0.21
(1,1120)	1:12:A:GLY:H	1:61:A:GLN:HB3	19	0.21
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	15	0.21
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	15	0.21
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	2	0.21
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	2	0.21
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	14	0.21
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	14	0.21
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	6	0.21
(1,1077)	1:4:A:TYR:HE1	1:51:A:CYS:HA	7	0.21
(1,1077)	1:4:A:TYR:HE2	1:51:A:CYS:HA	7	0.21
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	15	0.21
(1,1007)	1:90:A:PHE:HE1	1:129:A:GLN:HE21	19	0.21
(1,1007)	1:90:A:PHE:HE2	1:129:A:GLN:HE21	19	0.21
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA2	16	0.21
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA3	16	0.21
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA2	16	0.21
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA3	16	0.21
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA2	16	0.21
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA3	16	0.21
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA2	16	0.21
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA3	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA2	16	0.21
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA3	16	0.21
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA2	16	0.21
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA3	16	0.21
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	13	0.21
(1,989)	1:44:A:VAL:HG11	1:157:A:TYR:HE1	15	0.21
(1,989)	1:44:A:VAL:HG11	1:157:A:TYR:HE2	15	0.21
(1,989)	1:44:A:VAL:HG12	1:157:A:TYR:HE1	15	0.21
(1,989)	1:44:A:VAL:HG12	1:157:A:TYR:HE2	15	0.21
(1,989)	1:44:A:VAL:HG13	1:157:A:TYR:HE1	15	0.21
(1,989)	1:44:A:VAL:HG13	1:157:A:TYR:HE2	15	0.21
(1,965)	1:43:A:GLN:HE22	1:50:A:THR:HB	13	0.21
(1,964)	1:43:A:GLN:HA	1:43:A:GLN:HE22	11	0.21
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	5	0.21
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	5	0.21
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	5	0.21
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	5	0.21
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	5	0.21
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	5	0.21
(1,940)	1:26:A:ASN:H	1:26:A:ASN:HD22	14	0.21
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	10	0.21
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	10	0.21
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	18	0.21
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	18	0.21
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	15	0.21
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	15	0.21
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	2	0.21
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	2	0.21
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	12	0.21
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	12	0.21
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	6	0.21
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	9	0.21
(1,750)	1:63:A:GLU:HG2	1:64:A:TYR:H	15	0.21
(1,750)	1:63:A:GLU:HG3	1:64:A:TYR:H	15	0.21
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	3	0.21
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	3	0.21
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	3	0.21
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	3	0.21
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	3	0.21
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	3	0.21
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	4	0.21
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	4	0.21
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	4	0.21
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	4	0.21
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	4	0.21
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	15	0.21
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	7	0.21
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	17	0.21
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB2	11	0.21
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB3	11	0.21
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB2	11	0.21
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB3	11	0.21
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB2	11	0.21
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB3	11	0.21
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB2	11	0.21
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB3	11	0.21
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB2	11	0.21
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB3	11	0.21
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB2	11	0.21
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB3	11	0.21
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	5	0.21
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	5	0.21
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	5	0.21
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	7	0.21
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	7	0.21
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	7	0.21
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	5	0.21
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	14	0.21
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	14	0.21
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	14	0.21
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	20	0.21
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	5	0.21
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	5	0.21
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	5	0.21
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	4	0.21
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	14	0.21
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	14	0.21
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	14	0.21
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	14	0.21
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	14	0.21
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	14	0.21
(1,113)	1:23:A:LEU:HD11	1:156:A:PHE:HE1	12	0.21
(1,113)	1:23:A:LEU:HD11	1:156:A:PHE:HE2	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:23:A:LEU:HD12	1:156:A:PHE:HE1	12	0.21
(1,113)	1:23:A:LEU:HD12	1:156:A:PHE:HE2	12	0.21
(1,113)	1:23:A:LEU:HD13	1:156:A:PHE:HE1	12	0.21
(1,113)	1:23:A:LEU:HD13	1:156:A:PHE:HE2	12	0.21
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	6	0.2
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	13	0.2
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	20	0.2
(1,3222)	1:114:A:VAL:HG11	1:116:A:ASN:H	7	0.2
(1,3222)	1:114:A:VAL:HG12	1:116:A:ASN:H	7	0.2
(1,3222)	1:114:A:VAL:HG13	1:116:A:ASN:H	7	0.2
(1,3222)	1:114:A:VAL:HG21	1:116:A:ASN:H	7	0.2
(1,3222)	1:114:A:VAL:HG22	1:116:A:ASN:H	7	0.2
(1,3222)	1:114:A:VAL:HG23	1:116:A:ASN:H	7	0.2
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	19	0.2
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	19	0.2
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	19	0.2
(1,3156)	1:120:A:LEU:H	1:120:A:LEU:HG	17	0.2
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	13	0.2
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	16	0.2
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	16	0.2
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	18	0.2
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	18	0.2
(1,3049)	1:127:A:THR:HB	1:141:A:PHE:HE1	12	0.2
(1,3049)	1:127:A:THR:HB	1:141:A:PHE:HE2	12	0.2
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	6	0.2
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	17	0.2
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	4	0.2
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	4	0.2
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	4	0.2
(1,2818)	1:113:A:LEU:HB3	1:142:A:ILE:H	15	0.2
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	2	0.2
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	2	0.2
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	6	0.2
(1,2769)	1:145:A:SER:H	1:150:A:GLN:HB2	1	0.2
(1,2683)	1:72:A:MET:H	1:75:A:GLY:H	10	0.2
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD1	5	0.2
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD2	5	0.2
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD1	5	0.2
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD2	5	0.2
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD1	5	0.2
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD2	5	0.2
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	1	0.2
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	1	0.2
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	17	0.2
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	1	0.2
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	1	0.2
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	3	0.2
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	3	0.2
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	12	0.2
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	12	0.2
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	12	0.2
(1,2532)	1:19:A:LEU:HA	1:152:A:VAL:HA	16	0.2
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	16	0.2
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	16	0.2
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	16	0.2
(1,2518)	1:164:A:ARG:H	1:165:A:LYS:HG2	13	0.2
(1,2512)	1:4:A:TYR:HE1	1:160:A:VAL:HA	11	0.2
(1,2512)	1:4:A:TYR:HE2	1:160:A:VAL:HA	11	0.2
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB1	11	0.2
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB2	11	0.2
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB3	11	0.2
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD2	14	0.2
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD3	14	0.2
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	2	0.2
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD2	11	0.2
(1,2431)	1:163:A:ILE:HA	1:164:A:ARG:HD3	11	0.2
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	14	0.2
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	3	0.2
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	3	0.2
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	3	0.2
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	3	0.2
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	3	0.2
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	3	0.2
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	13	0.2
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	15	0.2
(1,2328)	1:144:A:THR:HA	1:152:A:VAL:H	11	0.2
(1,2315)	1:151:A:GLY:H	1:154:A:ASP:HB2	3	0.2
(1,2312)	1:154:A:ASP:HA	1:157:A:TYR:HD1	4	0.2
(1,2312)	1:154:A:ASP:HA	1:157:A:TYR:HD2	4	0.2
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD1	20	0.2
(1,2304)	1:2:A:THR:HB	1:4:A:TYR:HD2	20	0.2
(1,2302)	1:23:A:LEU:HD21	1:153:A:ASP:HA	4	0.2
(1,2302)	1:23:A:LEU:HD22	1:153:A:ASP:HA	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2302)	1:23:A:LEU:HD23	1:153:A:ASP:HA	4	0.2
(1,2294)	1:112:A:VAL:HG11	1:159:A:LEU:H	4	0.2
(1,2294)	1:112:A:VAL:HG12	1:159:A:LEU:H	4	0.2
(1,2294)	1:112:A:VAL:HG13	1:159:A:LEU:H	4	0.2
(1,2272)	1:144:A:THR:HA	1:150:A:GLN:HG3	1	0.2
(1,2272)	1:144:A:THR:HA	1:150:A:GLN:HG3	3	0.2
(1,2267)	1:150:A:GLN:HG2	1:151:A:GLY:H	4	0.2
(1,2223)	1:114:A:VAL:HA	1:144:A:THR:H	9	0.2
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	12	0.2
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	12	0.2
(1,2190)	1:44:A:VAL:HG21	1:51:A:CYS:H	8	0.2
(1,2190)	1:44:A:VAL:HG22	1:51:A:CYS:H	8	0.2
(1,2190)	1:44:A:VAL:HG23	1:51:A:CYS:H	8	0.2
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	15	0.2
(1,2157)	1:15:A:GLY:H	1:17:A:SER:H	5	0.2
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	2	0.2
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	2	0.2
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	2	0.2
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	2	0.2
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	2	0.2
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	2	0.2
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	14	0.2
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	14	0.2
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	14	0.2
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	14	0.2
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	14	0.2
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	14	0.2
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	13	0.2
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB1	12	0.2
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB2	12	0.2
(1,2079)	1:113:A:LEU:HD11	1:130:A:ALA:HB3	12	0.2
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB1	12	0.2
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB2	12	0.2
(1,2079)	1:113:A:LEU:HD12	1:130:A:ALA:HB3	12	0.2
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB1	12	0.2
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB2	12	0.2
(1,2079)	1:113:A:LEU:HD13	1:130:A:ALA:HB3	12	0.2
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	13	0.2
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	13	0.2
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	13	0.2
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	9	0.2
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	9	0.2
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	9	0.2
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	9	0.2
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	9	0.2
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	18	0.2
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	18	0.2
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	18	0.2
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	18	0.2
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	18	0.2
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	18	0.2
(1,1940)	1:120:A:LEU:HD11	1:121:A:PRO:HG3	1	0.2
(1,1940)	1:120:A:LEU:HD12	1:121:A:PRO:HG3	1	0.2
(1,1940)	1:120:A:LEU:HD13	1:121:A:PRO:HG3	1	0.2
(1,1940)	1:120:A:LEU:HD21	1:121:A:PRO:HG3	1	0.2
(1,1940)	1:120:A:LEU:HD22	1:121:A:PRO:HG3	1	0.2
(1,1940)	1:120:A:LEU:HD23	1:121:A:PRO:HG3	1	0.2
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	8	0.2
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	8	0.2
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	19	0.2
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	19	0.2
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	5	0.2
(1,1823)	1:112:A:VAL:HA	1:162:A:GLU:HG3	19	0.2
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	4	0.2
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	4	0.2
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	18	0.2
(1,1693)	1:72:A:MET:HB2	1:103:A:VAL:HA	15	0.2
(1,1693)	1:72:A:MET:HB3	1:103:A:VAL:HA	15	0.2
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG2	6	0.2
(1,1688)	1:99:A:GLN:HA	1:102:A:ARG:HG3	6	0.2
(1,1664)	1:113:A:LEU:HB3	1:141:A:PHE:HE1	3	0.2
(1,1664)	1:113:A:LEU:HB3	1:141:A:PHE:HE2	3	0.2
(1,1589)	1:94:A:HIS:HB2	1:97:A:ARG:HD3	2	0.2
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	2	0.2
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	2	0.2
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	10	0.2
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	10	0.2
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	20	0.2
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	20	0.2
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	16	0.2
(1,1488)	1:99:A:GLN:HE21	1:103:A:VAL:H	13	0.2
(1,1488)	1:99:A:GLN:HE22	1:103:A:VAL:H	13	0.2
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	11	0.2
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	11	0.2
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	11	0.2
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	11	0.2
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	11	0.2
(1,1389)	1:75:A:GLY:HA2	1:76:A:GLU:HG2	7	0.2
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD1	13	0.2
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD2	13	0.2
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	13	0.2
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	13	0.2
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	13	0.2
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	9	0.2
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	9	0.2
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	15	0.2
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	12	0.2
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	12	0.2
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	2	0.2
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	19	0.2
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	19	0.2
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	19	0.2
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	19	0.2
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	19	0.2
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	19	0.2
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	19	0.2
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	19	0.2
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	19	0.2
(1,1171)	1:55:A:ILE:HG21	1:156:A:PHE:HZ	1	0.2
(1,1171)	1:55:A:ILE:HG22	1:156:A:PHE:HZ	1	0.2
(1,1171)	1:55:A:ILE:HG23	1:156:A:PHE:HZ	1	0.2
(1,1146)	1:149:A:ARG:H	1:152:A:VAL:HG11	9	0.2
(1,1146)	1:149:A:ARG:H	1:152:A:VAL:HG12	9	0.2
(1,1146)	1:149:A:ARG:H	1:152:A:VAL:HG13	9	0.2
(1,1146)	1:149:A:ARG:H	1:152:A:VAL:HG21	9	0.2
(1,1146)	1:149:A:ARG:H	1:152:A:VAL:HG22	9	0.2
(1,1146)	1:149:A:ARG:H	1:152:A:VAL:HG23	9	0.2
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	19	0.2
(1,1115)	1:51:A:CYS:HB3	1:52:A:LEU:H	3	0.2
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	5	0.2
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	11	0.2
(1,1050)	1:90:A:PHE:HD1	1:129:A:GLN:HE22	12	0.2
(1,1050)	1:90:A:PHE:HD2	1:129:A:GLN:HE22	12	0.2
(1,991)	1:83:A:ALA:HB1	1:85:A:ASN:HD21	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:83:A:ALA:HB2	1:85:A:ASN:HD21	14	0.2
(1,991)	1:83:A:ALA:HB3	1:85:A:ASN:HD21	14	0.2
(1,965)	1:43:A:GLN:HE22	1:50:A:THR:HB	14	0.2
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	14	0.2
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	14	0.2
(1,916)	1:22:A:GLN:HE21	1:27:A:HIS:HA	11	0.2
(1,916)	1:22:A:GLN:HE22	1:27:A:HIS:HA	11	0.2
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	4	0.2
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	14	0.2
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	14	0.2
(1,819)	1:142:A:ILE:HD11	1:154:A:ASP:H	11	0.2
(1,819)	1:142:A:ILE:HD12	1:154:A:ASP:H	11	0.2
(1,819)	1:142:A:ILE:HD13	1:154:A:ASP:H	11	0.2
(1,815)	1:41:A:ARG:HD2	1:52:A:LEU:HB3	7	0.2
(1,815)	1:41:A:ARG:HD3	1:52:A:LEU:HB3	7	0.2
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	17	0.2
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	17	0.2
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	17	0.2
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	17	0.2
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	17	0.2
(1,728)	1:65:A:SER:HA	1:66:A:ALA:H	2	0.2
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	8	0.2
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	18	0.2
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	19	0.2
(1,623)	1:32:A:TYR:HE1	1:34:A:PRO:HA	15	0.2
(1,623)	1:32:A:TYR:HE2	1:34:A:PRO:HA	15	0.2
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	14	0.2
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG11	11	0.2
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG12	11	0.2
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG13	11	0.2
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG21	11	0.2
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG22	11	0.2
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG23	11	0.2
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	5	0.2
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	5	0.2
(1,495)	1:29:A:VAL:HA	1:32:A:TYR:HD1	1	0.2
(1,495)	1:29:A:VAL:HA	1:32:A:TYR:HD2	1	0.2
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	5	0.2
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	10	0.2
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	18	0.2
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	18	0.2
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	3	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	3	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	3	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	8	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	8	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	8	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	11	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	11	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	11	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	18	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	18	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	18	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	19	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	19	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	19	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	20	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	20	0.2
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	20	0.2
(1,243)	1:5:A:LYS:H	1:5:A:LYS:HG2	20	0.2
(1,243)	1:5:A:LYS:H	1:5:A:LYS:HG3	20	0.2
(1,186)	1:41:A:ARG:HD2	1:52:A:LEU:HD11	3	0.2
(1,186)	1:41:A:ARG:HD2	1:52:A:LEU:HD12	3	0.2
(1,186)	1:41:A:ARG:HD2	1:52:A:LEU:HD13	3	0.2
(1,186)	1:41:A:ARG:HD2	1:52:A:LEU:HD21	3	0.2
(1,186)	1:41:A:ARG:HD2	1:52:A:LEU:HD22	3	0.2
(1,186)	1:41:A:ARG:HD2	1:52:A:LEU:HD23	3	0.2
(1,186)	1:41:A:ARG:HD3	1:52:A:LEU:HD11	3	0.2
(1,186)	1:41:A:ARG:HD3	1:52:A:LEU:HD12	3	0.2
(1,186)	1:41:A:ARG:HD3	1:52:A:LEU:HD13	3	0.2
(1,186)	1:41:A:ARG:HD3	1:52:A:LEU:HD21	3	0.2
(1,186)	1:41:A:ARG:HD3	1:52:A:LEU:HD22	3	0.2
(1,186)	1:41:A:ARG:HD3	1:52:A:LEU:HD23	3	0.2
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	5	0.2
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	5	0.2
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	5	0.2
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	5	0.2
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	5	0.2
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	5	0.2
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD11	15	0.2
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD12	15	0.2
(1,175)	1:90:A:PHE:HD1	1:93:A:ILE:HD13	15	0.2
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD11	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD12	15	0.2
(1,175)	1:90:A:PHE:HD2	1:93:A:ILE:HD13	15	0.2
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	9	0.2
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	9	0.2
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	9	0.2
(1,114)	1:164:A:ARG:HA	1:164:A:ARG:HE	5	0.2
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	2	0.2
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	2	0.2
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	2	0.2
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	2	0.2
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	2	0.2
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	2	0.2
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD11	5	0.2
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD12	5	0.2
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD13	5	0.2
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD11	5	0.2
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD12	5	0.2
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD13	5	0.2
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	17	0.2
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	17	0.2
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	17	0.2
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD11	14	0.2
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD12	14	0.2
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD13	14	0.2
(1,24)	1:106:A:SER:HB2	1:107:A:GLU:H	6	0.2
(3,2)	1:17:A:SER:OG	2:201:A:GNP:O2B	8	0.19
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG21	20	0.19
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG22	20	0.19
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG23	20	0.19
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG21	20	0.19
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG22	20	0.19
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG23	20	0.19
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	12	0.19
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	2	0.19
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	12	0.19
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	2	0.19
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	2	0.19
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	8	0.19
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	8	0.19
(1,3156)	1:120:A:LEU:H	1:120:A:LEU:HG	20	0.19
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	8	0.19
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	8	0.19
(1,3133)	1:1:A:MET:HB2	1:2:A:THR:HB	4	0.19
(1,3128)	1:1:A:MET:HA	1:51:A:CYS:HA	18	0.19
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG2	7	0.19
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG3	7	0.19
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG2	7	0.19
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG3	7	0.19
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	14	0.19
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	14	0.19
(1,3063)	1:45:A:VAL:HB	1:48:A:GLY:H	9	0.19
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	10	0.19
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	10	0.19
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	15	0.19
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	15	0.19
(1,3044)	1:90:A:PHE:HZ	1:129:A:GLN:H	12	0.19
(1,3008)	1:58:A:THR:HB	1:68:A:ARG:HE	20	0.19
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	11	0.19
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	15	0.19
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	15	0.19
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	15	0.19
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	15	0.19
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	15	0.19
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	15	0.19
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	6	0.19
(1,2869)	1:163:A:ILE:HG21	1:166:A:HIS:H	20	0.19
(1,2869)	1:163:A:ILE:HG22	1:166:A:HIS:H	20	0.19
(1,2869)	1:163:A:ILE:HG23	1:166:A:HIS:H	20	0.19
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	4	0.19
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	4	0.19
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	5	0.19
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	5	0.19
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	7	0.19
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	7	0.19
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	14	0.19
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	19	0.19
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	4	0.19
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	4	0.19
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	7	0.19
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	7	0.19
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	14	0.19
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	15	0.19
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	4	0.19
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	4	0.19
(1,2501)	1:159:A:LEU:HD11	1:163:A:ILE:H	14	0.19
(1,2501)	1:159:A:LEU:HD12	1:163:A:ILE:H	14	0.19
(1,2501)	1:159:A:LEU:HD13	1:163:A:ILE:H	14	0.19
(1,2501)	1:159:A:LEU:HD21	1:163:A:ILE:H	14	0.19
(1,2501)	1:159:A:LEU:HD22	1:163:A:ILE:H	14	0.19
(1,2501)	1:159:A:LEU:HD23	1:163:A:ILE:H	14	0.19
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	17	0.19
(1,2417)	1:4:A:TYR:HD1	1:163:A:ILE:HA	6	0.19
(1,2417)	1:4:A:TYR:HD2	1:163:A:ILE:HA	6	0.19
(1,2407)	1:162:A:GLU:HA	1:164:A:ARG:H	2	0.19
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD2	11	0.19
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD3	11	0.19
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	11	0.19
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	11	0.19
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	11	0.19
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	11	0.19
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	11	0.19
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	11	0.19
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	18	0.19
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	18	0.19
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	18	0.19
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	18	0.19
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	18	0.19
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	18	0.19
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	8	0.19
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	11	0.19
(1,2328)	1:144:A:THR:HA	1:152:A:VAL:H	10	0.19
(1,2307)	1:23:A:LEU:HD11	1:153:A:ASP:HA	9	0.19
(1,2307)	1:23:A:LEU:HD12	1:153:A:ASP:HA	9	0.19
(1,2307)	1:23:A:LEU:HD13	1:153:A:ASP:HA	9	0.19
(1,2294)	1:112:A:VAL:HG11	1:159:A:LEU:H	11	0.19
(1,2294)	1:112:A:VAL:HG12	1:159:A:LEU:H	11	0.19
(1,2294)	1:112:A:VAL:HG13	1:159:A:LEU:H	11	0.19
(1,2288)	1:143:A:GLU:HB3	1:151:A:GLY:HA3	14	0.19
(1,2280)	1:144:A:THR:HA	1:151:A:GLY:HA2	18	0.19
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	14	0.19
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	14	0.19
(1,2156)	1:111:A:MET:H	1:140:A:PRO:HD3	13	0.19
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	4	0.19
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	4	0.19
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	4	0.19
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	4	0.19
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	4	0.19
(1,2132)	1:45:A:VAL:HG11	1:51:A:CYS:H	20	0.19
(1,2132)	1:45:A:VAL:HG12	1:51:A:CYS:H	20	0.19
(1,2132)	1:45:A:VAL:HG13	1:51:A:CYS:H	20	0.19
(1,2132)	1:45:A:VAL:HG21	1:51:A:CYS:H	20	0.19
(1,2132)	1:45:A:VAL:HG22	1:51:A:CYS:H	20	0.19
(1,2132)	1:45:A:VAL:HG23	1:51:A:CYS:H	20	0.19
(1,2082)	1:131:A:GLN:HA	1:141:A:PHE:HB2	20	0.19
(1,2017)	1:127:A:THR:HG21	1:131:A:GLN:HE21	3	0.19
(1,2017)	1:127:A:THR:HG22	1:131:A:GLN:HE21	3	0.19
(1,2017)	1:127:A:THR:HG23	1:131:A:GLN:HE21	3	0.19
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	19	0.19
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	19	0.19
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	19	0.19
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	19	0.19
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	19	0.19
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	19	0.19
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	3	0.19
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	3	0.19
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	3	0.19
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	3	0.19
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	3	0.19
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	3	0.19
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG21	19	0.19
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG22	19	0.19
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG23	19	0.19
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	20	0.19
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	20	0.19
(1,1902)	1:116:A:ASN:HA	1:144:A:THR:HA	16	0.19
(1,1891)	1:44:A:VAL:HB	1:51:A:CYS:H	3	0.19
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	7	0.19
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	7	0.19
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	7	0.19
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD21	7	0.19
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD22	7	0.19
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD23	7	0.19
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	7	0.19
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	7	0.19
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD21	7	0.19
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD22	7	0.19
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD23	7	0.19
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	14	0.19
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	11	0.19
(1,1730)	1:78:A:PHE:HZ	1:104:A:LYS:HE3	7	0.19
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	8	0.19
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	8	0.19
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	8	0.19
(1,1685)	1:113:A:LEU:HD11	1:141:A:PHE:HA	15	0.19
(1,1685)	1:113:A:LEU:HD12	1:141:A:PHE:HA	15	0.19
(1,1685)	1:113:A:LEU:HD13	1:141:A:PHE:HA	15	0.19
(1,1684)	1:102:A:ARG:H	1:102:A:ARG:HD2	16	0.19
(1,1684)	1:102:A:ARG:H	1:102:A:ARG:HD3	16	0.19
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE2	16	0.19
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE3	16	0.19
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD1	5	0.19
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD2	5	0.19
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	12	0.19
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	6	0.19
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	5	0.19
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	5	0.19
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	11	0.19
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	11	0.19
(1,1509)	1:87:A:THR:HA	1:125:A:VAL:HB	10	0.19
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	15	0.19
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	15	0.19
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	15	0.19
(1,1489)	1:95:A:HIS:HE1	1:99:A:GLN:HE22	12	0.19
(1,1440)	1:26:A:ASN:H	1:27:A:HIS:HD2	13	0.19
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	4	0.19
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	4	0.19
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	4	0.19
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	18	0.19
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	18	0.19
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	18	0.19
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	2	0.19
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	2	0.19
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	2	0.19
(1,1395)	1:84:A:ILE:HD11	1:123:A:ARG:HG2	5	0.19
(1,1395)	1:84:A:ILE:HD12	1:123:A:ARG:HG2	5	0.19
(1,1395)	1:84:A:ILE:HD13	1:123:A:ARG:HG2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	8	0.19
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	8	0.19
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	8	0.19
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	9	0.19
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	9	0.19
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	9	0.19
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE1	10	0.19
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE2	10	0.19
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	5	0.19
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD1	2	0.19
(1,1260)	1:94:A:HIS:HE1	1:137:A:TYR:HD2	2	0.19
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	20	0.19
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	20	0.19
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	20	0.19
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	20	0.19
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	20	0.19
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	20	0.19
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	20	0.19
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	20	0.19
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	20	0.19
(1,1232)	1:94:A:HIS:HE1	1:97:A:ARG:HD3	18	0.19
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	17	0.19
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	4	0.19
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	9	0.19
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	9	0.19
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	9	0.19
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	17	0.19
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	17	0.19
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	9	0.19
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	9	0.19
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	9	0.19
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	4	0.19
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	4	0.19
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	4	0.19
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	20	0.19
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	20	0.19
(1,839)	1:4:A:TYR:HE1	1:52:A:LEU:H	15	0.19
(1,839)	1:4:A:TYR:HE2	1:52:A:LEU:H	15	0.19
(1,830)	1:146:A:ALA:HB1	2:201:A:GNP:HN1	3	0.19
(1,830)	1:146:A:ALA:HB2	2:201:A:GNP:HN1	3	0.19
(1,830)	1:146:A:ALA:HB3	2:201:A:GNP:HN1	3	0.19
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:120:A:LEU:HB2	2:201:A:GNP:HN1	16	0.19
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	11	0.19
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	11	0.19
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	11	0.19
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	11	0.19
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB2	17	0.19
(1,649)	1:78:A:PHE:H	1:159:A:LEU:HB3	17	0.19
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD11	5	0.19
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD12	5	0.19
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD13	5	0.19
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	3	0.19
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	11	0.19
(1,532)	1:166:A:HIS:HB2	1:168:A:GLU:H	19	0.19
(1,523)	1:29:A:VAL:HG11	1:31:A:GLU:H	9	0.19
(1,523)	1:29:A:VAL:HG12	1:31:A:GLU:H	9	0.19
(1,523)	1:29:A:VAL:HG13	1:31:A:GLU:H	9	0.19
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	16	0.19
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	16	0.19
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	16	0.19
(1,364)	1:24:A:ILE:HG21	1:41:A:ARG:H	18	0.19
(1,364)	1:24:A:ILE:HG22	1:41:A:ARG:H	18	0.19
(1,364)	1:24:A:ILE:HG23	1:41:A:ARG:H	18	0.19
(1,323)	1:44:A:VAL:H	1:52:A:LEU:HA	2	0.19
(1,319)	1:23:A:LEU:HB2	1:152:A:VAL:HB	11	0.19
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	19	0.19
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	19	0.19
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	19	0.19
(1,289)	1:24:A:ILE:HD11	1:40:A:TYR:HB2	10	0.19
(1,289)	1:24:A:ILE:HD12	1:40:A:TYR:HB2	10	0.19
(1,289)	1:24:A:ILE:HD13	1:40:A:TYR:HB2	10	0.19
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	17	0.19
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	4	0.19
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	4	0.19
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	4	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	4	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	4	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	4	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	6	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	6	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	6	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	13	0.19
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	13	0.19
(1,260)	1:7:A:VAL:HG11	1:72:A:MET:HA	11	0.19
(1,260)	1:7:A:VAL:HG12	1:72:A:MET:HA	11	0.19
(1,260)	1:7:A:VAL:HG13	1:72:A:MET:HA	11	0.19
(1,260)	1:7:A:VAL:HG21	1:72:A:MET:HA	11	0.19
(1,260)	1:7:A:VAL:HG22	1:72:A:MET:HA	11	0.19
(1,260)	1:7:A:VAL:HG23	1:72:A:MET:HA	11	0.19
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	18	0.19
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	18	0.19
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	18	0.19
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	18	0.19
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	18	0.19
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	18	0.19
(1,191)	1:43:A:GLN:HA	1:52:A:LEU:HD11	7	0.19
(1,191)	1:43:A:GLN:HA	1:52:A:LEU:HD12	7	0.19
(1,191)	1:43:A:GLN:HA	1:52:A:LEU:HD13	7	0.19
(1,191)	1:43:A:GLN:HA	1:52:A:LEU:HD21	7	0.19
(1,191)	1:43:A:GLN:HA	1:52:A:LEU:HD22	7	0.19
(1,191)	1:43:A:GLN:HA	1:52:A:LEU:HD23	7	0.19
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	4	0.19
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD11	11	0.19
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD12	11	0.19
(1,38)	1:80:A:CYS:HB2	1:93:A:ILE:HD13	11	0.19
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD11	11	0.19
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD12	11	0.19
(1,38)	1:80:A:CYS:HB3	1:93:A:ILE:HD13	11	0.19
(1,15)	1:108:A:ASP:H	1:109:A:VAL:H	15	0.19
(3,2)	1:17:A:SER:OG	2:201:A:GNP:O2B	19	0.18
(1,3332)	1:104:A:LYS:HE3	1:109:A:VAL:H	13	0.18
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	2	0.18
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	3	0.18
(1,3301)	1:120:A:LEU:HD11	1:122:A:SER:H	20	0.18
(1,3301)	1:120:A:LEU:HD12	1:122:A:SER:H	20	0.18
(1,3301)	1:120:A:LEU:HD13	1:122:A:SER:H	20	0.18
(1,3301)	1:120:A:LEU:HD21	1:122:A:SER:H	20	0.18
(1,3301)	1:120:A:LEU:HD22	1:122:A:SER:H	20	0.18
(1,3301)	1:120:A:LEU:HD23	1:122:A:SER:H	20	0.18
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD1	6	0.18
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD2	6	0.18
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD1	20	0.18
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD2	20	0.18
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB3	9	0.18
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG21	5	0.18
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG22	5	0.18
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG23	5	0.18
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	15	0.18
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	15	0.18
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	19	0.18
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	1	0.18
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	9	0.18
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	1	0.18
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	1	0.18
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	16	0.18
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	16	0.18
(1,3005)	1:90:A:PHE:HE1	1:131:A:GLN:H	12	0.18
(1,3005)	1:90:A:PHE:HE2	1:131:A:GLN:H	12	0.18
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	19	0.18
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	2	0.18
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	17	0.18
(1,2910)	1:166:A:HIS:H	1:166:A:HIS:HD2	6	0.18
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	2	0.18
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	2	0.18
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	8	0.18
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	8	0.18
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	13	0.18
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	13	0.18
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	17	0.18
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	17	0.18
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	5	0.18
(1,2768)	1:145:A:SER:H	1:150:A:GLN:HG3	10	0.18
(1,2768)	1:145:A:SER:H	1:150:A:GLN:HG3	18	0.18
(1,2762)	1:102:A:ARG:H	1:102:A:ARG:HE	3	0.18
(1,2759)	1:146:A:ALA:HB1	1:149:A:ARG:HA	3	0.18
(1,2759)	1:146:A:ALA:HB2	1:149:A:ARG:HA	3	0.18
(1,2759)	1:146:A:ALA:HB3	1:149:A:ARG:HA	3	0.18
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	10	0.18
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	10	0.18
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	10	0.18
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG21	2	0.18
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG22	2	0.18
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG23	2	0.18
(1,2710)	1:102:A:ARG:HB3	1:102:A:ARG:HE	18	0.18
(1,2682)	1:25:A:GLN:HA	1:27:A:HIS:HE1	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	14	0.18
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	14	0.18
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	14	0.18
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	19	0.18
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	19	0.18
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	19	0.18
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	13	0.18
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	13	0.18
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG12	5	0.18
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG13	5	0.18
(1,2581)	1:153:A:ASP:HB3	1:155:A:ALA:H	3	0.18
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	17	0.18
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	17	0.18
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	7	0.18
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	7	0.18
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	7	0.18
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	7	0.18
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	13	0.18
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	13	0.18
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	13	0.18
(1,2501)	1:159:A:LEU:HD11	1:163:A:ILE:H	12	0.18
(1,2501)	1:159:A:LEU:HD12	1:163:A:ILE:H	12	0.18
(1,2501)	1:159:A:LEU:HD13	1:163:A:ILE:H	12	0.18
(1,2501)	1:159:A:LEU:HD21	1:163:A:ILE:H	12	0.18
(1,2501)	1:159:A:LEU:HD22	1:163:A:ILE:H	12	0.18
(1,2501)	1:159:A:LEU:HD23	1:163:A:ILE:H	12	0.18
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD2	3	0.18
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD3	3	0.18
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	17	0.18
(1,2462)	1:164:A:ARG:HA	1:167:A:LYS:HB3	15	0.18
(1,2415)	1:77:A:GLY:HA3	1:163:A:ILE:HA	17	0.18
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	19	0.18
(1,2408)	1:110:A:PRO:HB2	1:162:A:GLU:HB2	19	0.18
(1,2408)	1:110:A:PRO:HB2	1:162:A:GLU:HB3	19	0.18
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	15	0.18
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	15	0.18
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	16	0.18
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	16	0.18
(1,2353)	1:123:A:ARG:HE	1:126:A:ASP:HA	4	0.18
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	18	0.18
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	18	0.18
(1,2328)	1:144:A:THR:HA	1:152:A:VAL:H	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	4	0.18
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	4	0.18
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	4	0.18
(1,2280)	1:144:A:THR:HA	1:151:A:GLY:HA2	13	0.18
(1,2271)	1:144:A:THR:HA	1:150:A:GLN:HG2	3	0.18
(1,2262)	1:149:A:ARG:HG2	1:152:A:VAL:HG11	20	0.18
(1,2262)	1:149:A:ARG:HG2	1:152:A:VAL:HG12	20	0.18
(1,2262)	1:149:A:ARG:HG2	1:152:A:VAL:HG13	20	0.18
(1,2262)	1:149:A:ARG:HG2	1:152:A:VAL:HG21	20	0.18
(1,2262)	1:149:A:ARG:HG2	1:152:A:VAL:HG22	20	0.18
(1,2262)	1:149:A:ARG:HG2	1:152:A:VAL:HG23	20	0.18
(1,2262)	1:149:A:ARG:HG3	1:152:A:VAL:HG11	20	0.18
(1,2262)	1:149:A:ARG:HG3	1:152:A:VAL:HG12	20	0.18
(1,2262)	1:149:A:ARG:HG3	1:152:A:VAL:HG13	20	0.18
(1,2262)	1:149:A:ARG:HG3	1:152:A:VAL:HG21	20	0.18
(1,2262)	1:149:A:ARG:HG3	1:152:A:VAL:HG22	20	0.18
(1,2262)	1:149:A:ARG:HG3	1:152:A:VAL:HG23	20	0.18
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	7	0.18
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	7	0.18
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	7	0.18
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG21	12	0.18
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG22	12	0.18
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG23	12	0.18
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	16	0.18
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	16	0.18
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG11	5	0.18
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG12	5	0.18
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG13	5	0.18
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG21	5	0.18
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG22	5	0.18
(1,2198)	1:10:A:GLY:HA2	1:81:A:VAL:HG23	5	0.18
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG11	5	0.18
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG12	5	0.18
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG13	5	0.18
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG21	5	0.18
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG22	5	0.18
(1,2198)	1:10:A:GLY:HA3	1:81:A:VAL:HG23	5	0.18
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	5	0.18
(1,2172)	1:114:A:VAL:HA	1:142:A:ILE:HB	12	0.18
(1,2172)	1:114:A:VAL:HA	1:142:A:ILE:HB	16	0.18
(1,2159)	1:140:A:PRO:HG3	1:162:A:GLU:HG2	11	0.18
(1,2150)	1:53:A:LEU:HD11	1:54:A:ASP:HA	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2150)	1:53:A:LEU:HD12	1:54:A:ASP:HA	2	0.18
(1,2150)	1:53:A:LEU:HD13	1:54:A:ASP:HA	2	0.18
(1,2150)	1:53:A:LEU:HD21	1:54:A:ASP:HA	2	0.18
(1,2150)	1:53:A:LEU:HD22	1:54:A:ASP:HA	2	0.18
(1,2150)	1:53:A:LEU:HD23	1:54:A:ASP:HA	2	0.18
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	11	0.18
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	11	0.18
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	11	0.18
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	11	0.18
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	11	0.18
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	11	0.18
(1,2132)	1:45:A:VAL:HG11	1:51:A:CYS:H	2	0.18
(1,2132)	1:45:A:VAL:HG12	1:51:A:CYS:H	2	0.18
(1,2132)	1:45:A:VAL:HG13	1:51:A:CYS:H	2	0.18
(1,2132)	1:45:A:VAL:HG21	1:51:A:CYS:H	2	0.18
(1,2132)	1:45:A:VAL:HG22	1:51:A:CYS:H	2	0.18
(1,2132)	1:45:A:VAL:HG23	1:51:A:CYS:H	2	0.18
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	16	0.18
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	16	0.18
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	16	0.18
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	16	0.18
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	16	0.18
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	16	0.18
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	5	0.18
(1,2080)	1:131:A:GLN:HA	1:141:A:PHE:HD1	10	0.18
(1,2080)	1:131:A:GLN:HA	1:141:A:PHE:HD2	10	0.18
(1,2067)	1:3:A:GLU:HA	1:4:A:TYR:HB2	7	0.18
(1,2056)	1:126:A:ASP:HB2	1:129:A:GLN:HG2	11	0.18
(1,2056)	1:126:A:ASP:HB3	1:129:A:GLN:HG2	11	0.18
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	6	0.18
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	6	0.18
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	3	0.18
(1,1752)	1:8:A:VAL:HG11	1:10:A:GLY:H	7	0.18
(1,1752)	1:8:A:VAL:HG12	1:10:A:GLY:H	7	0.18
(1,1752)	1:8:A:VAL:HG13	1:10:A:GLY:H	7	0.18
(1,1752)	1:8:A:VAL:HG21	1:10:A:GLY:H	7	0.18
(1,1752)	1:8:A:VAL:HG22	1:10:A:GLY:H	7	0.18
(1,1752)	1:8:A:VAL:HG23	1:10:A:GLY:H	7	0.18
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	8	0.18
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	8	0.18
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	2	0.18
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	2	0.18
(1,1690)	1:102:A:ARG:H	1:102:A:ARG:HG3	16	0.18
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	9	0.18
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	12	0.18
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	12	0.18
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	12	0.18
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	12	0.18
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	12	0.18
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	12	0.18
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG11	8	0.18
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG12	8	0.18
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG13	8	0.18
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG21	8	0.18
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG22	8	0.18
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG23	8	0.18
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG2	7	0.18
(1,1519)	1:87:A:THR:HB	1:91:A:GLU:HG3	7	0.18
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	13	0.18
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	13	0.18
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	13	0.18
(1,1411)	1:5:A:LYS:HB2	1:76:A:GLU:HG3	8	0.18
(1,1411)	1:5:A:LYS:HB3	1:76:A:GLU:HG3	8	0.18
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	15	0.18
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	6	0.18
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG22	6	0.18
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG23	6	0.18
(1,1338)	1:73:A:ARG:HA	1:73:A:ARG:HD2	15	0.18
(1,1294)	1:95:A:HIS:HD2	1:96:A:TYR:HA	13	0.18
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	16	0.18
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	17	0.18
(1,1251)	1:149:A:ARG:HB3	1:149:A:ARG:HE	17	0.18
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	17	0.18
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD21	16	0.18
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD22	16	0.18
(1,1208)	1:39:A:SER:H	1:56:A:LEU:HD23	16	0.18
(1,1195)	1:56:A:LEU:HD11	1:57:A:ASP:H	1	0.18
(1,1195)	1:56:A:LEU:HD12	1:57:A:ASP:H	1	0.18
(1,1195)	1:56:A:LEU:HD13	1:57:A:ASP:H	1	0.18
(1,1176)	1:23:A:LEU:HD11	1:156:A:PHE:HB3	12	0.18
(1,1176)	1:23:A:LEU:HD12	1:156:A:PHE:HB3	12	0.18
(1,1176)	1:23:A:LEU:HD13	1:156:A:PHE:HB3	12	0.18
(1,1160)	1:55:A:ILE:HG13	1:156:A:PHE:HZ	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	11	0.18
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	11	0.18
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	11	0.18
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	11	0.18
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	11	0.18
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	11	0.18
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	11	0.18
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	11	0.18
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	11	0.18
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	11	0.18
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	11	0.18
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	11	0.18
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	16	0.18
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	16	0.18
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	16	0.18
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	16	0.18
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	16	0.18
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	16	0.18
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	16	0.18
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	16	0.18
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	16	0.18
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	16	0.18
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	16	0.18
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	16	0.18
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	17	0.18
(1,1117)	1:46:A:ILE:HD11	1:51:A:CYS:HB3	20	0.18
(1,1117)	1:46:A:ILE:HD12	1:51:A:CYS:HB3	20	0.18
(1,1117)	1:46:A:ILE:HD13	1:51:A:CYS:HB3	20	0.18
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	9	0.18
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	9	0.18
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	16	0.18
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	16	0.18
(1,1009)	1:45:A:VAL:HG11	1:48:A:GLY:H	16	0.18
(1,1009)	1:45:A:VAL:HG12	1:48:A:GLY:H	16	0.18
(1,1009)	1:45:A:VAL:HG13	1:48:A:GLY:H	16	0.18
(1,1009)	1:45:A:VAL:HG21	1:48:A:GLY:H	16	0.18
(1,1009)	1:45:A:VAL:HG22	1:48:A:GLY:H	16	0.18
(1,1009)	1:45:A:VAL:HG23	1:48:A:GLY:H	16	0.18
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	9	0.18
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	9	0.18
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	19	0.18
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB2	18	0.18
(1,918)	1:25:A:GLN:HE22	1:40:A:TYR:HB3	18	0.18
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	20	0.18
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	20	0.18
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	20	0.18
(1,847)	1:41:A:ARG:H	1:41:A:ARG:HD2	10	0.18
(1,847)	1:41:A:ARG:H	1:41:A:ARG:HD3	10	0.18
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	16	0.18
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	16	0.18
(1,840)	1:41:A:ARG:HD2	1:54:A:ASP:HB2	16	0.18
(1,840)	1:41:A:ARG:HD2	1:54:A:ASP:HB3	16	0.18
(1,840)	1:41:A:ARG:HD3	1:54:A:ASP:HB2	16	0.18
(1,840)	1:41:A:ARG:HD3	1:54:A:ASP:HB3	16	0.18
(1,830)	1:146:A:ALA:HB1	2:201:A:GNP:HN1	6	0.18
(1,830)	1:146:A:ALA:HB2	2:201:A:GNP:HN1	6	0.18
(1,830)	1:146:A:ALA:HB3	2:201:A:GNP:HN1	6	0.18
(1,825)	1:120:A:LEU:H	2:201:A:GNP:HN1	3	0.18
(1,813)	1:41:A:ARG:HA	1:41:A:ARG:HD2	3	0.18
(1,631)	1:58:A:THR:HG21	1:68:A:ARG:H	7	0.18
(1,631)	1:58:A:THR:HG22	1:68:A:ARG:H	7	0.18
(1,631)	1:58:A:THR:HG23	1:68:A:ARG:H	7	0.18
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	1	0.18
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	1	0.18
(1,626)	1:68:A:ARG:H	1:68:A:ARG:HB3	8	0.18
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	10	0.18
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	10	0.18
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	10	0.18
(1,474)	1:22:A:GLN:HE22	1:28:A:PHE:HB3	1	0.18
(1,464)	1:21:A:ILE:HG21	1:27:A:HIS:HB3	11	0.18
(1,464)	1:21:A:ILE:HG22	1:27:A:HIS:HB3	11	0.18
(1,464)	1:21:A:ILE:HG23	1:27:A:HIS:HB3	11	0.18
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	11	0.18
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	5	0.18
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	12	0.18
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	12	0.18
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	12	0.18
(1,274)	1:1:A:MET:HG3	1:2:A:THR:H	6	0.18
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	1	0.18
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	1	0.18
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	1	0.18
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	10	0.18
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	10	0.18
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	20	0.18
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD11	1	0.18
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD12	1	0.18
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD13	1	0.18
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD21	1	0.18
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD22	1	0.18
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD23	1	0.18
(1,209)	1:6:A:LEU:HD11	1:54:A:ASP:H	11	0.18
(1,209)	1:6:A:LEU:HD12	1:54:A:ASP:H	11	0.18
(1,209)	1:6:A:LEU:HD13	1:54:A:ASP:H	11	0.18
(1,209)	1:6:A:LEU:HD21	1:54:A:ASP:H	11	0.18
(1,209)	1:6:A:LEU:HD22	1:54:A:ASP:H	11	0.18
(1,209)	1:6:A:LEU:HD23	1:54:A:ASP:H	11	0.18
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	5	0.18
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	5	0.18
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	13	0.18
(1,194)	1:15:A:GLY:HA3	2:201:A:GNP:H1'	17	0.18
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	11	0.18
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	11	0.18
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	11	0.18
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	11	0.18
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	11	0.18
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	11	0.18
(1,118)	1:97:A:ARG:HB3	1:98:A:GLU:H	3	0.18
(1,73)	1:102:A:ARG:H	1:104:A:LYS:H	5	0.18
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	9	0.18
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	18	0.17
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD11	15	0.17
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD12	15	0.17
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD13	15	0.17
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD21	15	0.17
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD22	15	0.17
(1,3211)	1:117:A:LYS:H	1:120:A:LEU:HD23	15	0.17
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB2	1	0.17
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB3	1	0.17
(1,3141)	1:120:A:LEU:HD11	1:122:A:SER:H	20	0.17
(1,3141)	1:120:A:LEU:HD12	1:122:A:SER:H	20	0.17
(1,3141)	1:120:A:LEU:HD13	1:122:A:SER:H	20	0.17
(1,3133)	1:1:A:MET:HB2	1:2:A:THR:HB	1	0.17
(1,3133)	1:1:A:MET:HB2	1:2:A:THR:HB	7	0.17
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	11	0.17
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	6	0.17
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	6	0.17
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	6	0.17
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	6	0.17
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	6	0.17
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	6	0.17
(1,2980)	1:132:A:ASP:H	1:132:A:ASP:HB3	12	0.17
(1,2942)	1:133:A:LEU:HG	1:134:A:ALA:H	14	0.17
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	18	0.17
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	15	0.17
(1,2887)	1:21:A:ILE:HG13	1:40:A:TYR:HE1	3	0.17
(1,2887)	1:21:A:ILE:HG13	1:40:A:TYR:HE2	3	0.17
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	12	0.17
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	12	0.17
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	12	0.17
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	12	0.17
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	12	0.17
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	12	0.17
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	10	0.17
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	10	0.17
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	13	0.17
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	15	0.17
(1,2764)	1:19:A:LEU:HG	1:146:A:ALA:H	5	0.17
(1,2745)	1:29:A:VAL:H	1:146:A:ALA:HB1	2	0.17
(1,2745)	1:29:A:VAL:H	1:146:A:ALA:HB2	2	0.17
(1,2745)	1:29:A:VAL:H	1:146:A:ALA:HB3	2	0.17
(1,2734)	1:147:A:LYS:H	1:149:A:ARG:HA	20	0.17
(1,2710)	1:102:A:ARG:HB3	1:102:A:ARG:HE	17	0.17
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	3	0.17
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE1	4	0.17
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE2	4	0.17
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE3	4	0.17
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE1	4	0.17
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE2	4	0.17
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE3	4	0.17
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE1	4	0.17
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE2	4	0.17
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE3	4	0.17
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	1	0.17
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	1	0.17
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	12	0.17
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	6	0.17
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	6	0.17
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	6	0.17
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	18	0.17
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	18	0.17
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	18	0.17
(1,2588)	1:153:A:ASP:HB2	1:155:A:ALA:H	11	0.17
(1,2588)	1:153:A:ASP:HB3	1:155:A:ALA:H	11	0.17
(1,2559)	1:17:A:SER:HA	1:20:A:THR:HA	4	0.17
(1,2519)	1:97:A:ARG:HA	1:100:A:ILE:HG21	18	0.17
(1,2519)	1:97:A:ARG:HA	1:100:A:ILE:HG22	18	0.17
(1,2519)	1:97:A:ARG:HA	1:100:A:ILE:HG23	18	0.17
(1,2501)	1:159:A:LEU:HD11	1:163:A:ILE:H	19	0.17
(1,2501)	1:159:A:LEU:HD12	1:163:A:ILE:H	19	0.17
(1,2501)	1:159:A:LEU:HD13	1:163:A:ILE:H	19	0.17
(1,2501)	1:159:A:LEU:HD21	1:163:A:ILE:H	19	0.17
(1,2501)	1:159:A:LEU:HD22	1:163:A:ILE:H	19	0.17
(1,2501)	1:159:A:LEU:HD23	1:163:A:ILE:H	19	0.17
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	18	0.17
(1,2407)	1:162:A:GLU:HA	1:164:A:ARG:H	6	0.17
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG2	7	0.17
(1,2397)	1:161:A:ARG:HA	1:164:A:ARG:HG3	7	0.17
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG21	11	0.17
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG22	11	0.17
(1,2359)	1:140:A:PRO:HG2	1:158:A:THR:HG23	11	0.17
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	6	0.17
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	17	0.17
(1,2294)	1:112:A:VAL:HG11	1:159:A:LEU:H	9	0.17
(1,2294)	1:112:A:VAL:HG12	1:159:A:LEU:H	9	0.17
(1,2294)	1:112:A:VAL:HG13	1:159:A:LEU:H	9	0.17
(1,2293)	1:143:A:GLU:HB3	1:144:A:THR:HA	17	0.17
(1,2275)	1:150:A:GLN:HA	1:150:A:GLN:HG2	5	0.17
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG21	16	0.17
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG22	16	0.17
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG23	16	0.17
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	20	0.17
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	20	0.17
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	20	0.17
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	13	0.17
(1,2166)	1:131:A:GLN:HG3	1:141:A:PHE:HB3	20	0.17
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	6	0.17
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	6	0.17
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	10	0.17
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	10	0.17
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	10	0.17
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	6	0.17
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	6	0.17
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	6	0.17
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	6	0.17
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	6	0.17
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	6	0.17
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	15	0.17
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	15	0.17
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	15	0.17
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	15	0.17
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	15	0.17
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	15	0.17
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	12	0.17
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	12	0.17
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	12	0.17
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	12	0.17
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	12	0.17
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	12	0.17
(1,2087)	1:153:A:ASP:HA	1:155:A:ALA:H	4	0.17
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB1	12	0.17
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB2	12	0.17
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB3	12	0.17
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB1	12	0.17
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB2	12	0.17
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB3	12	0.17
(1,2037)	1:129:A:GLN:HA	1:132:A:ASP:HB3	17	0.17
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	3	0.17
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	3	0.17
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	3	0.17
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	3	0.17
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	3	0.17
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	3	0.17
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	3	0.17
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	3	0.17
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	3	0.17
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	3	0.17
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	3	0.17
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	3	0.17
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	3	0.17
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	3	0.17
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	3	0.17
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	3	0.17
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	3	0.17
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	20	0.17
(1,1971)	1:6:A:LEU:HB2	1:78:A:PHE:HA	1	0.17
(1,1971)	1:6:A:LEU:HB3	1:78:A:PHE:HA	1	0.17
(1,1952)	1:123:A:ARG:HA	1:125:A:VAL:H	4	0.17
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD1	5	0.17
(1,1947)	1:2:A:THR:HG21	1:4:A:TYR:HD2	5	0.17
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD1	5	0.17
(1,1947)	1:2:A:THR:HG22	1:4:A:TYR:HD2	5	0.17
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD1	5	0.17
(1,1947)	1:2:A:THR:HG23	1:4:A:TYR:HD2	5	0.17
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD11	11	0.17
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD12	11	0.17
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD13	11	0.17
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD21	11	0.17
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD22	11	0.17
(1,1925)	1:85:A:ASN:HB2	1:120:A:LEU:HD23	11	0.17
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD11	11	0.17
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD12	11	0.17
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD13	11	0.17
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD21	11	0.17
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD22	11	0.17
(1,1925)	1:85:A:ASN:HB3	1:120:A:LEU:HD23	11	0.17
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	3	0.17
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	11	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	12	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	12	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	12	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD21	12	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD22	12	0.17
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD23	12	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	12	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	12	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	12	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD21	12	0.17
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD22	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD23	12	0.17
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	4	0.17
(1,1823)	1:112:A:VAL:HA	1:162:A:GLU:HG3	12	0.17
(1,1793)	1:130:A:ALA:HB1	1:131:A:GLN:HB2	1	0.17
(1,1793)	1:130:A:ALA:HB2	1:131:A:GLN:HB2	1	0.17
(1,1793)	1:130:A:ALA:HB3	1:131:A:GLN:HB2	1	0.17
(1,1693)	1:72:A:MET:HB2	1:103:A:VAL:HA	7	0.17
(1,1693)	1:72:A:MET:HB3	1:103:A:VAL:HA	7	0.17
(1,1685)	1:113:A:LEU:HD11	1:141:A:PHE:HA	14	0.17
(1,1685)	1:113:A:LEU:HD12	1:141:A:PHE:HA	14	0.17
(1,1685)	1:113:A:LEU:HD13	1:141:A:PHE:HA	14	0.17
(1,1685)	1:113:A:LEU:HD11	1:141:A:PHE:HA	16	0.17
(1,1685)	1:113:A:LEU:HD12	1:141:A:PHE:HA	16	0.17
(1,1685)	1:113:A:LEU:HD13	1:141:A:PHE:HA	16	0.17
(1,1685)	1:113:A:LEU:HD11	1:141:A:PHE:HA	20	0.17
(1,1685)	1:113:A:LEU:HD12	1:141:A:PHE:HA	20	0.17
(1,1685)	1:113:A:LEU:HD13	1:141:A:PHE:HA	20	0.17
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE2	10	0.17
(1,1675)	1:165:A:LYS:HA	1:165:A:LYS:HE3	10	0.17
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	20	0.17
(1,1576)	1:46:A:ILE:HG21	1:161:A:ARG:HG2	4	0.17
(1,1576)	1:46:A:ILE:HG21	1:161:A:ARG:HG3	4	0.17
(1,1576)	1:46:A:ILE:HG22	1:161:A:ARG:HG2	4	0.17
(1,1576)	1:46:A:ILE:HG22	1:161:A:ARG:HG3	4	0.17
(1,1576)	1:46:A:ILE:HG23	1:161:A:ARG:HG2	4	0.17
(1,1576)	1:46:A:ILE:HG23	1:161:A:ARG:HG3	4	0.17
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	9	0.17
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	16	0.17
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	16	0.17
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	16	0.17
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	16	0.17
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	16	0.17
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	16	0.17
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG11	6	0.17
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG12	6	0.17
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG13	6	0.17
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG21	6	0.17
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG22	6	0.17
(1,1521)	1:87:A:THR:HB	1:125:A:VAL:HG23	6	0.17
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	4	0.17
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	4	0.17
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	6	0.17
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	6	0.17
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	6	0.17
(1,1422)	1:84:A:ILE:HD11	1:126:A:ASP:HA	11	0.17
(1,1422)	1:84:A:ILE:HD12	1:126:A:ASP:HA	11	0.17
(1,1422)	1:84:A:ILE:HD13	1:126:A:ASP:HA	11	0.17
(1,1385)	1:84:A:ILE:HD11	1:123:A:ARG:HB3	3	0.17
(1,1385)	1:84:A:ILE:HD12	1:123:A:ARG:HB3	3	0.17
(1,1385)	1:84:A:ILE:HD13	1:123:A:ARG:HB3	3	0.17
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	19	0.17
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	19	0.17
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	19	0.17
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	18	0.17
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	18	0.17
(1,1302)	1:111:A:MET:HB3	1:139:A:ILE:HD11	12	0.17
(1,1302)	1:111:A:MET:HB3	1:139:A:ILE:HD12	12	0.17
(1,1302)	1:111:A:MET:HB3	1:139:A:ILE:HD13	12	0.17
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD1	15	0.17
(1,1297)	1:68:A:ARG:HD2	1:71:A:TYR:HD2	15	0.17
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD1	15	0.17
(1,1297)	1:68:A:ARG:HD3	1:71:A:TYR:HD2	15	0.17
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	17	0.17
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	17	0.17
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	19	0.17
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	19	0.17
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	3	0.17
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	11	0.17
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	16	0.17
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD11	11	0.17
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD12	11	0.17
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD13	11	0.17
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	9	0.17
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	10	0.17
(1,1244)	1:91:A:GLU:H	1:91:A:GLU:HG3	9	0.17
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	2	0.17
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	2	0.17
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	2	0.17
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	3	0.17
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	3	0.17
(1,1162)	1:40:A:TYR:HD1	1:55:A:ILE:HG12	17	0.17
(1,1162)	1:40:A:TYR:HD2	1:55:A:ILE:HG12	17	0.17
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	10	0.17
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	10	0.17
(1,1139)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	10	0.17
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	10	0.17
(1,1139)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	10	0.17
(1,1131)	1:1:A:MET:HE1	1:52:A:LEU:HB3	16	0.17
(1,1131)	1:1:A:MET:HE2	1:52:A:LEU:HB3	16	0.17
(1,1131)	1:1:A:MET:HE3	1:52:A:LEU:HB3	16	0.17
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	16	0.17
(1,1045)	1:129:A:GLN:HB2	1:129:A:GLN:HE22	20	0.17
(1,1033)	1:90:A:PHE:HB2	1:129:A:GLN:HE21	13	0.17
(1,1033)	1:90:A:PHE:HB3	1:129:A:GLN:HE21	13	0.17
(1,962)	1:43:A:GLN:H	1:43:A:GLN:HG3	9	0.17
(1,962)	1:43:A:GLN:H	1:43:A:GLN:HG3	20	0.17
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	20	0.17
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	20	0.17
(1,952)	1:1:A:MET:HE1	1:43:A:GLN:HE21	19	0.17
(1,952)	1:1:A:MET:HE2	1:43:A:GLN:HE21	19	0.17
(1,952)	1:1:A:MET:HE3	1:43:A:GLN:HE21	19	0.17
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	18	0.17
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	8	0.17
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	8	0.17
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	18	0.17
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	18	0.17
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	6	0.17
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	6	0.17
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	7	0.17
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	2	0.17
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	2	0.17
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	7	0.17
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	7	0.17
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	7	0.17
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	7	0.17
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	7	0.17
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	7	0.17
(1,532)	1:166:A:HIS:HB2	1:168:A:GLU:H	2	0.17
(1,532)	1:166:A:HIS:HB2	1:168:A:GLU:H	13	0.17
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	10	0.17
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	10	0.17
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	19	0.17
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	19	0.17
(1,377)	1:24:A:ILE:HD11	1:43:A:GLN:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:24:A:ILE:HD12	1:43:A:GLN:H	1	0.17
(1,377)	1:24:A:ILE:HD13	1:43:A:GLN:H	1	0.17
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	1	0.17
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	11	0.17
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE1	20	0.17
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE2	20	0.17
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	17	0.17
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	17	0.17
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	17	0.17
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	17	0.17
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	17	0.17
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	17	0.17
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	17	0.17
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	17	0.17
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	17	0.17
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	8	0.17
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE2	16	0.17
(1,88)	1:101:A:LYS:H	1:101:A:LYS:HE3	16	0.17
(1,84)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	6	0.17
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	3	0.17
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD22	3	0.17
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	1	0.17
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	1	0.17
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	1	0.17
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	1	0.17
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	1	0.17
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	1	0.17
(1,73)	1:102:A:ARG:H	1:104:A:LYS:H	2	0.17
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	1	0.17
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	1	0.17
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	1	0.17
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	1	0.17
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	1	0.17
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	1	0.17
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	6	0.17
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	9	0.17
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	9	0.17
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	9	0.17
(1,3329)	1:109:A:VAL:H	1:110:A:PRO:HD2	9	0.16
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG21	19	0.16
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG22	19	0.16
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG23	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG21	19	0.16
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG22	19	0.16
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG23	19	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG21	4	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG22	4	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG23	4	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG21	8	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG22	8	0.16
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG23	8	0.16
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB2	19	0.16
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB3	19	0.16
(1,3156)	1:120:A:LEU:H	1:120:A:LEU:HG	18	0.16
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE1	9	0.16
(1,3113)	1:18:A:ALA:HA	1:32:A:TYR:HE2	9	0.16
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG11	10	0.16
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG12	10	0.16
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG13	10	0.16
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG21	10	0.16
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG22	10	0.16
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG23	10	0.16
(1,3006)	1:32:A:TYR:HE1	1:34:A:PRO:HB2	2	0.16
(1,3006)	1:32:A:TYR:HE1	1:34:A:PRO:HB3	2	0.16
(1,3006)	1:32:A:TYR:HE2	1:34:A:PRO:HB2	2	0.16
(1,3006)	1:32:A:TYR:HE2	1:34:A:PRO:HB3	2	0.16
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	19	0.16
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	5	0.16
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	10	0.16
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	16	0.16
(1,2908)	1:135:A:ARG:HD2	1:136:A:SER:H	19	0.16
(1,2908)	1:135:A:ARG:HD3	1:136:A:SER:H	19	0.16
(1,2824)	1:18:A:ALA:HB1	1:28:A:PHE:HD1	20	0.16
(1,2824)	1:18:A:ALA:HB1	1:28:A:PHE:HD2	20	0.16
(1,2824)	1:18:A:ALA:HB2	1:28:A:PHE:HD1	20	0.16
(1,2824)	1:18:A:ALA:HB2	1:28:A:PHE:HD2	20	0.16
(1,2824)	1:18:A:ALA:HB3	1:28:A:PHE:HD1	20	0.16
(1,2824)	1:18:A:ALA:HB3	1:28:A:PHE:HD2	20	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	3	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	3	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	12	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	12	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	15	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	19	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	19	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	20	0.16
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	20	0.16
(1,2804)	1:83:A:ALA:HB1	1:86:A:ASN:HD21	5	0.16
(1,2804)	1:83:A:ALA:HB1	1:86:A:ASN:HD22	5	0.16
(1,2804)	1:83:A:ALA:HB2	1:86:A:ASN:HD21	5	0.16
(1,2804)	1:83:A:ALA:HB2	1:86:A:ASN:HD22	5	0.16
(1,2804)	1:83:A:ALA:HB3	1:86:A:ASN:HD21	5	0.16
(1,2804)	1:83:A:ALA:HB3	1:86:A:ASN:HD22	5	0.16
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	7	0.16
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG21	1	0.16
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG22	1	0.16
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG23	1	0.16
(1,2733)	1:11:A:ALA:HB1	1:92:A:ASP:H	20	0.16
(1,2733)	1:11:A:ALA:HB2	1:92:A:ASP:H	20	0.16
(1,2733)	1:11:A:ALA:HB3	1:92:A:ASP:H	20	0.16
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE1	15	0.16
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE2	15	0.16
(1,2676)	1:100:A:ILE:HD11	1:111:A:MET:HE3	15	0.16
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE1	15	0.16
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE2	15	0.16
(1,2676)	1:100:A:ILE:HD12	1:111:A:MET:HE3	15	0.16
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE1	15	0.16
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE2	15	0.16
(1,2676)	1:100:A:ILE:HD13	1:111:A:MET:HE3	15	0.16
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG2	14	0.16
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG3	14	0.16
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD11	7	0.16
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD12	7	0.16
(1,2655)	1:72:A:MET:HE1	1:100:A:ILE:HD13	7	0.16
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD11	7	0.16
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD12	7	0.16
(1,2655)	1:72:A:MET:HE2	1:100:A:ILE:HD13	7	0.16
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD11	7	0.16
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD12	7	0.16
(1,2655)	1:72:A:MET:HE3	1:100:A:ILE:HD13	7	0.16
(1,2652)	1:148:A:THR:HB	1:150:A:GLN:H	13	0.16
(1,2627)	1:47:A:ASP:HB2	1:161:A:ARG:HE	5	0.16
(1,2627)	1:47:A:ASP:HB3	1:161:A:ARG:HE	5	0.16
(1,2595)	1:21:A:ILE:HA	1:25:A:GLN:HB2	5	0.16
(1,2588)	1:153:A:ASP:HB2	1:155:A:ALA:H	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2588)	1:153:A:ASP:HB3	1:155:A:ALA:H	19	0.16
(1,2577)	1:106:A:SER:HB2	1:107:A:GLU:HA	10	0.16
(1,2577)	1:106:A:SER:HB3	1:107:A:GLU:HA	10	0.16
(1,2559)	1:17:A:SER:HA	1:20:A:THR:HA	3	0.16
(1,2518)	1:164:A:ARG:H	1:165:A:LYS:HG2	4	0.16
(1,2512)	1:4:A:TYR:HE1	1:160:A:VAL:HA	10	0.16
(1,2512)	1:4:A:TYR:HE2	1:160:A:VAL:HA	10	0.16
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB1	3	0.16
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB2	3	0.16
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB3	3	0.16
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	7	0.16
(1,2403)	1:167:A:LYS:H	1:167:A:LYS:HD2	8	0.16
(1,2403)	1:167:A:LYS:H	1:167:A:LYS:HD3	8	0.16
(1,2302)	1:23:A:LEU:HD21	1:153:A:ASP:HA	15	0.16
(1,2302)	1:23:A:LEU:HD22	1:153:A:ASP:HA	15	0.16
(1,2302)	1:23:A:LEU:HD23	1:153:A:ASP:HA	15	0.16
(1,2280)	1:144:A:THR:HA	1:151:A:GLY:HA2	11	0.16
(1,2272)	1:144:A:THR:HA	1:150:A:GLN:HG3	11	0.16
(1,2267)	1:150:A:GLN:HG2	1:151:A:GLY:H	11	0.16
(1,2223)	1:114:A:VAL:HA	1:144:A:THR:H	6	0.16
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	8	0.16
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	8	0.16
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	9	0.16
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	9	0.16
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	9	0.16
(1,2202)	1:144:A:THR:HG21	1:154:A:ASP:HB3	15	0.16
(1,2202)	1:144:A:THR:HG22	1:154:A:ASP:HB3	15	0.16
(1,2202)	1:144:A:THR:HG23	1:154:A:ASP:HB3	15	0.16
(1,2196)	1:118:A:SER:HB3	1:143:A:GLU:HG3	6	0.16
(1,2189)	1:4:A:TYR:HD1	1:52:A:LEU:H	7	0.16
(1,2189)	1:4:A:TYR:HD2	1:52:A:LEU:H	7	0.16
(1,1999)	1:132:A:ASP:HA	1:135:A:ARG:HE	13	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	8	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	8	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	8	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	8	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	8	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	8	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	8	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	8	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	8	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	8	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	8	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	8	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	8	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	8	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	8	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	8	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	8	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG11	11	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG12	11	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG13	11	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG21	11	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG22	11	0.16
(1,1980)	1:124:A:THR:HG21	1:125:A:VAL:HG23	11	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG11	11	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG12	11	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG13	11	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG21	11	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG22	11	0.16
(1,1980)	1:124:A:THR:HG22	1:125:A:VAL:HG23	11	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG11	11	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG12	11	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG13	11	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG21	11	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG22	11	0.16
(1,1980)	1:124:A:THR:HG23	1:125:A:VAL:HG23	11	0.16
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG21	8	0.16
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG22	8	0.16
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG23	8	0.16
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG21	9	0.16
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG22	9	0.16
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG23	9	0.16
(1,1971)	1:6:A:LEU:HB2	1:78:A:PHE:HA	7	0.16
(1,1971)	1:6:A:LEU:HB3	1:78:A:PHE:HA	7	0.16
(1,1937)	1:8:A:VAL:HA	1:78:A:PHE:HA	14	0.16
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	17	0.16
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	17	0.16
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	15	0.16
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	15	0.16
(1,1876)	1:114:A:VAL:HG11	1:144:A:THR:H	3	0.16
(1,1876)	1:114:A:VAL:HG12	1:144:A:THR:H	3	0.16
(1,1876)	1:114:A:VAL:HG13	1:144:A:THR:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1876)	1:114:A:VAL:HG21	1:144:A:THR:H	3	0.16
(1,1876)	1:114:A:VAL:HG22	1:144:A:THR:H	3	0.16
(1,1876)	1:114:A:VAL:HG23	1:144:A:THR:H	3	0.16
(1,1876)	1:114:A:VAL:HG11	1:144:A:THR:H	18	0.16
(1,1876)	1:114:A:VAL:HG12	1:144:A:THR:H	18	0.16
(1,1876)	1:114:A:VAL:HG13	1:144:A:THR:H	18	0.16
(1,1876)	1:114:A:VAL:HG21	1:144:A:THR:H	18	0.16
(1,1876)	1:114:A:VAL:HG22	1:144:A:THR:H	18	0.16
(1,1876)	1:114:A:VAL:HG23	1:144:A:THR:H	18	0.16
(1,1814)	1:100:A:ILE:HD11	1:111:A:MET:HG2	12	0.16
(1,1814)	1:100:A:ILE:HD12	1:111:A:MET:HG2	12	0.16
(1,1814)	1:100:A:ILE:HD13	1:111:A:MET:HG2	12	0.16
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	5	0.16
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	5	0.16
(1,1793)	1:130:A:ALA:HB1	1:131:A:GLN:HB2	11	0.16
(1,1793)	1:130:A:ALA:HB2	1:131:A:GLN:HB2	11	0.16
(1,1793)	1:130:A:ALA:HB3	1:131:A:GLN:HB2	11	0.16
(1,1793)	1:130:A:ALA:HB1	1:131:A:GLN:HB2	20	0.16
(1,1793)	1:130:A:ALA:HB2	1:131:A:GLN:HB2	20	0.16
(1,1793)	1:130:A:ALA:HB3	1:131:A:GLN:HB2	20	0.16
(1,1785)	1:131:A:GLN:H	1:141:A:PHE:HZ	12	0.16
(1,1751)	1:141:A:PHE:HZ	1:143:A:GLU:HG2	5	0.16
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	16	0.16
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	16	0.16
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	16	0.16
(1,1664)	1:113:A:LEU:HB3	1:141:A:PHE:HE1	12	0.16
(1,1664)	1:113:A:LEU:HB3	1:141:A:PHE:HE2	12	0.16
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE1	6	0.16
(1,1554)	1:68:A:ARG:HA	1:71:A:TYR:HE2	6	0.16
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	13	0.16
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	13	0.16
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	13	0.16
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	13	0.16
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	13	0.16
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	13	0.16
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE1	7	0.16
(1,1518)	1:97:A:ARG:HB3	1:137:A:TYR:HE2	7	0.16
(1,1497)	1:84:A:ILE:HG21	1:125:A:VAL:HG11	4	0.16
(1,1497)	1:84:A:ILE:HG21	1:125:A:VAL:HG12	4	0.16
(1,1497)	1:84:A:ILE:HG21	1:125:A:VAL:HG13	4	0.16
(1,1497)	1:84:A:ILE:HG21	1:125:A:VAL:HG21	4	0.16
(1,1497)	1:84:A:ILE:HG21	1:125:A:VAL:HG22	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1497)	1:84:A:ILE:HG21	1:125:A:VAL:HG23	4	0.16
(1,1497)	1:84:A:ILE:HG22	1:125:A:VAL:HG11	4	0.16
(1,1497)	1:84:A:ILE:HG22	1:125:A:VAL:HG12	4	0.16
(1,1497)	1:84:A:ILE:HG22	1:125:A:VAL:HG13	4	0.16
(1,1497)	1:84:A:ILE:HG22	1:125:A:VAL:HG21	4	0.16
(1,1497)	1:84:A:ILE:HG22	1:125:A:VAL:HG22	4	0.16
(1,1497)	1:84:A:ILE:HG22	1:125:A:VAL:HG23	4	0.16
(1,1497)	1:84:A:ILE:HG23	1:125:A:VAL:HG11	4	0.16
(1,1497)	1:84:A:ILE:HG23	1:125:A:VAL:HG12	4	0.16
(1,1497)	1:84:A:ILE:HG23	1:125:A:VAL:HG13	4	0.16
(1,1497)	1:84:A:ILE:HG23	1:125:A:VAL:HG21	4	0.16
(1,1497)	1:84:A:ILE:HG23	1:125:A:VAL:HG22	4	0.16
(1,1497)	1:84:A:ILE:HG23	1:125:A:VAL:HG23	4	0.16
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	18	0.16
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	18	0.16
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	18	0.16
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	14	0.16
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	14	0.16
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	14	0.16
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	14	0.16
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	14	0.16
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	14	0.16
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD1	5	0.16
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD2	5	0.16
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	17	0.16
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	17	0.16
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	7	0.16
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	7	0.16
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	9	0.16
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	6	0.16
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	12	0.16
(1,1249)	1:25:A:GLN:HB2	1:27:A:HIS:HD2	8	0.16
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE21	7	0.16
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE22	7	0.16
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE21	18	0.16
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE22	18	0.16
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	17	0.16
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	17	0.16
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	17	0.16
(1,1194)	1:56:A:LEU:HD11	1:57:A:ASP:H	12	0.16
(1,1194)	1:56:A:LEU:HD12	1:57:A:ASP:H	12	0.16
(1,1194)	1:56:A:LEU:HD13	1:57:A:ASP:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	1:56:A:LEU:HD21	1:57:A:ASP:H	12	0.16
(1,1194)	1:56:A:LEU:HD22	1:57:A:ASP:H	12	0.16
(1,1194)	1:56:A:LEU:HD23	1:57:A:ASP:H	12	0.16
(1,1186)	1:56:A:LEU:HD11	1:71:A:TYR:HB3	11	0.16
(1,1186)	1:56:A:LEU:HD12	1:71:A:TYR:HB3	11	0.16
(1,1186)	1:56:A:LEU:HD13	1:71:A:TYR:HB3	11	0.16
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	3	0.16
(1,1110)	1:90:A:PHE:H	1:125:A:VAL:HG11	19	0.16
(1,1110)	1:90:A:PHE:H	1:125:A:VAL:HG12	19	0.16
(1,1110)	1:90:A:PHE:H	1:125:A:VAL:HG13	19	0.16
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE1	1	0.16
(1,1094)	1:21:A:ILE:H	1:40:A:TYR:HE2	1	0.16
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	20	0.16
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	20	0.16
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	12	0.16
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	15	0.16
(1,985)	1:67:A:MET:HA	1:70:A:GLN:HE21	17	0.16
(1,985)	1:67:A:MET:HA	1:70:A:GLN:HE22	17	0.16
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	3	0.16
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	3	0.16
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	3	0.16
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	3	0.16
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	3	0.16
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	3	0.16
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	17	0.16
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	17	0.16
(1,913)	1:23:A:LEU:HG	1:42:A:LYS:HD3	9	0.16
(1,897)	1:79:A:LEU:HD11	1:157:A:TYR:H	19	0.16
(1,897)	1:79:A:LEU:HD12	1:157:A:TYR:H	19	0.16
(1,897)	1:79:A:LEU:HD13	1:157:A:TYR:H	19	0.16
(1,897)	1:79:A:LEU:HD21	1:157:A:TYR:H	19	0.16
(1,897)	1:79:A:LEU:HD22	1:157:A:TYR:H	19	0.16
(1,897)	1:79:A:LEU:HD23	1:157:A:TYR:H	19	0.16
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	13	0.16
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	6	0.16
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	10	0.16
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	12	0.16
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	16	0.16
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	12	0.16
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	12	0.16
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	12	0.16
(1,740)	1:64:A:TYR:HA	1:65:A:SER:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	11	0.16
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	11	0.16
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	11	0.16
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	11	0.16
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	11	0.16
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	11	0.16
(1,656)	1:36:A:ILE:HD11	1:37:A:GLU:HA	5	0.16
(1,656)	1:36:A:ILE:HD12	1:37:A:GLU:HA	5	0.16
(1,656)	1:36:A:ILE:HD13	1:37:A:GLU:HA	5	0.16
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	13	0.16
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD11	6	0.16
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD12	6	0.16
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD13	6	0.16
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD1	8	0.16
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD2	8	0.16
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD2	18	0.16
(1,628)	1:123:A:ARG:H	1:123:A:ARG:HD3	18	0.16
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	5	0.16
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	5	0.16
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	5	0.16
(1,377)	1:24:A:ILE:HD11	1:43:A:GLN:H	6	0.16
(1,377)	1:24:A:ILE:HD12	1:43:A:GLN:H	6	0.16
(1,377)	1:24:A:ILE:HD13	1:43:A:GLN:H	6	0.16
(1,377)	1:24:A:ILE:HD11	1:43:A:GLN:H	19	0.16
(1,377)	1:24:A:ILE:HD12	1:43:A:GLN:H	19	0.16
(1,377)	1:24:A:ILE:HD13	1:43:A:GLN:H	19	0.16
(1,323)	1:44:A:VAL:H	1:52:A:LEU:HA	7	0.16
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	10	0.16
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	10	0.16
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	10	0.16
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	8	0.16
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	8	0.16
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	8	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	1	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	1	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	1	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	1	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	1	0.16
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	1	0.16
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE1	18	0.16
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE2	18	0.16
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE1	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE2	18	0.16
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE1	18	0.16
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE2	18	0.16
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	10	0.16
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	10	0.16
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	10	0.16
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	10	0.16
(1,148)	1:28:A:PHE:HE1	2:201:A:GNP:H1'	9	0.16
(1,148)	1:28:A:PHE:HE2	2:201:A:GNP:H1'	9	0.16
(1,103)	1:16:A:LYS:HA	1:19:A:LEU:HB3	12	0.16
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	14	0.16
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	14	0.16
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	14	0.16
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	14	0.16
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	14	0.16
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	14	0.16
(1,86)	1:15:A:GLY:HA2	1:116:A:ASN:HD22	3	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	4	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	4	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	4	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	4	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	4	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	4	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	11	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	11	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	11	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	11	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	11	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	11	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG11	16	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG12	16	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG13	16	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG21	16	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG22	16	0.16
(1,78)	1:15:A:GLY:HA3	1:81:A:VAL:HG23	16	0.16
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	14	0.15
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	14	0.15
(1,3282)	1:111:A:MET:HB3	1:112:A:VAL:H	9	0.15
(1,3279)	1:45:A:VAL:HG21	1:49:A:GLU:H	2	0.15
(1,3279)	1:45:A:VAL:HG22	1:49:A:GLU:H	2	0.15
(1,3279)	1:45:A:VAL:HG23	1:49:A:GLU:H	2	0.15
(1,3259)	1:113:A:LEU:H	1:141:A:PHE:HB3	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3212)	1:3:A:GLU:HB2	1:4:A:TYR:H	16	0.15
(1,3212)	1:3:A:GLU:HB3	1:4:A:TYR:H	16	0.15
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB2	20	0.15
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB3	20	0.15
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	19	0.15
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	4	0.15
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	15	0.15
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	15	0.15
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	15	0.15
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	4	0.15
(1,3122)	1:1:A:MET:HA	1:2:A:THR:HG21	5	0.15
(1,3122)	1:1:A:MET:HA	1:2:A:THR:HG22	5	0.15
(1,3122)	1:1:A:MET:HA	1:2:A:THR:HG23	5	0.15
(1,3063)	1:45:A:VAL:HB	1:48:A:GLY:H	2	0.15
(1,3030)	1:32:A:TYR:HE1	1:34:A:PRO:HG3	9	0.15
(1,3030)	1:32:A:TYR:HE2	1:34:A:PRO:HG3	9	0.15
(1,3004)	1:90:A:PHE:HZ	1:131:A:GLN:H	20	0.15
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	5	0.15
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	3	0.15
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	16	0.15
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	19	0.15
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	2	0.15
(1,2897)	1:75:A:GLY:H	1:77:A:GLY:H	5	0.15
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	13	0.15
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	13	0.15
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	13	0.15
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	13	0.15
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	13	0.15
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	13	0.15
(1,2869)	1:163:A:ILE:HG21	1:166:A:HIS:H	6	0.15
(1,2869)	1:163:A:ILE:HG22	1:166:A:HIS:H	6	0.15
(1,2869)	1:163:A:ILE:HG23	1:166:A:HIS:H	6	0.15
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	11	0.15
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	11	0.15
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	14	0.15
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	14	0.15
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG2	16	0.15
(1,2807)	1:143:A:GLU:H	1:143:A:GLU:HG3	16	0.15
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	20	0.15
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	16	0.15
(1,2768)	1:145:A:SER:H	1:150:A:GLN:HG3	16	0.15
(1,2730)	1:118:A:SER:H	1:147:A:LYS:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2711)	1:11:A:ALA:HB1	1:12:A:GLY:H	4	0.15
(1,2711)	1:11:A:ALA:HB2	1:12:A:GLY:H	4	0.15
(1,2711)	1:11:A:ALA:HB3	1:12:A:GLY:H	4	0.15
(1,2711)	1:11:A:ALA:HB1	1:12:A:GLY:H	11	0.15
(1,2711)	1:11:A:ALA:HB2	1:12:A:GLY:H	11	0.15
(1,2711)	1:11:A:ALA:HB3	1:12:A:GLY:H	11	0.15
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	20	0.15
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	20	0.15
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	20	0.15
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	20	0.15
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	20	0.15
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	20	0.15
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB1	19	0.15
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB2	19	0.15
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB3	19	0.15
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB1	19	0.15
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB2	19	0.15
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB3	19	0.15
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB1	19	0.15
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB2	19	0.15
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB3	19	0.15
(1,2682)	1:25:A:GLN:HA	1:27:A:HIS:HE1	13	0.15
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	6	0.15
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	6	0.15
(1,2627)	1:47:A:ASP:HB2	1:161:A:ARG:HE	18	0.15
(1,2627)	1:47:A:ASP:HB3	1:161:A:ARG:HE	18	0.15
(1,2607)	1:21:A:ILE:HA	1:27:A:HIS:H	5	0.15
(1,2574)	1:84:A:ILE:HD11	1:123:A:ARG:HE	11	0.15
(1,2574)	1:84:A:ILE:HD12	1:123:A:ARG:HE	11	0.15
(1,2574)	1:84:A:ILE:HD13	1:123:A:ARG:HE	11	0.15
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	1	0.15
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	1	0.15
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	1	0.15
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	8	0.15
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	8	0.15
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	8	0.15
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	11	0.15
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	11	0.15
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	11	0.15
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	2	0.15
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	2	0.15
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	17	0.15
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	17	0.15
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	17	0.15
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	20	0.15
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	20	0.15
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	20	0.15
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	14	0.15
(1,2454)	1:162:A:GLU:HB2	1:165:A:LYS:HG2	4	0.15
(1,2454)	1:162:A:GLU:HB3	1:165:A:LYS:HG2	4	0.15
(1,2452)	1:162:A:GLU:HA	1:165:A:LYS:HG2	11	0.15
(1,2440)	1:160:A:VAL:HG11	1:164:A:ARG:HA	6	0.15
(1,2440)	1:160:A:VAL:HG12	1:164:A:ARG:HA	6	0.15
(1,2440)	1:160:A:VAL:HG13	1:164:A:ARG:HA	6	0.15
(1,2440)	1:160:A:VAL:HG21	1:164:A:ARG:HA	6	0.15
(1,2440)	1:160:A:VAL:HG22	1:164:A:ARG:HA	6	0.15
(1,2440)	1:160:A:VAL:HG23	1:164:A:ARG:HA	6	0.15
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	15	0.15
(1,2351)	1:4:A:TYR:HE1	1:164:A:ARG:HA	13	0.15
(1,2351)	1:4:A:TYR:HE2	1:164:A:ARG:HA	13	0.15
(1,2267)	1:150:A:GLN:HG2	1:151:A:GLY:H	10	0.15
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG21	11	0.15
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG22	11	0.15
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG23	11	0.15
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG2	20	0.15
(1,2211)	1:146:A:ALA:HA	1:149:A:ARG:HG3	20	0.15
(1,2190)	1:44:A:VAL:HG21	1:51:A:CYS:H	19	0.15
(1,2190)	1:44:A:VAL:HG22	1:51:A:CYS:H	19	0.15
(1,2190)	1:44:A:VAL:HG23	1:51:A:CYS:H	19	0.15
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	1	0.15
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	11	0.15
(1,2156)	1:111:A:MET:H	1:140:A:PRO:HD3	18	0.15
(1,2132)	1:45:A:VAL:HG11	1:51:A:CYS:H	4	0.15
(1,2132)	1:45:A:VAL:HG12	1:51:A:CYS:H	4	0.15
(1,2132)	1:45:A:VAL:HG13	1:51:A:CYS:H	4	0.15
(1,2132)	1:45:A:VAL:HG21	1:51:A:CYS:H	4	0.15
(1,2132)	1:45:A:VAL:HG22	1:51:A:CYS:H	4	0.15
(1,2132)	1:45:A:VAL:HG23	1:51:A:CYS:H	4	0.15
(1,2123)	1:154:A:ASP:HA	1:157:A:TYR:H	2	0.15
(1,2067)	1:3:A:GLU:HA	1:4:A:TYR:HB2	20	0.15
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	9	0.15
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	9	0.15
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	7	0.15
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG21	11	0.15
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG22	11	0.15
(1,1950)	1:122:A:SER:HB2	1:124:A:THR:HG23	11	0.15
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG21	11	0.15
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG22	11	0.15
(1,1950)	1:122:A:SER:HB3	1:124:A:THR:HG23	11	0.15
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	13	0.15
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	13	0.15
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE1	17	0.15
(1,1933)	1:12:A:GLY:H	1:96:A:TYR:HE2	17	0.15
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	18	0.15
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	19	0.15
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	15	0.15
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	15	0.15
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	15	0.15
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	7	0.15
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	7	0.15
(1,1859)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	7	0.15
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	7	0.15
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	7	0.15
(1,1859)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	7	0.15
(1,1811)	1:109:A:VAL:HG11	1:111:A:MET:HG3	13	0.15
(1,1811)	1:109:A:VAL:HG12	1:111:A:MET:HG3	13	0.15
(1,1811)	1:109:A:VAL:HG13	1:111:A:MET:HG3	13	0.15
(1,1811)	1:109:A:VAL:HG21	1:111:A:MET:HG3	13	0.15
(1,1811)	1:109:A:VAL:HG22	1:111:A:MET:HG3	13	0.15
(1,1811)	1:109:A:VAL:HG23	1:111:A:MET:HG3	13	0.15
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG11	18	0.15
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG12	18	0.15
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG13	18	0.15
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG21	18	0.15
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG22	18	0.15
(1,1770)	1:78:A:PHE:HZ	1:109:A:VAL:HG23	18	0.15
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	10	0.15
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	10	0.15
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	15	0.15
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	15	0.15
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	11	0.15
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	11	0.15
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	11	0.15
(1,1685)	1:113:A:LEU:HD11	1:141:A:PHE:HA	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:113:A:LEU:HD12	1:141:A:PHE:HA	18	0.15
(1,1685)	1:113:A:LEU:HD13	1:141:A:PHE:HA	18	0.15
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	16	0.15
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE1	2	0.15
(1,1568)	1:93:A:ILE:HA	1:96:A:TYR:HE2	2	0.15
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	1	0.15
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	1	0.15
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD11	3	0.15
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD12	3	0.15
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD13	3	0.15
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD11	3	0.15
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD12	3	0.15
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD13	3	0.15
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	13	0.15
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	13	0.15
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	13	0.15
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	13	0.15
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	13	0.15
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	13	0.15
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	1	0.15
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	1	0.15
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	14	0.15
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	14	0.15
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG2	10	0.15
(1,1282)	1:66:A:ALA:HB1	1:67:A:MET:HG3	10	0.15
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG2	10	0.15
(1,1282)	1:66:A:ALA:HB2	1:67:A:MET:HG3	10	0.15
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG2	10	0.15
(1,1282)	1:66:A:ALA:HB3	1:67:A:MET:HG3	10	0.15
(1,1281)	1:67:A:MET:HA	1:67:A:MET:HG3	1	0.15
(1,1281)	1:67:A:MET:HA	1:67:A:MET:HG3	3	0.15
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD11	18	0.15
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD12	18	0.15
(1,1259)	1:97:A:ARG:H	1:100:A:ILE:HD13	18	0.15
(1,1246)	1:94:A:HIS:HE1	1:133:A:LEU:HD11	3	0.15
(1,1246)	1:94:A:HIS:HE1	1:133:A:LEU:HD12	3	0.15
(1,1246)	1:94:A:HIS:HE1	1:133:A:LEU:HD13	3	0.15
(1,1246)	1:94:A:HIS:HE1	1:133:A:LEU:HD21	3	0.15
(1,1246)	1:94:A:HIS:HE1	1:133:A:LEU:HD22	3	0.15
(1,1246)	1:94:A:HIS:HE1	1:133:A:LEU:HD23	3	0.15
(1,1222)	1:58:A:THR:HG21	1:59:A:ALA:H	17	0.15
(1,1222)	1:58:A:THR:HG22	1:59:A:ALA:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:58:A:THR:HG23	1:59:A:ALA:H	17	0.15
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE1	10	0.15
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE2	10	0.15
(1,1196)	1:56:A:LEU:HD11	1:71:A:TYR:H	2	0.15
(1,1196)	1:56:A:LEU:HD12	1:71:A:TYR:H	2	0.15
(1,1196)	1:56:A:LEU:HD13	1:71:A:TYR:H	2	0.15
(1,1196)	1:56:A:LEU:HD21	1:71:A:TYR:H	2	0.15
(1,1196)	1:56:A:LEU:HD22	1:71:A:TYR:H	2	0.15
(1,1196)	1:56:A:LEU:HD23	1:71:A:TYR:H	2	0.15
(1,1188)	1:56:A:LEU:HD11	1:71:A:TYR:HD1	11	0.15
(1,1188)	1:56:A:LEU:HD11	1:71:A:TYR:HD2	11	0.15
(1,1188)	1:56:A:LEU:HD12	1:71:A:TYR:HD1	11	0.15
(1,1188)	1:56:A:LEU:HD12	1:71:A:TYR:HD2	11	0.15
(1,1188)	1:56:A:LEU:HD13	1:71:A:TYR:HD1	11	0.15
(1,1188)	1:56:A:LEU:HD13	1:71:A:TYR:HD2	11	0.15
(1,1115)	1:51:A:CYS:HB3	1:52:A:LEU:H	13	0.15
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	8	0.15
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	8	0.15
(1,1088)	1:51:A:CYS:HA	1:52:A:LEU:HG	6	0.15
(1,1080)	1:1:A:MET:HG3	1:51:A:CYS:HA	12	0.15
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	1	0.15
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	14	0.15
(1,1044)	1:125:A:VAL:HG11	1:129:A:GLN:HE22	5	0.15
(1,1044)	1:125:A:VAL:HG12	1:129:A:GLN:HE22	5	0.15
(1,1044)	1:125:A:VAL:HG13	1:129:A:GLN:HE22	5	0.15
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	12	0.15
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	16	0.15
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA2	19	0.15
(1,1005)	1:45:A:VAL:HG11	1:48:A:GLY:HA3	19	0.15
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA2	19	0.15
(1,1005)	1:45:A:VAL:HG12	1:48:A:GLY:HA3	19	0.15
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA2	19	0.15
(1,1005)	1:45:A:VAL:HG13	1:48:A:GLY:HA3	19	0.15
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA2	19	0.15
(1,1005)	1:45:A:VAL:HG21	1:48:A:GLY:HA3	19	0.15
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA2	19	0.15
(1,1005)	1:45:A:VAL:HG22	1:48:A:GLY:HA3	19	0.15
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA2	19	0.15
(1,1005)	1:45:A:VAL:HG23	1:48:A:GLY:HA3	19	0.15
(1,994)	1:159:A:LEU:HD11	1:163:A:ILE:HG12	14	0.15
(1,994)	1:159:A:LEU:HD11	1:163:A:ILE:HG13	14	0.15
(1,994)	1:159:A:LEU:HD12	1:163:A:ILE:HG12	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:159:A:LEU:HD12	1:163:A:ILE:HG13	14	0.15
(1,994)	1:159:A:LEU:HD13	1:163:A:ILE:HG12	14	0.15
(1,994)	1:159:A:LEU:HD13	1:163:A:ILE:HG13	14	0.15
(1,994)	1:159:A:LEU:HD21	1:163:A:ILE:HG12	14	0.15
(1,994)	1:159:A:LEU:HD21	1:163:A:ILE:HG13	14	0.15
(1,994)	1:159:A:LEU:HD22	1:163:A:ILE:HG12	14	0.15
(1,994)	1:159:A:LEU:HD22	1:163:A:ILE:HG13	14	0.15
(1,994)	1:159:A:LEU:HD23	1:163:A:ILE:HG12	14	0.15
(1,994)	1:159:A:LEU:HD23	1:163:A:ILE:HG13	14	0.15
(1,962)	1:43:A:GLN:H	1:43:A:GLN:HG3	19	0.15
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	15	0.15
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	15	0.15
(1,957)	1:43:A:GLN:HG2	1:44:A:VAL:H	18	0.15
(1,957)	1:43:A:GLN:HG3	1:44:A:VAL:H	18	0.15
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	14	0.15
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	14	0.15
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	14	0.15
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	14	0.15
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	14	0.15
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	14	0.15
(1,945)	1:43:A:GLN:HE21	1:52:A:LEU:HD11	3	0.15
(1,945)	1:43:A:GLN:HE21	1:52:A:LEU:HD12	3	0.15
(1,945)	1:43:A:GLN:HE21	1:52:A:LEU:HD13	3	0.15
(1,945)	1:43:A:GLN:HE21	1:52:A:LEU:HD21	3	0.15
(1,945)	1:43:A:GLN:HE21	1:52:A:LEU:HD22	3	0.15
(1,945)	1:43:A:GLN:HE21	1:52:A:LEU:HD23	3	0.15
(1,940)	1:26:A:ASN:H	1:26:A:ASN:HD22	15	0.15
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	16	0.15
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	16	0.15
(1,897)	1:79:A:LEU:HD11	1:157:A:TYR:H	11	0.15
(1,897)	1:79:A:LEU:HD12	1:157:A:TYR:H	11	0.15
(1,897)	1:79:A:LEU:HD13	1:157:A:TYR:H	11	0.15
(1,897)	1:79:A:LEU:HD21	1:157:A:TYR:H	11	0.15
(1,897)	1:79:A:LEU:HD22	1:157:A:TYR:H	11	0.15
(1,897)	1:79:A:LEU:HD23	1:157:A:TYR:H	11	0.15
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	10	0.15
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	10	0.15
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	10	0.15
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	4	0.15
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	8	0.15
(1,886)	1:44:A:VAL:HB	1:46:A:ILE:H	15	0.15
(1,879)	1:49:A:GLU:H	1:50:A:THR:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:41:A:ARG:HG2	1:52:A:LEU:HD11	3	0.15
(1,865)	1:41:A:ARG:HG2	1:52:A:LEU:HD12	3	0.15
(1,865)	1:41:A:ARG:HG2	1:52:A:LEU:HD13	3	0.15
(1,865)	1:41:A:ARG:HG2	1:52:A:LEU:HD21	3	0.15
(1,865)	1:41:A:ARG:HG2	1:52:A:LEU:HD22	3	0.15
(1,865)	1:41:A:ARG:HG2	1:52:A:LEU:HD23	3	0.15
(1,865)	1:41:A:ARG:HG3	1:52:A:LEU:HD11	3	0.15
(1,865)	1:41:A:ARG:HG3	1:52:A:LEU:HD12	3	0.15
(1,865)	1:41:A:ARG:HG3	1:52:A:LEU:HD13	3	0.15
(1,865)	1:41:A:ARG:HG3	1:52:A:LEU:HD21	3	0.15
(1,865)	1:41:A:ARG:HG3	1:52:A:LEU:HD22	3	0.15
(1,865)	1:41:A:ARG:HG3	1:52:A:LEU:HD23	3	0.15
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	5	0.15
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	5	0.15
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	13	0.15
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	13	0.15
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	14	0.15
(1,815)	1:41:A:ARG:HD2	1:52:A:LEU:HB3	6	0.15
(1,815)	1:41:A:ARG:HD3	1:52:A:LEU:HB3	6	0.15
(1,789)	1:58:A:THR:H	1:58:A:THR:HG21	9	0.15
(1,789)	1:58:A:THR:H	1:58:A:THR:HG22	9	0.15
(1,789)	1:58:A:THR:H	1:58:A:THR:HG23	9	0.15
(1,788)	1:8:A:VAL:HB	1:58:A:THR:H	13	0.15
(1,762)	1:61:A:GLN:H	1:63:A:GLU:H	15	0.15
(1,673)	1:35:A:SER:HA	1:36:A:ILE:H	14	0.15
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	1	0.15
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD11	13	0.15
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD12	13	0.15
(1,648)	1:78:A:PHE:H	1:100:A:ILE:HD13	13	0.15
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	8	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG11	1	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG12	1	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG13	1	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG21	1	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG22	1	0.15
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG23	1	0.15
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	20	0.15
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	20	0.15
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	20	0.15
(1,482)	1:24:A:ILE:HG21	1:26:A:ASN:H	17	0.15
(1,482)	1:24:A:ILE:HG22	1:26:A:ASN:H	17	0.15
(1,482)	1:24:A:ILE:HG23	1:26:A:ASN:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:25:A:GLN:HB3	1:26:A:ASN:H	19	0.15
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG21	11	0.15
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG22	11	0.15
(1,318)	1:44:A:VAL:H	1:50:A:THR:HG23	11	0.15
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG2	1	0.15
(1,291)	1:67:A:MET:HA	1:70:A:GLN:HG3	1	0.15
(1,286)	1:2:A:THR:H	1:52:A:LEU:HB2	14	0.15
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	15	0.15
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	14	0.15
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	14	0.15
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	8	0.15
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	8	0.15
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	8	0.15
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	18	0.15
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	18	0.15
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	18	0.15
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	20	0.15
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	20	0.15
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	20	0.15
(1,149)	1:28:A:PHE:HE1	2:201:A:GNP:H8	16	0.15
(1,149)	1:28:A:PHE:HE2	2:201:A:GNP:H8	16	0.15
(1,108)	1:166:A:HIS:HB3	1:167:A:LYS:H	10	0.15
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	20	0.15
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	20	0.15
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	20	0.15
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	2	0.15
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	2	0.15
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	2	0.15
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG21	9	0.14
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG22	9	0.14
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG23	9	0.14
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG21	9	0.14
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG22	9	0.14
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG23	9	0.14
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	16	0.14
(1,3324)	1:111:A:MET:H	1:139:A:ILE:HA	19	0.14
(1,3317)	1:110:A:PRO:HB3	1:111:A:MET:H	11	0.14
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	17	0.14
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	17	0.14
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	9	0.14
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	11	0.14
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG21	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG22	15	0.14
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG23	15	0.14
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG21	11	0.14
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG22	11	0.14
(1,3165)	1:1:A:MET:HG2	1:50:A:THR:HG23	11	0.14
(1,3157)	1:82:A:PHE:H	1:113:A:LEU:HD11	7	0.14
(1,3157)	1:82:A:PHE:H	1:113:A:LEU:HD12	7	0.14
(1,3157)	1:82:A:PHE:H	1:113:A:LEU:HD13	7	0.14
(1,3157)	1:82:A:PHE:H	1:113:A:LEU:HD21	7	0.14
(1,3157)	1:82:A:PHE:H	1:113:A:LEU:HD22	7	0.14
(1,3157)	1:82:A:PHE:H	1:113:A:LEU:HD23	7	0.14
(1,3145)	1:1:A:MET:HE1	1:44:A:VAL:H	15	0.14
(1,3145)	1:1:A:MET:HE2	1:44:A:VAL:H	15	0.14
(1,3145)	1:1:A:MET:HE3	1:44:A:VAL:H	15	0.14
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	12	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG11	5	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG12	5	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG13	5	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG21	5	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG22	5	0.14
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG23	5	0.14
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	7	0.14
(1,3045)	1:90:A:PHE:HE1	1:129:A:GLN:H	20	0.14
(1,3045)	1:90:A:PHE:HE2	1:129:A:GLN:H	20	0.14
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	5	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD11	6	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD12	6	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD13	6	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD21	6	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD22	6	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD23	6	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD11	14	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD12	14	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD13	14	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD21	14	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD22	14	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD23	14	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD11	18	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD12	18	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD13	18	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD21	18	0.14
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD22	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD23	18	0.14
(1,3019)	1:133:A:LEU:HD11	1:134:A:ALA:H	14	0.14
(1,3019)	1:133:A:LEU:HD12	1:134:A:ALA:H	14	0.14
(1,3019)	1:133:A:LEU:HD13	1:134:A:ALA:H	14	0.14
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	12	0.14
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	16	0.14
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	14	0.14
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	13	0.14
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	2	0.14
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	2	0.14
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	2	0.14
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG21	7	0.14
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG22	7	0.14
(1,2872)	1:5:A:LYS:H	1:163:A:ILE:HG23	7	0.14
(1,2803)	1:116:A:ASN:HA	1:144:A:THR:H	7	0.14
(1,2762)	1:102:A:ARG:H	1:102:A:ARG:HE	15	0.14
(1,2710)	1:102:A:ARG:HB3	1:102:A:ARG:HE	20	0.14
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	6	0.14
(1,2653)	1:75:A:GLY:H	1:78:A:PHE:HE1	5	0.14
(1,2653)	1:75:A:GLY:H	1:78:A:PHE:HE2	5	0.14
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD1	7	0.14
(1,2647)	1:72:A:MET:HE1	1:96:A:TYR:HD2	7	0.14
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD1	7	0.14
(1,2647)	1:72:A:MET:HE2	1:96:A:TYR:HD2	7	0.14
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD1	7	0.14
(1,2647)	1:72:A:MET:HE3	1:96:A:TYR:HD2	7	0.14
(1,2630)	1:150:A:GLN:HG3	1:152:A:VAL:H	13	0.14
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB1	10	0.14
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB2	10	0.14
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB3	10	0.14
(1,2562)	1:20:A:THR:HA	1:23:A:LEU:HG	17	0.14
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	17	0.14
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	17	0.14
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	17	0.14
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	9	0.14
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	9	0.14
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	9	0.14
(1,2487)	1:168:A:GLU:H	1:168:A:GLU:HG3	1	0.14
(1,2436)	1:76:A:GLU:HB3	1:163:A:ILE:HG12	20	0.14
(1,2436)	1:76:A:GLU:HB3	1:163:A:ILE:HG13	20	0.14
(1,2415)	1:77:A:GLY:HA3	1:163:A:ILE:HA	6	0.14
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD2	8	0.14
(1,2395)	1:161:A:ARG:HA	1:164:A:ARG:HD3	8	0.14
(1,2380)	1:159:A:LEU:HD11	1:163:A:ILE:HA	14	0.14
(1,2380)	1:159:A:LEU:HD12	1:163:A:ILE:HA	14	0.14
(1,2380)	1:159:A:LEU:HD13	1:163:A:ILE:HA	14	0.14
(1,2380)	1:159:A:LEU:HD21	1:163:A:ILE:HA	14	0.14
(1,2380)	1:159:A:LEU:HD22	1:163:A:ILE:HA	14	0.14
(1,2380)	1:159:A:LEU:HD23	1:163:A:ILE:HA	14	0.14
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	12	0.14
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	6	0.14
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	6	0.14
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	6	0.14
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	1	0.14
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	1	0.14
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	10	0.14
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	10	0.14
(1,2271)	1:144:A:THR:HA	1:150:A:GLN:HG2	9	0.14
(1,2250)	1:22:A:GLN:HE21	1:149:A:ARG:HB2	2	0.14
(1,2250)	1:22:A:GLN:HE21	1:149:A:ARG:HB3	2	0.14
(1,2250)	1:22:A:GLN:HE22	1:149:A:ARG:HB2	2	0.14
(1,2250)	1:22:A:GLN:HE22	1:149:A:ARG:HB3	2	0.14
(1,2229)	1:22:A:GLN:HE21	1:148:A:THR:HA	18	0.14
(1,2229)	1:22:A:GLN:HE22	1:148:A:THR:HA	18	0.14
(1,2223)	1:114:A:VAL:HA	1:144:A:THR:H	2	0.14
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	1	0.14
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	1	0.14
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	5	0.14
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	5	0.14
(1,2206)	1:32:A:TYR:HD1	1:34:A:PRO:HD2	6	0.14
(1,2206)	1:32:A:TYR:HD2	1:34:A:PRO:HD2	6	0.14
(1,2193)	1:143:A:GLU:HG3	1:144:A:THR:H	18	0.14
(1,2189)	1:4:A:TYR:HD1	1:52:A:LEU:H	15	0.14
(1,2189)	1:4:A:TYR:HD2	1:52:A:LEU:H	15	0.14
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	3	0.14
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE1	18	0.14
(1,2113)	1:47:A:ASP:H	1:157:A:TYR:HE2	18	0.14
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	4	0.14
(1,2067)	1:3:A:GLU:HA	1:4:A:TYR:HB2	6	0.14
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE1	5	0.14
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE2	5	0.14
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE1	12	0.14
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE2	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:132:A:ASP:HA	1:135:A:ARG:HE	2	0.14
(1,1999)	1:132:A:ASP:HA	1:135:A:ARG:HE	3	0.14
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG21	16	0.14
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG22	16	0.14
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG23	16	0.14
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG21	20	0.14
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG22	20	0.14
(1,1978)	1:43:A:GLN:HA	1:50:A:THR:HG23	20	0.14
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	9	0.14
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	9	0.14
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	12	0.14
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	12	0.14
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	19	0.14
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	19	0.14
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	15	0.14
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	6	0.14
(1,1902)	1:116:A:ASN:HA	1:144:A:THR:HA	7	0.14
(1,1847)	1:113:A:LEU:HB2	1:141:A:PHE:HB3	9	0.14
(1,1843)	1:111:A:MET:HA	1:139:A:ILE:HG12	17	0.14
(1,1822)	1:112:A:VAL:HA	1:139:A:ILE:HG12	4	0.14
(1,1814)	1:100:A:ILE:HD11	1:111:A:MET:HG2	9	0.14
(1,1814)	1:100:A:ILE:HD12	1:111:A:MET:HG2	9	0.14
(1,1814)	1:100:A:ILE:HD13	1:111:A:MET:HG2	9	0.14
(1,1792)	1:141:A:PHE:HZ	1:143:A:GLU:H	6	0.14
(1,1774)	1:24:A:ILE:HD11	1:41:A:ARG:HA	5	0.14
(1,1774)	1:24:A:ILE:HD12	1:41:A:ARG:HA	5	0.14
(1,1774)	1:24:A:ILE:HD13	1:41:A:ARG:HA	5	0.14
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	18	0.14
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	18	0.14
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	18	0.14
(1,1699)	1:72:A:MET:HG2	1:103:A:VAL:HB	15	0.14
(1,1699)	1:72:A:MET:HG3	1:103:A:VAL:HB	15	0.14
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE1	3	0.14
(1,1546)	1:137:A:TYR:H	1:137:A:TYR:HE2	3	0.14
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	2	0.14
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	2	0.14
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	2	0.14
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	2	0.14
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	2	0.14
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	2	0.14
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	11	0.14
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	11	0.14
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	11	0.14
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	11	0.14
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	11	0.14
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG2	2	0.14
(1,1508)	1:127:A:THR:HA	1:143:A:GLU:HG3	2	0.14
(1,1425)	1:79:A:LEU:HB2	1:81:A:VAL:HG11	3	0.14
(1,1425)	1:79:A:LEU:HB2	1:81:A:VAL:HG12	3	0.14
(1,1425)	1:79:A:LEU:HB2	1:81:A:VAL:HG13	3	0.14
(1,1425)	1:79:A:LEU:HB2	1:81:A:VAL:HG21	3	0.14
(1,1425)	1:79:A:LEU:HB2	1:81:A:VAL:HG22	3	0.14
(1,1425)	1:79:A:LEU:HB2	1:81:A:VAL:HG23	3	0.14
(1,1425)	1:79:A:LEU:HB3	1:81:A:VAL:HG11	3	0.14
(1,1425)	1:79:A:LEU:HB3	1:81:A:VAL:HG12	3	0.14
(1,1425)	1:79:A:LEU:HB3	1:81:A:VAL:HG13	3	0.14
(1,1425)	1:79:A:LEU:HB3	1:81:A:VAL:HG21	3	0.14
(1,1425)	1:79:A:LEU:HB3	1:81:A:VAL:HG22	3	0.14
(1,1425)	1:79:A:LEU:HB3	1:81:A:VAL:HG23	3	0.14
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	18	0.14
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	18	0.14
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	18	0.14
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	18	0.14
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	18	0.14
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	18	0.14
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG11	12	0.14
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG12	12	0.14
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG13	12	0.14
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG21	12	0.14
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG22	12	0.14
(1,1351)	1:73:A:ARG:HG2	1:103:A:VAL:HG23	12	0.14
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG11	12	0.14
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG12	12	0.14
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG13	12	0.14
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG21	12	0.14
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG22	12	0.14
(1,1351)	1:73:A:ARG:HG3	1:103:A:VAL:HG23	12	0.14
(1,1343)	1:135:A:ARG:H	1:135:A:ARG:HD2	16	0.14
(1,1343)	1:135:A:ARG:H	1:135:A:ARG:HD3	16	0.14
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD1	20	0.14
(1,1339)	1:95:A:HIS:HD2	1:96:A:TYR:HD2	20	0.14
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	2	0.14
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	2	0.14
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD1	16	0.14
(1,1287)	1:67:A:MET:HG2	1:71:A:TYR:HD2	16	0.14
(1,1281)	1:67:A:MET:HA	1:67:A:MET:HG3	10	0.14
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	7	0.14
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	18	0.14
(1,1251)	1:149:A:ARG:HB3	1:149:A:ARG:HE	12	0.14
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	4	0.14
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	4	0.14
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	4	0.14
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	4	0.14
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	4	0.14
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	4	0.14
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	4	0.14
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	4	0.14
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	4	0.14
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	3	0.14
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	3	0.14
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	3	0.14
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	3	0.14
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	3	0.14
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	3	0.14
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	3	0.14
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	3	0.14
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	3	0.14
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	3	0.14
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	3	0.14
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	3	0.14
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	3	0.14
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	3	0.14
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	3	0.14
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	3	0.14
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	3	0.14
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	3	0.14
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	15	0.14
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	15	0.14
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	15	0.14
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	15	0.14
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	15	0.14
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	15	0.14
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	15	0.14
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	15	0.14
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	15	0.14
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	15	0.14
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	15	0.14
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	15	0.14
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	15	0.14
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	15	0.14
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	15	0.14
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	15	0.14
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	15	0.14
(1,1205)	1:56:A:LEU:HD21	1:57:A:ASP:H	12	0.14
(1,1205)	1:56:A:LEU:HD22	1:57:A:ASP:H	12	0.14
(1,1205)	1:56:A:LEU:HD23	1:57:A:ASP:H	12	0.14
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	9	0.14
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	9	0.14
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	9	0.14
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	9	0.14
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	9	0.14
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	9	0.14
(1,1124)	1:113:A:LEU:HB2	1:142:A:ILE:H	17	0.14
(1,1107)	1:1:A:MET:HG3	1:51:A:CYS:HB3	9	0.14
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	10	0.14
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	10	0.14
(1,1081)	1:46:A:ILE:HD11	1:49:A:GLU:HB3	4	0.14
(1,1081)	1:46:A:ILE:HD12	1:49:A:GLU:HB3	4	0.14
(1,1081)	1:46:A:ILE:HD13	1:49:A:GLU:HB3	4	0.14
(1,1080)	1:1:A:MET:HG3	1:51:A:CYS:HA	3	0.14
(1,1074)	1:50:A:THR:HA	1:51:A:CYS:HB2	4	0.14
(1,1052)	1:128:A:LYS:H	1:131:A:GLN:HE22	3	0.14
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	19	0.14
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB2	5	0.14
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB3	5	0.14
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB2	5	0.14
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB3	5	0.14
(1,962)	1:43:A:GLN:H	1:43:A:GLN:HG3	15	0.14
(1,955)	1:43:A:GLN:H	1:43:A:GLN:HE21	4	0.14
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	9	0.14
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	9	0.14
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	13	0.14
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	13	0.14
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	20	0.14
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	5	0.14
(1,830)	1:146:A:ALA:HB1	2:201:A:GNP:HN1	9	0.14
(1,830)	1:146:A:ALA:HB2	2:201:A:GNP:HN1	9	0.14
(1,830)	1:146:A:ALA:HB3	2:201:A:GNP:HN1	9	0.14
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	1	0.14
(1,756)	1:64:A:TYR:H	1:65:A:SER:H	7	0.14
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG21	13	0.14
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG22	13	0.14
(1,733)	1:35:A:SER:HA	1:36:A:ILE:HG23	13	0.14
(1,663)	1:120:A:LEU:HA	1:121:A:PRO:HG2	12	0.14
(1,658)	1:120:A:LEU:HD11	1:121:A:PRO:HG2	9	0.14
(1,658)	1:120:A:LEU:HD12	1:121:A:PRO:HG2	9	0.14
(1,658)	1:120:A:LEU:HD13	1:121:A:PRO:HG2	9	0.14
(1,658)	1:120:A:LEU:HD21	1:121:A:PRO:HG2	9	0.14
(1,658)	1:120:A:LEU:HD22	1:121:A:PRO:HG2	9	0.14
(1,658)	1:120:A:LEU:HD23	1:121:A:PRO:HG2	9	0.14
(1,653)	1:34:A:PRO:HD3	1:35:A:SER:H	10	0.14
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB2	13	0.14
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB3	13	0.14
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB2	13	0.14
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB3	13	0.14
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB2	13	0.14
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB3	13	0.14
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB2	13	0.14
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB3	13	0.14
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB2	13	0.14
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB3	13	0.14
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB2	13	0.14
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB3	13	0.14
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	18	0.14
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	18	0.14
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	18	0.14
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	18	0.14
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	18	0.14
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	18	0.14
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG11	5	0.14
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG12	5	0.14
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG13	5	0.14
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG21	5	0.14
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG22	5	0.14
(1,577)	1:18:A:ALA:H	1:29:A:VAL:HG23	5	0.14
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD1	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:63:A:GLU:HG2	1:64:A:TYR:HD2	19	0.14
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD1	19	0.14
(1,563)	1:63:A:GLU:HG3	1:64:A:TYR:HD2	19	0.14
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	6	0.14
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	6	0.14
(1,482)	1:24:A:ILE:HG21	1:26:A:ASN:H	10	0.14
(1,482)	1:24:A:ILE:HG22	1:26:A:ASN:H	10	0.14
(1,482)	1:24:A:ILE:HG23	1:26:A:ASN:H	10	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG11	2	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG12	2	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG13	2	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG21	2	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG22	2	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG23	2	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG11	11	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG12	11	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG13	11	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG21	11	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG22	11	0.14
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG23	11	0.14
(1,478)	1:25:A:GLN:HB3	1:26:A:ASN:H	1	0.14
(1,478)	1:25:A:GLN:HB3	1:26:A:ASN:H	16	0.14
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	11	0.14
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	14	0.14
(1,319)	1:23:A:LEU:HB2	1:152:A:VAL:HB	19	0.14
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	15	0.14
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	15	0.14
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	15	0.14
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	5	0.14
(1,164)	1:83:A:ALA:H	1:86:A:ASN:HB2	9	0.14
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	1	0.14
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	1	0.14
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	1	0.14
(1,107)	1:96:A:TYR:HA	1:100:A:ILE:H	7	0.14
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	13	0.14
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	13	0.14
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	13	0.14
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	13	0.14
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	13	0.14
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	13	0.14
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG21	4	0.13
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG22	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3326)	1:10:A:GLY:HA2	1:93:A:ILE:HG23	4	0.13
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG21	4	0.13
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG22	4	0.13
(1,3326)	1:10:A:GLY:HA3	1:93:A:ILE:HG23	4	0.13
(1,3301)	1:120:A:LEU:HD11	1:122:A:SER:H	8	0.13
(1,3301)	1:120:A:LEU:HD12	1:122:A:SER:H	8	0.13
(1,3301)	1:120:A:LEU:HD13	1:122:A:SER:H	8	0.13
(1,3301)	1:120:A:LEU:HD21	1:122:A:SER:H	8	0.13
(1,3301)	1:120:A:LEU:HD22	1:122:A:SER:H	8	0.13
(1,3301)	1:120:A:LEU:HD23	1:122:A:SER:H	8	0.13
(1,3292)	1:120:A:LEU:H	1:120:A:LEU:HD11	16	0.13
(1,3292)	1:120:A:LEU:H	1:120:A:LEU:HD12	16	0.13
(1,3292)	1:120:A:LEU:H	1:120:A:LEU:HD13	16	0.13
(1,3292)	1:120:A:LEU:H	1:120:A:LEU:HD21	16	0.13
(1,3292)	1:120:A:LEU:H	1:120:A:LEU:HD22	16	0.13
(1,3292)	1:120:A:LEU:H	1:120:A:LEU:HD23	16	0.13
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG21	9	0.13
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG22	9	0.13
(1,3238)	1:115:A:GLY:H	1:144:A:THR:HG23	9	0.13
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB2	2	0.13
(1,3189)	1:118:A:SER:H	1:145:A:SER:HB3	2	0.13
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	19	0.13
(1,3175)	1:1:A:MET:HG2	1:51:A:CYS:HA	17	0.13
(1,3131)	1:124:A:THR:H	1:126:A:ASP:H	20	0.13
(1,3128)	1:1:A:MET:HA	1:51:A:CYS:HA	5	0.13
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	2	0.13
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	4	0.13
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	14	0.13
(1,3027)	1:130:A:ALA:H	1:131:A:GLN:HE21	9	0.13
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	18	0.13
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	18	0.13
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	18	0.13
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	18	0.13
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	18	0.13
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	18	0.13
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	4	0.13
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	9	0.13
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	18	0.13
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD1	16	0.13
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD2	16	0.13
(1,2927)	1:90:A:PHE:HZ	1:134:A:ALA:H	10	0.13
(1,2918)	1:133:A:LEU:HD11	1:136:A:SER:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2918)	1:133:A:LEU:HD12	1:136:A:SER:H	13	0.13
(1,2918)	1:133:A:LEU:HD13	1:136:A:SER:H	13	0.13
(1,2918)	1:133:A:LEU:HD21	1:136:A:SER:H	13	0.13
(1,2918)	1:133:A:LEU:HD22	1:136:A:SER:H	13	0.13
(1,2918)	1:133:A:LEU:HD23	1:136:A:SER:H	13	0.13
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	12	0.13
(1,2837)	1:113:A:LEU:H	1:142:A:ILE:H	6	0.13
(1,2803)	1:116:A:ASN:HA	1:144:A:THR:H	15	0.13
(1,2797)	1:143:A:GLU:HG2	1:144:A:THR:H	9	0.13
(1,2797)	1:143:A:GLU:HG3	1:144:A:THR:H	9	0.13
(1,2747)	1:118:A:SER:H	1:146:A:ALA:H	6	0.13
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG21	3	0.13
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG22	3	0.13
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG23	3	0.13
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG21	18	0.13
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG22	18	0.13
(1,2743)	1:146:A:ALA:H	1:148:A:THR:HG23	18	0.13
(1,2735)	1:117:A:LYS:HA	1:146:A:ALA:H	10	0.13
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	13	0.13
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	13	0.13
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	13	0.13
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	13	0.13
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	13	0.13
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	13	0.13
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	18	0.13
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	18	0.13
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	18	0.13
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	18	0.13
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	18	0.13
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	18	0.13
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE1	3	0.13
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE2	3	0.13
(1,2677)	1:97:A:ARG:HA	1:111:A:MET:HE3	3	0.13
(1,2652)	1:148:A:THR:HB	1:150:A:GLN:H	15	0.13
(1,2650)	1:72:A:MET:HE1	1:100:A:ILE:H	14	0.13
(1,2650)	1:72:A:MET:HE2	1:100:A:ILE:H	14	0.13
(1,2650)	1:72:A:MET:HE3	1:100:A:ILE:H	14	0.13
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	11	0.13
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	11	0.13
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	11	0.13
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	12	0.13
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	12	0.13
(1,2607)	1:21:A:ILE:HA	1:27:A:HIS:H	12	0.13
(1,2569)	1:156:A:PHE:H	1:156:A:PHE:HE1	2	0.13
(1,2569)	1:156:A:PHE:H	1:156:A:PHE:HE2	2	0.13
(1,2554)	1:100:A:ILE:HG21	1:111:A:MET:HG3	11	0.13
(1,2554)	1:100:A:ILE:HG22	1:111:A:MET:HG3	11	0.13
(1,2554)	1:100:A:ILE:HG23	1:111:A:MET:HG3	11	0.13
(1,2554)	1:100:A:ILE:HG21	1:111:A:MET:HG3	12	0.13
(1,2554)	1:100:A:ILE:HG22	1:111:A:MET:HG3	12	0.13
(1,2554)	1:100:A:ILE:HG23	1:111:A:MET:HG3	12	0.13
(1,2546)	1:78:A:PHE:HE1	1:100:A:ILE:HA	10	0.13
(1,2546)	1:78:A:PHE:HE2	1:100:A:ILE:HA	10	0.13
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	12	0.13
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	12	0.13
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	12	0.13
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	14	0.13
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	14	0.13
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	14	0.13
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	7	0.13
(1,2514)	1:157:A:TYR:HA	1:160:A:VAL:HA	19	0.13
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	10	0.13
(1,2417)	1:4:A:TYR:HD1	1:163:A:ILE:HA	17	0.13
(1,2417)	1:4:A:TYR:HD2	1:163:A:ILE:HA	17	0.13
(1,2417)	1:4:A:TYR:HD1	1:163:A:ILE:HA	19	0.13
(1,2417)	1:4:A:TYR:HD2	1:163:A:ILE:HA	19	0.13
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	4	0.13
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	4	0.13
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	17	0.13
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	17	0.13
(1,2306)	1:135:A:ARG:H	1:135:A:ARG:HE	18	0.13
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	18	0.13
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	18	0.13
(1,2267)	1:150:A:GLN:HG2	1:151:A:GLY:H	13	0.13
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	2	0.13
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	2	0.13
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	2	0.13
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	8	0.13
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	6	0.13
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	3	0.13
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	3	0.13
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	3	0.13
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	17	0.13
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	17	0.13
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	17	0.13
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	17	0.13
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	17	0.13
(1,2117)	1:16:A:LYS:HB3	1:17:A:SER:H	9	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	13	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	13	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	13	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	13	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	13	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	13	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	15	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	15	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	15	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	15	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	15	0.13
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	15	0.13
(1,2093)	1:159:A:LEU:HA	1:162:A:GLU:HG3	11	0.13
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB1	10	0.13
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB2	10	0.13
(1,2073)	1:90:A:PHE:HD1	1:130:A:ALA:HB3	10	0.13
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB1	10	0.13
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB2	10	0.13
(1,2073)	1:90:A:PHE:HD2	1:130:A:ALA:HB3	10	0.13
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE1	3	0.13
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE2	3	0.13
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	19	0.13
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	19	0.13
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	19	0.13
(1,2050)	1:128:A:LYS:H	1:129:A:GLN:HG2	15	0.13
(1,2036)	1:129:A:GLN:HA	1:132:A:ASP:HB2	20	0.13
(1,2036)	1:129:A:GLN:HA	1:132:A:ASP:HB3	20	0.13
(1,1971)	1:6:A:LEU:HB2	1:78:A:PHE:HA	8	0.13
(1,1971)	1:6:A:LEU:HB3	1:78:A:PHE:HA	8	0.13
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	2	0.13
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	2	0.13
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG21	6	0.13
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG22	6	0.13
(1,1869)	1:116:A:ASN:HA	1:144:A:THR:HG23	6	0.13
(1,1808)	1:80:A:CYS:HB2	1:111:A:MET:HG2	19	0.13
(1,1808)	1:80:A:CYS:HB3	1:111:A:MET:HG2	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1731)	1:100:A:ILE:HG21	1:104:A:LYS:HE2	16	0.13
(1,1731)	1:100:A:ILE:HG22	1:104:A:LYS:HE2	16	0.13
(1,1731)	1:100:A:ILE:HG23	1:104:A:LYS:HE2	16	0.13
(1,1693)	1:72:A:MET:HB2	1:103:A:VAL:HA	1	0.13
(1,1693)	1:72:A:MET:HB3	1:103:A:VAL:HA	1	0.13
(1,1645)	1:128:A:LYS:HG2	1:129:A:GLN:HB2	11	0.13
(1,1645)	1:128:A:LYS:HG3	1:129:A:GLN:HB2	11	0.13
(1,1640)	1:97:A:ARG:HG2	1:98:A:GLU:HG2	13	0.13
(1,1640)	1:97:A:ARG:HG2	1:98:A:GLU:HG3	13	0.13
(1,1640)	1:97:A:ARG:HG3	1:98:A:GLU:HG2	13	0.13
(1,1640)	1:97:A:ARG:HG3	1:98:A:GLU:HG3	13	0.13
(1,1623)	1:150:A:GLN:HB3	1:151:A:GLY:HA3	17	0.13
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	4	0.13
(1,1584)	1:93:A:ILE:HG21	1:137:A:TYR:HD1	14	0.13
(1,1584)	1:93:A:ILE:HG21	1:137:A:TYR:HD2	14	0.13
(1,1584)	1:93:A:ILE:HG22	1:137:A:TYR:HD1	14	0.13
(1,1584)	1:93:A:ILE:HG22	1:137:A:TYR:HD2	14	0.13
(1,1584)	1:93:A:ILE:HG23	1:137:A:TYR:HD1	14	0.13
(1,1584)	1:93:A:ILE:HG23	1:137:A:TYR:HD2	14	0.13
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG21	11	0.13
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG22	11	0.13
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG23	11	0.13
(1,1547)	1:82:A:PHE:HA	1:90:A:PHE:HA	17	0.13
(1,1525)	1:77:A:GLY:H	1:163:A:ILE:HD11	8	0.13
(1,1525)	1:77:A:GLY:H	1:163:A:ILE:HD12	8	0.13
(1,1525)	1:77:A:GLY:H	1:163:A:ILE:HD13	8	0.13
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	19	0.13
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	19	0.13
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	19	0.13
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	19	0.13
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	19	0.13
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	19	0.13
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	19	0.13
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	19	0.13
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	19	0.13
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	19	0.13
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	19	0.13
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	19	0.13
(1,1436)	1:79:A:LEU:HD11	1:156:A:PHE:HB3	10	0.13
(1,1436)	1:79:A:LEU:HD12	1:156:A:PHE:HB3	10	0.13
(1,1436)	1:79:A:LEU:HD13	1:156:A:PHE:HB3	10	0.13
(1,1436)	1:79:A:LEU:HD21	1:156:A:PHE:HB3	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:79:A:LEU:HD22	1:156:A:PHE:HB3	10	0.13
(1,1436)	1:79:A:LEU:HD23	1:156:A:PHE:HB3	10	0.13
(1,1412)	1:75:A:GLY:HA3	1:76:A:GLU:HG3	9	0.13
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	10	0.13
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	18	0.13
(1,1396)	1:99:A:GLN:H	1:100:A:ILE:HB	15	0.13
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG21	16	0.13
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG22	16	0.13
(1,1367)	1:56:A:LEU:HD11	1:74:A:THR:HG23	16	0.13
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG21	16	0.13
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG22	16	0.13
(1,1367)	1:56:A:LEU:HD12	1:74:A:THR:HG23	16	0.13
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG21	16	0.13
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG22	16	0.13
(1,1367)	1:56:A:LEU:HD13	1:74:A:THR:HG23	16	0.13
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG21	16	0.13
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG22	16	0.13
(1,1367)	1:56:A:LEU:HD21	1:74:A:THR:HG23	16	0.13
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG21	16	0.13
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG22	16	0.13
(1,1367)	1:56:A:LEU:HD22	1:74:A:THR:HG23	16	0.13
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG21	16	0.13
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG22	16	0.13
(1,1367)	1:56:A:LEU:HD23	1:74:A:THR:HG23	16	0.13
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD2	6	0.13
(1,1340)	1:99:A:GLN:HA	1:102:A:ARG:HD3	6	0.13
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE2	2	0.13
(1,1334)	1:101:A:LYS:HA	1:101:A:LYS:HE3	2	0.13
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG11	10	0.13
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG12	10	0.13
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG13	10	0.13
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG21	10	0.13
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG22	10	0.13
(1,1333)	1:101:A:LYS:HA	1:109:A:VAL:HG23	10	0.13
(1,1331)	1:95:A:HIS:HA	1:99:A:GLN:H	3	0.13
(1,1281)	1:67:A:MET:HA	1:67:A:MET:HG3	13	0.13
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	10	0.13
(1,1268)	1:96:A:TYR:H	1:97:A:ARG:HB3	12	0.13
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE21	2	0.13
(1,1227)	1:61:A:GLN:HA	1:61:A:GLN:HE22	2	0.13
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE1	6	0.13
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD11	20	0.13
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD12	20	0.13
(1,1201)	1:9:A:VAL:HB	1:100:A:ILE:HD13	20	0.13
(1,1199)	1:56:A:LEU:HD11	1:59:A:ALA:H	17	0.13
(1,1199)	1:56:A:LEU:HD12	1:59:A:ALA:H	17	0.13
(1,1199)	1:56:A:LEU:HD13	1:59:A:ALA:H	17	0.13
(1,1199)	1:56:A:LEU:HD21	1:59:A:ALA:H	17	0.13
(1,1199)	1:56:A:LEU:HD22	1:59:A:ALA:H	17	0.13
(1,1199)	1:56:A:LEU:HD23	1:59:A:ALA:H	17	0.13
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	19	0.13
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	19	0.13
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	19	0.13
(1,1130)	1:51:A:CYS:HB2	1:52:A:LEU:HB2	3	0.13
(1,1079)	1:2:A:THR:HB	1:51:A:CYS:HA	14	0.13
(1,1077)	1:4:A:TYR:HE1	1:51:A:CYS:HA	20	0.13
(1,1077)	1:4:A:TYR:HE2	1:51:A:CYS:HA	20	0.13
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	7	0.13
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	19	0.13
(1,1036)	1:46:A:ILE:HB	1:49:A:GLU:HB2	3	0.13
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB2	11	0.13
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB3	11	0.13
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB2	11	0.13
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB3	11	0.13
(1,980)	1:44:A:VAL:HB	1:46:A:ILE:HD11	16	0.13
(1,980)	1:44:A:VAL:HB	1:46:A:ILE:HD12	16	0.13
(1,980)	1:44:A:VAL:HB	1:46:A:ILE:HD13	16	0.13
(1,957)	1:43:A:GLN:HG2	1:44:A:VAL:H	12	0.13
(1,957)	1:43:A:GLN:HG3	1:44:A:VAL:H	12	0.13
(1,955)	1:43:A:GLN:H	1:43:A:GLN:HE21	12	0.13
(1,952)	1:1:A:MET:HE1	1:43:A:GLN:HE21	14	0.13
(1,952)	1:1:A:MET:HE2	1:43:A:GLN:HE21	14	0.13
(1,952)	1:1:A:MET:HE3	1:43:A:GLN:HE21	14	0.13
(1,947)	1:83:A:ALA:H	1:90:A:PHE:H	18	0.13
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	17	0.13
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	1	0.13
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	1	0.13
(1,922)	1:42:A:LYS:HE2	1:43:A:GLN:H	7	0.13
(1,922)	1:42:A:LYS:HE3	1:43:A:GLN:H	7	0.13
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	12	0.13
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	12	0.13
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	12	0.13
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	10	0.13
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	11	0.13
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	17	0.13
(1,885)	1:161:A:ARG:HA	1:164:A:ARG:HE	13	0.13
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	2	0.13
(1,843)	1:41:A:ARG:HD2	1:54:A:ASP:HA	7	0.13
(1,843)	1:41:A:ARG:HD3	1:54:A:ASP:HA	7	0.13
(1,829)	1:146:A:ALA:H	2:201:A:GNP:HN1	16	0.13
(1,824)	1:119:A:ASP:H	2:201:A:GNP:HN1	7	0.13
(1,821)	1:117:A:LYS:H	2:201:A:GNP:HN1	12	0.13
(1,742)	1:65:A:SER:H	1:65:A:SER:HB2	3	0.13
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	14	0.13
(1,643)	1:78:A:PHE:H	1:110:A:PRO:HB2	5	0.13
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB2	9	0.13
(1,594)	1:6:A:LEU:HD11	1:54:A:ASP:HB3	9	0.13
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB2	9	0.13
(1,594)	1:6:A:LEU:HD12	1:54:A:ASP:HB3	9	0.13
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB2	9	0.13
(1,594)	1:6:A:LEU:HD13	1:54:A:ASP:HB3	9	0.13
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB2	9	0.13
(1,594)	1:6:A:LEU:HD21	1:54:A:ASP:HB3	9	0.13
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB2	9	0.13
(1,594)	1:6:A:LEU:HD22	1:54:A:ASP:HB3	9	0.13
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB2	9	0.13
(1,594)	1:6:A:LEU:HD23	1:54:A:ASP:HB3	9	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	10	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	10	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	10	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	10	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	10	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	10	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	20	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	20	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	20	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	20	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	20	0.13
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	20	0.13
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	5	0.13
(1,579)	1:15:A:GLY:H	1:18:A:ALA:H	11	0.13
(1,498)	1:28:A:PHE:HD1	1:29:A:VAL:HA	2	0.13
(1,498)	1:28:A:PHE:HD2	1:29:A:VAL:HA	2	0.13
(1,482)	1:24:A:ILE:HG21	1:26:A:ASN:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:24:A:ILE:HG22	1:26:A:ASN:H	11	0.13
(1,482)	1:24:A:ILE:HG23	1:26:A:ASN:H	11	0.13
(1,478)	1:25:A:GLN:HB3	1:26:A:ASN:H	12	0.13
(1,478)	1:25:A:GLN:HB3	1:26:A:ASN:H	14	0.13
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	13	0.13
(1,377)	1:24:A:ILE:HD11	1:43:A:GLN:H	4	0.13
(1,377)	1:24:A:ILE:HD12	1:43:A:GLN:H	4	0.13
(1,377)	1:24:A:ILE:HD13	1:43:A:GLN:H	4	0.13
(1,323)	1:44:A:VAL:H	1:52:A:LEU:HA	8	0.13
(1,312)	1:7:A:VAL:H	1:77:A:GLY:HA2	10	0.13
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE1	16	0.13
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE2	16	0.13
(1,289)	1:24:A:ILE:HD11	1:40:A:TYR:HB2	5	0.13
(1,289)	1:24:A:ILE:HD12	1:40:A:TYR:HB2	5	0.13
(1,289)	1:24:A:ILE:HD13	1:40:A:TYR:HB2	5	0.13
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	7	0.13
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	8	0.13
(1,285)	1:2:A:THR:H	1:51:A:CYS:H	9	0.13
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE1	12	0.13
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE2	12	0.13
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE1	17	0.13
(1,284)	1:2:A:THR:H	1:4:A:TYR:HE2	17	0.13
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD11	16	0.13
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD12	16	0.13
(1,264)	1:24:A:ILE:HA	1:24:A:ILE:HD13	16	0.13
(1,263)	1:3:A:GLU:H	1:52:A:LEU:HB2	3	0.13
(1,258)	1:7:A:VAL:HG11	1:72:A:MET:HA	5	0.13
(1,258)	1:7:A:VAL:HG12	1:72:A:MET:HA	5	0.13
(1,258)	1:7:A:VAL:HG13	1:72:A:MET:HA	5	0.13
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	1	0.13
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	1	0.13
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	1	0.13
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	6	0.13
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	6	0.13
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	6	0.13
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	6	0.13
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	6	0.13
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	6	0.13
(1,241)	1:24:A:ILE:HD11	1:40:A:TYR:HA	18	0.13
(1,241)	1:24:A:ILE:HD12	1:40:A:TYR:HA	18	0.13
(1,241)	1:24:A:ILE:HD13	1:40:A:TYR:HA	18	0.13
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD11	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD12	18	0.13
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD13	18	0.13
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD21	18	0.13
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD22	18	0.13
(1,212)	1:41:A:ARG:HE	1:52:A:LEU:HD23	18	0.13
(1,197)	1:92:A:ASP:H	1:93:A:ILE:HD11	14	0.13
(1,197)	1:92:A:ASP:H	1:93:A:ILE:HD12	14	0.13
(1,197)	1:92:A:ASP:H	1:93:A:ILE:HD13	14	0.13
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	9	0.13
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	9	0.13
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	9	0.13
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	9	0.13
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	9	0.13
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	9	0.13
(1,179)	1:19:A:LEU:HD11	1:81:A:VAL:HA	18	0.13
(1,179)	1:19:A:LEU:HD12	1:81:A:VAL:HA	18	0.13
(1,179)	1:19:A:LEU:HD13	1:81:A:VAL:HA	18	0.13
(1,179)	1:19:A:LEU:HD21	1:81:A:VAL:HA	18	0.13
(1,179)	1:19:A:LEU:HD22	1:81:A:VAL:HA	18	0.13
(1,179)	1:19:A:LEU:HD23	1:81:A:VAL:HA	18	0.13
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	6	0.13
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	6	0.13
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	6	0.13
(1,150)	1:28:A:PHE:HZ	2:201:A:GNP:H1'	13	0.13
(1,129)	1:97:A:ARG:H	1:97:A:ARG:HB2	3	0.13
(1,103)	1:16:A:LYS:HA	1:19:A:LEU:HB3	5	0.13
(1,86)	1:15:A:GLY:HA2	1:116:A:ASN:HD22	6	0.13
(1,46)	1:18:A:ALA:HB1	2:201:A:GNP:H1'	18	0.13
(1,46)	1:18:A:ALA:HB2	2:201:A:GNP:H1'	18	0.13
(1,46)	1:18:A:ALA:HB3	2:201:A:GNP:H1'	18	0.13
(1,20)	1:107:A:GLU:HB2	1:108:A:ASP:H	8	0.13
(1,20)	1:107:A:GLU:HB3	1:108:A:ASP:H	8	0.13
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	10	0.12
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG2	5	0.12
(1,3311)	1:7:A:VAL:HG11	1:72:A:MET:HG3	5	0.12
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG2	5	0.12
(1,3311)	1:7:A:VAL:HG12	1:72:A:MET:HG3	5	0.12
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG2	5	0.12
(1,3311)	1:7:A:VAL:HG13	1:72:A:MET:HG3	5	0.12
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG2	5	0.12
(1,3311)	1:7:A:VAL:HG21	1:72:A:MET:HG3	5	0.12
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:7:A:VAL:HG22	1:72:A:MET:HG3	5	0.12
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG2	5	0.12
(1,3311)	1:7:A:VAL:HG23	1:72:A:MET:HG3	5	0.12
(1,3302)	1:120:A:LEU:HD21	1:122:A:SER:H	4	0.12
(1,3302)	1:120:A:LEU:HD22	1:122:A:SER:H	4	0.12
(1,3302)	1:120:A:LEU:HD23	1:122:A:SER:H	4	0.12
(1,3301)	1:120:A:LEU:HD11	1:122:A:SER:H	14	0.12
(1,3301)	1:120:A:LEU:HD12	1:122:A:SER:H	14	0.12
(1,3301)	1:120:A:LEU:HD13	1:122:A:SER:H	14	0.12
(1,3301)	1:120:A:LEU:HD21	1:122:A:SER:H	14	0.12
(1,3301)	1:120:A:LEU:HD22	1:122:A:SER:H	14	0.12
(1,3301)	1:120:A:LEU:HD23	1:122:A:SER:H	14	0.12
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD1	18	0.12
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD2	18	0.12
(1,3214)	1:114:A:VAL:HB	1:116:A:ASN:H	3	0.12
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD11	12	0.12
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD12	12	0.12
(1,3160)	1:120:A:LEU:H	1:120:A:LEU:HD13	12	0.12
(1,3158)	1:1:A:MET:HA	1:1:A:MET:HG3	10	0.12
(1,3144)	1:1:A:MET:HE1	1:52:A:LEU:H	16	0.12
(1,3144)	1:1:A:MET:HE2	1:52:A:LEU:H	16	0.12
(1,3144)	1:1:A:MET:HE3	1:52:A:LEU:H	16	0.12
(1,3142)	1:1:A:MET:HB3	1:50:A:THR:HG21	18	0.12
(1,3142)	1:1:A:MET:HB3	1:50:A:THR:HG22	18	0.12
(1,3142)	1:1:A:MET:HB3	1:50:A:THR:HG23	18	0.12
(1,3139)	1:41:A:ARG:HE	1:42:A:LYS:H	2	0.12
(1,3136)	1:1:A:MET:HB3	1:51:A:CYS:HA	15	0.12
(1,3128)	1:1:A:MET:HA	1:51:A:CYS:HA	2	0.12
(1,3116)	1:85:A:ASN:HB2	1:124:A:THR:H	16	0.12
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	11	0.12
(1,2998)	1:129:A:GLN:H	1:132:A:ASP:HB2	20	0.12
(1,2998)	1:129:A:GLN:H	1:132:A:ASP:HB3	20	0.12
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	3	0.12
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	3	0.12
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	3	0.12
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	3	0.12
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	3	0.12
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	3	0.12
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	18	0.12
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	19	0.12
(1,2944)	1:134:A:ALA:HA	1:139:A:ILE:HG12	7	0.12
(1,2918)	1:133:A:LEU:HD11	1:136:A:SER:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2918)	1:133:A:LEU:HD12	1:136:A:SER:H	19	0.12
(1,2918)	1:133:A:LEU:HD13	1:136:A:SER:H	19	0.12
(1,2918)	1:133:A:LEU:HD21	1:136:A:SER:H	19	0.12
(1,2918)	1:133:A:LEU:HD22	1:136:A:SER:H	19	0.12
(1,2918)	1:133:A:LEU:HD23	1:136:A:SER:H	19	0.12
(1,2911)	1:48:A:GLY:H	1:49:A:GLU:HB2	3	0.12
(1,2897)	1:75:A:GLY:H	1:77:A:GLY:H	2	0.12
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	7	0.12
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	7	0.12
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	7	0.12
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	7	0.12
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	7	0.12
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	7	0.12
(1,2818)	1:113:A:LEU:HB3	1:142:A:ILE:H	6	0.12
(1,2818)	1:113:A:LEU:HB3	1:142:A:ILE:H	16	0.12
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	16	0.12
(1,2788)	1:116:A:ASN:HA	1:145:A:SER:H	10	0.12
(1,2768)	1:145:A:SER:H	1:150:A:GLN:HG3	4	0.12
(1,2735)	1:117:A:LYS:HA	1:146:A:ALA:H	6	0.12
(1,2712)	1:11:A:ALA:HB1	1:89:A:SER:H	20	0.12
(1,2712)	1:11:A:ALA:HB2	1:89:A:SER:H	20	0.12
(1,2712)	1:11:A:ALA:HB3	1:89:A:SER:H	20	0.12
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	1	0.12
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	1	0.12
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	1	0.12
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	1	0.12
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	1	0.12
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	1	0.12
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB1	7	0.12
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB2	7	0.12
(1,2702)	1:130:A:ALA:HB1	1:134:A:ALA:HB3	7	0.12
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB1	7	0.12
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB2	7	0.12
(1,2702)	1:130:A:ALA:HB2	1:134:A:ALA:HB3	7	0.12
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB1	7	0.12
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB2	7	0.12
(1,2702)	1:130:A:ALA:HB3	1:134:A:ALA:HB3	7	0.12
(1,2690)	1:148:A:THR:H	1:150:A:GLN:HB2	9	0.12
(1,2690)	1:148:A:THR:H	1:150:A:GLN:HB2	12	0.12
(1,2683)	1:72:A:MET:H	1:75:A:GLY:H	15	0.12
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG2	6	0.12
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2666)	1:22:A:GLN:HE21	1:150:A:GLN:H	11	0.12
(1,2666)	1:22:A:GLN:HE22	1:150:A:GLN:H	11	0.12
(1,2650)	1:72:A:MET:HE1	1:100:A:ILE:H	13	0.12
(1,2650)	1:72:A:MET:HE2	1:100:A:ILE:H	13	0.12
(1,2650)	1:72:A:MET:HE3	1:100:A:ILE:H	13	0.12
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	10	0.12
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	10	0.12
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	10	0.12
(1,2648)	1:142:A:ILE:HD11	1:151:A:GLY:H	20	0.12
(1,2648)	1:142:A:ILE:HD12	1:151:A:GLY:H	20	0.12
(1,2648)	1:142:A:ILE:HD13	1:151:A:GLY:H	20	0.12
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	19	0.12
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	19	0.12
(1,2630)	1:150:A:GLN:HG3	1:152:A:VAL:H	10	0.12
(1,2606)	1:21:A:ILE:HA	1:40:A:TYR:HD1	19	0.12
(1,2606)	1:21:A:ILE:HA	1:40:A:TYR:HD2	19	0.12
(1,2588)	1:153:A:ASP:HB2	1:155:A:ALA:H	7	0.12
(1,2588)	1:153:A:ASP:HB3	1:155:A:ALA:H	7	0.12
(1,2572)	1:72:A:MET:HG2	1:100:A:ILE:HG21	2	0.12
(1,2572)	1:72:A:MET:HG2	1:100:A:ILE:HG22	2	0.12
(1,2572)	1:72:A:MET:HG2	1:100:A:ILE:HG23	2	0.12
(1,2572)	1:72:A:MET:HG3	1:100:A:ILE:HG21	2	0.12
(1,2572)	1:72:A:MET:HG3	1:100:A:ILE:HG22	2	0.12
(1,2572)	1:72:A:MET:HG3	1:100:A:ILE:HG23	2	0.12
(1,2559)	1:17:A:SER:HA	1:20:A:THR:HA	12	0.12
(1,2542)	1:100:A:ILE:HG21	1:104:A:LYS:HA	14	0.12
(1,2542)	1:100:A:ILE:HG22	1:104:A:LYS:HA	14	0.12
(1,2542)	1:100:A:ILE:HG23	1:104:A:LYS:HA	14	0.12
(1,2540)	1:72:A:MET:HE1	1:100:A:ILE:HA	14	0.12
(1,2540)	1:72:A:MET:HE2	1:100:A:ILE:HA	14	0.12
(1,2540)	1:72:A:MET:HE3	1:100:A:ILE:HA	14	0.12
(1,2528)	1:4:A:TYR:HE1	1:164:A:ARG:H	20	0.12
(1,2528)	1:4:A:TYR:HE2	1:164:A:ARG:H	20	0.12
(1,2523)	1:163:A:ILE:HD11	1:164:A:ARG:H	10	0.12
(1,2523)	1:163:A:ILE:HD12	1:164:A:ARG:H	10	0.12
(1,2523)	1:163:A:ILE:HD13	1:164:A:ARG:H	10	0.12
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB1	19	0.12
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB2	19	0.12
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB3	19	0.12
(1,2482)	1:168:A:GLU:HA	1:169:A:LYS:H	1	0.12
(1,2477)	1:164:A:ARG:HA	1:167:A:LYS:HG2	1	0.12
(1,2477)	1:164:A:ARG:HA	1:167:A:LYS:HG3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2473)	1:58:A:THR:HB	1:59:A:ALA:H	4	0.12
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	6	0.12
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	9	0.12
(1,2415)	1:77:A:GLY:HA3	1:163:A:ILE:HA	5	0.12
(1,2415)	1:77:A:GLY:HA3	1:163:A:ILE:HA	7	0.12
(1,2415)	1:77:A:GLY:HA3	1:163:A:ILE:HA	8	0.12
(1,2411)	1:144:A:THR:HB	1:152:A:VAL:HB	3	0.12
(1,2406)	1:157:A:TYR:HD1	1:160:A:VAL:H	5	0.12
(1,2406)	1:157:A:TYR:HD2	1:160:A:VAL:H	5	0.12
(1,2312)	1:154:A:ASP:HA	1:157:A:TYR:HD1	3	0.12
(1,2312)	1:154:A:ASP:HA	1:157:A:TYR:HD2	3	0.12
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG21	20	0.12
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG22	20	0.12
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG23	20	0.12
(1,2223)	1:114:A:VAL:HA	1:144:A:THR:H	17	0.12
(1,2220)	1:147:A:LYS:HG2	1:148:A:THR:HA	1	0.12
(1,2220)	1:147:A:LYS:HG3	1:148:A:THR:HA	1	0.12
(1,2175)	1:148:A:THR:H	2:201:A:GNP:HN1	7	0.12
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	14	0.12
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG21	5	0.12
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG22	5	0.12
(1,2142)	1:140:A:PRO:HB3	1:158:A:THR:HG23	5	0.12
(1,2121)	1:134:A:ALA:HB1	1:139:A:ILE:HB	20	0.12
(1,2121)	1:134:A:ALA:HB2	1:139:A:ILE:HB	20	0.12
(1,2121)	1:134:A:ALA:HB3	1:139:A:ILE:HB	20	0.12
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	2	0.12
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	2	0.12
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	2	0.12
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	2	0.12
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	2	0.12
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	2	0.12
(1,2078)	1:129:A:GLN:HB2	1:130:A:ALA:HB1	11	0.12
(1,2078)	1:129:A:GLN:HB2	1:130:A:ALA:HB2	11	0.12
(1,2078)	1:129:A:GLN:HB2	1:130:A:ALA:HB3	11	0.12
(1,2074)	1:90:A:PHE:HE1	1:130:A:ALA:HB1	12	0.12
(1,2074)	1:90:A:PHE:HE1	1:130:A:ALA:HB2	12	0.12
(1,2074)	1:90:A:PHE:HE1	1:130:A:ALA:HB3	12	0.12
(1,2074)	1:90:A:PHE:HE2	1:130:A:ALA:HB1	12	0.12
(1,2074)	1:90:A:PHE:HE2	1:130:A:ALA:HB2	12	0.12
(1,2074)	1:90:A:PHE:HE2	1:130:A:ALA:HB3	12	0.12
(1,2067)	1:3:A:GLU:HA	1:4:A:TYR:HB2	19	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	8	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	8	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	12	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	12	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	12	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	20	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	20	0.12
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	20	0.12
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG11	16	0.12
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG12	16	0.12
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG13	16	0.12
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG21	16	0.12
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG22	16	0.12
(1,1993)	1:85:A:ASN:HA	1:125:A:VAL:HG23	16	0.12
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	8	0.12
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	16	0.12
(1,1977)	1:85:A:ASN:HA	1:124:A:THR:HA	17	0.12
(1,1931)	1:10:A:GLY:HA2	1:12:A:GLY:H	18	0.12
(1,1931)	1:10:A:GLY:HA3	1:12:A:GLY:H	18	0.12
(1,1920)	1:12:A:GLY:H	1:60:A:GLY:H	13	0.12
(1,1907)	1:117:A:LYS:H	1:118:A:SER:HB2	11	0.12
(1,1907)	1:117:A:LYS:H	1:118:A:SER:HB3	11	0.12
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	5	0.12
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	5	0.12
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	14	0.12
(1,1823)	1:112:A:VAL:HA	1:162:A:GLU:HG3	11	0.12
(1,1817)	1:112:A:VAL:HA	1:139:A:ILE:HA	10	0.12
(1,1793)	1:130:A:ALA:HB1	1:131:A:GLN:HB2	15	0.12
(1,1793)	1:130:A:ALA:HB2	1:131:A:GLN:HB2	15	0.12
(1,1793)	1:130:A:ALA:HB3	1:131:A:GLN:HB2	15	0.12
(1,1774)	1:24:A:ILE:HD11	1:41:A:ARG:HA	6	0.12
(1,1774)	1:24:A:ILE:HD12	1:41:A:ARG:HA	6	0.12
(1,1774)	1:24:A:ILE:HD13	1:41:A:ARG:HA	6	0.12
(1,1774)	1:24:A:ILE:HD11	1:41:A:ARG:HA	7	0.12
(1,1774)	1:24:A:ILE:HD12	1:41:A:ARG:HA	7	0.12
(1,1774)	1:24:A:ILE:HD13	1:41:A:ARG:HA	7	0.12
(1,1744)	1:108:A:ASP:HA	1:109:A:VAL:H	16	0.12
(1,1729)	1:78:A:PHE:HZ	1:104:A:LYS:HE2	19	0.12
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	11	0.12
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	11	0.12
(1,1714)	1:75:A:GLY:HA2	1:104:A:LYS:HD2	7	0.12
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD11	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD12	11	0.12
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD13	11	0.12
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD11	18	0.12
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD12	18	0.12
(1,1619)	1:97:A:ARG:HA	1:100:A:ILE:HD13	18	0.12
(1,1608)	1:9:A:VAL:HB	1:96:A:TYR:HB3	14	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG21	10	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG22	10	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG23	10	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG21	16	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG22	16	0.12
(1,1581)	1:80:A:CYS:HB2	1:93:A:ILE:HG23	16	0.12
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	13	0.12
(1,1537)	1:135:A:ARG:HA	1:137:A:TYR:H	1	0.12
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	9	0.12
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	9	0.12
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	9	0.12
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	9	0.12
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	9	0.12
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	9	0.12
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	15	0.12
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	15	0.12
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	15	0.12
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	15	0.12
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	15	0.12
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	15	0.12
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG11	13	0.12
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG12	13	0.12
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG13	13	0.12
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG21	13	0.12
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG22	13	0.12
(1,1455)	1:99:A:GLN:HE21	1:103:A:VAL:HG23	13	0.12
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG11	13	0.12
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG12	13	0.12
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG13	13	0.12
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG21	13	0.12
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG22	13	0.12
(1,1455)	1:99:A:GLN:HE22	1:103:A:VAL:HG23	13	0.12
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	3	0.12
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	3	0.12
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	3	0.12
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE1	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1413)	1:11:A:ALA:HB1	1:96:A:TYR:HE2	15	0.12
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE1	15	0.12
(1,1413)	1:11:A:ALA:HB2	1:96:A:TYR:HE2	15	0.12
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE1	15	0.12
(1,1413)	1:11:A:ALA:HB3	1:96:A:TYR:HE2	15	0.12
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	1	0.12
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	13	0.12
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	20	0.12
(1,1385)	1:84:A:ILE:HD11	1:123:A:ARG:HB3	9	0.12
(1,1385)	1:84:A:ILE:HD12	1:123:A:ARG:HB3	9	0.12
(1,1385)	1:84:A:ILE:HD13	1:123:A:ARG:HB3	9	0.12
(1,1272)	1:9:A:VAL:HG11	1:96:A:TYR:H	1	0.12
(1,1272)	1:9:A:VAL:HG12	1:96:A:TYR:H	1	0.12
(1,1272)	1:9:A:VAL:HG13	1:96:A:TYR:H	1	0.12
(1,1272)	1:9:A:VAL:HG21	1:96:A:TYR:H	1	0.12
(1,1272)	1:9:A:VAL:HG22	1:96:A:TYR:H	1	0.12
(1,1272)	1:9:A:VAL:HG23	1:96:A:TYR:H	1	0.12
(1,1272)	1:9:A:VAL:HG11	1:96:A:TYR:H	19	0.12
(1,1272)	1:9:A:VAL:HG12	1:96:A:TYR:H	19	0.12
(1,1272)	1:9:A:VAL:HG13	1:96:A:TYR:H	19	0.12
(1,1272)	1:9:A:VAL:HG21	1:96:A:TYR:H	19	0.12
(1,1272)	1:9:A:VAL:HG22	1:96:A:TYR:H	19	0.12
(1,1272)	1:9:A:VAL:HG23	1:96:A:TYR:H	19	0.12
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE1	14	0.12
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE2	14	0.12
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE1	17	0.12
(1,1267)	1:94:A:HIS:HE1	1:137:A:TYR:HE2	17	0.12
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG11	16	0.12
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG12	16	0.12
(1,1248)	1:87:A:THR:HG21	1:125:A:VAL:HG13	16	0.12
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG11	16	0.12
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG12	16	0.12
(1,1248)	1:87:A:THR:HG22	1:125:A:VAL:HG13	16	0.12
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG11	16	0.12
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG12	16	0.12
(1,1248)	1:87:A:THR:HG23	1:125:A:VAL:HG13	16	0.12
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	9	0.12
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	9	0.12
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	9	0.12
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	9	0.12
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	9	0.12
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	9	0.12
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	9	0.12
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	9	0.12
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	9	0.12
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	9	0.12
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	9	0.12
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	9	0.12
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	9	0.12
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	9	0.12
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	9	0.12
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	9	0.12
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	9	0.12
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE1	14	0.12
(1,1213)	1:94:A:HIS:HD2	1:137:A:TYR:HE2	14	0.12
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	18	0.12
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	18	0.12
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	18	0.12
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	18	0.12
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	18	0.12
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	18	0.12
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	18	0.12
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	18	0.12
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	18	0.12
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	18	0.12
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	18	0.12
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	18	0.12
(1,1115)	1:51:A:CYS:HB3	1:52:A:LEU:H	2	0.12
(1,1115)	1:51:A:CYS:HB3	1:52:A:LEU:H	6	0.12
(1,1115)	1:51:A:CYS:HB3	1:52:A:LEU:H	10	0.12
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD1	4	0.12
(1,1093)	1:21:A:ILE:H	1:40:A:TYR:HD2	4	0.12
(1,1080)	1:1:A:MET:HG3	1:51:A:CYS:HA	19	0.12
(1,1062)	1:131:A:GLN:HA	1:131:A:GLN:HE21	2	0.12
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG21	5	0.12
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG22	5	0.12
(1,1020)	1:45:A:VAL:HG11	1:50:A:THR:HG23	5	0.12
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG21	5	0.12
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG22	5	0.12
(1,1020)	1:45:A:VAL:HG12	1:50:A:THR:HG23	5	0.12
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG21	5	0.12
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG22	5	0.12
(1,1020)	1:45:A:VAL:HG13	1:50:A:THR:HG23	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG21	5	0.12
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG22	5	0.12
(1,1020)	1:45:A:VAL:HG21	1:50:A:THR:HG23	5	0.12
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG21	5	0.12
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG22	5	0.12
(1,1020)	1:45:A:VAL:HG22	1:50:A:THR:HG23	5	0.12
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG21	5	0.12
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG22	5	0.12
(1,1020)	1:45:A:VAL:HG23	1:50:A:THR:HG23	5	0.12
(1,988)	1:85:A:ASN:HD21	1:117:A:LYS:HB2	17	0.12
(1,988)	1:85:A:ASN:HD21	1:117:A:LYS:HB3	17	0.12
(1,988)	1:85:A:ASN:HD22	1:117:A:LYS:HB2	17	0.12
(1,988)	1:85:A:ASN:HD22	1:117:A:LYS:HB3	17	0.12
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG2	13	0.12
(1,961)	1:43:A:GLN:H	1:43:A:GLN:HG3	13	0.12
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG21	19	0.12
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG22	19	0.12
(1,949)	1:43:A:GLN:HB2	1:50:A:THR:HG23	19	0.12
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG21	19	0.12
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG22	19	0.12
(1,949)	1:43:A:GLN:HB3	1:50:A:THR:HG23	19	0.12
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD1	19	0.12
(1,938)	1:97:A:ARG:HB2	1:137:A:TYR:HD2	19	0.12
(1,900)	1:90:A:PHE:HE1	1:129:A:GLN:HG2	8	0.12
(1,900)	1:90:A:PHE:HE2	1:129:A:GLN:HG2	8	0.12
(1,897)	1:79:A:LEU:HD11	1:157:A:TYR:H	14	0.12
(1,897)	1:79:A:LEU:HD12	1:157:A:TYR:H	14	0.12
(1,897)	1:79:A:LEU:HD13	1:157:A:TYR:H	14	0.12
(1,897)	1:79:A:LEU:HD21	1:157:A:TYR:H	14	0.12
(1,897)	1:79:A:LEU:HD22	1:157:A:TYR:H	14	0.12
(1,897)	1:79:A:LEU:HD23	1:157:A:TYR:H	14	0.12
(1,896)	1:24:A:ILE:HD11	1:42:A:LYS:HB3	8	0.12
(1,896)	1:24:A:ILE:HD12	1:42:A:LYS:HB3	8	0.12
(1,896)	1:24:A:ILE:HD13	1:42:A:LYS:HB3	8	0.12
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	1	0.12
(1,888)	1:45:A:VAL:HB	1:46:A:ILE:H	18	0.12
(1,860)	1:41:A:ARG:HG2	1:53:A:LEU:H	3	0.12
(1,860)	1:41:A:ARG:HG3	1:53:A:LEU:H	3	0.12
(1,789)	1:58:A:THR:H	1:58:A:THR:HG21	8	0.12
(1,789)	1:58:A:THR:H	1:58:A:THR:HG22	8	0.12
(1,789)	1:58:A:THR:H	1:58:A:THR:HG23	8	0.12
(1,788)	1:8:A:VAL:HB	1:58:A:THR:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,788)	1:8:A:VAL:HB	1:58:A:THR:H	6	0.12
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	5	0.12
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	5	0.12
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	5	0.12
(1,745)	1:67:A:MET:HA	1:70:A:GLN:H	9	0.12
(1,741)	1:65:A:SER:H	1:65:A:SER:HB2	9	0.12
(1,741)	1:65:A:SER:H	1:65:A:SER:HB3	9	0.12
(1,714)	1:36:A:ILE:HG12	1:37:A:GLU:H	20	0.12
(1,714)	1:36:A:ILE:HG13	1:37:A:GLU:H	20	0.12
(1,673)	1:35:A:SER:HA	1:36:A:ILE:H	2	0.12
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	3	0.12
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	3	0.12
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	3	0.12
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	3	0.12
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	3	0.12
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	3	0.12
(1,538)	1:20:A:THR:HG21	1:21:A:ILE:H	9	0.12
(1,538)	1:20:A:THR:HG22	1:21:A:ILE:H	9	0.12
(1,538)	1:20:A:THR:HG23	1:21:A:ILE:H	9	0.12
(1,507)	1:169:A:LYS:H	1:169:A:LYS:HB2	8	0.12
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD1	3	0.12
(1,505)	1:29:A:VAL:HB	1:32:A:TYR:HD2	3	0.12
(1,491)	1:29:A:VAL:HA	1:31:A:GLU:H	2	0.12
(1,489)	1:160:A:VAL:HG11	1:164:A:ARG:HE	16	0.12
(1,489)	1:160:A:VAL:HG12	1:164:A:ARG:HE	16	0.12
(1,489)	1:160:A:VAL:HG13	1:164:A:ARG:HE	16	0.12
(1,489)	1:160:A:VAL:HG21	1:164:A:ARG:HE	16	0.12
(1,489)	1:160:A:VAL:HG22	1:164:A:ARG:HE	16	0.12
(1,489)	1:160:A:VAL:HG23	1:164:A:ARG:HE	16	0.12
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	20	0.12
(1,448)	1:22:A:GLN:HE22	1:28:A:PHE:H	13	0.12
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD11	5	0.12
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD12	5	0.12
(1,422)	1:96:A:TYR:HD1	1:100:A:ILE:HD13	5	0.12
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD11	5	0.12
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD12	5	0.12
(1,422)	1:96:A:TYR:HD2	1:100:A:ILE:HD13	5	0.12
(1,337)	1:23:A:LEU:HD21	1:156:A:PHE:HB3	12	0.12
(1,337)	1:23:A:LEU:HD22	1:156:A:PHE:HB3	12	0.12
(1,337)	1:23:A:LEU:HD23	1:156:A:PHE:HB3	12	0.12
(1,319)	1:23:A:LEU:HB2	1:152:A:VAL:HB	13	0.12
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE1	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE2	3	0.12
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE1	4	0.12
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE2	4	0.12
(1,283)	1:2:A:THR:H	1:50:A:THR:HG21	6	0.12
(1,283)	1:2:A:THR:H	1:50:A:THR:HG22	6	0.12
(1,283)	1:2:A:THR:H	1:50:A:THR:HG23	6	0.12
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	9	0.12
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	9	0.12
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	9	0.12
(1,249)	1:142:A:ILE:HG21	1:144:A:THR:H	13	0.12
(1,249)	1:142:A:ILE:HG22	1:144:A:THR:H	13	0.12
(1,249)	1:142:A:ILE:HG23	1:144:A:THR:H	13	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	4	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	4	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	4	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	4	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	4	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	4	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	10	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	10	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	10	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	10	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	10	0.12
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	10	0.12
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD11	12	0.12
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD12	12	0.12
(1,218)	1:23:A:LEU:HD11	1:24:A:ILE:HD13	12	0.12
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD11	12	0.12
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD12	12	0.12
(1,218)	1:23:A:LEU:HD12	1:24:A:ILE:HD13	12	0.12
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD11	12	0.12
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD12	12	0.12
(1,218)	1:23:A:LEU:HD13	1:24:A:ILE:HD13	12	0.12
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD11	12	0.12
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD12	12	0.12
(1,218)	1:23:A:LEU:HD21	1:24:A:ILE:HD13	12	0.12
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD11	12	0.12
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD12	12	0.12
(1,218)	1:23:A:LEU:HD22	1:24:A:ILE:HD13	12	0.12
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD11	12	0.12
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD12	12	0.12
(1,218)	1:23:A:LEU:HD23	1:24:A:ILE:HD13	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	4	0.12
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	4	0.12
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	4	0.12
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	7	0.12
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	7	0.12
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	7	0.12
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	12	0.12
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	12	0.12
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	12	0.12
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	13	0.12
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	13	0.12
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	13	0.12
(1,151)	1:29:A:VAL:HG11	2:201:A:GNP:H2'	17	0.12
(1,151)	1:29:A:VAL:HG12	2:201:A:GNP:H2'	17	0.12
(1,151)	1:29:A:VAL:HG13	2:201:A:GNP:H2'	17	0.12
(1,148)	1:28:A:PHE:HE1	2:201:A:GNP:H1'	10	0.12
(1,148)	1:28:A:PHE:HE2	2:201:A:GNP:H1'	10	0.12
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG11	9	0.12
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG12	9	0.12
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG13	9	0.12
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG21	9	0.12
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG22	9	0.12
(1,94)	1:15:A:GLY:HA2	1:81:A:VAL:HG23	9	0.12
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD21	15	0.12
(1,83)	1:15:A:GLY:HA2	1:116:A:ASN:HD22	15	0.12
(1,73)	1:102:A:ARG:H	1:104:A:LYS:H	20	0.12
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	10	0.12
(1,42)	1:105:A:ASP:H	1:106:A:SER:H	13	0.12
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD11	13	0.12
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD12	13	0.12
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD13	13	0.12
(1,1)	1:10:A:GLY:HA2	1:81:A:VAL:HB	11	0.12
(1,1)	1:10:A:GLY:HA3	1:81:A:VAL:HB	11	0.12
(3,2)	1:17:A:SER:OG	2:201:A:GNP:O2B	17	0.11
(2,2)	3:202:A:MG:MG	2:201:A:GNP:O2B	4	0.11
(2,2)	3:202:A:MG:MG	2:201:A:GNP:O2B	5	0.11
(1,3302)	1:120:A:LEU:HD21	1:122:A:SER:H	3	0.11
(1,3302)	1:120:A:LEU:HD22	1:122:A:SER:H	3	0.11
(1,3302)	1:120:A:LEU:HD23	1:122:A:SER:H	3	0.11
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	5	0.11
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	5	0.11
(1,3295)	1:78:A:PHE:HD1	1:112:A:VAL:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3295)	1:78:A:PHE:HD2	1:112:A:VAL:H	9	0.11
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD1	9	0.11
(1,3265)	1:9:A:VAL:HB	1:78:A:PHE:HD2	9	0.11
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB2	2	0.11
(1,3209)	1:117:A:LYS:H	1:145:A:SER:HB3	2	0.11
(1,3198)	1:109:A:VAL:HA	1:166:A:HIS:HD2	17	0.11
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG21	6	0.11
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG22	6	0.11
(1,3177)	1:119:A:ASP:H	1:148:A:THR:HG23	6	0.11
(1,3173)	1:1:A:MET:HG2	1:2:A:THR:H	19	0.11
(1,3158)	1:1:A:MET:HA	1:1:A:MET:HG3	5	0.11
(1,3140)	1:1:A:MET:HB3	1:2:A:THR:H	16	0.11
(1,3129)	1:123:A:ARG:HE	1:124:A:THR:H	7	0.11
(1,3128)	1:1:A:MET:HA	1:51:A:CYS:HA	13	0.11
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG2	15	0.11
(1,3120)	1:85:A:ASN:HB2	1:123:A:ARG:HG3	15	0.11
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG2	15	0.11
(1,3120)	1:85:A:ASN:HB3	1:123:A:ARG:HG3	15	0.11
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	6	0.11
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	6	0.11
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	14	0.11
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	14	0.11
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE1	16	0.11
(1,3105)	1:64:A:TYR:H	1:64:A:TYR:HE2	16	0.11
(1,3093)	1:125:A:VAL:H	1:126:A:ASP:H	6	0.11
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD11	1	0.11
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD12	1	0.11
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD13	1	0.11
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD21	1	0.11
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD22	1	0.11
(1,3022)	1:91:A:GLU:H	1:133:A:LEU:HD23	1	0.11
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	4	0.11
(1,3009)	1:129:A:GLN:HG2	1:130:A:ALA:H	8	0.11
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE1	4	0.11
(1,2992)	1:18:A:ALA:HB1	1:32:A:TYR:HE2	4	0.11
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE1	4	0.11
(1,2992)	1:18:A:ALA:HB2	1:32:A:TYR:HE2	4	0.11
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE1	4	0.11
(1,2992)	1:18:A:ALA:HB3	1:32:A:TYR:HE2	4	0.11
(1,2986)	1:131:A:GLN:HB3	1:132:A:ASP:H	14	0.11
(1,2979)	1:131:A:GLN:HG3	1:134:A:ALA:HB1	4	0.11
(1,2979)	1:131:A:GLN:HG3	1:134:A:ALA:HB2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2979)	1:131:A:GLN:HG3	1:134:A:ALA:HB3	4	0.11
(1,2962)	1:132:A:ASP:HB2	1:133:A:LEU:H	7	0.11
(1,2954)	1:31:A:GLU:H	1:32:A:TYR:H	2	0.11
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD1	3	0.11
(1,2950)	1:64:A:TYR:H	1:64:A:TYR:HD2	3	0.11
(1,2919)	1:132:A:ASP:HA	1:135:A:ARG:H	4	0.11
(1,2892)	1:21:A:ILE:HG13	1:25:A:GLN:HB2	19	0.11
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD2	3	0.11
(1,2874)	1:163:A:ILE:HG21	1:167:A:LYS:HD3	3	0.11
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD2	3	0.11
(1,2874)	1:163:A:ILE:HG22	1:167:A:LYS:HD3	3	0.11
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD2	3	0.11
(1,2874)	1:163:A:ILE:HG23	1:167:A:LYS:HD3	3	0.11
(1,2869)	1:163:A:ILE:HG21	1:166:A:HIS:H	5	0.11
(1,2869)	1:163:A:ILE:HG22	1:166:A:HIS:H	5	0.11
(1,2869)	1:163:A:ILE:HG23	1:166:A:HIS:H	5	0.11
(1,2785)	1:117:A:LYS:H	1:145:A:SER:H	16	0.11
(1,2753)	1:146:A:ALA:HB1	1:147:A:LYS:HB3	11	0.11
(1,2753)	1:146:A:ALA:HB2	1:147:A:LYS:HB3	11	0.11
(1,2753)	1:146:A:ALA:HB3	1:147:A:LYS:HB3	11	0.11
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	8	0.11
(1,2709)	1:27:A:HIS:H	1:27:A:HIS:HE1	10	0.11
(1,2705)	1:145:A:SER:HA	1:148:A:THR:H	4	0.11
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD1	2	0.11
(1,2704)	1:134:A:ALA:HB1	1:137:A:TYR:HD2	2	0.11
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD1	2	0.11
(1,2704)	1:134:A:ALA:HB2	1:137:A:TYR:HD2	2	0.11
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD1	2	0.11
(1,2704)	1:134:A:ALA:HB3	1:137:A:TYR:HD2	2	0.11
(1,2703)	1:22:A:GLN:HE21	1:148:A:THR:H	11	0.11
(1,2703)	1:22:A:GLN:HE22	1:148:A:THR:H	11	0.11
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG2	1	0.11
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG3	1	0.11
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG2	12	0.11
(1,2674)	1:149:A:ARG:H	1:149:A:ARG:HG3	12	0.11
(1,2665)	1:1:A:MET:HE1	1:51:A:CYS:HA	6	0.11
(1,2665)	1:1:A:MET:HE2	1:51:A:CYS:HA	6	0.11
(1,2665)	1:1:A:MET:HE3	1:51:A:CYS:HA	6	0.11
(1,2646)	1:150:A:GLN:HB3	1:151:A:GLY:H	14	0.11
(1,2634)	1:80:A:CYS:HB2	1:112:A:VAL:HB	2	0.11
(1,2634)	1:80:A:CYS:HB3	1:112:A:VAL:HB	2	0.11
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB1	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB2	4	0.11
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB3	4	0.11
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG12	7	0.11
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG13	7	0.11
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	12	0.11
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	12	0.11
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	12	0.11
(1,2600)	1:20:A:THR:HG21	1:21:A:ILE:HA	13	0.11
(1,2600)	1:20:A:THR:HG22	1:21:A:ILE:HA	13	0.11
(1,2600)	1:20:A:THR:HG23	1:21:A:ILE:HA	13	0.11
(1,2536)	1:144:A:THR:HA	1:152:A:VAL:HA	4	0.11
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD2	13	0.11
(1,2491)	1:169:A:LYS:HA	1:169:A:LYS:HD3	13	0.11
(1,2461)	1:167:A:LYS:HB3	1:168:A:GLU:H	6	0.11
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	4	0.11
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	11	0.11
(1,2437)	1:162:A:GLU:H	1:162:A:GLU:HG3	12	0.11
(1,2398)	1:161:A:ARG:HA	1:165:A:LYS:H	12	0.11
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	20	0.11
(1,2319)	1:142:A:ILE:HD11	1:154:A:ASP:HB2	3	0.11
(1,2319)	1:142:A:ILE:HD12	1:154:A:ASP:HB2	3	0.11
(1,2319)	1:142:A:ILE:HD13	1:154:A:ASP:HB2	3	0.11
(1,2305)	1:44:A:VAL:H	1:51:A:CYS:H	20	0.11
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE1	8	0.11
(1,2298)	1:153:A:ASP:HA	1:156:A:PHE:HE2	8	0.11
(1,2294)	1:112:A:VAL:HG11	1:159:A:LEU:H	7	0.11
(1,2294)	1:112:A:VAL:HG12	1:159:A:LEU:H	7	0.11
(1,2294)	1:112:A:VAL:HG13	1:159:A:LEU:H	7	0.11
(1,2294)	1:112:A:VAL:HG11	1:159:A:LEU:H	12	0.11
(1,2294)	1:112:A:VAL:HG12	1:159:A:LEU:H	12	0.11
(1,2294)	1:112:A:VAL:HG13	1:159:A:LEU:H	12	0.11
(1,2267)	1:150:A:GLN:HG2	1:151:A:GLY:H	2	0.11
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG21	15	0.11
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG22	15	0.11
(1,2257)	1:114:A:VAL:HA	1:142:A:ILE:HG23	15	0.11
(1,2220)	1:147:A:LYS:HG2	1:148:A:THR:HA	15	0.11
(1,2220)	1:147:A:LYS:HG3	1:148:A:THR:HA	15	0.11
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	2	0.11
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG21	20	0.11
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG22	20	0.11
(1,2134)	1:137:A:TYR:HD1	1:139:A:ILE:HG23	20	0.11
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG21	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG22	20	0.11
(1,2134)	1:137:A:TYR:HD2	1:139:A:ILE:HG23	20	0.11
(1,2121)	1:134:A:ALA:HB1	1:139:A:ILE:HB	7	0.11
(1,2121)	1:134:A:ALA:HB2	1:139:A:ILE:HB	7	0.11
(1,2121)	1:134:A:ALA:HB3	1:139:A:ILE:HB	7	0.11
(1,2095)	1:132:A:ASP:H	1:133:A:LEU:HD11	17	0.11
(1,2095)	1:132:A:ASP:H	1:133:A:LEU:HD12	17	0.11
(1,2095)	1:132:A:ASP:H	1:133:A:LEU:HD13	17	0.11
(1,2095)	1:132:A:ASP:H	1:133:A:LEU:HD21	17	0.11
(1,2095)	1:132:A:ASP:H	1:133:A:LEU:HD22	17	0.11
(1,2095)	1:132:A:ASP:H	1:133:A:LEU:HD23	17	0.11
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE1	8	0.11
(1,2077)	1:44:A:VAL:HB	1:157:A:TYR:HE2	8	0.11
(1,2067)	1:3:A:GLU:HA	1:4:A:TYR:HB2	2	0.11
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE1	15	0.11
(1,2061)	1:153:A:ASP:HA	1:157:A:TYR:HE2	15	0.11
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB1	15	0.11
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB2	15	0.11
(1,2059)	1:129:A:GLN:HG3	1:130:A:ALA:HB3	15	0.11
(1,1984)	1:124:A:THR:HG21	1:125:A:VAL:H	3	0.11
(1,1984)	1:124:A:THR:HG22	1:125:A:VAL:H	3	0.11
(1,1984)	1:124:A:THR:HG23	1:125:A:VAL:H	3	0.11
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD1	20	0.11
(1,1930)	1:153:A:ASP:HB3	1:157:A:TYR:HD2	20	0.11
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	3	0.11
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	6	0.11
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	9	0.11
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	10	0.11
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	12	0.11
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG21	7	0.11
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG22	7	0.11
(1,1913)	1:119:A:ASP:HA	1:148:A:THR:HG23	7	0.11
(1,1878)	1:114:A:VAL:HG11	1:116:A:ASN:HA	3	0.11
(1,1878)	1:114:A:VAL:HG12	1:116:A:ASN:HA	3	0.11
(1,1878)	1:114:A:VAL:HG13	1:116:A:ASN:HA	3	0.11
(1,1878)	1:114:A:VAL:HG21	1:116:A:ASN:HA	3	0.11
(1,1878)	1:114:A:VAL:HG22	1:116:A:ASN:HA	3	0.11
(1,1878)	1:114:A:VAL:HG23	1:116:A:ASN:HA	3	0.11
(1,1876)	1:114:A:VAL:HG11	1:144:A:THR:H	6	0.11
(1,1876)	1:114:A:VAL:HG12	1:144:A:THR:H	6	0.11
(1,1876)	1:114:A:VAL:HG13	1:144:A:THR:H	6	0.11
(1,1876)	1:114:A:VAL:HG21	1:144:A:THR:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1876)	1:114:A:VAL:HG22	1:144:A:THR:H	6	0.11
(1,1876)	1:114:A:VAL:HG23	1:144:A:THR:H	6	0.11
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD11	6	0.11
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD12	6	0.11
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD13	6	0.11
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD21	6	0.11
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD22	6	0.11
(1,1853)	1:90:A:PHE:HE1	1:113:A:LEU:HD23	6	0.11
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD11	6	0.11
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD12	6	0.11
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD13	6	0.11
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD21	6	0.11
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD22	6	0.11
(1,1853)	1:90:A:PHE:HE2	1:113:A:LEU:HD23	6	0.11
(1,1823)	1:112:A:VAL:HA	1:162:A:GLU:HG3	1	0.11
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	13	0.11
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	13	0.11
(1,1700)	1:100:A:ILE:HG21	1:103:A:VAL:HB	3	0.11
(1,1700)	1:100:A:ILE:HG22	1:103:A:VAL:HB	3	0.11
(1,1700)	1:100:A:ILE:HG23	1:103:A:VAL:HB	3	0.11
(1,1685)	1:113:A:LEU:HD11	1:141:A:PHE:HA	10	0.11
(1,1685)	1:113:A:LEU:HD12	1:141:A:PHE:HA	10	0.11
(1,1685)	1:113:A:LEU:HD13	1:141:A:PHE:HA	10	0.11
(1,1597)	1:8:A:VAL:H	1:58:A:THR:H	2	0.11
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD11	10	0.11
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD12	10	0.11
(1,1534)	1:4:A:TYR:HE1	1:163:A:ILE:HD13	10	0.11
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD11	10	0.11
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD12	10	0.11
(1,1534)	1:4:A:TYR:HE2	1:163:A:ILE:HD13	10	0.11
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD11	8	0.11
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD12	8	0.11
(1,1500)	1:159:A:LEU:HG	1:163:A:ILE:HD13	8	0.11
(1,1444)	1:79:A:LEU:HD21	1:155:A:ALA:HA	5	0.11
(1,1444)	1:79:A:LEU:HD22	1:155:A:ALA:HA	5	0.11
(1,1444)	1:79:A:LEU:HD23	1:155:A:ALA:HA	5	0.11
(1,1417)	1:84:A:ILE:HD11	1:85:A:ASN:HA	18	0.11
(1,1417)	1:84:A:ILE:HD12	1:85:A:ASN:HA	18	0.11
(1,1417)	1:84:A:ILE:HD13	1:85:A:ASN:HA	18	0.11
(1,1406)	1:76:A:GLU:HG2	1:77:A:GLY:H	19	0.11
(1,1393)	1:75:A:GLY:HA3	1:76:A:GLU:HG2	20	0.11
(1,1385)	1:84:A:ILE:HD11	1:123:A:ARG:HB3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:84:A:ILE:HD12	1:123:A:ARG:HB3	14	0.11
(1,1385)	1:84:A:ILE:HD13	1:123:A:ARG:HB3	14	0.11
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	5	0.11
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	5	0.11
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	5	0.11
(1,1321)	1:56:A:LEU:HD11	1:71:A:TYR:HA	3	0.11
(1,1321)	1:56:A:LEU:HD12	1:71:A:TYR:HA	3	0.11
(1,1321)	1:56:A:LEU:HD13	1:71:A:TYR:HA	3	0.11
(1,1321)	1:56:A:LEU:HD21	1:71:A:TYR:HA	3	0.11
(1,1321)	1:56:A:LEU:HD22	1:71:A:TYR:HA	3	0.11
(1,1321)	1:56:A:LEU:HD23	1:71:A:TYR:HA	3	0.11
(1,1309)	1:95:A:HIS:HD2	1:99:A:GLN:HG2	9	0.11
(1,1309)	1:95:A:HIS:HD2	1:99:A:GLN:HG3	9	0.11
(1,1294)	1:95:A:HIS:HD2	1:96:A:TYR:HA	20	0.11
(1,1274)	1:67:A:MET:HA	1:67:A:MET:HG2	15	0.11
(1,1270)	1:65:A:SER:H	1:65:A:SER:HB3	10	0.11
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	1	0.11
(1,1228)	1:61:A:GLN:HA	1:61:A:GLN:HE22	12	0.11
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD11	20	0.11
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD12	20	0.11
(1,1198)	1:39:A:SER:H	1:56:A:LEU:HD13	20	0.11
(1,1143)	1:90:A:PHE:HZ	1:132:A:ASP:H	18	0.11
(1,1131)	1:1:A:MET:HE1	1:52:A:LEU:HB3	14	0.11
(1,1131)	1:1:A:MET:HE2	1:52:A:LEU:HB3	14	0.11
(1,1131)	1:1:A:MET:HE3	1:52:A:LEU:HB3	14	0.11
(1,1080)	1:1:A:MET:HG3	1:51:A:CYS:HA	1	0.11
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	16	0.11
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	16	0.11
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	16	0.11
(1,1040)	1:55:A:ILE:HD11	1:156:A:PHE:HB2	17	0.11
(1,1040)	1:55:A:ILE:HD12	1:156:A:PHE:HB2	17	0.11
(1,1040)	1:55:A:ILE:HD13	1:156:A:PHE:HB2	17	0.11
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	8	0.11
(1,1001)	1:164:A:ARG:H	1:164:A:ARG:HE	11	0.11
(1,955)	1:43:A:GLN:H	1:43:A:GLN:HE21	13	0.11
(1,942)	1:25:A:GLN:HB3	1:26:A:ASN:HD21	9	0.11
(1,940)	1:26:A:ASN:H	1:26:A:ASN:HD22	16	0.11
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB2	15	0.11
(1,917)	1:146:A:ALA:HA	1:149:A:ARG:HB3	15	0.11
(1,897)	1:79:A:LEU:HD11	1:157:A:TYR:H	10	0.11
(1,897)	1:79:A:LEU:HD12	1:157:A:TYR:H	10	0.11
(1,897)	1:79:A:LEU:HD13	1:157:A:TYR:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,897)	1:79:A:LEU:HD21	1:157:A:TYR:H	10	0.11
(1,897)	1:79:A:LEU:HD22	1:157:A:TYR:H	10	0.11
(1,897)	1:79:A:LEU:HD23	1:157:A:TYR:H	10	0.11
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	9	0.11
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	1	0.11
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	1	0.11
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	3	0.11
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	3	0.11
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD2	10	0.11
(1,844)	1:41:A:ARG:HA	1:41:A:ARG:HD3	10	0.11
(1,819)	1:142:A:ILE:HD11	1:154:A:ASP:H	19	0.11
(1,819)	1:142:A:ILE:HD12	1:154:A:ASP:H	19	0.11
(1,819)	1:142:A:ILE:HD13	1:154:A:ASP:H	19	0.11
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE1	20	0.11
(1,785)	1:59:A:ALA:H	1:71:A:TYR:HE2	20	0.11
(1,783)	1:142:A:ILE:HD11	1:143:A:GLU:HB2	19	0.11
(1,783)	1:142:A:ILE:HD12	1:143:A:GLU:HB2	19	0.11
(1,783)	1:142:A:ILE:HD13	1:143:A:GLU:HB2	19	0.11
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD11	7	0.11
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD12	7	0.11
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD13	7	0.11
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD21	7	0.11
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD22	7	0.11
(1,778)	1:39:A:SER:HA	1:56:A:LEU:HD23	7	0.11
(1,776)	1:90:A:PHE:H	1:125:A:VAL:HG21	6	0.11
(1,776)	1:90:A:PHE:H	1:125:A:VAL:HG22	6	0.11
(1,776)	1:90:A:PHE:H	1:125:A:VAL:HG23	6	0.11
(1,756)	1:64:A:TYR:H	1:65:A:SER:H	2	0.11
(1,756)	1:64:A:TYR:H	1:65:A:SER:H	13	0.11
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB2	3	0.11
(1,711)	1:36:A:ILE:HD11	1:40:A:TYR:HB3	3	0.11
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB2	3	0.11
(1,711)	1:36:A:ILE:HD12	1:40:A:TYR:HB3	3	0.11
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB2	3	0.11
(1,711)	1:36:A:ILE:HD13	1:40:A:TYR:HB3	3	0.11
(1,681)	1:78:A:PHE:HZ	1:110:A:PRO:HD2	2	0.11
(1,605)	1:36:A:ILE:HD11	1:37:A:GLU:H	13	0.11
(1,605)	1:36:A:ILE:HD12	1:37:A:GLU:H	13	0.11
(1,605)	1:36:A:ILE:HD13	1:37:A:GLU:H	13	0.11
(1,533)	1:66:A:ALA:HA	1:69:A:ASP:HB2	9	0.11
(1,533)	1:66:A:ALA:HA	1:69:A:ASP:HB3	9	0.11
(1,498)	1:28:A:PHE:HD1	1:29:A:VAL:HA	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:28:A:PHE:HD2	1:29:A:VAL:HA	3	0.11
(1,483)	1:29:A:VAL:HA	1:32:A:TYR:HB3	16	0.11
(1,461)	1:27:A:HIS:HB2	1:28:A:PHE:H	10	0.11
(1,381)	1:112:A:VAL:HB	1:162:A:GLU:HG3	6	0.11
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE1	8	0.11
(1,310)	1:23:A:LEU:HA	1:156:A:PHE:HE2	8	0.11
(1,289)	1:24:A:ILE:HD11	1:40:A:TYR:HB2	18	0.11
(1,289)	1:24:A:ILE:HD12	1:40:A:TYR:HB2	18	0.11
(1,289)	1:24:A:ILE:HD13	1:40:A:TYR:HB2	18	0.11
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	10	0.11
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	10	0.11
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	10	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	12	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	12	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	12	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	12	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	12	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	12	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	13	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	13	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	13	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	13	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	13	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	13	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG11	14	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG12	14	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG13	14	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG21	14	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG22	14	0.11
(1,246)	1:16:A:LYS:H	1:81:A:VAL:HG23	14	0.11
(1,206)	1:32:A:TYR:HE1	2:201:A:GNP:H8	3	0.11
(1,206)	1:32:A:TYR:HE2	2:201:A:GNP:H8	3	0.11
(1,203)	1:30:A:ASP:HA	2:201:A:GNP:H2'	20	0.11
(1,198)	1:52:A:LEU:HD11	1:53:A:LEU:H	2	0.11
(1,198)	1:52:A:LEU:HD12	1:53:A:LEU:H	2	0.11
(1,198)	1:52:A:LEU:HD13	1:53:A:LEU:H	2	0.11
(1,198)	1:52:A:LEU:HD21	1:53:A:LEU:H	2	0.11
(1,198)	1:52:A:LEU:HD22	1:53:A:LEU:H	2	0.11
(1,198)	1:52:A:LEU:HD23	1:53:A:LEU:H	2	0.11
(1,128)	1:18:A:ALA:HA	1:21:A:ILE:HG21	4	0.11
(1,128)	1:18:A:ALA:HA	1:21:A:ILE:HG22	4	0.11
(1,128)	1:18:A:ALA:HA	1:21:A:ILE:HG23	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:95:A:HIS:HA	1:98:A:GLU:H	14	0.11
(1,108)	1:166:A:HIS:HB3	1:167:A:LYS:H	4	0.11
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	19	0.11
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	19	0.11
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	19	0.11
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	19	0.11
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	19	0.11
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	19	0.11
(1,40)	1:106:A:SER:H	1:107:A:GLU:H	4	0.11
(1,40)	1:106:A:SER:H	1:107:A:GLU:H	9	0.11
(1,40)	1:106:A:SER:H	1:107:A:GLU:H	10	0.11
(1,40)	1:106:A:SER:H	1:107:A:GLU:H	13	0.11
(1,3312)	1:111:A:MET:H	1:159:A:LEU:HA	7	0.1
(1,3302)	1:120:A:LEU:HD21	1:122:A:SER:H	8	0.1
(1,3302)	1:120:A:LEU:HD22	1:122:A:SER:H	8	0.1
(1,3302)	1:120:A:LEU:HD23	1:122:A:SER:H	8	0.1
(1,3200)	1:161:A:ARG:H	1:161:A:ARG:HE	15	0.1
(1,3176)	1:119:A:ASP:H	1:120:A:LEU:HG	9	0.1
(1,3158)	1:1:A:MET:HA	1:1:A:MET:HG3	6	0.1
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG11	20	0.1
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG12	20	0.1
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG13	20	0.1
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG21	20	0.1
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG22	20	0.1
(1,3100)	1:102:A:ARG:H	1:103:A:VAL:HG23	20	0.1
(1,3063)	1:45:A:VAL:HB	1:48:A:GLY:H	5	0.1
(1,3005)	1:90:A:PHE:HE1	1:131:A:GLN:H	16	0.1
(1,3005)	1:90:A:PHE:HE2	1:131:A:GLN:H	16	0.1
(1,2986)	1:131:A:GLN:HB3	1:132:A:ASP:H	4	0.1
(1,2876)	1:149:A:ARG:HG2	1:150:A:GLN:HE21	19	0.1
(1,2876)	1:149:A:ARG:HG3	1:150:A:GLN:HE21	19	0.1
(1,2799)	1:143:A:GLU:HB3	1:144:A:THR:H	3	0.1
(1,2735)	1:117:A:LYS:HA	1:146:A:ALA:H	9	0.1
(1,2653)	1:75:A:GLY:H	1:78:A:PHE:HE1	3	0.1
(1,2653)	1:75:A:GLY:H	1:78:A:PHE:HE2	3	0.1
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB1	18	0.1
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB2	18	0.1
(1,2616)	1:153:A:ASP:H	1:155:A:ALA:HB3	18	0.1
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG12	8	0.1
(1,2602)	1:21:A:ILE:HA	1:24:A:ILE:HG13	8	0.1
(1,2569)	1:156:A:PHE:H	1:156:A:PHE:HE1	9	0.1
(1,2569)	1:156:A:PHE:H	1:156:A:PHE:HE2	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	1:75:A:GLY:H	1:76:A:GLU:HG2	19	0.1
(1,2532)	1:19:A:LEU:HA	1:152:A:VAL:HA	4	0.1
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB1	2	0.1
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB2	2	0.1
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB3	2	0.1
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB1	18	0.1
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB2	18	0.1
(1,2497)	1:58:A:THR:HB	1:59:A:ALA:HB3	18	0.1
(1,2495)	1:169:A:LYS:H	1:169:A:LYS:HB3	5	0.1
(1,2416)	1:110:A:PRO:HA	1:163:A:ILE:HA	5	0.1
(1,2398)	1:161:A:ARG:HA	1:165:A:LYS:H	19	0.1
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB2	14	0.1
(1,2360)	1:158:A:THR:HG21	1:159:A:LEU:HB3	14	0.1
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB2	14	0.1
(1,2360)	1:158:A:THR:HG22	1:159:A:LEU:HB3	14	0.1
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB2	14	0.1
(1,2360)	1:158:A:THR:HG23	1:159:A:LEU:HB3	14	0.1
(1,2329)	1:156:A:PHE:HB2	1:159:A:LEU:H	13	0.1
(1,2275)	1:150:A:GLN:HA	1:150:A:GLN:HG2	14	0.1
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG21	20	0.1
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG22	20	0.1
(1,2258)	1:114:A:VAL:HA	1:144:A:THR:HG23	20	0.1
(1,2178)	1:110:A:PRO:HG2	1:166:A:HIS:HE1	4	0.1
(1,2174)	1:147:A:LYS:HG3	2:201:A:GNP:HN1	2	0.1
(1,2173)	1:147:A:LYS:HD2	2:201:A:GNP:HN1	10	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	5	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	5	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	5	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	5	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	5	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	5	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD11	8	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD12	8	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD13	8	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD21	8	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD22	8	0.1
(1,2102)	1:130:A:ALA:HA	1:133:A:LEU:HD23	8	0.1
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	12	0.1
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	18	0.1
(1,1922)	1:11:A:ALA:H	1:12:A:GLY:H	19	0.1
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD1	17	0.1
(1,1919)	1:46:A:ILE:HG12	1:157:A:TYR:HD2	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:118:A:SER:HB2	1:143:A:GLU:HB3	17	0.1
(1,1906)	1:118:A:SER:HB3	1:143:A:GLU:HB3	17	0.1
(1,1870)	1:81:A:VAL:HA	1:114:A:VAL:HB	3	0.1
(1,1823)	1:112:A:VAL:HA	1:162:A:GLU:HG3	5	0.1
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG12	18	0.1
(1,1791)	1:110:A:PRO:HG3	1:163:A:ILE:HG13	18	0.1
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG21	20	0.1
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG22	20	0.1
(1,1789)	1:110:A:PRO:HG3	1:163:A:ILE:HG23	20	0.1
(1,1752)	1:8:A:VAL:HG11	1:10:A:GLY:H	20	0.1
(1,1752)	1:8:A:VAL:HG12	1:10:A:GLY:H	20	0.1
(1,1752)	1:8:A:VAL:HG13	1:10:A:GLY:H	20	0.1
(1,1752)	1:8:A:VAL:HG21	1:10:A:GLY:H	20	0.1
(1,1752)	1:8:A:VAL:HG22	1:10:A:GLY:H	20	0.1
(1,1752)	1:8:A:VAL:HG23	1:10:A:GLY:H	20	0.1
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE1	3	0.1
(1,1728)	1:116:A:ASN:H	1:141:A:PHE:HE2	3	0.1
(1,1661)	1:101:A:LYS:HD2	1:107:A:GLU:HA	11	0.1
(1,1661)	1:101:A:LYS:HD3	1:107:A:GLU:HA	11	0.1
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD1	12	0.1
(1,1633)	1:47:A:ASP:H	1:157:A:TYR:HD2	12	0.1
(1,1579)	1:80:A:CYS:HB3	1:93:A:ILE:HG21	11	0.1
(1,1579)	1:80:A:CYS:HB3	1:93:A:ILE:HG22	11	0.1
(1,1579)	1:80:A:CYS:HB3	1:93:A:ILE:HG23	11	0.1
(1,1559)	1:61:A:GLN:HB2	1:62:A:GLU:HA	5	0.1
(1,1533)	1:88:A:LYS:HA	1:91:A:GLU:HG2	4	0.1
(1,1533)	1:88:A:LYS:HA	1:91:A:GLU:HG3	4	0.1
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD11	19	0.1
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD12	19	0.1
(1,1526)	1:137:A:TYR:HE1	1:139:A:ILE:HD13	19	0.1
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD11	19	0.1
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD12	19	0.1
(1,1526)	1:137:A:TYR:HE2	1:139:A:ILE:HD13	19	0.1
(1,1394)	1:75:A:GLY:HA3	1:77:A:GLY:H	9	0.1
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD11	11	0.1
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD12	11	0.1
(1,1329)	1:138:A:GLY:H	1:139:A:ILE:HD13	11	0.1
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB2	11	0.1
(1,1311)	1:95:A:HIS:HD2	1:99:A:GLN:HB3	11	0.1
(1,1263)	1:64:A:TYR:H	1:64:A:TYR:HB3	10	0.1
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG21	18	0.1
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG22	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:56:A:LEU:HD11	1:58:A:THR:HG23	18	0.1
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG21	18	0.1
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG22	18	0.1
(1,1218)	1:56:A:LEU:HD12	1:58:A:THR:HG23	18	0.1
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG21	18	0.1
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG22	18	0.1
(1,1218)	1:56:A:LEU:HD13	1:58:A:THR:HG23	18	0.1
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG21	18	0.1
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG22	18	0.1
(1,1218)	1:56:A:LEU:HD21	1:58:A:THR:HG23	18	0.1
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG21	18	0.1
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG22	18	0.1
(1,1218)	1:56:A:LEU:HD22	1:58:A:THR:HG23	18	0.1
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG21	18	0.1
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG22	18	0.1
(1,1218)	1:56:A:LEU:HD23	1:58:A:THR:HG23	18	0.1
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD1	17	0.1
(1,1144)	1:53:A:LEU:HD11	1:157:A:TYR:HD2	17	0.1
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD1	17	0.1
(1,1144)	1:53:A:LEU:HD12	1:157:A:TYR:HD2	17	0.1
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD1	17	0.1
(1,1144)	1:53:A:LEU:HD13	1:157:A:TYR:HD2	17	0.1
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD1	17	0.1
(1,1144)	1:53:A:LEU:HD21	1:157:A:TYR:HD2	17	0.1
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD1	17	0.1
(1,1144)	1:53:A:LEU:HD22	1:157:A:TYR:HD2	17	0.1
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD1	17	0.1
(1,1144)	1:53:A:LEU:HD23	1:157:A:TYR:HD2	17	0.1
(1,1128)	1:3:A:GLU:HA	1:52:A:LEU:HB3	11	0.1
(1,1080)	1:1:A:MET:HG3	1:51:A:CYS:HA	2	0.1
(1,1033)	1:90:A:PHE:HB2	1:129:A:GLN:HE21	15	0.1
(1,1033)	1:90:A:PHE:HB3	1:129:A:GLN:HE21	15	0.1
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB2	4	0.1
(1,1004)	1:86:A:ASN:HD21	1:89:A:SER:HB3	4	0.1
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB2	4	0.1
(1,1004)	1:86:A:ASN:HD22	1:89:A:SER:HB3	4	0.1
(1,884)	1:25:A:GLN:HA	1:27:A:HIS:HD2	10	0.1
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD1	17	0.1
(1,633)	1:68:A:ARG:H	1:71:A:TYR:HD2	17	0.1
(1,596)	1:14:A:VAL:H	1:82:A:PHE:HA	6	0.1
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG11	16	0.1
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG12	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG13	16	0.1
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG21	16	0.1
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG22	16	0.1
(1,582)	1:14:A:VAL:H	1:81:A:VAL:HG23	16	0.1
(1,558)	1:37:A:GLU:H	1:37:A:GLU:HB3	12	0.1
(1,508)	1:21:A:ILE:HD11	1:24:A:ILE:H	12	0.1
(1,508)	1:21:A:ILE:HD12	1:24:A:ILE:H	12	0.1
(1,508)	1:21:A:ILE:HD13	1:24:A:ILE:H	12	0.1
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG11	17	0.1
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG12	17	0.1
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG13	17	0.1
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG21	17	0.1
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG22	17	0.1
(1,481)	1:73:A:ARG:H	1:103:A:VAL:HG23	17	0.1
(1,374)	1:21:A:ILE:HA	1:24:A:ILE:HB	12	0.1
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG21	20	0.1
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG22	20	0.1
(1,276)	1:72:A:MET:HA	1:100:A:ILE:HG23	20	0.1
(1,252)	1:21:A:ILE:HG21	1:25:A:GLN:HE21	3	0.1
(1,252)	1:21:A:ILE:HG22	1:25:A:GLN:HE21	3	0.1
(1,252)	1:21:A:ILE:HG23	1:25:A:GLN:HE21	3	0.1
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE1	4	0.1
(1,238)	1:20:A:THR:HG21	1:40:A:TYR:HE2	4	0.1
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE1	4	0.1
(1,238)	1:20:A:THR:HG22	1:40:A:TYR:HE2	4	0.1
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE1	4	0.1
(1,238)	1:20:A:THR:HG23	1:40:A:TYR:HE2	4	0.1
(1,230)	1:4:A:TYR:HD1	1:5:A:LYS:H	14	0.1
(1,230)	1:4:A:TYR:HD2	1:5:A:LYS:H	14	0.1
(1,60)	1:14:A:VAL:HG11	1:89:A:SER:H	11	0.1
(1,60)	1:14:A:VAL:HG12	1:89:A:SER:H	11	0.1
(1,60)	1:14:A:VAL:HG13	1:89:A:SER:H	11	0.1
(1,60)	1:14:A:VAL:HG21	1:89:A:SER:H	11	0.1
(1,60)	1:14:A:VAL:HG22	1:89:A:SER:H	11	0.1
(1,60)	1:14:A:VAL:HG23	1:89:A:SER:H	11	0.1
(1,40)	1:106:A:SER:H	1:107:A:GLU:H	2	0.1
(1,40)	1:106:A:SER:H	1:107:A:GLU:H	3	0.1
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG21	14	0.1
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG22	14	0.1
(1,36)	1:111:A:MET:HB2	1:139:A:ILE:HG23	14	0.1
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD11	18	0.1
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD12	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:82:A:PHE:HB2	1:93:A:ILE:HD13	18	0.1

10 Dihedral-angle violation analysis

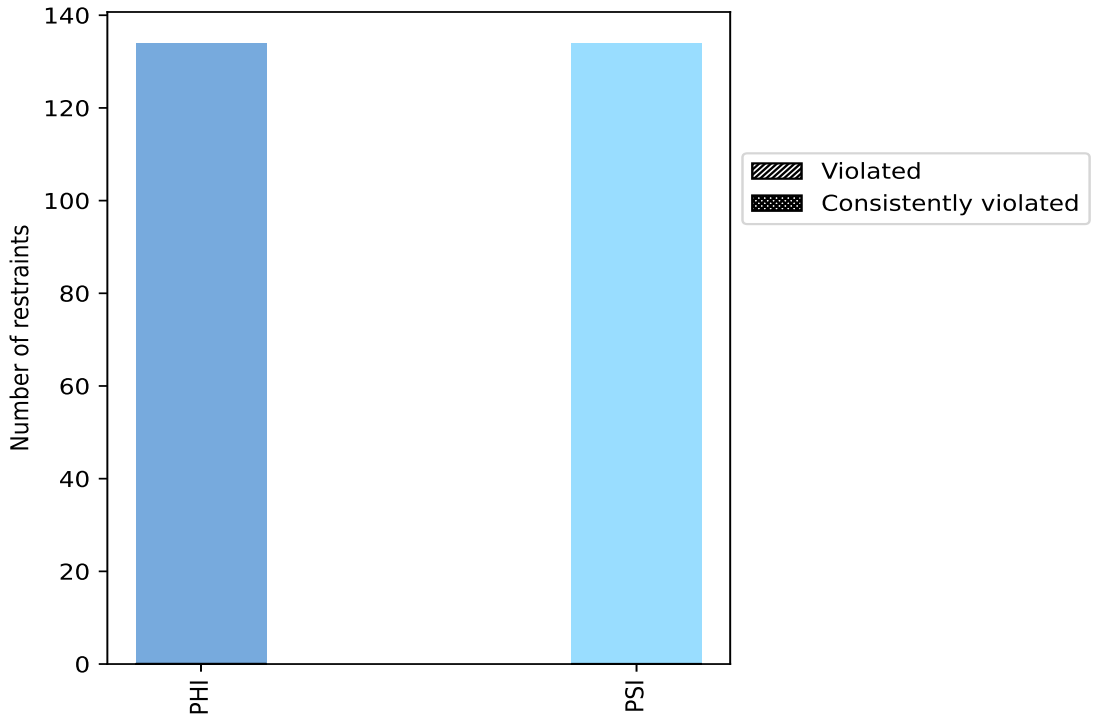
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	134	50.0	0	0.0	0.0	0	0.0	0.0
PSI	134	50.0	0	0.0	0.0	0	0.0	0.0
Total	268	100.0	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

No violations found

10.3 Dihedral-angle violation statistics for the ensemble (i)

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble (i)

No violations found

10.5 All violated dihedral-angle restraints (i)

No violations found