Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 04:32 PM EDT

PDB ID	:	6UHW
BMRB ID	:	30677
Title	:	Solution structure of an organic hydroperoxide resistance protein from Burkholderia pseudomallei. Seattle Structural Genomics Center for Infectious Disease target BupsA.00074.a.
Authors	:	Buchko, G.W.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2019-09-29

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 (1)) were used in the production of this report:

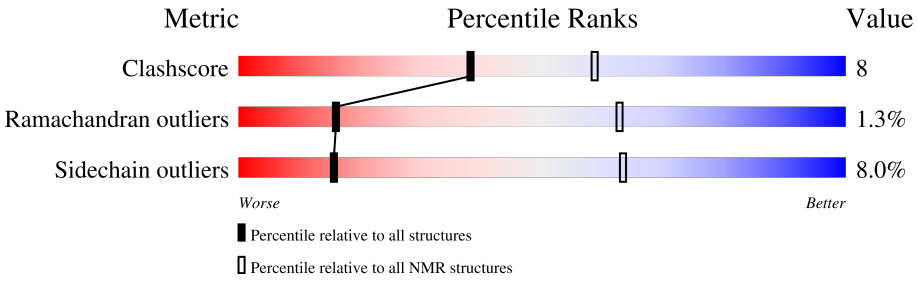
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 40%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	139	84% 14% ·
1	B	139	82% 14% ··

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:139, B:1-B:124, B:128-B:139 (275)	1.07	4

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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4037 atoms, of which 2016 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Organic hydroperoxide resistance protein.

Mol	Chain	Residues	Atoms						Trace
1	A	139	Total	C	H	N	O	S	0
			2019	625	1009	183	198	4	
1	B	139	Total	C	H	N	O	S	0
			2018	625	1007	183	199	4	

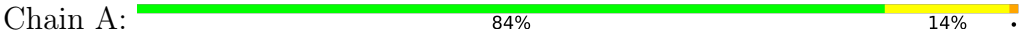
4 Residue-property plots

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.

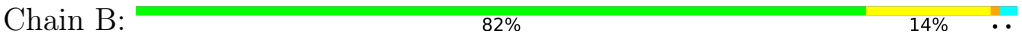
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

Chain B:



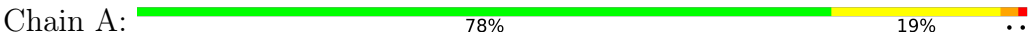
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

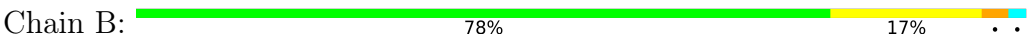
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

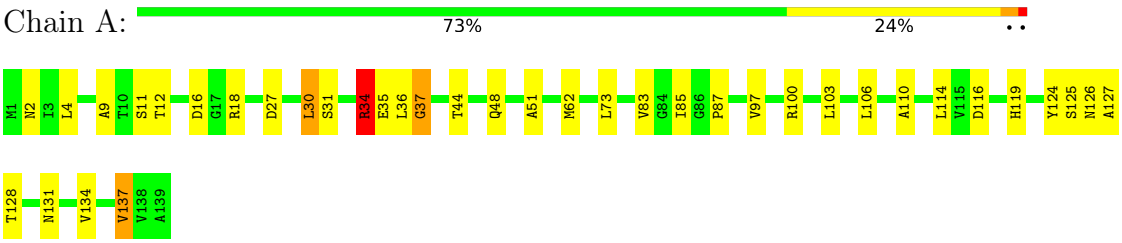
Chain B:



4.2.2 Score per residue for model 2

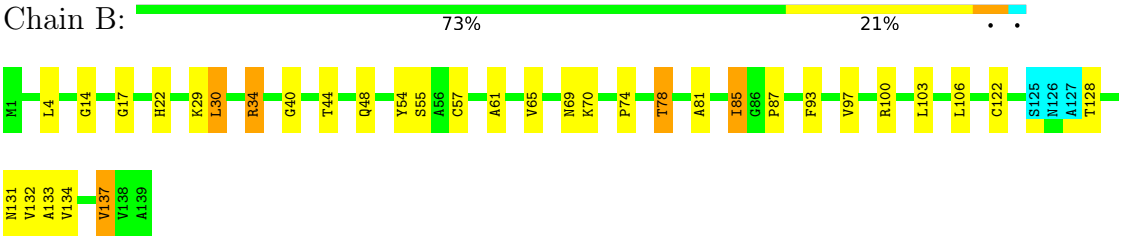
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

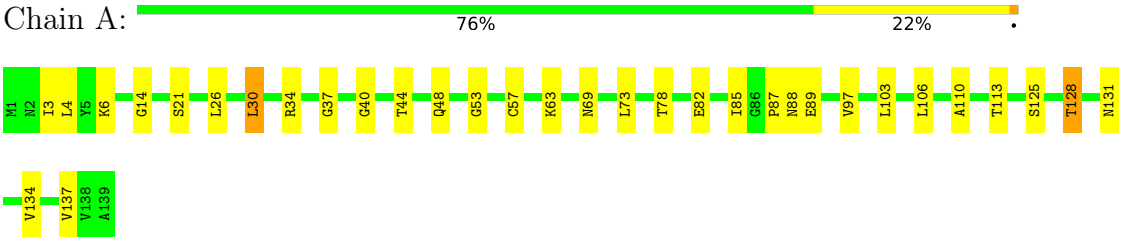
Chain B:



4.2.3 Score per residue for model 3

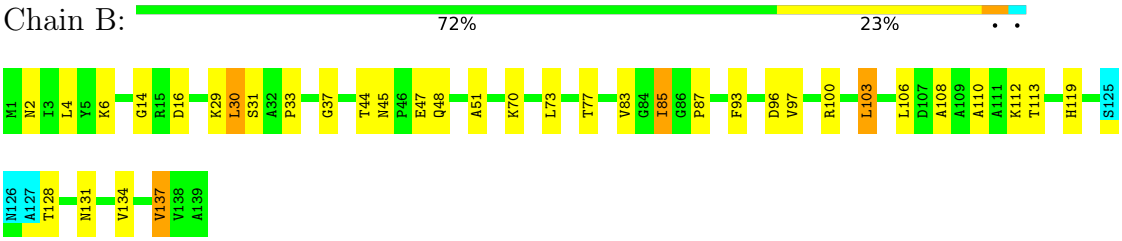
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

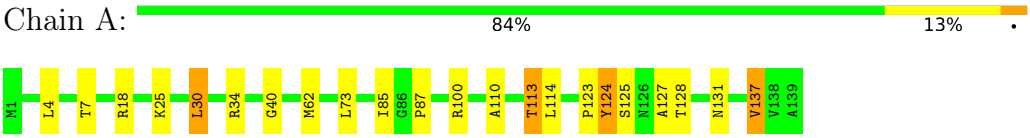
Chain B:



4.2.4 Score per residue for model 4 (medoid)

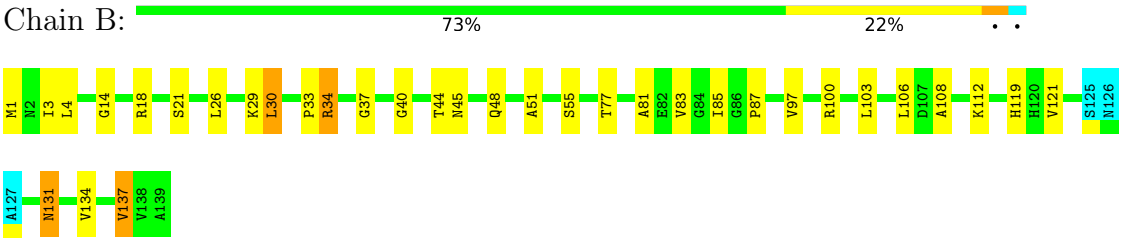
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

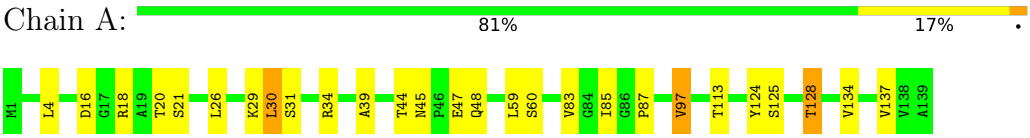
Chain B:



4.2.5 Score per residue for model 5

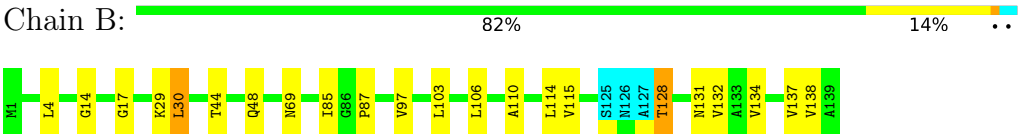
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

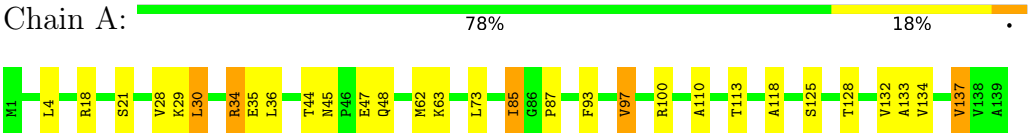
Chain B:



4.2.6 Score per residue for model 6

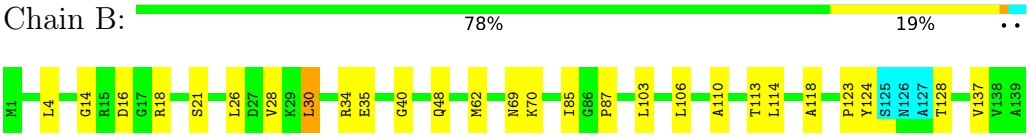
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

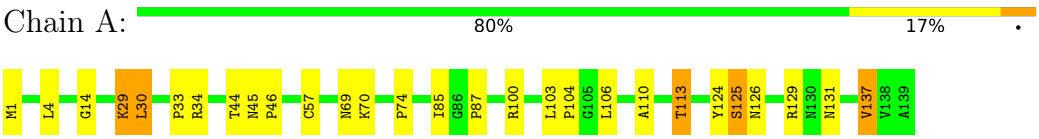
Chain B:



4.2.7 Score per residue for model 7

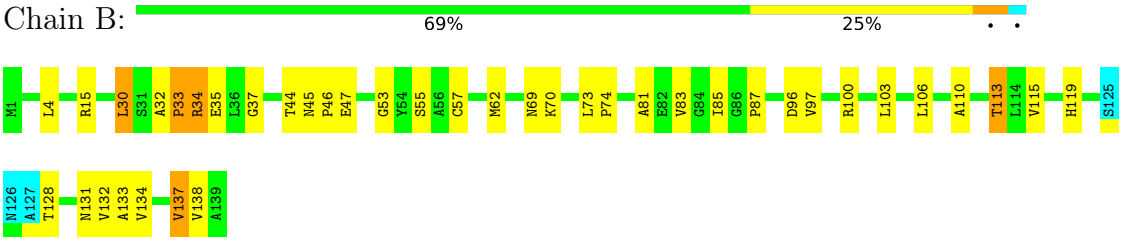
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

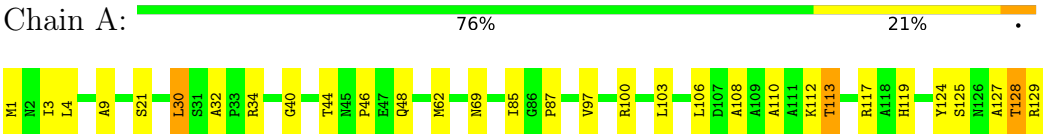
Chain B:



4.2.8 Score per residue for model 8

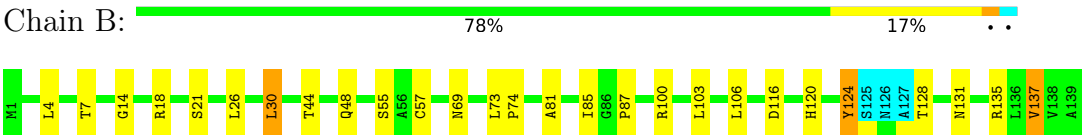
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

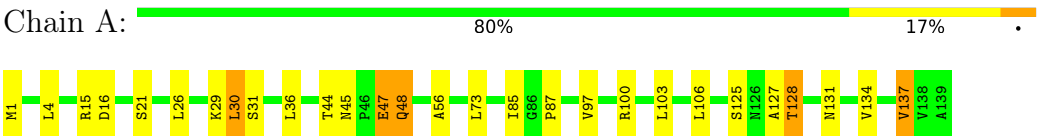
Chain B:



4.2.9 Score per residue for model 9

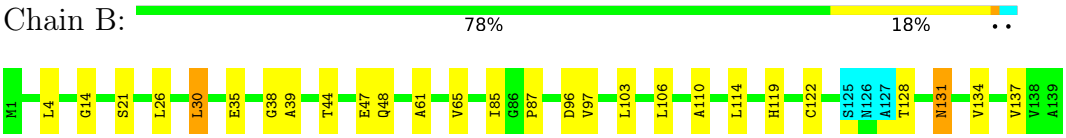
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

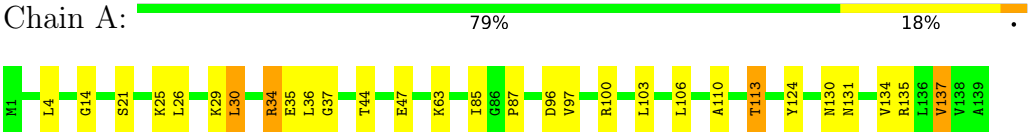
Chain B:



4.2.10 Score per residue for model 10

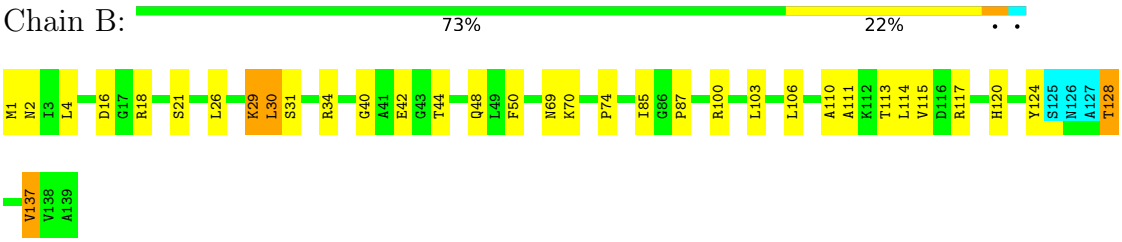
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

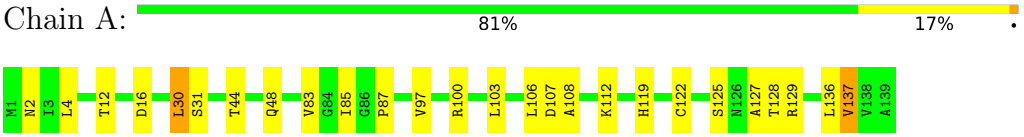
Chain B:



4.2.11 Score per residue for model 11

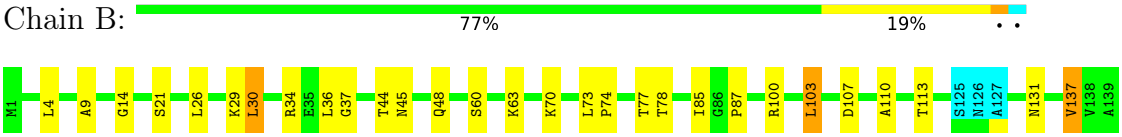
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

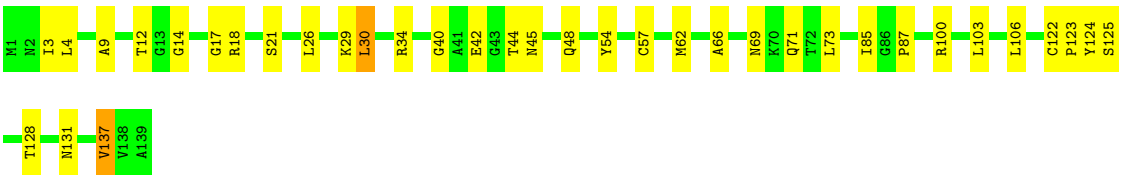
Chain B:



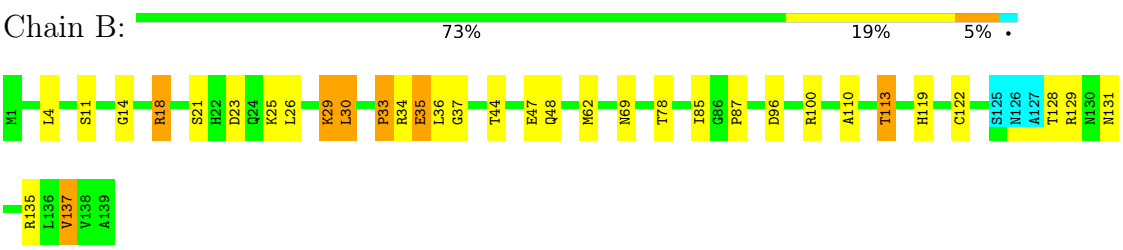
4.2.12 Score per residue for model 12

• Molecule 1: Organic hydroperoxide resistance protein

Chain A:

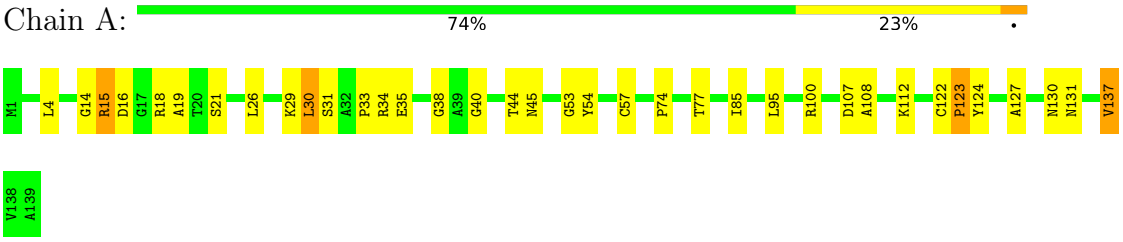


• Molecule 1: Organic hydroperoxide resistance protein

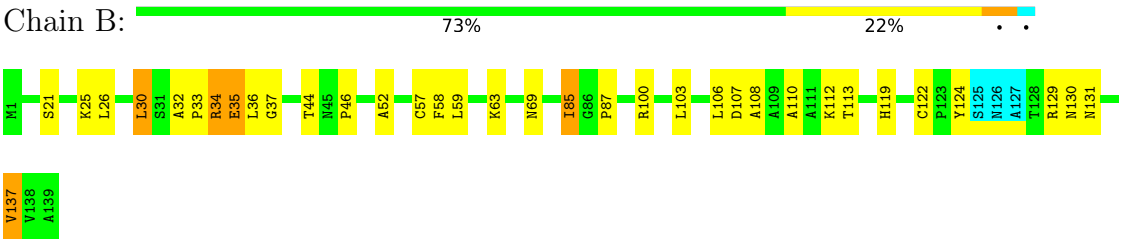


4.2.13 Score per residue for model 13

• Molecule 1: Organic hydroperoxide resistance protein

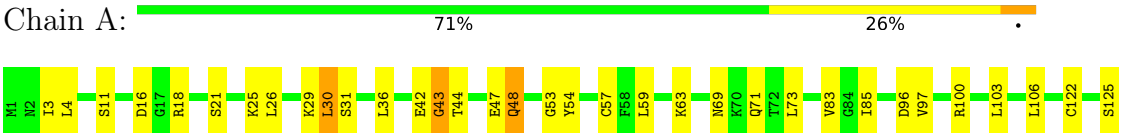


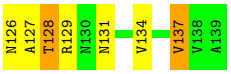
• Molecule 1: Organic hydroperoxide resistance protein



4.2.14 Score per residue for model 14

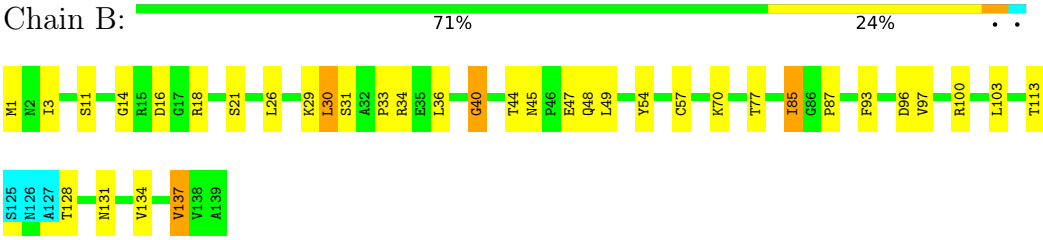
• Molecule 1: Organic hydroperoxide resistance protein





• Molecule 1: Organic hydroperoxide resistance protein

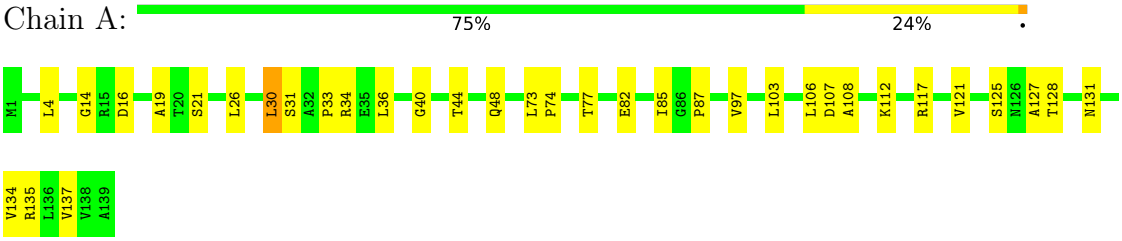
Chain B:



4.2.15 Score per residue for model 15

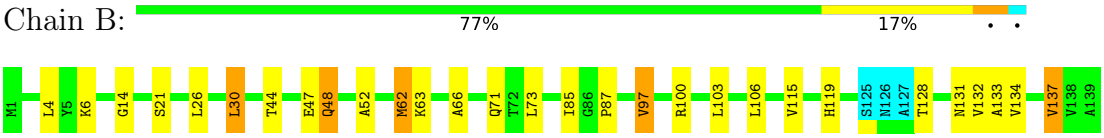
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

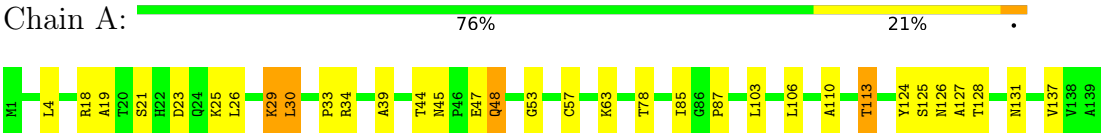
Chain B:



4.2.16 Score per residue for model 16

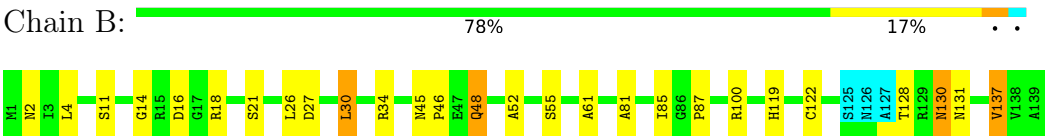
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

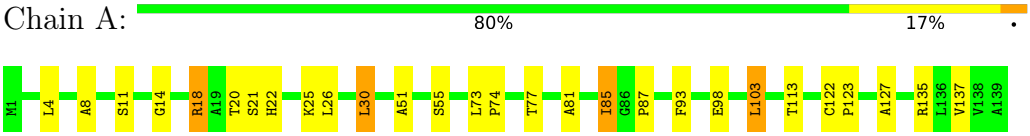
Chain B:



4.2.17 Score per residue for model 17

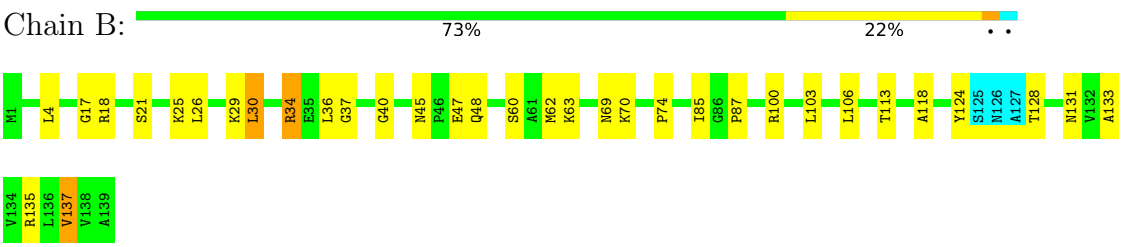
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

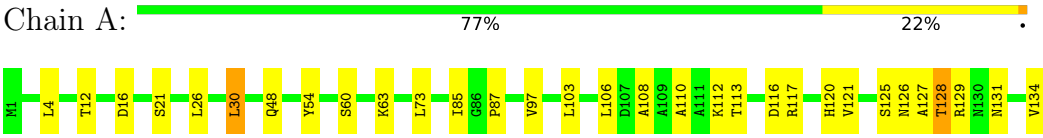
Chain B:



4.2.18 Score per residue for model 18

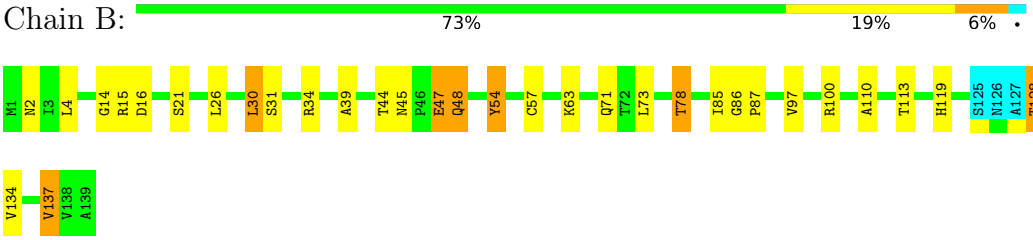
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

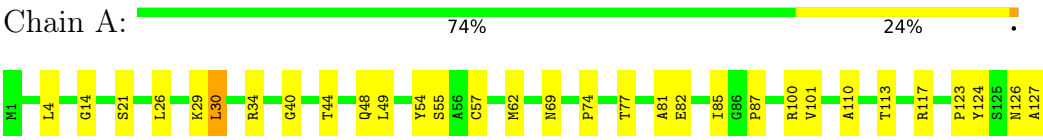
Chain B:



4.2.19 Score per residue for model 19

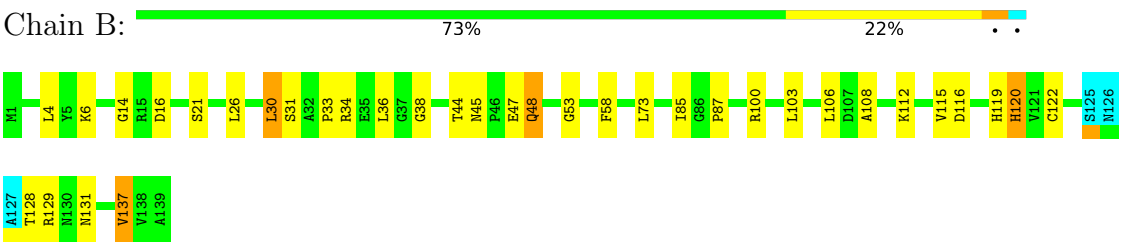
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

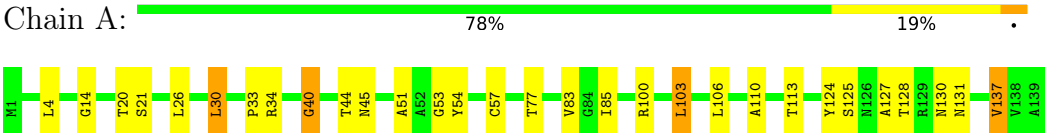
Chain B:



4.2.20 Score per residue for model 20

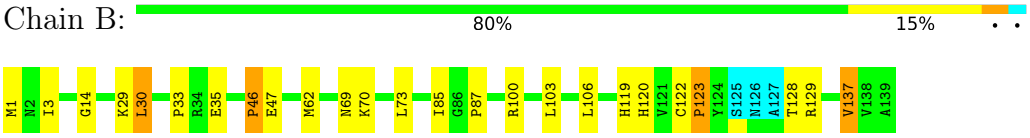
• Molecule 1: Organic hydroperoxide resistance protein

Chain A:



• Molecule 1: Organic hydroperoxide resistance protein

Chain B:



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	refinement	2.1
CYANA	structure calculation	

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	1396
Number of shifts mapped to atoms	1396
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

6 Model quality

6.1 Standard geometry

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	1010	1009	1006	19±4
1	B	992	991	990	18±4
All	All	40040	40000	39920	643

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:PHE:HE2	1:B:122:CYS:HG	0.90	1.09	13	1
1:A:54:TYR:HA	1:A:57:CYS:SG	0.79	2.18	12	3
1:B:57:CYS:HG	1:B:124:TYR:HE2	0.78	1.20	8	2
1:A:103:LEU:HD23	1:A:106:LEU:HD22	0.74	1.58	3	11
1:B:54:TYR:HA	1:B:57:CYS:SG	0.73	2.24	2	3
1:A:46:PRO:HB3	1:B:57:CYS:SG	0.71	2.26	1	2
1:B:97:VAL:HB	1:B:134:VAL:HG22	0.65	1.67	18	7
1:B:103:LEU:HD23	1:B:106:LEU:HD22	0.65	1.66	2	12
1:A:57:CYS:SG	1:B:46:PRO:HB3	0.64	2.31	7	4
1:B:30:LEU:HA	1:B:44:THR:H	0.64	1.52	11	14
1:A:97:VAL:HB	1:A:134:VAL:HG22	0.64	1.69	8	4
1:B:97:VAL:HG13	1:B:134:VAL:HG22	0.63	1.69	1	2
1:A:97:VAL:HG13	1:A:134:VAL:HG22	0.63	1.69	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ALA:HB2	1:B:48:GLN:HE21	0.62	1.54	12	1
1:A:30:LEU:HA	1:A:44:THR:H	0.62	1.53	19	9
1:B:32:ALA:O	1:B:34:ARG:HD3	0.61	1.96	7	1
1:B:130:ASN:HD22	1:B:131:ASN:N	0.61	1.93	16	1
1:A:4:LEU:HG	1:B:87:PRO:HD3	0.60	1.73	4	20
1:B:122:CYS:SG	1:B:129:ARG:NE	0.60	2.75	19	1
1:B:62:MET:HG2	1:B:73:LEU:HD12	0.60	1.73	15	1
1:B:62:MET:SD	1:B:63:LYS:N	0.60	2.75	15	1
1:A:127:ALA:O	1:A:131:ASN:HB3	0.58	1.98	15	11
1:B:119:HIS:HA	1:B:122:CYS:SG	0.58	2.39	13	1
1:A:55:SER:OG	1:A:81:ALA:HB2	0.57	2.00	19	2
1:A:54:TYR:O	1:A:57:CYS:SG	0.57	2.61	19	1
1:B:34:ARG:HB2	1:B:40:GLY:HA3	0.56	1.75	14	3
1:B:45:ASN:HB2	1:B:48:GLN:HB3	0.56	1.74	17	5
1:B:62:MET:HE2	1:B:73:LEU:HD12	0.56	1.75	15	1
1:A:21:SER:HB3	1:A:26:LEU:N	0.56	2.16	20	11
1:A:34:ARG:O	1:A:36:LEU:N	0.56	2.38	2	3
1:A:87:PRO:HD3	1:B:4:LEU:HG	0.55	1.77	17	17
1:A:116:ASP:HA	1:A:119:HIS:CD2	0.55	2.36	2	1
1:B:30:LEU:HD13	1:B:30:LEU:N	0.54	2.17	6	20
1:A:45:ASN:HB2	1:A:48:GLN:HB3	0.54	1.79	9	4
1:A:9:ALA:HA	1:A:21:SER:HA	0.54	1.80	8	1
1:B:133:ALA:HB1	1:B:135:ARG:NH1	0.54	2.18	17	1
1:A:57:CYS:SG	1:A:124:TYR:CE2	0.53	3.01	19	1
1:A:30:LEU:HD13	1:A:30:LEU:N	0.53	2.17	14	20
1:B:53:GLY:O	1:B:57:CYS:SG	0.53	2.66	1	2
1:A:125:SER:O	1:A:128:THR:HG22	0.53	2.04	3	13
1:B:122:CYS:SG	1:B:128:THR:HG21	0.52	2.44	12	2
1:A:30:LEU:HB2	1:A:44:THR:O	0.52	2.04	1	6
1:B:74:PRO:HD2	1:B:103:LEU:HD11	0.52	1.81	2	6
1:B:33:PRO:HG2	1:B:35:GLU:HG3	0.52	1.80	12	1
1:A:97:VAL:O	1:A:134:VAL:HA	0.52	2.03	6	5
1:B:62:MET:SD	1:B:118:ALA:HB1	0.52	2.44	17	2
1:B:30:LEU:HB2	1:B:44:THR:O	0.52	2.03	7	3
1:A:9:ALA:HB2	1:B:48:GLN:NE2	0.52	2.20	12	2
1:A:125:SER:O	1:A:129:ARG:HG2	0.52	2.04	11	1
1:B:116:ASP:O	1:B:120:HIS:HB2	0.52	2.05	8	2
1:A:119:HIS:CE1	1:A:128:THR:HG23	0.52	2.39	11	1
1:B:57:CYS:SG	1:B:124:TYR:HE2	0.52	2.28	13	1
1:A:21:SER:CB	1:A:26:LEU:HB3	0.51	2.35	18	3
1:B:100:ARG:HA	1:B:137:VAL:O	0.51	2.05	7	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:VAL:HG12	1:A:97:VAL:HB	0.51	1.83	5	1
1:A:34:ARG:HB2	1:A:40:GLY:HA3	0.51	1.83	13	3
1:B:11:SER:HA	1:B:18:ARG:O	0.51	2.05	16	3
1:B:130:ASN:HD22	1:B:131:ASN:H	0.51	1.47	16	1
1:A:110:ALA:O	1:A:113:THR:HG22	0.51	2.06	3	11
1:B:62:MET:HG3	1:B:73:LEU:HD11	0.51	1.83	7	2
1:A:33:PRO:HB2	1:A:35:GLU:HG2	0.51	1.81	13	1
1:A:100:ARG:HA	1:A:137:VAL:O	0.51	2.06	9	14
1:B:34:ARG:O	1:B:36:LEU:N	0.51	2.44	13	1
1:A:48:GLN:OE1	1:B:21:SER:HB2	0.51	2.06	14	2
1:A:126:ASN:HB3	1:B:131:ASN:HD21	0.50	1.65	2	1
1:B:124:TYR:HB3	1:B:128:THR:HG21	0.50	1.82	17	2
1:A:34:ARG:HB2	1:A:40:GLY:N	0.50	2.21	12	2
1:A:25:LYS:HG3	1:B:48:GLN:HE22	0.50	1.67	14	1
1:A:11:SER:HA	1:A:18:ARG:O	0.50	2.07	14	3
1:A:128:THR:OG1	1:A:134:VAL:HG21	0.50	2.06	14	1
1:A:15:ARG:NE	1:A:15:ARG:HA	0.49	2.21	9	2
1:A:119:HIS:HB3	1:A:129:ARG:HD2	0.49	1.83	8	1
1:A:125:SER:HA	1:A:128:THR:HG22	0.49	1.83	9	1
1:A:53:GLY:O	1:A:57:CYS:SG	0.49	2.70	20	4
1:A:4:LEU:HG	1:B:86:GLY:HA2	0.49	1.83	18	1
1:A:132:VAL:HG12	1:A:133:ALA:H	0.49	1.68	6	1
1:A:3:ILE:HD11	1:B:96:ASP:HB3	0.49	1.84	12	3
1:A:96:ASP:HB3	1:B:3:ILE:HD11	0.49	1.84	14	1
1:B:33:PRO:HG3	1:B:45:ASN:HD21	0.49	1.67	14	1
1:B:9:ALA:HA	1:B:21:SER:HA	0.49	1.83	11	1
1:B:119:HIS:CE1	1:B:128:THR:HG23	0.49	2.42	12	1
1:B:48:GLN:HA	1:B:48:GLN:HE21	0.49	1.67	15	1
1:B:21:SER:HB3	1:B:26:LEU:N	0.49	2.22	13	13
1:B:97:VAL:CG1	1:B:134:VAL:HG22	0.49	2.38	1	2
1:A:30:LEU:HB3	1:A:44:THR:HB	0.49	1.85	2	2
1:A:74:PRO:HB2	1:A:104:PRO:HG2	0.48	1.84	7	1
1:A:126:ASN:O	1:A:129:ARG:HG2	0.48	2.07	7	4
1:A:83:VAL:HG23	1:A:97:VAL:HG22	0.48	1.85	14	1
1:B:21:SER:HB2	1:B:26:LEU:HB3	0.48	1.85	9	2
1:A:34:ARG:HD2	1:A:40:GLY:HA2	0.48	1.84	20	1
1:A:18:ARG:HG3	1:A:28:VAL:O	0.48	2.09	6	1
1:A:33:PRO:HD3	1:A:45:ASN:ND2	0.48	2.23	13	1
1:B:45:ASN:ND2	1:B:48:GLN:HB2	0.48	2.24	19	1
1:A:87:PRO:HD2	1:B:2:ASN:O	0.48	2.09	16	4
1:B:110:ALA:O	1:B:113:THR:HG22	0.48	2.08	18	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:LYS:HE3	1:B:42:GLU:HG3	0.48	1.85	10	1
1:A:19:ALA:HB1	1:B:52:ALA:HB1	0.48	1.85	16	3
1:A:30:LEU:HB3	1:A:44:THR:OG1	0.48	2.09	20	2
1:B:59:LEU:O	1:B:63:LYS:HG2	0.48	2.08	13	1
1:A:103:LEU:HD12	1:A:106:LEU:HB2	0.48	1.86	15	1
1:B:62:MET:HE3	1:B:73:LEU:HB2	0.48	1.85	15	1
1:A:34:ARG:HB2	1:A:40:GLY:CA	0.47	2.39	3	2
1:B:34:ARG:HB2	1:B:40:GLY:N	0.47	2.24	6	1
1:A:1:MET:SD	1:B:96:ASP:HB2	0.47	2.48	9	2
1:A:124:TYR:O	1:A:125:SER:HB2	0.47	2.09	7	1
1:B:122:CYS:N	1:B:123:PRO:HD3	0.47	2.24	20	1
1:B:33:PRO:HD2	1:B:45:ASN:OD1	0.47	2.10	3	1
1:B:108:ALA:O	1:B:112:LYS:HG3	0.47	2.09	4	3
1:B:131:ASN:HD22	1:B:132:VAL:HG13	0.47	1.68	5	1
1:A:46:PRO:HB2	1:B:57:CYS:SG	0.47	2.49	8	1
1:B:128:THR:O	1:B:134:VAL:HG23	0.47	2.09	15	1
1:A:108:ALA:O	1:A:112:LYS:HG3	0.47	2.10	18	3
1:B:115:VAL:O	1:B:119:HIS:HB2	0.47	2.10	15	1
1:A:29:LYS:NZ	1:A:29:LYS:HB3	0.47	2.24	7	1
1:B:85:ILE:HD11	1:B:93:PHE:CD2	0.46	2.45	2	3
1:A:128:THR:O	1:A:134:VAL:HG23	0.46	2.10	6	1
1:B:103:LEU:HB3	1:B:106:LEU:HD23	0.46	1.86	4	3
1:A:18:ARG:HA	1:A:29:LYS:HA	0.46	1.86	16	4
1:A:122:CYS:N	1:A:123:PRO:HD3	0.46	2.25	17	3
1:A:12:THR:HA	1:B:78:THR:HG22	0.46	1.86	18	4
1:A:15:ARG:HA	1:A:15:ARG:HE	0.46	1.70	13	1
1:B:108:ALA:O	1:B:112:LYS:HG2	0.46	2.10	19	1
1:A:62:MET:HG3	1:A:73:LEU:HD11	0.46	1.88	2	1
1:A:34:ARG:HH11	1:A:37:GLY:HA2	0.46	1.69	2	1
1:A:32:ALA:HA	1:A:46:PRO:HD2	0.46	1.87	8	1
1:B:62:MET:SD	1:B:62:MET:C	0.46	2.94	15	1
1:A:77:THR:OG1	1:A:103:LEU:HD22	0.46	2.11	17	1
1:B:62:MET:HG2	1:B:73:LEU:CD1	0.46	2.40	15	1
1:A:54:TYR:HD1	1:A:57:CYS:SG	0.46	2.34	12	1
1:B:29:LYS:NZ	1:B:29:LYS:HB3	0.45	2.26	12	2
1:B:115:VAL:HG21	1:B:138:VAL:HG12	0.45	1.88	7	2
1:A:15:ARG:HA	1:A:15:ARG:NE	0.45	2.26	13	1
1:B:61:ALA:HB1	1:B:122:CYS:SG	0.45	2.52	2	2
1:B:1:MET:HE3	1:B:3:ILE:HD13	0.45	1.88	20	2
1:A:108:ALA:O	1:A:112:LYS:HG2	0.45	2.11	13	2
1:A:74:PRO:O	1:A:77:THR:HG22	0.45	2.11	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:30:LEU:HA	1:B:44:THR:N	0.45	2.26	14	1
1:A:82:GLU:HG2	1:B:6:LYS:HD3	0.45	1.87	19	3
1:A:63:LYS:NZ	1:B:16:ASP:HA	0.45	2.26	14	2
1:B:111:ALA:O	1:B:115:VAL:HG23	0.45	2.12	10	1
1:A:96:ASP:HB2	1:B:1:MET:SD	0.45	2.51	10	2
1:B:60:SER:HA	1:B:63:LYS:HD3	0.45	1.88	11	1
1:B:36:LEU:HG	1:B:85:ILE:HD12	0.45	1.88	13	1
1:A:103:LEU:HB2	1:A:106:LEU:HD23	0.45	1.88	11	1
1:A:101:VAL:HB	1:A:138:VAL:HG13	0.45	1.87	19	1
1:A:57:CYS:HG	1:A:124:TYR:HE2	0.45	1.53	7	1
1:A:25:LYS:NZ	1:B:45:ASN:OD1	0.45	2.50	17	1
1:A:116:ASP:O	1:A:120:HIS:HB2	0.45	2.12	18	1
1:A:63:LYS:HZ2	1:A:63:LYS:HB2	0.45	1.71	3	1
1:B:124:TYR:CD2	1:B:124:TYR:N	0.45	2.85	13	2
1:B:60:SER:O	1:B:63:LYS:HB3	0.45	2.12	17	1
1:A:21:SER:OG	1:B:48:GLN:NE2	0.44	2.50	6	2
1:B:35:GLU:HB2	1:B:36:LEU:HD22	0.44	1.90	12	1
1:A:51:ALA:HB2	1:A:83:VAL:HG11	0.44	1.88	2	2
1:B:55:SER:HB3	1:B:81:ALA:HB2	0.44	1.89	7	2
1:A:48:GLN:OE1	1:B:7:THR:HG23	0.44	2.12	8	1
1:A:16:ASP:HB3	1:A:31:SER:HA	0.44	1.89	2	7
1:B:66:ALA:HB1	1:B:71:GLN:O	0.44	2.12	15	1
1:B:45:ASN:HB3	1:B:47:GLU:OE1	0.44	2.12	18	1
1:B:21:SER:CB	1:B:26:LEU:HB3	0.44	2.41	9	1
1:A:63:LYS:NZ	1:B:16:ASP:OD1	0.44	2.50	18	1
1:A:59:LEU:HD12	1:A:60:SER:N	0.44	2.28	5	1
1:B:45:ASN:HB2	1:B:48:GLN:CB	0.44	2.43	18	2
1:B:128:THR:OG1	1:B:134:VAL:HG21	0.44	2.11	18	1
1:A:122:CYS:O	1:A:125:SER:HB2	0.44	2.12	11	1
1:A:110:ALA:O	1:A:114:LEU:HG	0.44	2.13	4	2
1:A:45:ASN:HB2	1:A:48:GLN:CB	0.44	2.43	6	2
1:B:36:LEU:N	1:B:36:LEU:HD22	0.44	2.28	17	3
1:A:122:CYS:HB2	1:A:125:SER:OG	0.44	2.13	14	1
1:B:97:VAL:O	1:B:134:VAL:HA	0.43	2.12	18	4
1:A:1:MET:HE3	1:A:3:ILE:HD13	0.43	1.90	8	1
1:B:21:SER:OG	1:B:25:LYS:HB2	0.43	2.13	13	2
1:B:77:THR:CB	1:B:103:LEU:HD22	0.43	2.42	3	2
1:A:98:GLU:HG2	1:A:135:ARG:HD3	0.43	1.89	17	1
1:B:45:ASN:HD21	1:B:48:GLN:HB2	0.43	1.71	19	1
1:A:97:VAL:CG1	1:A:134:VAL:HG22	0.43	2.43	5	2
1:A:132:VAL:HG12	1:A:133:ALA:N	0.43	2.28	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:ARG:HD3	1:B:34:ARG:N	0.43	2.28	7	1
1:A:20:THR:HG23	1:A:26:LEU:O	0.43	2.13	20	2
1:B:18:ARG:HA	1:B:29:LYS:HA	0.43	1.90	14	2
1:A:83:VAL:HG12	1:A:97:VAL:HG13	0.43	1.89	11	1
1:A:124:TYR:O	1:A:128:THR:HB	0.43	2.14	12	1
1:A:77:THR:HB	1:A:103:LEU:HD22	0.43	1.90	20	2
1:A:36:LEU:HD22	1:A:36:LEU:N	0.43	2.28	9	3
1:B:77:THR:HB	1:B:103:LEU:HD13	0.43	1.91	14	1
1:B:70:LYS:N	1:B:70:LYS:HD3	0.43	2.29	17	1
1:B:119:HIS:CD2	1:B:129:ARG:HB3	0.43	2.48	20	1
1:A:123:PRO:O	1:A:124:TYR:HB2	0.43	2.13	1	1
1:B:74:PRO:O	1:B:77:THR:HG22	0.43	2.13	1	1
1:B:77:THR:HB	1:B:103:LEU:HD22	0.43	1.90	4	1
1:A:96:ASP:CB	1:B:3:ILE:HD11	0.43	2.44	14	1
1:A:51:ALA:HB1	1:A:81:ALA:HB1	0.43	1.89	17	1
1:B:34:ARG:HB2	1:B:40:GLY:CA	0.43	2.44	6	4
1:A:53:GLY:HA3	1:B:49:LEU:HD12	0.43	1.91	14	1
1:B:33:PRO:HB2	1:B:35:GLU:HG2	0.43	1.89	20	1
1:A:113:THR:O	1:A:117:ARG:HG2	0.42	2.14	1	3
1:A:59:LEU:O	1:A:63:LYS:HD3	0.42	2.14	14	1
1:B:55:SER:OG	1:B:81:ALA:HB2	0.42	2.13	16	4
1:B:103:LEU:HD12	1:B:106:LEU:HB2	0.42	1.91	4	1
1:A:47:GLU:H	1:A:47:GLU:CD	0.42	2.17	1	2
1:B:17:GLY:O	1:B:29:LYS:HG3	0.42	2.14	5	3
1:B:110:ALA:O	1:B:114:LEU:HG	0.42	2.15	10	4
1:A:33:PRO:HG3	1:A:45:ASN:ND2	0.42	2.28	20	2
1:B:83:VAL:HG23	1:B:97:VAL:HG22	0.42	1.90	7	1
1:A:103:LEU:HB3	1:A:106:LEU:HD23	0.42	1.92	20	3
1:B:18:ARG:HG3	1:B:28:VAL:O	0.42	2.14	6	1
1:B:38:GLY:O	1:B:39:ALA:HB3	0.42	2.15	9	1
1:A:124:TYR:O	1:A:125:SER:HB3	0.42	2.14	12	1
1:A:6:LYS:HG3	1:B:83:VAL:O	0.42	2.15	3	1
1:B:23:ASP:HB2	1:B:25:LYS:HG2	0.42	1.92	12	1
1:A:18:ARG:NH1	1:A:20:THR:OG1	0.42	2.52	5	1
1:A:62:MET:SD	1:A:118:ALA:HB1	0.42	2.55	6	1
1:A:21:SER:HB3	1:A:26:LEU:HB3	0.42	1.92	20	1
1:A:128:THR:HG23	1:A:134:VAL:HG21	0.42	1.90	6	1
1:B:103:LEU:HD23	1:B:106:LEU:CD2	0.42	2.44	9	2
1:A:42:GLU:HG3	1:A:43:GLY:N	0.42	2.30	14	1
1:B:120:HIS:HB2	1:B:129:ARG:NH1	0.42	2.29	20	1
1:A:135:ARG:CD	1:A:135:ARG:N	0.41	2.83	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ALA:HB1	1:A:71:GLN:O	0.41	2.15	12	1
1:A:60:SER:O	1:A:63:LYS:HB3	0.41	2.15	18	1
1:B:115:VAL:HG13	1:B:119:HIS:CD2	0.41	2.50	19	1
1:A:33:PRO:HD3	1:A:45:ASN:HB2	0.41	1.91	16	1
1:A:125:SER:HB3	1:A:128:THR:HB	0.41	1.90	16	1
1:A:2:ASN:O	1:B:87:PRO:HD2	0.41	2.15	2	2
1:B:119:HIS:NE2	1:B:128:THR:HG23	0.41	2.29	16	2
1:A:34:ARG:HG3	1:A:40:GLY:N	0.41	2.31	1	2
1:B:33:PRO:HG3	1:B:45:ASN:ND2	0.41	2.30	4	1
1:B:103:LEU:O	1:B:106:LEU:HB3	0.41	2.14	8	1
1:A:17:GLY:O	1:A:29:LYS:HG3	0.41	2.14	12	1
1:B:132:VAL:HG12	1:B:133:ALA:N	0.41	2.30	2	3
1:B:16:ASP:HB3	1:B:31:SER:HA	0.41	1.92	14	5
1:B:33:PRO:O	1:B:35:GLU:N	0.41	2.54	7	1
1:A:45:ASN:HB3	1:A:47:GLU:OE1	0.41	2.15	9	1
1:B:117:ARG:O	1:B:120:HIS:HB3	0.41	2.15	10	1
1:A:3:ILE:HD11	1:B:96:ASP:CB	0.41	2.46	14	1
1:B:128:THR:HA	1:B:132:VAL:HB	0.41	1.92	1	1
1:A:7:THR:HG23	1:B:48:GLN:OE1	0.41	2.14	4	1
1:B:32:ALA:O	1:B:34:ARG:N	0.41	2.51	13	1
1:A:16:ASP:CB	1:A:31:SER:HA	0.41	2.45	2	1
1:A:56:ALA:HB1	1:B:30:LEU:HD21	0.41	1.91	9	1
1:A:25:LYS:NZ	1:B:48:GLN:OE1	0.41	2.54	16	1
1:B:33:PRO:HG2	1:B:36:LEU:HD23	0.41	1.91	19	1
1:B:61:ALA:O	1:B:65:VAL:HG23	0.41	2.16	9	2
1:A:97:VAL:HG13	1:A:134:VAL:HG13	0.41	1.93	15	1
1:A:126:ASN:OD1	1:A:127:ALA:N	0.41	2.53	16	1
1:A:8:ALA:O	1:A:22:HIS:ND1	0.41	2.54	17	1
1:B:51:ALA:HB2	1:B:83:VAL:HG11	0.41	1.93	4	2
1:B:33:PRO:O	1:B:35:GLU:HG2	0.41	2.16	13	1
1:A:71:GLN:HE22	1:A:73:LEU:HD21	0.41	1.75	14	1
1:B:77:THR:OG1	1:B:103:LEU:HD22	0.40	2.16	14	1
1:A:7:THR:OG1	1:A:25:LYS:NZ	0.40	2.52	4	1
1:A:124:TYR:HH	1:B:50:PHE:HD2	0.40	1.59	10	1
1:A:119:HIS:ND1	1:A:136:LEU:HD11	0.40	2.31	11	1
1:A:117:ARG:O	1:A:121:VAL:HG22	0.40	2.16	15	2
1:A:49:LEU:HD12	1:B:53:GLY:HA3	0.40	1.91	19	1
1:B:65:VAL:HG13	1:B:69:ASN:ND2	0.40	2.31	2	1
1:A:85:ILE:HD11	1:A:93:PHE:CD2	0.40	2.51	17	2
1:A:25:LYS:HE3	1:B:48:GLN:OE1	0.40	2.17	10	1
1:A:33:PRO:HG2	1:A:36:LEU:HD23	0.40	1.93	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:66:ALA:HA	1:B:71:GLN:HG3	0.40	1.92	15	1
1:A:21:SER:HB2	1:A:26:LEU:HB3	0.40	1.93	18	1
1:B:34:ARG:HG2	1:B:40:GLY:CA	0.40	2.46	2	1
1:A:88:ASN:OD1	1:A:89:GLU:N	0.40	2.54	3	1
1:A:63:LYS:NZ	1:B:16:ASP:O	0.40	2.54	6	1
1:A:48:GLN:NE2	1:B:21:SER:HB2	0.40	2.31	12	1
1:B:36:LEU:HD22	1:B:36:LEU:N	0.40	2.31	19	1
1:A:34:ARG:NH1	1:A:37:GLY:HA2	0.40	2.30	2	1
1:A:16:ASP:O	1:B:63:LYS:NZ	0.40	2.55	18	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	137/139 (99%)	126±2 (92±2%)	9±2 (7±1%)	2±1 (1±1%)	16	63
1	B	134/139 (96%)	124±3 (93±2%)	8±3 (6±2%)	2±1 (1±1%)	16	63
All	All	5420/5560 (97%)	5004 (92%)	345 (6%)	71 (1%)	16	63

All 25 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	14	GLY	16
1	A	14	GLY	10
1	B	37	GLY	7
1	A	37	GLY	4
1	A	123	PRO	4
1	A	34	ARG	3
1	A	35	GLU	3
1	A	124	TYR	2
1	A	39	ALA	2
1	B	123	PRO	2
1	B	33	PRO	2
1	B	34	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	40	GLY	2
1	A	33	PRO	1
1	B	43	GLY	1
1	B	121	VAL	1
1	A	125	SER	1
1	A	42	GLU	1
1	A	38	GLY	1
1	B	35	GLU	1
1	A	43	GLY	1
1	B	40	GLY	1
1	B	39	ALA	1
1	B	38	GLY	1
1	B	46	PRO	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	102/102 (100%)	94±1 (92±1%)	8±1 (8±1%)	16	64
1	B	100/102 (98%)	92±2 (92±2%)	8±2 (8±2%)	15	62
All	All	4040/4080 (99%)	3718 (92%)	322 (8%)	16	63

All 61 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	30	LEU	20
1	A	85	ILE	20
1	A	137	VAL	20
1	B	30	LEU	20
1	B	85	ILE	20
1	B	137	VAL	20
1	B	47	GLU	11
1	A	48	GLN	10
1	B	69	ASN	10
1	A	124	TYR	8
1	B	34	ARG	8

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Mol	Chain	Res	Type	Models (Total)
1	B	70	LYS	8
1	A	73	LEU	8
1	B	48	GLN	7
1	A	113	THR	7
1	A	29	LYS	7
1	B	73	LEU	6
1	A	69	ASN	6
1	A	128	THR	6
1	A	131	ASN	6
1	A	62	MET	5
1	B	113	THR	5
1	A	34	ARG	5
1	B	29	LYS	5
1	B	131	ASN	5
1	A	47	GLU	5
1	B	128	THR	4
1	B	18	ARG	4
1	A	130	ASN	4
1	B	35	GLU	3
1	A	107	ASP	3
1	A	54	TYR	3
1	B	130	ASN	3
1	B	97	VAL	2
1	B	78	THR	2
1	A	78	THR	2
1	B	103	LEU	2
1	A	18	ARG	2
1	A	97	VAL	2
1	B	124	TYR	2
1	B	15	ARG	2
1	B	135	ARG	2
1	B	107	ASP	2
1	B	62	MET	2
1	A	103	LEU	2
1	A	22	HIS	1
1	B	100	ARG	1
1	A	27	ASP	1
1	B	22	HIS	1
1	A	70	LYS	1
1	B	45	ASN	1
1	A	63	LYS	1
1	A	15	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	95	LEU	1
1	A	135	ARG	1
1	A	23	ASP	1
1	B	27	ASP	1
1	B	54	TYR	1
1	B	71	GLN	1
1	B	58	PHE	1
1	B	120	HIS	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

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 40% for the well-defined parts and 40% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *B74_2019_BMRB_CYANA_StereoRFINAL.txt*

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	1396
Number of shifts mapped to atoms	1396
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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	130	-0.18 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	109	-0.05 ± 0.24	None needed (< 0.5 ppm)
$^{13}C'$	112	0.34 ± 0.19	None needed (< 0.5 ppm)
^{15}N	128	-0.34 ± 0.39	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 40%, i.e. 1395 atoms were assigned a chemical shift out of a possible 3489. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	629/1379 (46%)	259/566 (46%)	242/550 (44%)	128/263 (49%)
Sidechain	722/1928 (37%)	498/1265 (39%)	218/588 (37%)	6/75 (8%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	44/182 (24%)	22/88 (25%)	22/82 (27%)	0/12 (0%)
Overall	1395/3489 (40%)	779/1919 (41%)	482/1220 (40%)	134/350 (38%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 1395 atoms were assigned a chemical shift out of a possible 3518. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	629/1394 (45%)	259/572 (45%)	242/556 (44%)	128/266 (48%)
Sidechain	722/1942 (37%)	498/1274 (39%)	218/592 (37%)	6/76 (8%)
Aromatic	44/182 (24%)	22/88 (25%)	22/82 (27%)	0/12 (0%)
Overall	1395/3518 (40%)	779/1934 (40%)	482/1230 (39%)	134/354 (38%)

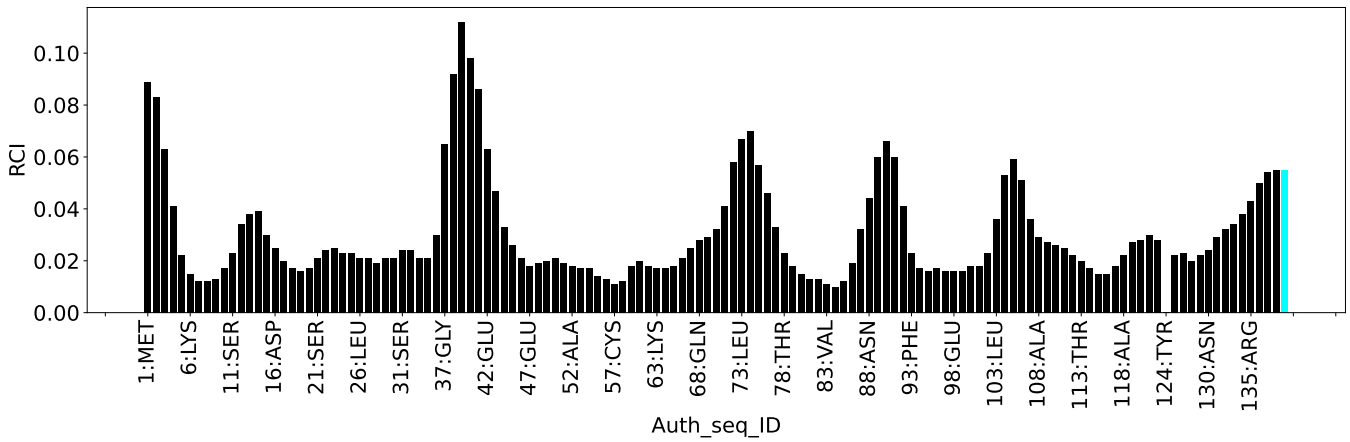
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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:



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	1772
Intra-residue (|i-j|=0)	437
Sequential (|i-j|=1)	569
Medium range (|i-j|>1 and |i-j|<5)	305
Long range (|i-j|≥5)	367
Inter-chain	0
Hydrogen bond restraints	94
Disulfide bond restraints	0
Total dihedral-angle restraints	404
Number of unmapped restraints	4
Number of restraints per residue	7.8
Number of long range restraints per residue[1]	1.5

[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)	49.3	0.2
0.2-0.5 (Medium)	18.8	0.32
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.7	1.9
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

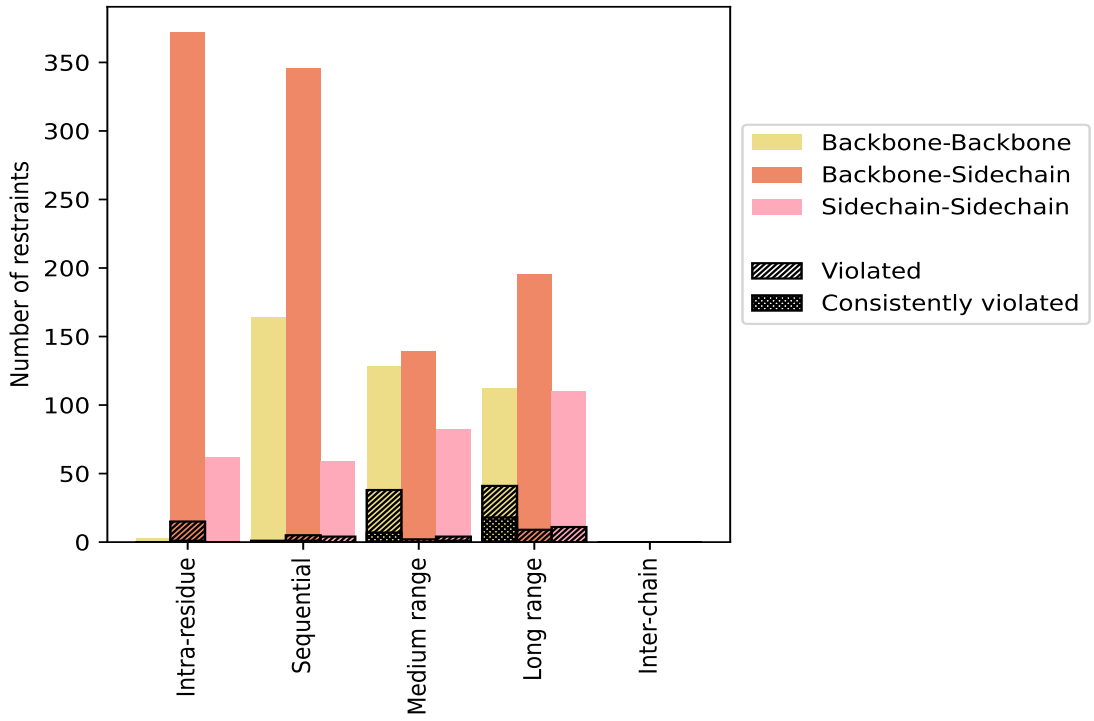
9.1 Summary of distance violations (i)

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)	437	24.7	15	3.4	0.8	1	0.2	0.1
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	372	21.0	15	4.0	0.8	1	0.3	0.1
Sidechain-Sidechain	62	3.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	569	32.1	10	1.8	0.6	1	0.2	0.1
Backbone-Backbone	164	9.3	1	0.6	0.1	0	0.0	0.0
Backbone-Sidechain	346	19.5	5	1.4	0.3	1	0.3	0.1
Sidechain-Sidechain	59	3.3	4	6.8	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	305	17.2	7	2.3	0.4	1	0.3	0.1
Backbone-Backbone	84	4.7	1	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	139	7.8	2	1.4	0.1	0	0.0	0.0
Sidechain-Sidechain	82	4.6	4	4.9	0.2	1	1.2	0.1
Long range (|i-j|≥5)	367	20.7	20	5.4	1.1	0	0.0	0.0
Backbone-Backbone	62	3.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	195	11.0	9	4.6	0.5	0	0.0	0.0
Sidechain-Sidechain	110	6.2	11	10.0	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	94	5.3	78	83.0	4.4	25	26.6	1.4
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1772	100.0	130	7.3	7.3	28	1.6	1.6
Backbone-Backbone	407	23.0	80	19.7	4.5	25	6.1	1.4
Backbone-Sidechain	1052	59.4	31	2.9	1.7	2	0.2	0.1
Sidechain-Sidechain	313	17.7	19	6.1	1.1	1	0.3	0.1

[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	4	2	29	38	0	73	0.18	0.32	0.05	0.18
2	1	4	28	36	0	69	0.18	0.32	0.05	0.17
3	4	4	29	30	0	67	0.18	0.32	0.05	0.17
4	4	2	27	34	0	67	0.18	0.31	0.06	0.16
5	1	5	26	33	0	65	0.18	0.31	0.05	0.18
6	1	4	24	38	0	67	0.18	0.31	0.05	0.16
7	2	4	27	36	0	69	0.18	0.32	0.06	0.18
8	3	4	29	37	0	73	0.18	0.32	0.05	0.17
9	5	4	24	35	0	68	0.18	0.31	0.05	0.16
10	4	4	22	35	0	65	0.18	0.32	0.06	0.18
11	9	2	28	35	0	74	0.18	0.31	0.05	0.18

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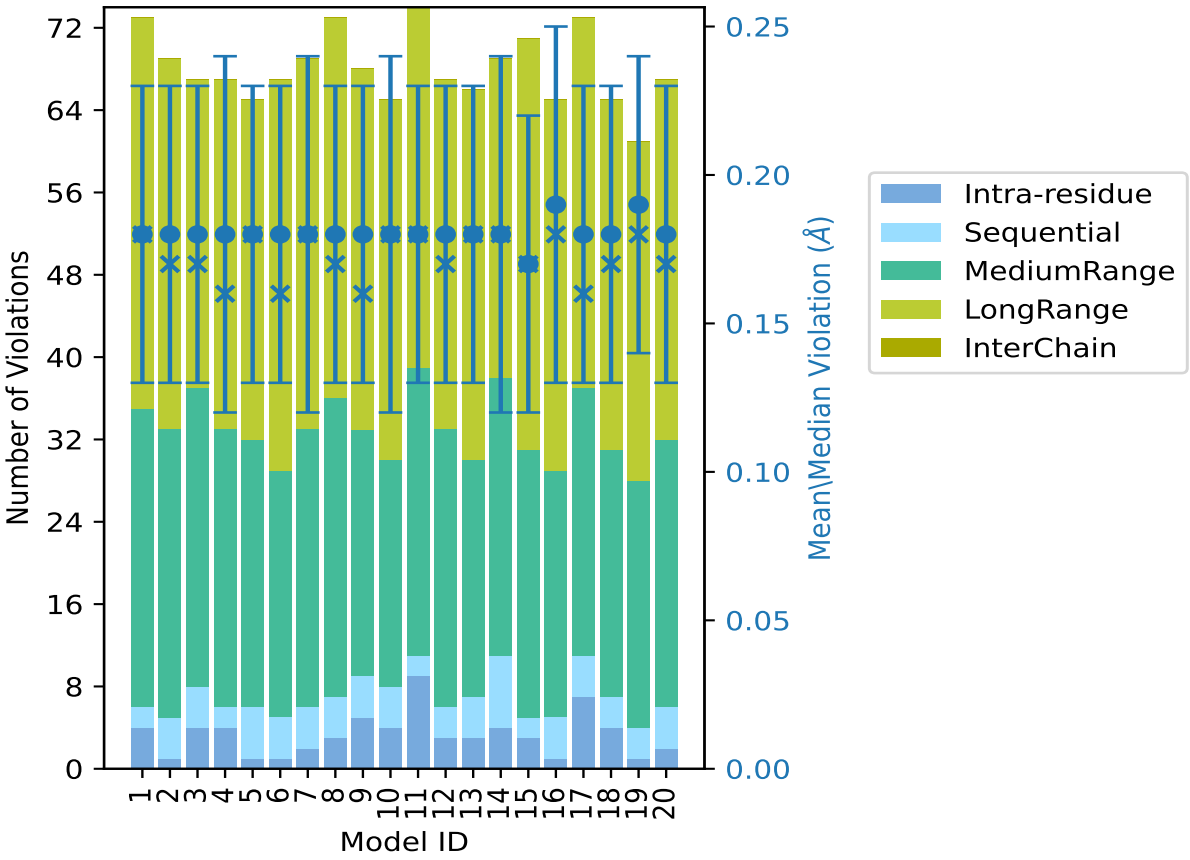
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	3	27	34	0	67	0.18	0.31	0.05	0.17
13	3	4	23	36	0	66	0.18	0.32	0.05	0.18
14	4	7	27	31	0	69	0.18	0.31	0.06	0.18
15	3	2	26	40	0	71	0.17	0.32	0.05	0.17
16	1	4	24	36	0	65	0.19	0.31	0.06	0.18
17	7	4	26	36	0	73	0.18	0.31	0.05	0.16
18	4	3	24	34	0	65	0.18	0.32	0.05	0.17
19	1	3	24	33	0	61	0.19	0.32	0.05	0.18
20	2	4	26	35	0	67	0.18	0.31	0.05	0.17

[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

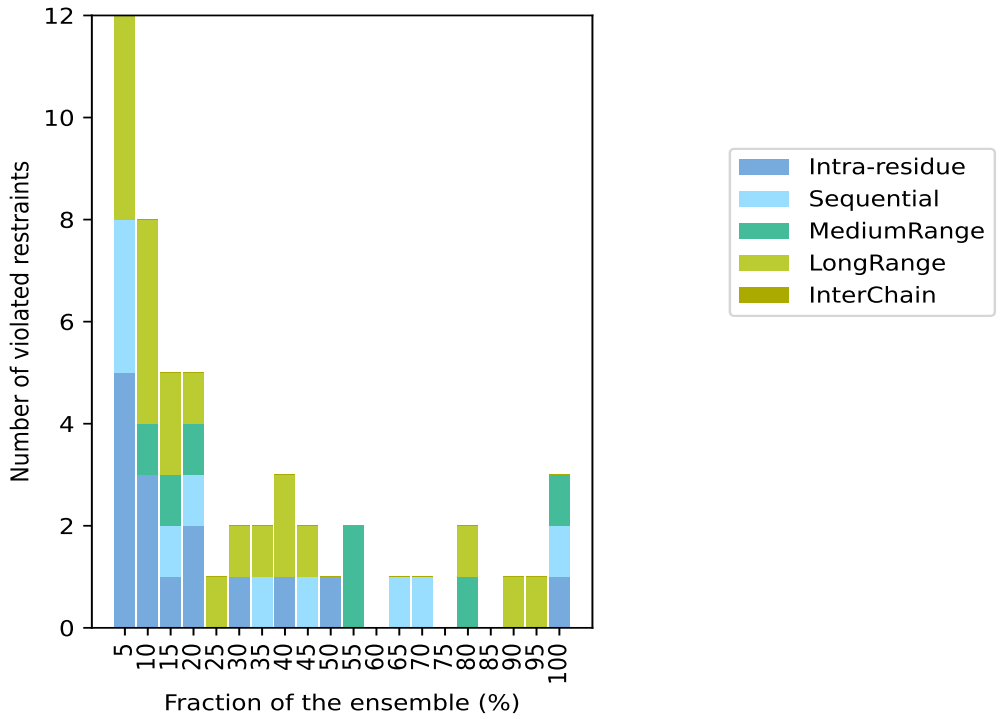
9.3 Distance violation statistics for the ensemble (i)

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, 1626(IR:422, SQ:559, MR:298, LR:347, IC:0) 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]	%
5	3	0	4	0	12	1	5.0
3	0	1	4	0	8	2	10.0
1	1	1	2	0	5	3	15.0
2	1	1	1	0	5	4	20.0
0	0	0	1	0	1	5	25.0
1	0	0	1	0	2	6	30.0
0	1	0	1	0	2	7	35.0
1	0	0	2	0	3	8	40.0
0	1	0	1	0	2	9	45.0
1	0	0	0	0	1	10	50.0
0	0	2	0	0	2	11	55.0
0	0	0	0	0	0	12	60.0
0	1	0	0	0	1	13	65.0
0	1	0	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	1	1	0	2	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	1	0	1	18	90.0
0	0	0	1	0	1	19	95.0
1	1	1	0	0	3	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

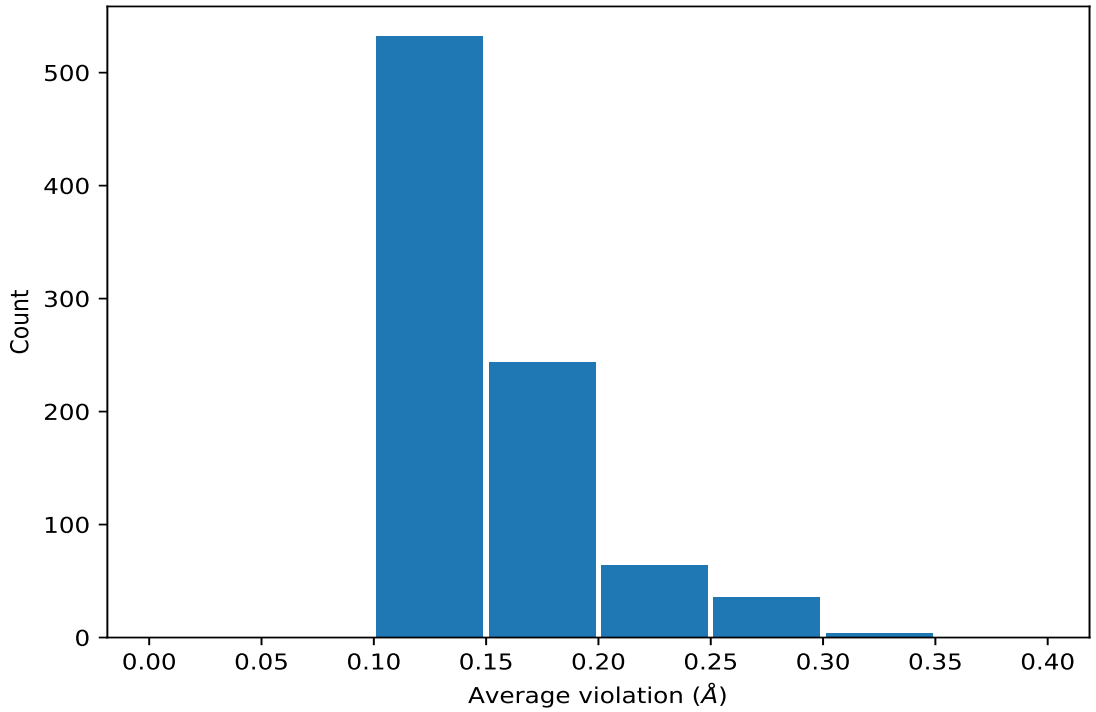
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 the violation 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)
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	20	0.31	0.01	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	20	0.31	0.01	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	20	0.31	0.01	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	20	0.31	0.01	0.32
(1,10)	1:A:10:THR:N	1:A:20:THR:O	20	0.29	0.01	0.29
(1,10)	1:A:10:THR:N	1:B:20:THR:O	20	0.29	0.01	0.29
(1,10)	1:B:10:THR:N	1:A:20:THR:O	20	0.29	0.01	0.29
(1,10)	1:B:10:THR:N	1:B:20:THR:O	20	0.29	0.01	0.29
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	20	0.28	0.02	0.28
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	20	0.28	0.02	0.28
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	20	0.28	0.02	0.28
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	20	0.28	0.02	0.28
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	20	0.28	0.02	0.28
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	20	0.28	0.02	0.28
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	20	0.28	0.02	0.28
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	20	0.28	0.02	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	20	0.27	0.02	0.27
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	20	0.27	0.02	0.27
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	20	0.27	0.02	0.27
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	20	0.27	0.02	0.27
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	20	0.27	0.02	0.27
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	20	0.27	0.02	0.27
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	20	0.27	0.02	0.27
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	20	0.27	0.02	0.27
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	20	0.26	0.04	0.28
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	20	0.26	0.04	0.28
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	20	0.26	0.04	0.28
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	20	0.26	0.04	0.28
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	20	0.25	0.04	0.26
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	20	0.25	0.04	0.26
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	20	0.25	0.04	0.26
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	20	0.25	0.04	0.26
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	20	0.25	0.03	0.24
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	20	0.25	0.03	0.24
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	20	0.25	0.03	0.24
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	20	0.25	0.03	0.24
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	20	0.25	0.02	0.25
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	20	0.25	0.02	0.25
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	20	0.25	0.02	0.25
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	20	0.25	0.02	0.25
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	20	0.24	0.03	0.24
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	20	0.24	0.03	0.24
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	20	0.24	0.03	0.24
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	20	0.24	0.03	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	20	0.24	0.02	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	20	0.24	0.02	0.24
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	20	0.24	0.02	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	20	0.24	0.02	0.24
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	20	0.21	0.03	0.21
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	20	0.21	0.03	0.21
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	20	0.21	0.03	0.21
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	20	0.21	0.03	0.21
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	20	0.21	0.03	0.21
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	20	0.21	0.03	0.21
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	20	0.21	0.03	0.21
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	20	0.21	0.03	0.21
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	20	0.21	0.03	0.22
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	20	0.21	0.03	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	20	0.21	0.03	0.22
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	20	0.21	0.03	0.22
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	20	0.21	0.03	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	20	0.21	0.03	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	20	0.21	0.03	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	20	0.21	0.03	0.21
(1,2)	1:A:10:THR:O	1:A:20:THR:N	20	0.2	0.03	0.21
(1,2)	1:A:10:THR:O	1:B:20:THR:N	20	0.2	0.03	0.21
(1,2)	1:B:10:THR:O	1:A:20:THR:N	20	0.2	0.03	0.21
(1,2)	1:B:10:THR:O	1:B:20:THR:N	20	0.2	0.03	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	20	0.2	0.01	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	20	0.2	0.01	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	20	0.2	0.01	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	20	0.2	0.01	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	20	0.2	0.01	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	20	0.2	0.01	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	20	0.2	0.01	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	20	0.2	0.01	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	20	0.2	0.01	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	20	0.2	0.01	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	20	0.2	0.01	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	20	0.2	0.01	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	20	0.2	0.01	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	20	0.2	0.01	0.2
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	20	0.2	0.03	0.19
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	20	0.2	0.03	0.19
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	20	0.2	0.03	0.19
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	20	0.2	0.03	0.19
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	20	0.19	0.01	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	20	0.19	0.01	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	20	0.19	0.01	0.2
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	20	0.19	0.04	0.19
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	20	0.19	0.04	0.19
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	20	0.19	0.04	0.19
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	20	0.19	0.04	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	20	0.18	0.02	0.18
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	20	0.18	0.02	0.18
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	20	0.18	0.02	0.18
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	20	0.18	0.02	0.18
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	20	0.18	0.02	0.18
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	20	0.18	0.02	0.18
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	20	0.18	0.02	0.18
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	20	0.18	0.02	0.18
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	20	0.17	0.02	0.18
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	20	0.17	0.02	0.18
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	20	0.17	0.02	0.18
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	20	0.17	0.02	0.18
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	20	0.16	0.03	0.17
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	20	0.16	0.03	0.17
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	20	0.16	0.03	0.17
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	20	0.16	0.03	0.17
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	20	0.16	0.03	0.16
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	20	0.16	0.03	0.16
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	20	0.16	0.03	0.16
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	20	0.16	0.03	0.16
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	20	0.15	0.03	0.15
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	20	0.15	0.03	0.15
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	20	0.15	0.03	0.15
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	20	0.15	0.03	0.15
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	19	0.22	0.03	0.22
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	19	0.22	0.03	0.22
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	19	0.22	0.03	0.22
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	19	0.22	0.03	0.22
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	19	0.21	0.04	0.21
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	19	0.21	0.04	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	19	0.21	0.04	0.21
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	19	0.21	0.04	0.21
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	19	0.17	0.02	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	19	0.17	0.02	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	19	0.17	0.02	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	19	0.17	0.02	0.17
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	19	0.16	0.03	0.16
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	19	0.16	0.03	0.16
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	19	0.16	0.03	0.16
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	19	0.16	0.03	0.16
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	18	0.18	0.03	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	18	0.18	0.03	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	18	0.18	0.03	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	18	0.18	0.03	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	18	0.18	0.03	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	18	0.18	0.03	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	18	0.18	0.03	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	18	0.18	0.03	0.2
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	18	0.17	0.02	0.17
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	18	0.17	0.02	0.17
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	18	0.17	0.02	0.17
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	18	0.17	0.02	0.17
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	18	0.17	0.03	0.16
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	18	0.17	0.03	0.16
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	18	0.17	0.03	0.16
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	18	0.17	0.03	0.16
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	18	0.15	0.03	0.16
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	18	0.15	0.03	0.16
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	18	0.15	0.03	0.16
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	18	0.15	0.03	0.16
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	18	0.15	0.03	0.14
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	18	0.15	0.03	0.14
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	18	0.15	0.03	0.14
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	18	0.15	0.03	0.14
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	18	0.14	0.02	0.15
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	18	0.14	0.02	0.15
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	18	0.14	0.02	0.15
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	18	0.14	0.02	0.15
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	18	0.14	0.02	0.14
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	18	0.14	0.02	0.14
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	18	0.14	0.02	0.14
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	18	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,20)	1:A:31:SER:N	1:A:44:THR:O	18	0.14	0.03	0.14
(1,20)	1:A:31:SER:N	1:B:44:THR:O	18	0.14	0.03	0.14
(1,20)	1:B:31:SER:N	1:A:44:THR:O	18	0.14	0.03	0.14
(1,20)	1:B:31:SER:N	1:B:44:THR:O	18	0.14	0.03	0.14
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	18	0.14	0.02	0.14
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	18	0.14	0.02	0.14
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	18	0.14	0.02	0.14
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	18	0.14	0.02	0.14
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	18	0.14	0.02	0.14
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	18	0.14	0.02	0.14
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	18	0.14	0.02	0.14
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	18	0.14	0.02	0.14
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	17	0.19	0.04	0.2
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	17	0.19	0.04	0.2
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	17	0.19	0.04	0.2
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	17	0.19	0.04	0.2
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	17	0.18	0.02	0.19
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	17	0.18	0.02	0.19
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	17	0.18	0.02	0.19
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	17	0.18	0.02	0.19
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	17	0.15	0.03	0.14
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	17	0.15	0.03	0.14
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	17	0.15	0.03	0.14
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	17	0.15	0.03	0.14
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	17	0.14	0.02	0.14
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	17	0.14	0.02	0.14
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	17	0.14	0.02	0.14
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	17	0.14	0.02	0.14
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	16	0.19	0.04	0.2
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	16	0.19	0.04	0.2
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	16	0.19	0.04	0.2
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	16	0.19	0.04	0.2
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	16	0.19	0.03	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	16	0.19	0.03	0.18
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	16	0.19	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	16	0.16	0.03	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	16	0.16	0.03	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	16	0.16	0.03	0.18
(1,9)	1:A:10:THR:H	1:A:20:THR:O	16	0.15	0.02	0.16
(1,9)	1:A:10:THR:H	1:B:20:THR:O	16	0.15	0.02	0.16
(1,9)	1:B:10:THR:H	1:A:20:THR:O	16	0.15	0.02	0.16
(1,9)	1:B:10:THR:H	1:B:20:THR:O	16	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	15	0.14	0.02	0.13
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	15	0.14	0.02	0.13
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	15	0.14	0.02	0.13
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	15	0.14	0.02	0.13
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	14	0.18	0.03	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	14	0.18	0.03	0.2
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	14	0.15	0.03	0.16
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	14	0.15	0.03	0.16
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	14	0.15	0.03	0.16
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	14	0.15	0.03	0.16
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	14	0.14	0.03	0.13
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	14	0.14	0.03	0.13
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	14	0.14	0.03	0.13
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	14	0.14	0.03	0.13
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	13	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	13	0.14	0.02	0.14
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	13	0.14	0.02	0.14
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	13	0.14	0.02	0.14
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	13	0.14	0.02	0.14
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	13	0.14	0.02	0.14
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	13	0.14	0.02	0.14
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	12	0.14	0.02	0.15
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	12	0.14	0.02	0.15
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	12	0.14	0.02	0.15
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	12	0.14	0.02	0.15
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	12	0.13	0.01	0.13
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	12	0.13	0.01	0.13
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	12	0.13	0.01	0.13
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	12	0.13	0.01	0.13
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	12	0.12	0.01	0.12
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	12	0.12	0.01	0.12
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	12	0.12	0.01	0.12
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	12	0.12	0.01	0.12
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	11	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	11	0.17	0.03	0.17
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	11	0.17	0.03	0.17
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	11	0.15	0.03	0.14
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	11	0.15	0.03	0.14
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	11	0.15	0.03	0.14
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	11	0.15	0.03	0.14
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	11	0.13	0.02	0.12
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	11	0.13	0.02	0.12
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	11	0.13	0.02	0.12
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	11	0.13	0.02	0.12
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	11	0.13	0.02	0.12
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	11	0.13	0.02	0.12
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	11	0.13	0.02	0.12
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	11	0.13	0.02	0.12
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	10	0.16	0.06	0.16
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	10	0.16	0.06	0.16
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	10	0.16	0.06	0.16
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	10	0.16	0.06	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	10	0.14	0.02	0.14
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	10	0.14	0.02	0.14
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	10	0.14	0.02	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	10	0.14	0.02	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	10	0.14	0.02	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	10	0.14	0.02	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	10	0.14	0.02	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	10	0.14	0.02	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	10	0.14	0.02	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	10	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	10	0.14	0.02	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	10	0.14	0.02	0.14
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	9	0.16	0.04	0.19
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	9	0.16	0.04	0.19
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	9	0.16	0.04	0.19
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	9	0.16	0.04	0.19
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	9	0.16	0.04	0.19
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	9	0.16	0.04	0.19
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	9	0.16	0.04	0.19
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	9	0.16	0.04	0.19
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	9	0.16	0.04	0.19
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	9	0.16	0.04	0.19
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	9	0.16	0.04	0.19
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	9	0.16	0.04	0.19
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	9	0.15	0.03	0.15
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	9	0.15	0.03	0.15
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	9	0.15	0.03	0.15
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	9	0.15	0.03	0.15
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	9	0.15	0.03	0.15
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	9	0.15	0.03	0.15
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	9	0.15	0.03	0.15
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	9	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	8	0.15	0.03	0.15
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	8	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	8	0.15	0.03	0.15
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	8	0.15	0.03	0.15
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	8	0.15	0.03	0.14
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	8	0.15	0.03	0.14
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	8	0.14	0.02	0.14
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	8	0.14	0.02	0.14
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	8	0.14	0.02	0.14
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	8	0.14	0.02	0.14
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	8	0.13	0.01	0.13
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	8	0.13	0.01	0.13
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	8	0.13	0.01	0.13
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	8	0.13	0.01	0.13
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	8	0.12	0.02	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	8	0.12	0.02	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	8	0.12	0.02	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	8	0.12	0.02	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	8	0.12	0.02	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	8	0.12	0.02	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	8	0.12	0.02	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	8	0.12	0.02	0.12
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	7	0.16	0.04	0.14
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	7	0.16	0.04	0.14
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	7	0.16	0.04	0.14
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	7	0.16	0.04	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	7	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	7	0.15	0.02	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	7	0.15	0.02	0.14
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	7	0.12	0.0	0.12
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	7	0.12	0.0	0.12
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	7	0.12	0.0	0.12
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	7	0.12	0.0	0.12
(2,257)	1:A:42:GLU:H	1:A:42:GLU:HG2	6	0.15	0.02	0.15
(2,257)	1:A:42:GLU:H	1:B:42:GLU:HG2	6	0.15	0.02	0.15
(2,257)	1:B:42:GLU:H	1:A:42:GLU:HG2	6	0.15	0.02	0.15
(2,257)	1:B:42:GLU:H	1:B:42:GLU:HG2	6	0.15	0.02	0.15
(1,31)	1:A:51:ALA:O	1:A:55:SER:H	6	0.13	0.02	0.13
(1,31)	1:A:51:ALA:O	1:B:55:SER:H	6	0.13	0.02	0.13
(1,31)	1:B:51:ALA:O	1:A:55:SER:H	6	0.13	0.02	0.13
(1,31)	1:B:51:ALA:O	1:B:55:SER:H	6	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,34)	1:A:52:ALA:O	1:A:56:ALA:N	6	0.13	0.02	0.12
(1,34)	1:A:52:ALA:O	1:B:56:ALA:N	6	0.13	0.02	0.12
(1,34)	1:B:52:ALA:O	1:A:56:ALA:N	6	0.13	0.02	0.12
(1,34)	1:B:52:ALA:O	1:B:56:ALA:N	6	0.13	0.02	0.12
(1,82)	1:A:113:THR:O	1:A:117:ARG:N	6	0.13	0.01	0.12
(1,82)	1:A:113:THR:O	1:B:117:ARG:N	6	0.13	0.01	0.12
(1,82)	1:B:113:THR:O	1:A:117:ARG:N	6	0.13	0.01	0.12
(1,82)	1:B:113:THR:O	1:B:117:ARG:N	6	0.13	0.01	0.12
(1,84)	1:A:114:LEU:O	1:A:118:ALA:N	6	0.12	0.01	0.12
(1,84)	1:A:114:LEU:O	1:B:118:ALA:N	6	0.12	0.01	0.12
(1,84)	1:B:114:LEU:O	1:A:118:ALA:N	6	0.12	0.01	0.12
(1,84)	1:B:114:LEU:O	1:B:118:ALA:N	6	0.12	0.01	0.12
(1,64)	1:A:99:LEU:O	1:A:137:VAL:N	6	0.12	0.01	0.12
(1,64)	1:A:99:LEU:O	1:B:137:VAL:N	6	0.12	0.01	0.12
(1,64)	1:B:99:LEU:O	1:A:137:VAL:N	6	0.12	0.01	0.12
(1,64)	1:B:99:LEU:O	1:B:137:VAL:N	6	0.12	0.01	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB1	6	0.12	0.01	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB2	6	0.12	0.01	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB3	6	0.12	0.01	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB1	6	0.12	0.01	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB2	6	0.12	0.01	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB3	6	0.12	0.01	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB1	6	0.12	0.01	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB2	6	0.12	0.01	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB3	6	0.12	0.01	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB1	6	0.12	0.01	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB2	6	0.12	0.01	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB3	6	0.12	0.01	0.12
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	5	0.15	0.03	0.15
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	5	0.15	0.03	0.15
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	5	0.15	0.03	0.15
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	5	0.15	0.03	0.15
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	5	0.15	0.03	0.15
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	5	0.15	0.03	0.15
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	5	0.15	0.03	0.15
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	5	0.15	0.03	0.15
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	5	0.15	0.03	0.15
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	5	0.15	0.03	0.15
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	5	0.15	0.03	0.15
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	5	0.15	0.03	0.15
(1,42)	1:A:60:SER:O	1:A:64:PHE:N	5	0.13	0.01	0.12
(1,42)	1:A:60:SER:O	1:B:64:PHE:N	5	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,42)	1:B:60:SER:O	1:A:64:PHE:N	5	0.13	0.01	0.12
(1,42)	1:B:60:SER:O	1:B:64:PHE:N	5	0.13	0.01	0.12
(1,39)	1:A:58:PHE:O	1:A:62:MET:H	5	0.12	0.02	0.11
(1,39)	1:A:58:PHE:O	1:B:62:MET:H	5	0.12	0.02	0.11
(1,39)	1:B:58:PHE:O	1:A:62:MET:H	5	0.12	0.02	0.11
(1,39)	1:B:58:PHE:O	1:B:62:MET:H	5	0.12	0.02	0.11
(2,1208)	1:A:107:ASP:HB3	1:A:110:ALA:H	4	0.17	0.01	0.16
(2,1208)	1:A:107:ASP:HB3	1:B:110:ALA:H	4	0.17	0.01	0.16
(2,1208)	1:B:107:ASP:HB3	1:A:110:ALA:H	4	0.17	0.01	0.16
(2,1208)	1:B:107:ASP:HB3	1:B:110:ALA:H	4	0.17	0.01	0.16
(2,162)	1:A:12:THR:HG21	1:A:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:A:12:THR:HG21	1:B:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:A:12:THR:HG22	1:A:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:A:12:THR:HG22	1:B:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:A:12:THR:HG23	1:A:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:A:12:THR:HG23	1:B:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:B:12:THR:HG21	1:A:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:B:12:THR:HG21	1:B:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:B:12:THR:HG22	1:A:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:B:12:THR:HG22	1:B:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:B:12:THR:HG23	1:A:13:GLY:H	4	0.14	0.02	0.14
(2,162)	1:B:12:THR:HG23	1:B:13:GLY:H	4	0.14	0.02	0.14
(1,93)	1:A:101:VAL:H	1:A:137:VAL:O	4	0.13	0.01	0.13
(1,93)	1:A:101:VAL:H	1:B:137:VAL:O	4	0.13	0.01	0.13
(1,93)	1:B:101:VAL:H	1:A:137:VAL:O	4	0.13	0.01	0.13
(1,93)	1:B:101:VAL:H	1:B:137:VAL:O	4	0.13	0.01	0.13
(1,5)	1:A:17:GLY:O	1:A:30:LEU:H	4	0.12	0.01	0.12
(1,5)	1:A:17:GLY:O	1:B:30:LEU:H	4	0.12	0.01	0.12
(1,5)	1:B:17:GLY:O	1:A:30:LEU:H	4	0.12	0.01	0.12
(1,5)	1:B:17:GLY:O	1:B:30:LEU:H	4	0.12	0.01	0.12
(2,1245)	1:A:117:ARG:H	1:A:117:ARG:HG2	4	0.12	0.02	0.11
(2,1245)	1:A:117:ARG:H	1:B:117:ARG:HG2	4	0.12	0.02	0.11
(2,1245)	1:B:117:ARG:H	1:A:117:ARG:HG2	4	0.12	0.02	0.11
(2,1245)	1:B:117:ARG:H	1:B:117:ARG:HG2	4	0.12	0.02	0.11
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD22	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD23	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD22	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD23	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD22	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD23	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD22	4	0.12	0.01	0.12
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD23	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD22	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD23	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD22	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD23	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD22	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD23	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD21	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD22	4	0.12	0.01	0.12
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD23	4	0.12	0.01	0.12
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG11	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG12	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG13	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG21	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG22	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG23	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG11	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG12	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG13	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG21	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG22	4	0.11	0.0	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG23	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG11	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG12	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG13	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG21	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG22	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG23	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG11	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG12	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG13	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG21	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG22	4	0.11	0.0	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG23	4	0.11	0.0	0.11
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE3	3	0.16	0.03	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE3	3	0.16	0.03	0.14
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE3	3	0.16	0.03	0.14
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE3	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE3	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE3	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE3	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE2	3	0.16	0.03	0.14
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE3	3	0.16	0.03	0.14
(2,1276)	1:A:129:ARG:HG3	1:A:130:ASN:H	3	0.15	0.03	0.13
(2,1276)	1:A:129:ARG:HG3	1:B:130:ASN:H	3	0.15	0.03	0.13
(2,1276)	1:B:129:ARG:HG3	1:A:130:ASN:H	3	0.15	0.03	0.13
(2,1276)	1:B:129:ARG:HG3	1:B:130:ASN:H	3	0.15	0.03	0.13
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG13	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG13	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG13	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG13	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG13	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG13	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG13	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG11	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG12	3	0.14	0.02	0.15
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG13	3	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,87)	1:A:117:ARG:O	1:A:121:VAL:H	3	0.13	0.02	0.14
(1,87)	1:A:117:ARG:O	1:B:121:VAL:H	3	0.13	0.02	0.14
(1,87)	1:B:117:ARG:O	1:A:121:VAL:H	3	0.13	0.02	0.14
(1,87)	1:B:117:ARG:O	1:B:121:VAL:H	3	0.13	0.02	0.14
(2,53)	1:A:77:THR:HA	1:A:104:PRO:HD3	3	0.13	0.0	0.13
(2,53)	1:A:77:THR:HA	1:B:104:PRO:HD3	3	0.13	0.0	0.13
(2,53)	1:B:77:THR:HA	1:A:104:PRO:HD3	3	0.13	0.0	0.13
(2,53)	1:B:77:THR:HA	1:B:104:PRO:HD3	3	0.13	0.0	0.13
(1,85)	1:A:115:VAL:O	1:A:119:HIS:H	3	0.12	0.0	0.12
(1,85)	1:A:115:VAL:O	1:B:119:HIS:H	3	0.12	0.0	0.12
(1,85)	1:B:115:VAL:O	1:A:119:HIS:H	3	0.12	0.0	0.12
(1,85)	1:B:115:VAL:O	1:B:119:HIS:H	3	0.12	0.0	0.12
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG2	3	0.12	0.01	0.12
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG3	3	0.12	0.01	0.12
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG2	3	0.12	0.01	0.12
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG3	3	0.12	0.01	0.12
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG2	3	0.12	0.01	0.12
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG3	3	0.12	0.01	0.12
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG2	3	0.12	0.01	0.12
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG3	3	0.12	0.01	0.12
(1,81)	1:A:113:THR:O	1:A:117:ARG:H	3	0.12	0.01	0.12
(1,81)	1:A:113:THR:O	1:B:117:ARG:H	3	0.12	0.01	0.12
(1,81)	1:B:113:THR:O	1:A:117:ARG:H	3	0.12	0.01	0.12
(1,81)	1:B:113:THR:O	1:B:117:ARG:H	3	0.12	0.01	0.12
(1,80)	1:A:110:ALA:O	1:A:114:LEU:N	3	0.11	0.0	0.11
(1,80)	1:A:110:ALA:O	1:B:114:LEU:N	3	0.11	0.0	0.11
(1,80)	1:B:110:ALA:O	1:A:114:LEU:N	3	0.11	0.0	0.11
(1,80)	1:B:110:ALA:O	1:B:114:LEU:N	3	0.11	0.0	0.11
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD11	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD12	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD13	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD21	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD22	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD23	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD11	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD12	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD13	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD21	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD22	2	0.16	0.01	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD23	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD11	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD12	2	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD13	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD21	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD22	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD23	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD11	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD12	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD13	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD21	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD22	2	0.16	0.01	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD23	2	0.16	0.01	0.16
(1,61)	1:A:82:GLU:H	1:A:98:GLU:O	2	0.14	0.02	0.14
(1,61)	1:A:82:GLU:H	1:B:98:GLU:O	2	0.14	0.02	0.14
(1,61)	1:B:82:GLU:H	1:A:98:GLU:O	2	0.14	0.02	0.14
(1,61)	1:B:82:GLU:H	1:B:98:GLU:O	2	0.14	0.02	0.14
(1,1)	1:A:10:THR:O	1:A:20:THR:H	2	0.14	0.02	0.14
(1,1)	1:A:10:THR:O	1:B:20:THR:H	2	0.14	0.02	0.14
(1,1)	1:B:10:THR:O	1:A:20:THR:H	2	0.14	0.02	0.14
(1,1)	1:B:10:THR:O	1:B:20:THR:H	2	0.14	0.02	0.14
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	2	0.14	0.02	0.14
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	2	0.14	0.02	0.14
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	2	0.14	0.02	0.14
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	2	0.14	0.02	0.14
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	2	0.14	0.02	0.14
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	2	0.14	0.02	0.14
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	2	0.14	0.02	0.14
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	2	0.14	0.02	0.14
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	2	0.14	0.02	0.14
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	2	0.14	0.02	0.14
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	2	0.14	0.02	0.14
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	2	0.14	0.02	0.14
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB3	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB3	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB1	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB2	2	0.12	0.01	0.12
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB3	2	0.12	0.01	0.12
(2,1531)	1:A:80:THR:HB	1:A:100:ARG:HB2	2	0.12	0.01	0.12
(2,1531)	1:A:80:THR:HB	1:A:100:ARG:HB3	2	0.12	0.01	0.12
(2,1531)	1:A:80:THR:HB	1:B:100:ARG:HB2	2	0.12	0.01	0.12
(2,1531)	1:A:80:THR:HB	1:B:100:ARG:HB3	2	0.12	0.01	0.12
(2,1531)	1:B:80:THR:HB	1:A:100:ARG:HB2	2	0.12	0.01	0.12
(2,1531)	1:B:80:THR:HB	1:A:100:ARG:HB3	2	0.12	0.01	0.12
(2,1531)	1:B:80:THR:HB	1:B:100:ARG:HB2	2	0.12	0.01	0.12
(2,1531)	1:B:80:THR:HB	1:B:100:ARG:HB3	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG21	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG23	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG21	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG23	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG21	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG23	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG21	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG23	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG21	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG23	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG21	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG23	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG21	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG23	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG21	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG22	2	0.12	0.01	0.12
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG23	2	0.12	0.01	0.12
(2,383)	1:A:80:THR:HB	1:A:100:ARG:HB2	2	0.12	0.0	0.12
(2,383)	1:A:80:THR:HB	1:B:100:ARG:HB2	2	0.12	0.0	0.12
(2,383)	1:B:80:THR:HB	1:A:100:ARG:HB2	2	0.12	0.0	0.12
(2,383)	1:B:80:THR:HB	1:B:100:ARG:HB2	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD11	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD12	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD13	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD21	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD22	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD23	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD11	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD12	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD13	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD21	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD22	2	0.12	0.0	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD23	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD11	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD12	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD13	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD21	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD22	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD23	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD11	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD12	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD13	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD21	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD22	2	0.12	0.0	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD23	2	0.12	0.0	0.12

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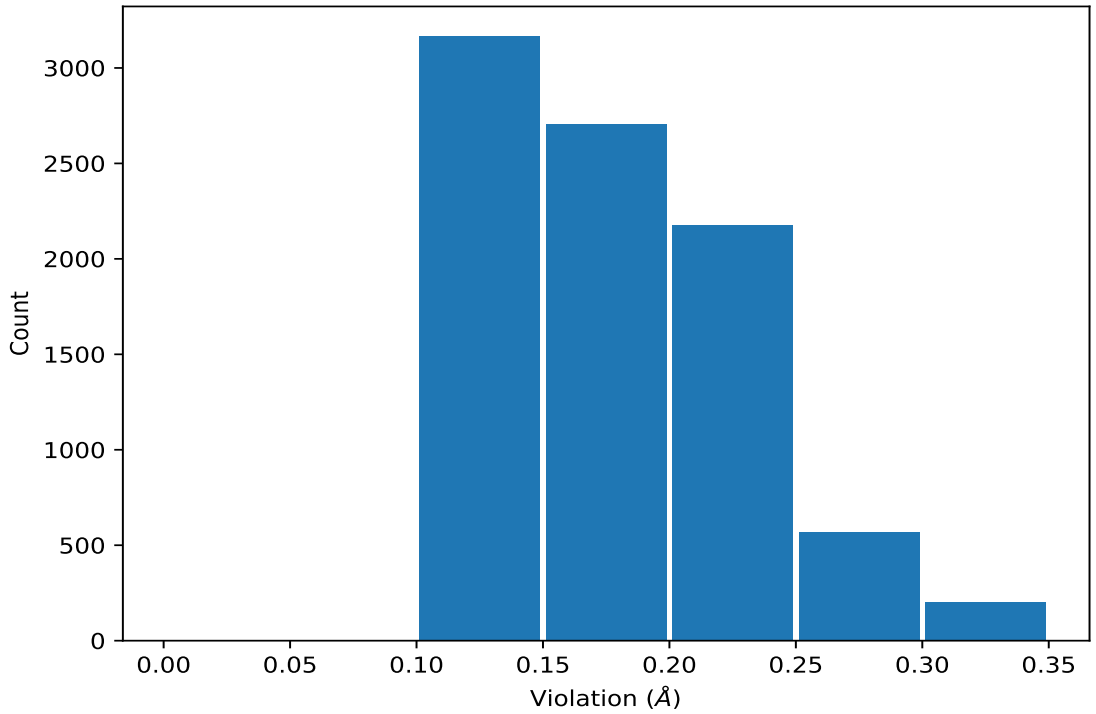
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD11	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD12	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD13	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD21	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD22	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD23	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD11	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD12	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD13	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD21	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD22	2	0.11	0.0	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD23	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD11	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD12	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD13	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD21	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD22	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD23	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD11	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD12	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD13	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD21	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD22	2	0.11	0.0	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD23	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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 (i)

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)
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	1	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	1	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	1	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	1	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	2	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	2	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	2	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	2	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	3	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	3	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	3	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	3	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	7	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	7	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	7	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	8	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	8	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	8	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	8	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	10	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	10	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	10	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	10	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	13	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	13	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	13	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	13	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	15	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	15	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	15	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	15	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	18	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	18	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	18	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	18	0.32
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	19	0.32
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	19	0.32
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	19	0.32
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	19	0.32
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	4	0.31
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	4	0.31
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	4	0.31
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	4	0.31
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	7	0.31
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	7	0.31
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	7	0.31
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	7	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	5	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	5	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	5	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	5	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	6	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	6	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	6	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	6	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	9	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	9	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	9	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	11	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	11	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	11	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	11	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	12	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	12	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	12	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	12	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	14	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	14	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	14	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	14	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	16	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	16	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	16	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	16	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	17	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	17	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	17	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	17	0.31
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	20	0.31
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	20	0.31
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	20	0.31
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	20	0.31
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	2	0.3
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	2	0.3
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	2	0.3
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	2	0.3
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	8	0.3
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	8	0.3
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	8	0.3
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	8	0.3
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	13	0.3
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	13	0.3
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	13	0.3
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	13	0.3
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	18	0.3
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	18	0.3
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	18	0.3
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	19	0.3
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	19	0.3
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	19	0.3
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	19	0.3
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	4	0.3
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	4	0.3
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	4	0.3
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	4	0.3
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	7	0.3
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	7	0.3
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	7	0.3
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	7	0.3
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	14	0.3
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	14	0.3
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	14	0.3
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	14	0.3
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	18	0.3
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	18	0.3
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	18	0.3
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	18	0.3
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	7	0.3
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	7	0.3
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	7	0.3
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	7	0.3
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	14	0.3
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	14	0.3
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	14	0.3
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	14	0.3
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	1	0.3
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	1	0.3
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	1	0.3
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	1	0.3
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	3	0.3
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	3	0.3
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	3	0.3
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	3	0.3
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	4	0.3
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	4	0.3
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	4	0.3
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	4	0.3
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	6	0.3
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	6	0.3
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	6	0.3
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	7	0.3
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	7	0.3
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	7	0.3
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	7	0.3
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	8	0.3
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	8	0.3
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	8	0.3
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	8	0.3
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	16	0.3
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	16	0.3
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	16	0.3
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	16	0.3
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	10	0.3
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	10	0.3
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	10	0.3
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	10	0.3
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	14	0.3
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	14	0.3
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	14	0.3
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	14	0.3
(1,14)	1:A:21:SER:N	1:A:26:LEU:O	4	0.3
(1,14)	1:A:21:SER:N	1:B:26:LEU:O	4	0.3
(1,14)	1:B:21:SER:N	1:A:26:LEU:O	4	0.3
(1,14)	1:B:21:SER:N	1:B:26:LEU:O	4	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	2	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	2	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	2	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	2	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	8	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	8	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	8	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	8	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	9	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	9	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	9	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	9	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	10	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	10	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	10	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:A:10:THR:N	1:A:20:THR:O	11	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	11	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	11	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	11	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	12	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	12	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	12	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	12	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	14	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	14	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	14	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	14	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	16	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	16	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	16	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	16	0.3
(1,10)	1:A:10:THR:N	1:A:20:THR:O	19	0.3
(1,10)	1:A:10:THR:N	1:B:20:THR:O	19	0.3
(1,10)	1:B:10:THR:N	1:A:20:THR:O	19	0.3
(1,10)	1:B:10:THR:N	1:B:20:THR:O	19	0.3
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	16	0.29
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	16	0.29
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	16	0.29
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	16	0.29
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	1	0.29
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	1	0.29
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	1	0.29
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	1	0.29
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	15	0.29
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	15	0.29
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	15	0.29
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	15	0.29
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	20	0.29
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	20	0.29
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	20	0.29
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	20	0.29
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	7	0.29
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	7	0.29
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	7	0.29
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	7	0.29
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	5	0.29
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	5	0.29
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	5	0.29
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	8	0.29
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	8	0.29
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	8	0.29
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	8	0.29
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	15	0.29
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	15	0.29
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	15	0.29
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	15	0.29
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	16	0.29
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	16	0.29
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	16	0.29
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	16	0.29
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	5	0.29
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	5	0.29
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	5	0.29
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	5	0.29
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	8	0.29
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	8	0.29
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	8	0.29
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	8	0.29
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	12	0.29
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	12	0.29
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	12	0.29
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	12	0.29
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	14	0.29
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	14	0.29
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	14	0.29
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	14	0.29
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	1	0.29
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	1	0.29
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	1	0.29
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	1	0.29
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	4	0.29
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	4	0.29
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	4	0.29
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	4	0.29
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	17	0.29
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	17	0.29
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	17	0.29
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	4	0.29
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	4	0.29
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	4	0.29
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	4	0.29
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	7	0.29
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	7	0.29
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	7	0.29
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	7	0.29
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	14	0.29
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	14	0.29
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	14	0.29
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	14	0.29
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	15	0.29
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	15	0.29
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	15	0.29
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	15	0.29
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	12	0.29
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	12	0.29
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	12	0.29
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	12	0.29
(1,10)	1:A:10:THR:N	1:A:20:THR:O	4	0.29
(1,10)	1:A:10:THR:N	1:B:20:THR:O	4	0.29
(1,10)	1:B:10:THR:N	1:A:20:THR:O	4	0.29
(1,10)	1:B:10:THR:N	1:B:20:THR:O	4	0.29
(1,10)	1:A:10:THR:N	1:A:20:THR:O	13	0.29
(1,10)	1:A:10:THR:N	1:B:20:THR:O	13	0.29
(1,10)	1:B:10:THR:N	1:A:20:THR:O	13	0.29
(1,10)	1:B:10:THR:N	1:B:20:THR:O	13	0.29
(1,10)	1:A:10:THR:N	1:A:20:THR:O	20	0.29
(1,10)	1:A:10:THR:N	1:B:20:THR:O	20	0.29
(1,10)	1:B:10:THR:N	1:A:20:THR:O	20	0.29
(1,10)	1:B:10:THR:N	1:B:20:THR:O	20	0.29
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	16	0.28
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	16	0.28
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	16	0.28
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	16	0.28
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	3	0.28
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	3	0.28
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	3	0.28
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	3	0.28
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	5	0.28
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	5	0.28
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	5	0.28
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	10	0.28
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	10	0.28
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	10	0.28
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	10	0.28
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	12	0.28
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	12	0.28
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	12	0.28
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	12	0.28
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	20	0.28
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	20	0.28
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	20	0.28
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	20	0.28
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	5	0.28
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	5	0.28
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	5	0.28
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	5	0.28
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	6	0.28
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	6	0.28
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	6	0.28
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	6	0.28
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	8	0.28
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	8	0.28
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	8	0.28
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	8	0.28
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	11	0.28
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	11	0.28
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	11	0.28
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	11	0.28
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	3	0.28
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	3	0.28
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	3	0.28
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	3	0.28
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	6	0.28
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	6	0.28
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	6	0.28
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	6	0.28
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	7	0.28
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	7	0.28
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	7	0.28
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	11	0.28
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	11	0.28
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	11	0.28
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	11	0.28
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	17	0.28
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	17	0.28
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	17	0.28
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	17	0.28
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	5	0.28
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	5	0.28
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	5	0.28
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	5	0.28
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	9	0.28
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	9	0.28
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	9	0.28
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	9	0.28
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	11	0.28
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	11	0.28
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	11	0.28
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	11	0.28
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	14	0.28
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	14	0.28
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	14	0.28
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	14	0.28
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	15	0.28
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	15	0.28
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	15	0.28
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	15	0.28
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	16	0.28
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	16	0.28
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	16	0.28
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	16	0.28
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	2	0.28
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	2	0.28
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	2	0.28
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	2	0.28
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	17	0.28
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	17	0.28
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	17	0.28
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	17	0.28
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	19	0.28
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	19	0.28
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	19	0.28
(1,10)	1:A:10:THR:N	1:A:20:THR:O	6	0.28
(1,10)	1:A:10:THR:N	1:B:20:THR:O	6	0.28
(1,10)	1:B:10:THR:N	1:A:20:THR:O	6	0.28
(1,10)	1:B:10:THR:N	1:B:20:THR:O	6	0.28
(1,10)	1:A:10:THR:N	1:A:20:THR:O	7	0.28
(1,10)	1:A:10:THR:N	1:B:20:THR:O	7	0.28
(1,10)	1:B:10:THR:N	1:A:20:THR:O	7	0.28
(1,10)	1:B:10:THR:N	1:B:20:THR:O	7	0.28
(1,10)	1:A:10:THR:N	1:A:20:THR:O	15	0.28
(1,10)	1:A:10:THR:N	1:B:20:THR:O	15	0.28
(1,10)	1:B:10:THR:N	1:A:20:THR:O	15	0.28
(1,10)	1:B:10:THR:N	1:B:20:THR:O	15	0.28
(1,10)	1:A:10:THR:N	1:A:20:THR:O	18	0.28
(1,10)	1:A:10:THR:N	1:B:20:THR:O	18	0.28
(1,10)	1:B:10:THR:N	1:A:20:THR:O	18	0.28
(1,10)	1:B:10:THR:N	1:B:20:THR:O	18	0.28
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	2	0.27
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	2	0.27
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	2	0.27
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	2	0.27
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	4	0.27
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	4	0.27
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	4	0.27
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	4	0.27
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	11	0.27
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	11	0.27
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	11	0.27
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	11	0.27
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	12	0.27
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	12	0.27
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	12	0.27
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	12	0.27
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	18	0.27
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	18	0.27
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	18	0.27
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	18	0.27
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	11	0.27
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	11	0.27
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	11	0.27
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	14	0.27
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	14	0.27
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	14	0.27
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	14	0.27
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	2	0.27
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	2	0.27
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	2	0.27
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	2	0.27
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	10	0.27
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	10	0.27
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	10	0.27
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	10	0.27
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	12	0.27
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	12	0.27
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	12	0.27
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	12	0.27
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	13	0.27
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	13	0.27
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	13	0.27
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	13	0.27
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	19	0.27
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	19	0.27
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	19	0.27
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	19	0.27
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	11	0.27
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	11	0.27
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	11	0.27
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	11	0.27
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	1	0.27
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	1	0.27
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	1	0.27
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	1	0.27
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	10	0.27
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	10	0.27
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	10	0.27
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	10	0.27
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	13	0.27
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	13	0.27
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	13	0.27
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	13	0.27
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	18	0.27
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	18	0.27
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	18	0.27
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	20	0.27
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	20	0.27
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	20	0.27
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	20	0.27
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	1	0.27
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	1	0.27
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	1	0.27
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	1	0.27
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	20	0.27
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	20	0.27
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	20	0.27
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	20	0.27
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	2	0.27
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	2	0.27
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	2	0.27
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	2	0.27
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	10	0.27
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	10	0.27
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	10	0.27
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	10	0.27
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	1	0.27
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	1	0.27
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	1	0.27
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	1	0.27
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	1	0.27
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	1	0.27
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	1	0.27
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	1	0.27
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	3	0.27
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	3	0.27
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	3	0.27
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	3	0.27
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	9	0.27
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	9	0.27
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	9	0.27
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	9	0.27
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	13	0.27
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	13	0.27
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	13	0.27
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	16	0.27
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	16	0.27
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	16	0.27
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	16	0.27
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	17	0.27
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	17	0.27
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	17	0.27
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	17	0.27
(1,10)	1:A:10:THR:N	1:A:20:THR:O	3	0.27
(1,10)	1:A:10:THR:N	1:B:20:THR:O	3	0.27
(1,10)	1:B:10:THR:N	1:A:20:THR:O	3	0.27
(1,10)	1:B:10:THR:N	1:B:20:THR:O	3	0.27
(1,10)	1:A:10:THR:N	1:A:20:THR:O	5	0.27
(1,10)	1:A:10:THR:N	1:B:20:THR:O	5	0.27
(1,10)	1:B:10:THR:N	1:A:20:THR:O	5	0.27
(1,10)	1:B:10:THR:N	1:B:20:THR:O	5	0.27
(1,10)	1:A:10:THR:N	1:A:20:THR:O	17	0.27
(1,10)	1:A:10:THR:N	1:B:20:THR:O	17	0.27
(1,10)	1:B:10:THR:N	1:A:20:THR:O	17	0.27
(1,10)	1:B:10:THR:N	1:B:20:THR:O	17	0.27
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	19	0.26
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	19	0.26
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	19	0.26
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	19	0.26
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	4	0.26
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	4	0.26
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	4	0.26
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	4	0.26
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	1	0.26
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	1	0.26
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	1	0.26
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	1	0.26
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	5	0.26
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	5	0.26
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	5	0.26
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	5	0.26
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	6	0.26
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	6	0.26
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	6	0.26
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	6	0.26
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	9	0.26
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	9	0.26
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	9	0.26
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	16	0.26
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	16	0.26
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	16	0.26
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	16	0.26
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	17	0.26
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	17	0.26
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	17	0.26
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	17	0.26
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	9	0.26
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	9	0.26
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	9	0.26
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	9	0.26
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	16	0.26
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	16	0.26
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	16	0.26
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	16	0.26
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	8	0.26
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	8	0.26
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	8	0.26
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	8	0.26
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	2	0.26
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	2	0.26
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	2	0.26
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	2	0.26
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	4	0.26
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	4	0.26
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	4	0.26
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	4	0.26
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	19	0.26
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	19	0.26
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	19	0.26
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	19	0.26
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	3	0.26
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	3	0.26
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	3	0.26
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	3	0.26
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	10	0.26
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	10	0.26
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	10	0.26
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	19	0.26
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	19	0.26
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	19	0.26
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	19	0.26
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	2	0.26
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	2	0.26
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	2	0.26
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	2	0.26
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	7	0.26
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	7	0.26
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	7	0.26
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	7	0.26
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	12	0.26
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	12	0.26
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	12	0.26
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	12	0.26
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	19	0.26
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	19	0.26
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	19	0.26
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	19	0.26
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	7	0.26
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	7	0.26
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	7	0.26
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	7	0.26
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	5	0.26
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	5	0.26
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	5	0.26
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	5	0.26
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	11	0.26
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	11	0.26
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	11	0.26
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	11	0.26
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	18	0.26
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	18	0.26
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	18	0.26
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	18	0.26
(1,2)	1:A:10:THR:O	1:A:20:THR:N	6	0.26
(1,2)	1:A:10:THR:O	1:B:20:THR:N	6	0.26
(1,2)	1:B:10:THR:O	1:A:20:THR:N	6	0.26
(1,2)	1:B:10:THR:O	1:B:20:THR:N	6	0.26
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	2	0.26
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	2	0.26
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	2	0.26
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	10	0.26
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	10	0.26
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	10	0.26
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	10	0.26
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	11	0.26
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	11	0.26
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	11	0.26
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	11	0.26
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	9	0.25
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	9	0.25
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	9	0.25
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	9	0.25
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	17	0.25
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	17	0.25
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	17	0.25
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	17	0.25
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	18	0.25
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	18	0.25
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	18	0.25
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	18	0.25
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	18	0.25
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	18	0.25
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	18	0.25
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	18	0.25
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	8	0.25
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	8	0.25
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	8	0.25
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	8	0.25
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	10	0.25
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	10	0.25
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	10	0.25
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	10	0.25
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	15	0.25
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	15	0.25
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	15	0.25
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	15	0.25
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	4	0.25
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	4	0.25
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	4	0.25
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	10	0.25
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	10	0.25
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	10	0.25
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	10	0.25
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	12	0.25
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	12	0.25
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	12	0.25
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	12	0.25
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	1	0.25
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	1	0.25
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	1	0.25
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	1	0.25
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	9	0.25
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	9	0.25
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	9	0.25
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	9	0.25
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	9	0.25
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	9	0.25
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	9	0.25
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	9	0.25
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	12	0.25
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	12	0.25
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	12	0.25
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	12	0.25
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	6	0.25
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	6	0.25
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	6	0.25
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	6	0.25
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	4	0.25
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	4	0.25
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	4	0.25
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	4	0.25
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	13	0.25
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	13	0.25
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	13	0.25
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	13	0.25
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	8	0.25
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	8	0.25
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	8	0.25
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	8	0.25
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	13	0.25
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	13	0.25
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	13	0.25
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	19	0.25
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	19	0.25
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	19	0.25
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	19	0.25
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	16	0.25
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	16	0.25
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	16	0.25
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	16	0.25
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	20	0.25
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	20	0.25
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	20	0.25
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	20	0.25
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	8	0.25
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	8	0.25
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	8	0.25
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	8	0.25
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	4	0.25
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	4	0.25
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	4	0.25
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	4	0.25
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	5	0.25
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	5	0.25
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	5	0.25
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	5	0.25
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	17	0.25
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	17	0.25
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	17	0.25
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	17	0.25
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	8	0.25
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	8	0.25
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	8	0.25
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	8	0.25
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	19	0.25
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	19	0.25
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	19	0.25
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	19	0.25
(1,10)	1:A:10:THR:N	1:A:20:THR:O	1	0.25
(1,10)	1:A:10:THR:N	1:B:20:THR:O	1	0.25
(1,10)	1:B:10:THR:N	1:A:20:THR:O	1	0.25
(1,10)	1:B:10:THR:N	1:B:20:THR:O	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	8	0.24
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	8	0.24
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	8	0.24
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	8	0.24
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	8	0.24
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	8	0.24
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	8	0.24
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	8	0.24
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	8	0.24
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	8	0.24
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	8	0.24
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	8	0.24
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	8	0.24
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	8	0.24
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	8	0.24
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	8	0.24
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	8	0.24
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	8	0.24
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	8	0.24
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	8	0.24
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	8	0.24
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	8	0.24
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	8	0.24
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	8	0.24
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	20	0.24
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	20	0.24
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	20	0.24
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	20	0.24
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	12	0.24
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	12	0.24
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	12	0.24
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	12	0.24
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	18	0.24
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	18	0.24
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	18	0.24
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	18	0.24
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	2	0.24
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	2	0.24
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	2	0.24
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	2	0.24
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	9	0.24
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	9	0.24
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	9	0.24
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	19	0.24
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	19	0.24
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	19	0.24
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	19	0.24
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	3	0.24
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	3	0.24
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	3	0.24
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	3	0.24
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	7	0.24
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	7	0.24
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	7	0.24
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	7	0.24
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	1	0.24
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	1	0.24
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	1	0.24
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	1	0.24
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	9	0.24
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	9	0.24
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	9	0.24
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	9	0.24
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	20	0.24
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	20	0.24
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	20	0.24
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	20	0.24
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	8	0.24
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	8	0.24
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	8	0.24
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	8	0.24
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	17	0.24
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	17	0.24
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	17	0.24
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	17	0.24
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	12	0.24
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	12	0.24
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	12	0.24
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	12	0.24
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	20	0.24
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	20	0.24
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	20	0.24
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	11	0.24
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	11	0.24
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	11	0.24
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	11	0.24
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	17	0.24
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	17	0.24
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	17	0.24
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	17	0.24
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	20	0.24
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	20	0.24
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	20	0.24
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	20	0.24
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	1	0.24
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	1	0.24
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	1	0.24
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	1	0.24
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	16	0.24
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	16	0.24
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	16	0.24
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	16	0.24
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	3	0.24
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	3	0.24
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	3	0.24
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	3	0.24
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	20	0.24
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	20	0.24
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	20	0.24
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	20	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	4	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	4	0.24
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	4	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	4	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	6	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	6	0.24
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	6	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	6	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	9	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	9	0.24
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	9	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	9	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	11	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	11	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	11	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	15	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	15	0.24
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	15	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	15	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	17	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	17	0.24
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	17	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	17	0.24
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	20	0.24
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	20	0.24
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	20	0.24
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	20	0.24
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	8	0.24
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	8	0.24
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	8	0.24
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	8	0.24
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	12	0.24
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	12	0.24
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	12	0.24
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	12	0.24
(1,2)	1:A:10:THR:O	1:A:20:THR:N	4	0.24
(1,2)	1:A:10:THR:O	1:B:20:THR:N	4	0.24
(1,2)	1:B:10:THR:O	1:A:20:THR:N	4	0.24
(1,2)	1:B:10:THR:O	1:B:20:THR:N	4	0.24
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	6	0.24
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	6	0.24
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	6	0.24
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	6	0.24
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	6	0.24
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	6	0.24
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	6	0.24
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	6	0.24
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	13	0.24
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	13	0.24
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	13	0.24
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	13	0.24
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	20	0.24
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	20	0.24
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	20	0.24
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	11	0.23
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	11	0.23
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	11	0.23
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	11	0.23
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	17	0.23
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	17	0.23
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	17	0.23
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	17	0.23
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	11	0.23
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	11	0.23
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	11	0.23
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	11	0.23
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	7	0.23
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	7	0.23
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	7	0.23
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	7	0.23
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	14	0.23
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	14	0.23
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	14	0.23
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	14	0.23
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	2	0.23
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	2	0.23
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	2	0.23
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	2	0.23
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	10	0.23
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	10	0.23
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	10	0.23
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	10	0.23
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	8	0.23
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	8	0.23
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	8	0.23
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	8	0.23
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	16	0.23
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	16	0.23
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	16	0.23
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	16	0.23
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	1	0.23
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	1	0.23
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	1	0.23
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	1	0.23
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	14	0.23
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	14	0.23
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	14	0.23
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	19	0.23
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	19	0.23
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	19	0.23
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	19	0.23
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	20	0.23
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	20	0.23
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	20	0.23
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	20	0.23
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	11	0.23
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	11	0.23
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	11	0.23
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	11	0.23
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	16	0.23
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	16	0.23
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	16	0.23
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	16	0.23
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	15	0.23
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	15	0.23
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	15	0.23
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	15	0.23
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	6	0.23
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	6	0.23
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	6	0.23
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	6	0.23
(1,58)	1:A:97:VAL:O	1:A:135:ARG:N	15	0.23
(1,58)	1:A:97:VAL:O	1:B:135:ARG:N	15	0.23
(1,58)	1:B:97:VAL:O	1:A:135:ARG:N	15	0.23
(1,58)	1:B:97:VAL:O	1:B:135:ARG:N	15	0.23
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	3	0.23
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	3	0.23
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	3	0.23
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	3	0.23
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	17	0.23
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	17	0.23
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	17	0.23
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	17	0.23
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	2	0.23
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	2	0.23
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	2	0.23
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	4	0.23
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	4	0.23
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	4	0.23
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	4	0.23
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	16	0.23
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	16	0.23
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	16	0.23
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	16	0.23
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	6	0.23
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	6	0.23
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	6	0.23
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	6	0.23
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	10	0.23
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	10	0.23
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	10	0.23
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	10	0.23
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	12	0.23
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	12	0.23
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	12	0.23
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	12	0.23
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	14	0.23
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	14	0.23
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	14	0.23
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	14	0.23
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	15	0.23
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	15	0.23
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	15	0.23
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	15	0.23
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	17	0.23
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	17	0.23
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	17	0.23
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	17	0.23
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	19	0.23
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	19	0.23
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	19	0.23
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	19	0.23
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	5	0.23
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	5	0.23
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	5	0.23
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	5	0.23
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	9	0.23
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	9	0.23
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	9	0.23
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	11	0.23
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	11	0.23
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	11	0.23
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	11	0.23
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	13	0.23
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	13	0.23
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	13	0.23
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	13	0.23
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	19	0.23
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	19	0.23
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	19	0.23
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	19	0.23
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	3	0.23
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	3	0.23
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	3	0.23
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	3	0.23
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	5	0.23
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	5	0.23
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	5	0.23
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	5	0.23
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	6	0.23
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	6	0.23
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	6	0.23
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	6	0.23
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	12	0.23
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	12	0.23
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	12	0.23
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	12	0.23
(1,2)	1:A:10:THR:O	1:A:20:THR:N	5	0.23
(1,2)	1:A:10:THR:O	1:B:20:THR:N	5	0.23
(1,2)	1:B:10:THR:O	1:A:20:THR:N	5	0.23
(1,2)	1:B:10:THR:O	1:B:20:THR:N	5	0.23
(1,2)	1:A:10:THR:O	1:A:20:THR:N	11	0.23
(1,2)	1:A:10:THR:O	1:B:20:THR:N	11	0.23
(1,2)	1:B:10:THR:O	1:A:20:THR:N	11	0.23
(1,2)	1:B:10:THR:O	1:B:20:THR:N	11	0.23
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	1	0.23
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	1	0.23
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	1	0.23
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	7	0.23
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	7	0.23
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	7	0.23
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	7	0.23
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	3	0.23
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	3	0.23
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	3	0.23
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	3	0.23
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	5	0.23
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	5	0.23
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	5	0.23
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	5	0.23
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	7	0.23
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	7	0.23
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	7	0.23
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	7	0.23
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	15	0.23
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	15	0.23
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	15	0.23
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	15	0.23
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	11	0.22
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	11	0.22
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	11	0.22
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	11	0.22
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	11	0.22
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	11	0.22
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	11	0.22
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	11	0.22
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	11	0.22
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	11	0.22
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	11	0.22
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	11	0.22
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	11	0.22
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	11	0.22
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	11	0.22
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	11	0.22
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	11	0.22
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	11	0.22
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	11	0.22
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	11	0.22
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	11	0.22
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	11	0.22
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	11	0.22
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	14	0.22
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	14	0.22
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	14	0.22
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	14	0.22
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	14	0.22
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	14	0.22
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	14	0.22
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	14	0.22
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	14	0.22
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	14	0.22
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	14	0.22
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	14	0.22
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	14	0.22
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	14	0.22
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	14	0.22
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	14	0.22
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	14	0.22
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	14	0.22
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	14	0.22
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	14	0.22
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	14	0.22
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	14	0.22
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	14	0.22
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	14	0.22
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	7	0.22
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	7	0.22
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	7	0.22
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	7	0.22
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	14	0.22
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	14	0.22
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	14	0.22
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	14	0.22
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	20	0.22
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	20	0.22
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	20	0.22
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	20	0.22
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	7	0.22
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	7	0.22
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	7	0.22
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	15	0.22
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	15	0.22
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	15	0.22
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	15	0.22
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	17	0.22
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	17	0.22
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	17	0.22
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	17	0.22
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	16	0.22
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	16	0.22
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	16	0.22
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	16	0.22
(1,56)	1:A:84:GLY:N	1:A:96:ASP:O	17	0.22
(1,56)	1:A:84:GLY:N	1:B:96:ASP:O	17	0.22
(1,56)	1:B:84:GLY:N	1:A:96:ASP:O	17	0.22
(1,56)	1:B:84:GLY:N	1:B:96:ASP:O	17	0.22
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	10	0.22
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	10	0.22
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	10	0.22
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	10	0.22
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	19	0.22
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	19	0.22
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	19	0.22
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	19	0.22
(1,50)	1:A:86:GLY:O	1:A:94:ALA:N	14	0.22
(1,50)	1:A:86:GLY:O	1:B:94:ALA:N	14	0.22
(1,50)	1:B:86:GLY:O	1:A:94:ALA:N	14	0.22
(1,50)	1:B:86:GLY:O	1:B:94:ALA:N	14	0.22
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	6	0.22
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	6	0.22
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	6	0.22
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	6	0.22
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	20	0.22
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	20	0.22
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	20	0.22
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	20	0.22
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	7	0.22
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	7	0.22
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	7	0.22
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	7	0.22
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	9	0.22
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	9	0.22
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	9	0.22
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	11	0.22
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	11	0.22
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	11	0.22
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	11	0.22
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	16	0.22
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	16	0.22
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	16	0.22
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	16	0.22
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	15	0.22
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	15	0.22
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	15	0.22
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	15	0.22
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	2	0.22
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	2	0.22
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	2	0.22
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	2	0.22
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	10	0.22
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	10	0.22
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	10	0.22
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	10	0.22
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	12	0.22
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	12	0.22
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	12	0.22
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	12	0.22
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	14	0.22
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	14	0.22
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	14	0.22
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	14	0.22
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	5	0.22
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	5	0.22
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	5	0.22
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	5	0.22
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	16	0.22
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	16	0.22
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	16	0.22
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	16	0.22
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	2	0.22
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	2	0.22
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	2	0.22
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	3	0.22
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	3	0.22
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	3	0.22
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	3	0.22
(1,2)	1:A:10:THR:O	1:A:20:THR:N	1	0.22
(1,2)	1:A:10:THR:O	1:B:20:THR:N	1	0.22
(1,2)	1:B:10:THR:O	1:A:20:THR:N	1	0.22
(1,2)	1:B:10:THR:O	1:B:20:THR:N	1	0.22
(1,2)	1:A:10:THR:O	1:A:20:THR:N	12	0.22
(1,2)	1:A:10:THR:O	1:B:20:THR:N	12	0.22
(1,2)	1:B:10:THR:O	1:A:20:THR:N	12	0.22
(1,2)	1:B:10:THR:O	1:B:20:THR:N	12	0.22
(1,2)	1:A:10:THR:O	1:A:20:THR:N	13	0.22
(1,2)	1:A:10:THR:O	1:B:20:THR:N	13	0.22
(1,2)	1:B:10:THR:O	1:A:20:THR:N	13	0.22
(1,2)	1:B:10:THR:O	1:B:20:THR:N	13	0.22
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	12	0.22
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	12	0.22
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	12	0.22
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	12	0.22
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	20	0.22
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	20	0.22
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	20	0.22
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	20	0.22
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	4	0.22
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	4	0.22
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	4	0.22
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	4	0.22
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	18	0.22
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	18	0.22
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	18	0.22
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	18	0.22
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	2	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	2	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	2	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	2	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	2	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	2	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	2	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	2	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	2	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	2	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	2	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	5	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	5	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	5	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	5	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	5	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	5	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	5	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	5	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	5	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	5	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	5	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	5	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	7	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	7	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	7	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	7	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	7	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	7	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	7	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	7	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	7	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	7	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	7	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	7	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	8	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	8	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	8	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	8	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	8	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	8	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	8	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	8	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	8	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	8	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	8	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	8	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	9	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	9	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	9	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	9	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	9	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	9	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	9	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	9	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	9	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	9	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	9	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	10	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	10	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	10	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	10	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	10	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	10	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	10	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	10	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	10	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	10	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	10	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	10	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	11	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	11	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	11	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	11	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	11	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	11	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	11	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	11	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	11	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	11	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	11	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	11	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	13	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	13	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	13	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	13	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	13	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	13	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	13	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	13	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	13	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	13	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	13	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	17	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	17	0.21
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	17	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	17	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	17	0.21
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	17	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	17	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	17	0.21
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	17	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	17	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	17	0.21
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	17	0.21
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	17	0.21
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	17	0.21
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	17	0.21
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	17	0.21
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	17	0.21
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	17	0.21
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	17	0.21
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	17	0.21
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	15	0.21
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	15	0.21
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	15	0.21
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	15	0.21
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	15	0.21
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	15	0.21
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	15	0.21
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	15	0.21
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	15	0.21
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	15	0.21
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	15	0.21
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	15	0.21
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	15	0.21
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	15	0.21
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	15	0.21
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	15	0.21
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	15	0.21
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	15	0.21
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	15	0.21
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	15	0.21
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	15	0.21
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	15	0.21
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	15	0.21
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	7	0.21
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	7	0.21
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	7	0.21
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	7	0.21
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	7	0.21
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	7	0.21
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	7	0.21
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	7	0.21
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	7	0.21
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	7	0.21
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	7	0.21
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	7	0.21
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	7	0.21
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	7	0.21
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	7	0.21
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	7	0.21
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	7	0.21
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	7	0.21
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	7	0.21
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	7	0.21
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	7	0.21
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	7	0.21
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	7	0.21
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	7	0.21
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	12	0.21
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	12	0.21
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	12	0.21
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	12	0.21
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	12	0.21
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	12	0.21
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	12	0.21
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	12	0.21
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	12	0.21
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	12	0.21
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	12	0.21
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	12	0.21
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	12	0.21
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	12	0.21
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	12	0.21
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	12	0.21
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	12	0.21
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	12	0.21
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	12	0.21
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	12	0.21
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	12	0.21
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	12	0.21
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	12	0.21
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	16	0.21
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	16	0.21
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	16	0.21
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	16	0.21
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	1	0.21
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	1	0.21
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	1	0.21
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	1	0.21
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	14	0.21
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	14	0.21
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	14	0.21
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	14	0.21
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	19	0.21
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	19	0.21
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	19	0.21
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	19	0.21
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	5	0.21
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	5	0.21
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	5	0.21
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	5	0.21
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	6	0.21
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	6	0.21
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	6	0.21
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	6	0.21
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	19	0.21
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	19	0.21
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	19	0.21
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	19	0.21
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	20	0.21
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	20	0.21
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	20	0.21
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	13	0.21
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	13	0.21
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	13	0.21
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	13	0.21
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	1	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	1	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	1	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	1	0.21
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	8	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	8	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	8	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	8	0.21
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	11	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	11	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	11	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	11	0.21
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	12	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	12	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	12	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	12	0.21
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	13	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	13	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	13	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	13	0.21
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	16	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	16	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	16	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	16	0.21
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	19	0.21
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	19	0.21
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	19	0.21
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	19	0.21
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	3	0.21
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	3	0.21
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	3	0.21
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	3	0.21
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	11	0.21
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	11	0.21
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	11	0.21
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	11	0.21
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	13	0.21
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	13	0.21
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	13	0.21
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	4	0.21
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	4	0.21
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	4	0.21
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	4	0.21
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	5	0.21
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	5	0.21
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	5	0.21
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	5	0.21
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	8	0.21
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	8	0.21
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	8	0.21
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	8	0.21
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	19	0.21
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	19	0.21
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	19	0.21
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	19	0.21
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	2	0.21
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	2	0.21
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	2	0.21
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	2	0.21
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	5	0.21
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	5	0.21
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	5	0.21
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	5	0.21
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	13	0.21
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	13	0.21
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	13	0.21
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	13	0.21
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	18	0.21
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	18	0.21
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	18	0.21
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	18	0.21
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	19	0.21
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	19	0.21
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	19	0.21
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	19	0.21
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	20	0.21
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	20	0.21
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	20	0.21
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	5	0.21
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	5	0.21
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	5	0.21
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	5	0.21
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	13	0.21
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	13	0.21
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	13	0.21
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	13	0.21
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	14	0.21
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	14	0.21
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	14	0.21
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	14	0.21
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	9	0.21
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	9	0.21
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	9	0.21
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	9	0.21
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	18	0.21
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	18	0.21
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	18	0.21
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	18	0.21
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	15	0.21
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	15	0.21
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	15	0.21
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	15	0.21
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	2	0.21
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	2	0.21
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	2	0.21
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	2	0.21
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	13	0.21
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	13	0.21
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	13	0.21
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	13	0.21
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	19	0.21
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	19	0.21
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	19	0.21
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	19	0.21
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	12	0.21
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	12	0.21
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	12	0.21
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	12	0.21
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	14	0.21
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	14	0.21
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	14	0.21
(1,30)	1:A:50:PHE:O	1:A:54:TYR:N	18	0.21
(1,30)	1:A:50:PHE:O	1:B:54:TYR:N	18	0.21
(1,30)	1:B:50:PHE:O	1:A:54:TYR:N	18	0.21
(1,30)	1:B:50:PHE:O	1:B:54:TYR:N	18	0.21
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	9	0.21
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	9	0.21
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	9	0.21
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	9	0.21
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	20	0.21
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	20	0.21
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	20	0.21
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	20	0.21
(1,2)	1:A:10:THR:O	1:A:20:THR:N	7	0.21
(1,2)	1:A:10:THR:O	1:B:20:THR:N	7	0.21
(1,2)	1:B:10:THR:O	1:A:20:THR:N	7	0.21
(1,2)	1:B:10:THR:O	1:B:20:THR:N	7	0.21
(1,2)	1:A:10:THR:O	1:A:20:THR:N	8	0.21
(1,2)	1:A:10:THR:O	1:B:20:THR:N	8	0.21
(1,2)	1:B:10:THR:O	1:A:20:THR:N	8	0.21
(1,2)	1:B:10:THR:O	1:B:20:THR:N	8	0.21
(1,2)	1:A:10:THR:O	1:A:20:THR:N	10	0.21
(1,2)	1:A:10:THR:O	1:B:20:THR:N	10	0.21
(1,2)	1:B:10:THR:O	1:A:20:THR:N	10	0.21
(1,2)	1:B:10:THR:O	1:B:20:THR:N	10	0.21
(1,2)	1:A:10:THR:O	1:A:20:THR:N	16	0.21
(1,2)	1:A:10:THR:O	1:B:20:THR:N	16	0.21
(1,2)	1:B:10:THR:O	1:A:20:THR:N	16	0.21
(1,2)	1:B:10:THR:O	1:B:20:THR:N	16	0.21
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	2	0.21
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	2	0.21
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	2	0.21
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	2	0.21
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	8	0.21
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	8	0.21
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	8	0.21
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	8	0.21
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	19	0.21
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	19	0.21
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	19	0.21
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	5	0.2
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	5	0.2
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	5	0.2
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	5	0.2
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	6	0.2
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	6	0.2
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	6	0.2
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	6	0.2
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	2	0.2
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	2	0.2
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	2	0.2
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	2	0.2
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	2	0.2
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	2	0.2
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	2	0.2
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	2	0.2
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	2	0.2
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	2	0.2
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	2	0.2
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	2	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	2	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	2	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	2	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	2	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	2	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	2	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	2	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	2	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	2	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	2	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	2	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	2	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	8	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	8	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	8	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	8	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	8	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	8	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	8	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	8	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	8	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	8	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	8	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	16	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	16	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	16	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	16	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	16	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	16	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	16	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	16	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	16	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	16	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	16	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	16	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	18	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	18	0.2
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	18	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	18	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	18	0.2
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	18	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	18	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	18	0.2
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	18	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	18	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	18	0.2
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	18	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	1	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	1	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	1	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	1	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	1	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	1	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	1	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	1	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	1	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	1	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	1	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	1	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	2	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	2	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	2	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	2	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	2	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	2	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	2	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	2	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	2	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	2	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	2	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	3	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	3	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	3	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	3	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	3	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	3	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	3	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	3	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	3	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	3	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	3	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	3	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	4	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	4	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	4	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	4	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	4	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	4	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	4	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	4	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	4	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	4	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	4	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	4	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	5	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	5	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	5	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	5	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	5	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	5	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	5	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	5	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	5	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	5	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	5	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	6	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	6	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	6	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	6	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	6	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	6	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	6	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	6	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	6	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	6	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	6	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	6	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	8	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	8	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	8	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	8	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	8	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	8	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	8	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	8	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	8	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	8	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	8	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	8	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	11	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	11	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	11	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	11	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	11	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	11	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	11	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	11	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	11	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	11	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	11	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	11	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	12	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	12	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	12	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	12	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	12	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	12	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	12	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	12	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	12	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	12	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	12	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	13	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	13	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	13	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	13	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	13	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	13	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	13	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	13	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	13	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	13	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	13	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	13	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	14	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	14	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	14	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	14	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	14	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	14	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	14	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	14	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	14	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	14	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	14	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	14	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	15	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	15	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	15	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	15	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	15	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	15	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	15	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	15	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	15	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	15	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	15	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	16	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	16	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	16	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	16	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	16	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	16	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	16	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	16	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	16	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	16	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	16	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	16	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	17	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	17	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	17	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	17	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	17	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	17	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	17	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	17	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	17	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	17	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	17	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	17	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	18	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	18	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	18	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	18	0.2
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	18	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	18	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	18	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	18	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	18	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	18	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	18	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	18	0.2
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	19	0.2
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	19	0.2
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	19	0.2
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	19	0.2
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	19	0.2
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	19	0.2
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	19	0.2
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	19	0.2
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	19	0.2
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	19	0.2
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	19	0.2
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	9	0.2
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	9	0.2
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	9	0.2
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	9	0.2
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	13	0.2
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	13	0.2
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	13	0.2
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	13	0.2
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	14	0.2
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	14	0.2
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	14	0.2
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	14	0.2
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	15	0.2
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	15	0.2
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	15	0.2
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	15	0.2
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	18	0.2
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	18	0.2
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	18	0.2
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	18	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	1	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	1	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	1	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	1	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	1	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	1	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	1	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	1	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	1	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	1	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	1	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	1	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	6	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	6	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	6	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	6	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	6	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	6	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	6	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	6	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	6	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	6	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	6	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	12	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	12	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	12	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	12	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	12	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	12	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	12	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	12	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	12	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	12	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	12	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	12	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	14	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	14	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	14	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	14	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	14	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	14	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	14	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	14	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	14	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	14	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	14	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	14	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	15	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	15	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	15	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	15	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	15	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	15	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	15	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	15	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	15	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	15	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	15	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	18	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	18	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	18	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	18	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	18	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	18	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	18	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	18	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	18	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	18	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	18	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	18	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	19	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	19	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	19	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	19	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	19	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	19	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	19	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	19	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	19	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	19	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	19	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	19	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	20	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	20	0.2
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	20	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	20	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	20	0.2
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	20	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	20	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	20	0.2
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	20	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	20	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	20	0.2
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	20	0.2
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	14	0.2
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	14	0.2
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	14	0.2
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	14	0.2
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	14	0.2
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	14	0.2
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	14	0.2
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	1	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	1	0.2
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	2	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	2	0.2
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	7	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	7	0.2
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	8	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	8	0.2
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	9	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	10	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	10	0.2
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	15	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	15	0.2
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	18	0.2
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	18	0.2
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	20	0.2
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	20	0.2
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	20	0.2
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	20	0.2
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	20	0.2
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	20	0.2
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	20	0.2
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	20	0.2
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	20	0.2
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	20	0.2
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	20	0.2
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	20	0.2
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	20	0.2
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	20	0.2
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	20	0.2
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	20	0.2
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	20	0.2
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	20	0.2
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	20	0.2
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	20	0.2
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	20	0.2
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	20	0.2
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	20	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	3	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	3	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	3	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	3	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	3	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	3	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	3	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	3	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	3	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	3	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	3	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	3	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	3	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	3	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	3	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	3	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	3	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	3	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	3	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	3	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	3	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	3	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	3	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	3	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	8	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	8	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	8	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	8	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	8	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	8	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	8	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	8	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	8	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	8	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	8	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	8	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	8	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	8	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	8	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	8	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	8	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	8	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	8	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	8	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	8	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	8	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	8	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	14	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	14	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	14	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	14	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	14	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	14	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	14	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	14	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	14	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	14	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	14	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	14	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	14	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	14	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	14	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	14	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	14	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	14	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	14	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	14	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	14	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	14	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	14	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	17	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	17	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	17	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	17	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	17	0.2
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	17	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	17	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	17	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	17	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	17	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	17	0.2
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	17	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	17	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	17	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	17	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	17	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	17	0.2
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	17	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	17	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	17	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	17	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	17	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	17	0.2
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	17	0.2
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	5	0.2
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	5	0.2
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	5	0.2
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	5	0.2
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	5	0.2
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	5	0.2
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	5	0.2
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	5	0.2
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	5	0.2
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	5	0.2
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	5	0.2
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	5	0.2
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	5	0.2
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	5	0.2
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	5	0.2
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	5	0.2
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	5	0.2
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	5	0.2
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	5	0.2
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	5	0.2
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	5	0.2
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	5	0.2
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	5	0.2
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	13	0.2
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	13	0.2
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	13	0.2
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	13	0.2
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	13	0.2
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	13	0.2
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	13	0.2
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	13	0.2
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	13	0.2
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	13	0.2
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	13	0.2
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	13	0.2
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	13	0.2
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	13	0.2
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	13	0.2
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	13	0.2
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	13	0.2
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	13	0.2
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	13	0.2
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	13	0.2
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	13	0.2
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	13	0.2
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	13	0.2
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	13	0.2
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE2	8	0.2
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE3	8	0.2
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE2	8	0.2
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE3	8	0.2
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE2	8	0.2
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE3	8	0.2
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE2	8	0.2
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE3	8	0.2
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE2	8	0.2
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE3	8	0.2
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE2	8	0.2
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE3	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE2	8	0.2
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE3	8	0.2
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE2	8	0.2
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE3	8	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	1	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	1	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	1	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	1	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	1	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	1	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	1	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	1	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	3	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	3	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	3	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	3	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	3	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	3	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	3	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	3	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	5	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	5	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	5	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	5	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	5	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	5	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	5	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	5	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	11	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	11	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	11	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	11	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	11	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	11	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	11	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	11	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	12	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	12	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	12	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	12	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	12	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	12	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	12	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	13	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	13	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	13	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	13	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	13	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	13	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	13	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	13	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	14	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	14	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	14	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	14	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	14	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	14	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	14	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	14	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	15	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	15	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	15	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	15	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	15	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	15	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	15	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	15	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	16	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	16	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	16	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	16	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	16	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	16	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	16	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	16	0.2
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	19	0.2
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	19	0.2
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	19	0.2
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	19	0.2
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	19	0.2
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	19	0.2
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	19	0.2
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	2	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	2	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	2	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	2	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	2	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	2	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	2	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	2	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	2	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	2	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	2	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	2	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	3	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	3	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	3	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	3	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	3	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	3	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	3	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	3	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	3	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	3	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	3	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	3	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	5	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	5	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	5	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	5	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	5	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	5	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	5	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	5	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	5	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	5	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	5	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	5	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	6	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	6	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	6	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	6	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	6	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	6	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	6	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	6	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	6	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	6	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	6	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	7	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	7	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	7	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	7	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	7	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	7	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	7	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	7	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	7	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	7	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	7	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	7	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	8	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	8	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	8	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	8	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	8	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	8	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	8	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	8	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	8	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	8	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	8	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	8	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	9	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	9	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	9	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	9	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	9	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	9	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	9	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	9	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	9	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	9	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	9	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	11	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	11	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	11	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	11	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	11	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	11	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	11	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	11	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	11	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	11	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	11	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	11	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	12	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	12	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	12	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	12	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	12	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	12	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	12	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	12	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	12	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	12	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	12	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	12	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	14	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	14	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	14	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	14	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	14	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	14	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	14	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	14	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	14	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	14	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	14	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	14	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	15	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	15	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	15	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	15	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	15	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	15	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	15	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	15	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	15	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	15	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	15	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	16	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	16	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	16	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	16	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	16	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	16	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	16	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	16	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	16	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	16	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	16	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	16	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	18	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	18	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	18	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	18	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	18	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	18	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	18	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	18	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	18	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	18	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	18	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	18	0.2
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	19	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	19	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	19	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	19	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	19	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	19	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	19	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	19	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	19	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	19	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	19	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	20	0.2
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	20	0.2
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	20	0.2
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	20	0.2
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	20	0.2
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	20	0.2
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	20	0.2
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	20	0.2
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	20	0.2
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	20	0.2
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	20	0.2
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	20	0.2
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	16	0.2
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	16	0.2
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	16	0.2
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	16	0.2
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	16	0.2
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	16	0.2
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	16	0.2
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	16	0.2
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	16	0.2
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	16	0.2
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	16	0.2
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	16	0.2
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	16	0.2
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	16	0.2
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	16	0.2
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	16	0.2
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	16	0.2
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	16	0.2
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	16	0.2
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	16	0.2
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	16	0.2
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	16	0.2
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	16	0.2
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	16	0.2
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	16	0.2
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	16	0.2
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	16	0.2
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	16	0.2
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	16	0.2
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	16	0.2
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	16	0.2
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	16	0.2
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	16	0.2
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	16	0.2
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	16	0.2
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	5	0.2
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	5	0.2
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	5	0.2
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	5	0.2
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	7	0.2
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	7	0.2
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	7	0.2
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	7	0.2
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	14	0.2
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	14	0.2
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	14	0.2
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	14	0.2
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	5	0.2
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	5	0.2
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	5	0.2
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	5	0.2
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	6	0.2
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	6	0.2
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	6	0.2
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	6	0.2
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	12	0.2
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	12	0.2
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	12	0.2
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	12	0.2
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	3	0.2
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	3	0.2
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	3	0.2
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	3	0.2
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	12	0.2
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	12	0.2
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	12	0.2
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	12	0.2
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	15	0.2
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	15	0.2
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	15	0.2
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	10	0.2
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	10	0.2
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	10	0.2
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	10	0.2
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	13	0.2
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	13	0.2
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	13	0.2
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	13	0.2
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	1	0.2
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	1	0.2
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	1	0.2
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	1	0.2
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	2	0.2
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	2	0.2
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	2	0.2
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	2	0.2
(1,66)	1:A:101:VAL:O	1:A:139:ALA:N	17	0.2
(1,66)	1:A:101:VAL:O	1:B:139:ALA:N	17	0.2
(1,66)	1:B:101:VAL:O	1:A:139:ALA:N	17	0.2
(1,66)	1:B:101:VAL:O	1:B:139:ALA:N	17	0.2
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	4	0.2
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	4	0.2
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	4	0.2
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	4	0.2
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	11	0.2
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	11	0.2
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	11	0.2
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	11	0.2
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	16	0.2
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	16	0.2
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	16	0.2
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	16	0.2
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	6	0.2
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	6	0.2
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	6	0.2
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	6	0.2
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	14	0.2
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	14	0.2
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	14	0.2
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	14	0.2
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	3	0.2
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	3	0.2
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	3	0.2
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	6	0.2
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	6	0.2
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	6	0.2
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	6	0.2
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	16	0.2
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	16	0.2
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	16	0.2
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	16	0.2
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	3	0.2
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	3	0.2
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	3	0.2
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	3	0.2
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	18	0.2
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	18	0.2
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	18	0.2
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	18	0.2
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	2	0.2
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	2	0.2
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	2	0.2
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	2	0.2
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	9	0.2
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	9	0.2
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	9	0.2
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	9	0.2
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	11	0.2
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	11	0.2
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	11	0.2
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	11	0.2
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	16	0.2
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	16	0.2
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	16	0.2
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	16	0.2
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	8	0.2
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	8	0.2
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	8	0.2
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	8	0.2
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	7	0.2
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	7	0.2
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	7	0.2
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	10	0.2
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	10	0.2
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	10	0.2
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	10	0.2
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	17	0.2
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	17	0.2
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	17	0.2
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	17	0.2
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	18	0.2
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	18	0.2
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	18	0.2
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	18	0.2
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	9	0.2
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	9	0.2
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	9	0.2
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	9	0.2
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	1	0.2
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	1	0.2
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	1	0.2
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	1	0.2
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	5	0.2
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	5	0.2
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	5	0.2
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	5	0.2
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	14	0.2
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	14	0.2
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	14	0.2
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	14	0.2
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	16	0.2
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	16	0.2
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	16	0.2
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	16	0.2
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	18	0.2
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	18	0.2
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	18	0.2
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	18	0.2
(1,20)	1:A:31:SER:N	1:A:44:THR:O	1	0.2
(1,20)	1:A:31:SER:N	1:B:44:THR:O	1	0.2
(1,20)	1:B:31:SER:N	1:A:44:THR:O	1	0.2
(1,20)	1:B:31:SER:N	1:B:44:THR:O	1	0.2
(1,2)	1:A:10:THR:O	1:A:20:THR:N	9	0.2
(1,2)	1:A:10:THR:O	1:B:20:THR:N	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:B:10:THR:O	1:A:20:THR:N	9	0.2
(1,2)	1:B:10:THR:O	1:B:20:THR:N	9	0.2
(1,2)	1:A:10:THR:O	1:A:20:THR:N	14	0.2
(1,2)	1:A:10:THR:O	1:B:20:THR:N	14	0.2
(1,2)	1:B:10:THR:O	1:A:20:THR:N	14	0.2
(1,2)	1:B:10:THR:O	1:B:20:THR:N	14	0.2
(1,2)	1:A:10:THR:O	1:A:20:THR:N	19	0.2
(1,2)	1:A:10:THR:O	1:B:20:THR:N	19	0.2
(1,2)	1:B:10:THR:O	1:A:20:THR:N	19	0.2
(1,2)	1:B:10:THR:O	1:B:20:THR:N	19	0.2
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	3	0.2
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	3	0.2
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	3	0.2
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	3	0.2
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	9	0.2
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	9	0.2
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	9	0.2
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	9	0.2
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	10	0.2
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	10	0.2
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	10	0.2
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	10	0.2
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	11	0.2
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	11	0.2
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	11	0.2
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	11	0.2
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	9	0.2
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	9	0.2
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	9	0.2
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	9	0.2
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	6	0.2
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	6	0.2
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	6	0.2
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	6	0.2
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	9	0.19
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	9	0.19
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	9	0.19
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	9	0.19
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	10	0.19
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	10	0.19
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	10	0.19
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	10	0.19
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	10	0.19
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	10	0.19
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	10	0.19
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	10	0.19
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	10	0.19
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	10	0.19
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	10	0.19
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	6	0.19
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	6	0.19
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	6	0.19
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	6	0.19
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	6	0.19
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	6	0.19
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	6	0.19
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	6	0.19
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	6	0.19
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	6	0.19
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	6	0.19
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	6	0.19
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	7	0.19
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	7	0.19
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	7	0.19
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	7	0.19
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	7	0.19
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	7	0.19
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	7	0.19
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	7	0.19
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	7	0.19
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	7	0.19
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	7	0.19
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	7	0.19
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	10	0.19
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	10	0.19
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	10	0.19
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	10	0.19
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	10	0.19
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	10	0.19
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	10	0.19
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	10	0.19
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	10	0.19
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	10	0.19
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	10	0.19
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	20	0.19
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	20	0.19
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	20	0.19
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	20	0.19
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	20	0.19
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	20	0.19
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	20	0.19
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	20	0.19
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	20	0.19
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	20	0.19
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	20	0.19
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	20	0.19
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	20	0.19
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	20	0.19
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	20	0.19
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	20	0.19
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	20	0.19
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	20	0.19
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	20	0.19
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	20	0.19
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	20	0.19
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	20	0.19
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	20	0.19
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	20	0.19
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	10	0.19
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	10	0.19
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	10	0.19
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	10	0.19
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	11	0.19
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	11	0.19
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	11	0.19
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	11	0.19
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	18	0.19
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	18	0.19
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	18	0.19
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	18	0.19
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	18	0.19
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	18	0.19
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	18	0.19
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	18	0.19
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	18	0.19
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	18	0.19
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	18	0.19
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	18	0.19
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	18	0.19
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	18	0.19
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	18	0.19
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	18	0.19
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	18	0.19
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	18	0.19
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	18	0.19
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	18	0.19
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	18	0.19
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	18	0.19
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	18	0.19
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	18	0.19
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	18	0.19
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	18	0.19
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	18	0.19
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	18	0.19
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	18	0.19
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	18	0.19
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	18	0.19
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	18	0.19
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	18	0.19
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	18	0.19
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	18	0.19
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	3	0.19
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	3	0.19
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	3	0.19
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	3	0.19
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	3	0.19
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	3	0.19
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	3	0.19
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	3	0.19
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	3	0.19
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	3	0.19
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	3	0.19
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	3	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	4	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	4	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	4	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	4	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	4	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	4	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	4	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	4	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	4	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	4	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	4	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	4	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	4	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	4	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	4	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	4	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	4	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	4	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	4	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	4	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	4	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	4	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	4	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	10	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	10	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	10	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	10	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	10	0.19
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	10	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	10	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	10	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	10	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	10	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	10	0.19
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	10	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	10	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	10	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	10	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	10	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	10	0.19
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	10	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	10	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	10	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	10	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	10	0.19
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	10	0.19
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	4	0.19
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	4	0.19
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	4	0.19
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	4	0.19
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	4	0.19
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	4	0.19
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	4	0.19
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	4	0.19
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	4	0.19
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	4	0.19
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	4	0.19
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	4	0.19
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	4	0.19
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	4	0.19
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	4	0.19
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	4	0.19
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	4	0.19
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	4	0.19
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	4	0.19
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	4	0.19
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	4	0.19
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	4	0.19
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	4	0.19
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	4	0.19
(2,1462)	1:A:34:ARG:HG2	1:A:40:GLY:HA2	7	0.19
(2,1462)	1:A:34:ARG:HG2	1:A:40:GLY:HA3	7	0.19
(2,1462)	1:A:34:ARG:HG2	1:B:40:GLY:HA2	7	0.19
(2,1462)	1:A:34:ARG:HG2	1:B:40:GLY:HA3	7	0.19
(2,1462)	1:A:34:ARG:HG3	1:A:40:GLY:HA2	7	0.19
(2,1462)	1:A:34:ARG:HG3	1:A:40:GLY:HA3	7	0.19
(2,1462)	1:A:34:ARG:HG3	1:B:40:GLY:HA2	7	0.19
(2,1462)	1:A:34:ARG:HG3	1:B:40:GLY:HA3	7	0.19
(2,1462)	1:B:34:ARG:HG2	1:A:40:GLY:HA2	7	0.19
(2,1462)	1:B:34:ARG:HG2	1:A:40:GLY:HA3	7	0.19
(2,1462)	1:B:34:ARG:HG2	1:B:40:GLY:HA2	7	0.19
(2,1462)	1:B:34:ARG:HG2	1:B:40:GLY:HA3	7	0.19
(2,1462)	1:B:34:ARG:HG3	1:A:40:GLY:HA2	7	0.19
(2,1462)	1:B:34:ARG:HG3	1:A:40:GLY:HA3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1462)	1:B:34:ARG:HG3	1:B:40:GLY:HA2	7	0.19
(2,1462)	1:B:34:ARG:HG3	1:B:40:GLY:HA3	7	0.19
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	2	0.19
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	2	0.19
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	2	0.19
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	2	0.19
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	2	0.19
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	2	0.19
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	2	0.19
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	2	0.19
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	6	0.19
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	6	0.19
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	6	0.19
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	6	0.19
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	6	0.19
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	6	0.19
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	6	0.19
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	6	0.19
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	7	0.19
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	7	0.19
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	7	0.19
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	7	0.19
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	7	0.19
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	7	0.19
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	7	0.19
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	7	0.19
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	10	0.19
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	10	0.19
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	10	0.19
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	10	0.19
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	10	0.19
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	10	0.19
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	10	0.19
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	10	0.19
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	1	0.19
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	1	0.19
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	1	0.19
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	1	0.19
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	1	0.19
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	1	0.19
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	1	0.19
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	1	0.19
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	1	0.19
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	1	0.19
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	1	0.19
(2,1276)	1:A:129:ARG:HG3	1:A:130:ASN:H	17	0.19
(2,1276)	1:A:129:ARG:HG3	1:B:130:ASN:H	17	0.19
(2,1276)	1:B:129:ARG:HG3	1:A:130:ASN:H	17	0.19
(2,1276)	1:B:129:ARG:HG3	1:B:130:ASN:H	17	0.19
(2,1208)	1:A:107:ASP:HB3	1:A:110:ALA:H	8	0.19
(2,1208)	1:A:107:ASP:HB3	1:B:110:ALA:H	8	0.19
(2,1208)	1:B:107:ASP:HB3	1:A:110:ALA:H	8	0.19
(2,1208)	1:B:107:ASP:HB3	1:B:110:ALA:H	8	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	2	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	2	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	2	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	2	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	2	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	2	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	2	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	2	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	2	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	2	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	2	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	2	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	2	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	2	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	2	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	2	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	2	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	2	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	2	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	2	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	2	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	2	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	2	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	2	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	2	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	2	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	2	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	2	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	2	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	2	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	2	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	2	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	2	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	2	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	2	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	8	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	8	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	8	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	8	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	8	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	8	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	8	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	8	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	8	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	8	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	8	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	8	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	8	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	8	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	8	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	8	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	8	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	8	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	8	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	8	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	8	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	8	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	8	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	8	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	8	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	8	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	8	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	8	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	8	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	8	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	8	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	8	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	8	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	8	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	8	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	20	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	20	0.19
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	20	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	20	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	20	0.19
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	20	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	20	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	20	0.19
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	20	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	20	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	20	0.19
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	20	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	20	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	20	0.19
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	20	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	20	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	20	0.19
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	20	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	20	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	20	0.19
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	20	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	20	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	20	0.19
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	20	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	20	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	20	0.19
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	20	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	20	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	20	0.19
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	20	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	20	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	20	0.19
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	20	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	20	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	20	0.19
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	20	0.19
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	6	0.19
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	6	0.19
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	6	0.19
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	6	0.19
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	18	0.19
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	18	0.19
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	18	0.19
(1,9)	1:A:10:THR:H	1:A:20:THR:O	7	0.19
(1,9)	1:A:10:THR:H	1:B:20:THR:O	7	0.19
(1,9)	1:B:10:THR:H	1:A:20:THR:O	7	0.19
(1,9)	1:B:10:THR:H	1:B:20:THR:O	7	0.19
(1,9)	1:A:10:THR:H	1:A:20:THR:O	13	0.19
(1,9)	1:A:10:THR:H	1:B:20:THR:O	13	0.19
(1,9)	1:B:10:THR:H	1:A:20:THR:O	13	0.19
(1,9)	1:B:10:THR:H	1:B:20:THR:O	13	0.19
(1,9)	1:A:10:THR:H	1:A:20:THR:O	20	0.19
(1,9)	1:A:10:THR:H	1:B:20:THR:O	20	0.19
(1,9)	1:B:10:THR:H	1:A:20:THR:O	20	0.19
(1,9)	1:B:10:THR:H	1:B:20:THR:O	20	0.19
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	8	0.19
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	8	0.19
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	8	0.19
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	8	0.19
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	2	0.19
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	2	0.19
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	2	0.19
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	2	0.19
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	17	0.19
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	17	0.19
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	17	0.19
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	17	0.19
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	1	0.19
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	1	0.19
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	1	0.19
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	1	0.19
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	13	0.19
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	13	0.19
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	13	0.19
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	13	0.19
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	1	0.19
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	1	0.19
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	1	0.19
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	1	0.19
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	3	0.19
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	3	0.19
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	3	0.19
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	11	0.19
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	11	0.19
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	11	0.19
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	11	0.19
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	15	0.19
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	15	0.19
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	15	0.19
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	15	0.19
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	11	0.19
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	11	0.19
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	11	0.19
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	11	0.19
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	15	0.19
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	15	0.19
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	15	0.19
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	15	0.19
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	20	0.19
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	20	0.19
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	20	0.19
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	20	0.19
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	9	0.19
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	9	0.19
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	9	0.19
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	9	0.19
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	15	0.19
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	15	0.19
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	15	0.19
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	15	0.19
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	17	0.19
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	17	0.19
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	17	0.19
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	17	0.19
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	12	0.19
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	12	0.19
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	12	0.19
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	12	0.19
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	13	0.19
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	13	0.19
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	13	0.19
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	13	0.19
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	11	0.19
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	11	0.19
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	11	0.19
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	5	0.19
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	5	0.19
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	5	0.19
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	5	0.19
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	6	0.19
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	6	0.19
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	6	0.19
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	6	0.19
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	12	0.19
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	12	0.19
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	12	0.19
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	12	0.19
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	18	0.19
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	18	0.19
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	18	0.19
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	18	0.19
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	19	0.19
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	19	0.19
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	19	0.19
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	19	0.19
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	7	0.19
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	7	0.19
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	7	0.19
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	7	0.19
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	12	0.19
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	12	0.19
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	12	0.19
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	12	0.19
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	14	0.19
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	14	0.19
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	14	0.19
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	14	0.19
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	17	0.19
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	17	0.19
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	17	0.19
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	17	0.19
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	7	0.19
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	7	0.19
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	7	0.19
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	11	0.19
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	11	0.19
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	11	0.19
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	11	0.19
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	13	0.19
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	13	0.19
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	13	0.19
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	13	0.19
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	7	0.19
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	7	0.19
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	7	0.19
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	7	0.19
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	18	0.19
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	18	0.19
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	18	0.19
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	18	0.19
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	3	0.19
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	3	0.19
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	3	0.19
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	3	0.19
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	5	0.19
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	5	0.19
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	5	0.19
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	5	0.19
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	1	0.19
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	1	0.19
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	1	0.19
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	1	0.19
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	4	0.19
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	4	0.19
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	4	0.19
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	4	0.19
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	12	0.19
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	12	0.19
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	12	0.19
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	12	0.19
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	14	0.19
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	14	0.19
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	14	0.19
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	14	0.19
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	17	0.19
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	17	0.19
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	17	0.19
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	13	0.19
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	13	0.19
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	13	0.19
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	13	0.19
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	8	0.19
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	8	0.19
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	8	0.19
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	8	0.19
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	10	0.19
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	10	0.19
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	10	0.19
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	10	0.19
(1,4)	1:A:12:THR:O	1:A:18:ARG:N	18	0.19
(1,4)	1:A:12:THR:O	1:B:18:ARG:N	18	0.19
(1,4)	1:B:12:THR:O	1:A:18:ARG:N	18	0.19
(1,4)	1:B:12:THR:O	1:B:18:ARG:N	18	0.19
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	6	0.19
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	6	0.19
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	6	0.19
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	6	0.19
(1,36)	1:A:53:GLY:O	1:A:57:CYS:N	18	0.19
(1,36)	1:A:53:GLY:O	1:B:57:CYS:N	18	0.19
(1,36)	1:B:53:GLY:O	1:A:57:CYS:N	18	0.19
(1,36)	1:B:53:GLY:O	1:B:57:CYS:N	18	0.19
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	9	0.19
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	9	0.19
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	9	0.19
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	9	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	3	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	3	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	3	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	3	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	4	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	4	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	4	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	4	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	7	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	7	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	7	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	13	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	13	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	13	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	13	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	15	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	15	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	15	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	15	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	16	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	16	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	16	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	16	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	17	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	17	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	17	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	17	0.19
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	20	0.19
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	20	0.19
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	20	0.19
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	20	0.19
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	6	0.19
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	6	0.19
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	6	0.19
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	6	0.19
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	7	0.19
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	7	0.19
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	7	0.19
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	7	0.19
(1,20)	1:A:31:SER:N	1:A:44:THR:O	5	0.19
(1,20)	1:A:31:SER:N	1:B:44:THR:O	5	0.19
(1,20)	1:B:31:SER:N	1:A:44:THR:O	5	0.19
(1,20)	1:B:31:SER:N	1:B:44:THR:O	5	0.19
(1,20)	1:A:31:SER:N	1:A:44:THR:O	13	0.19
(1,20)	1:A:31:SER:N	1:B:44:THR:O	13	0.19
(1,20)	1:B:31:SER:N	1:A:44:THR:O	13	0.19
(1,20)	1:B:31:SER:N	1:B:44:THR:O	13	0.19
(1,2)	1:A:10:THR:O	1:A:20:THR:N	3	0.19
(1,2)	1:A:10:THR:O	1:B:20:THR:N	3	0.19
(1,2)	1:B:10:THR:O	1:A:20:THR:N	3	0.19
(1,2)	1:B:10:THR:O	1:B:20:THR:N	3	0.19
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	15	0.19
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	15	0.19
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	15	0.19
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	16	0.19
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	16	0.19
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	16	0.19
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	16	0.19
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	1	0.18
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	1	0.18
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	1	0.18
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	1	0.18
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	3	0.18
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	3	0.18
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	3	0.18
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	3	0.18
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	3	0.18
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	3	0.18
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	3	0.18
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	3	0.18
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	3	0.18
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	3	0.18
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	3	0.18
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	3	0.18
(2,489)	1:A:106:LEU:HD11	1:A:107:ASP:H	9	0.18
(2,489)	1:A:106:LEU:HD11	1:B:107:ASP:H	9	0.18
(2,489)	1:A:106:LEU:HD12	1:A:107:ASP:H	9	0.18
(2,489)	1:A:106:LEU:HD12	1:B:107:ASP:H	9	0.18
(2,489)	1:A:106:LEU:HD13	1:A:107:ASP:H	9	0.18
(2,489)	1:A:106:LEU:HD13	1:B:107:ASP:H	9	0.18
(2,489)	1:B:106:LEU:HD11	1:A:107:ASP:H	9	0.18
(2,489)	1:B:106:LEU:HD11	1:B:107:ASP:H	9	0.18
(2,489)	1:B:106:LEU:HD12	1:A:107:ASP:H	9	0.18
(2,489)	1:B:106:LEU:HD12	1:B:107:ASP:H	9	0.18
(2,489)	1:B:106:LEU:HD13	1:A:107:ASP:H	9	0.18
(2,489)	1:B:106:LEU:HD13	1:B:107:ASP:H	9	0.18
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	17	0.18
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	17	0.18
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	17	0.18
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	17	0.18
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	1	0.18
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	1	0.18
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	1	0.18
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	1	0.18
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	1	0.18
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	1	0.18
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	1	0.18
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	1	0.18
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	1	0.18
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	1	0.18
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	1	0.18
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	1	0.18
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	1	0.18
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	1	0.18
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	1	0.18
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	1	0.18
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	1	0.18
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	1	0.18
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	1	0.18
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	1	0.18
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	1	0.18
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	1	0.18
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	1	0.18
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	1	0.18
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	1	0.18
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	1	0.18
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	1	0.18
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	1	0.18
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	1	0.18
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	1	0.18
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	1	0.18
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	1	0.18
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	1	0.18
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	1	0.18
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	1	0.18
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	4	0.18
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	4	0.18
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	4	0.18
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	4	0.18
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	4	0.18
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	4	0.18
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	4	0.18
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	4	0.18
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	4	0.18
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	4	0.18
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	4	0.18
(2,1649)	1:A:130:ASN:HA	1:A:130:ASN:HD21	11	0.18
(2,1649)	1:A:130:ASN:HA	1:A:130:ASN:HD22	11	0.18
(2,1649)	1:A:130:ASN:HA	1:B:130:ASN:HD21	11	0.18
(2,1649)	1:A:130:ASN:HA	1:B:130:ASN:HD22	11	0.18
(2,1649)	1:B:130:ASN:HA	1:A:130:ASN:HD21	11	0.18
(2,1649)	1:B:130:ASN:HA	1:A:130:ASN:HD22	11	0.18
(2,1649)	1:B:130:ASN:HA	1:B:130:ASN:HD21	11	0.18
(2,1649)	1:B:130:ASN:HA	1:B:130:ASN:HD22	11	0.18
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	17	0.18
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	17	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	11	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	11	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	11	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	11	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	11	0.18
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	11	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	11	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	11	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	11	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	11	0.18
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	11	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	11	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	11	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	11	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	11	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	11	0.18
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	11	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	11	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	11	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	11	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	11	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	11	0.18
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	11	0.18
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	2	0.18
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	2	0.18
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	2	0.18
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	2	0.18
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	2	0.18
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	2	0.18
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	2	0.18
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	2	0.18
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	2	0.18
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	2	0.18
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	2	0.18
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	2	0.18
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	2	0.18
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	2	0.18
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	2	0.18
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	2	0.18
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	2	0.18
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	2	0.18
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	2	0.18
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	2	0.18
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	2	0.18
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	2	0.18
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	2	0.18
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	2	0.18
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	19	0.18
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	19	0.18
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	19	0.18
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	19	0.18
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	19	0.18
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	19	0.18
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	19	0.18
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	19	0.18
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	19	0.18
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	19	0.18
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	19	0.18
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	19	0.18
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	19	0.18
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	19	0.18
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	19	0.18
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	19	0.18
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	19	0.18
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	19	0.18
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	19	0.18
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	19	0.18
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	19	0.18
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	19	0.18
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	19	0.18
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	13	0.18
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	13	0.18
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	13	0.18
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	13	0.18
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	13	0.18
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	13	0.18
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	13	0.18
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	13	0.18
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	13	0.18
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	13	0.18
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	13	0.18
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	13	0.18
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	17	0.18
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	17	0.18
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	17	0.18
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	17	0.18
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	17	0.18
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	17	0.18
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	17	0.18
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	17	0.18
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	17	0.18
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	17	0.18
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	17	0.18
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	14	0.18
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	14	0.18
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	14	0.18
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	14	0.18
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	14	0.18
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	14	0.18
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	14	0.18
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	14	0.18
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	14	0.18
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	14	0.18
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	14	0.18
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	14	0.18
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	14	0.18
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	14	0.18
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	14	0.18
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	14	0.18
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	14	0.18
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	14	0.18
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	14	0.18
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	14	0.18
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	14	0.18
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	14	0.18
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	14	0.18
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	14	0.18
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	14	0.18
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	14	0.18
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	14	0.18
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	14	0.18
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	14	0.18
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	14	0.18
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	14	0.18
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	14	0.18
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	14	0.18
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	14	0.18
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	14	0.18
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	14	0.18
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	2	0.18
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	2	0.18
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	2	0.18
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	4	0.18
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	4	0.18
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	4	0.18
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	4	0.18
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	1	0.18
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	1	0.18
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	1	0.18
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	1	0.18
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	13	0.18
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	13	0.18
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	13	0.18
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	13	0.18
(1,9)	1:A:10:THR:H	1:A:20:THR:O	5	0.18
(1,9)	1:A:10:THR:H	1:B:20:THR:O	5	0.18
(1,9)	1:B:10:THR:H	1:A:20:THR:O	5	0.18
(1,9)	1:B:10:THR:H	1:B:20:THR:O	5	0.18
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	11	0.18
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	11	0.18
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	11	0.18
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	11	0.18
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	3	0.18
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	3	0.18
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	3	0.18
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	3	0.18
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	4	0.18
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	4	0.18
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	4	0.18
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	4	0.18
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	9	0.18
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	9	0.18
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	9	0.18
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	9	0.18
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	14	0.18
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	14	0.18
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	14	0.18
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	14	0.18
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	16	0.18
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	16	0.18
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	16	0.18
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	20	0.18
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	20	0.18
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	20	0.18
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	20	0.18
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	8	0.18
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	8	0.18
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	8	0.18
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	8	0.18
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	10	0.18
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	10	0.18
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	10	0.18
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	10	0.18
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	12	0.18
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	12	0.18
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	12	0.18
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	12	0.18
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	10	0.18
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	10	0.18
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	10	0.18
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	10	0.18
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	14	0.18
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	14	0.18
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	14	0.18
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	14	0.18
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	9	0.18
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	9	0.18
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	9	0.18
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	9	0.18
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	10	0.18
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	10	0.18
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	10	0.18
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	10	0.18
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	19	0.18
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	19	0.18
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	19	0.18
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	19	0.18
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	2	0.18
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	2	0.18
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	2	0.18
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	2	0.18
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	10	0.18
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	10	0.18
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	10	0.18
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	1	0.18
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	1	0.18
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	1	0.18
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	1	0.18
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	1	0.18
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	1	0.18
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	1	0.18
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	1	0.18
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	19	0.18
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	19	0.18
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	19	0.18
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	19	0.18
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	4	0.18
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	4	0.18
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	4	0.18
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	4	0.18
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	5	0.18
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	5	0.18
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	5	0.18
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	5	0.18
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	7	0.18
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	7	0.18
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	7	0.18
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	7	0.18
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	15	0.18
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	15	0.18
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	15	0.18
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	15	0.18
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	15	0.18
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	15	0.18
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	15	0.18
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	15	0.18
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	20	0.18
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	20	0.18
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	20	0.18
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	20	0.18
(1,48)	1:A:65:VAL:O	1:A:69:ASN:N	15	0.18
(1,48)	1:A:65:VAL:O	1:B:69:ASN:N	15	0.18
(1,48)	1:B:65:VAL:O	1:A:69:ASN:N	15	0.18
(1,48)	1:B:65:VAL:O	1:B:69:ASN:N	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	1	0.18
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	1	0.18
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	1	0.18
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	1	0.18
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	10	0.18
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	10	0.18
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	10	0.18
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	10	0.18
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	6	0.18
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	6	0.18
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	6	0.18
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	6	0.18
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	10	0.18
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	10	0.18
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	10	0.18
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	10	0.18
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	15	0.18
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	15	0.18
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	15	0.18
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	15	0.18
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	1	0.18
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	1	0.18
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	1	0.18
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	1	0.18
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	18	0.18
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	18	0.18
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	18	0.18
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	18	0.18
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	6	0.18
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	6	0.18
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	6	0.18
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	6	0.18
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	1	0.18
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	1	0.18
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	1	0.18
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	1	0.18
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	11	0.18
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	11	0.18
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	11	0.18
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	11	0.18
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	2	0.18
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	2	0.18
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	2	0.18
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	3	0.18
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	3	0.18
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	3	0.18
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	3	0.18
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	12	0.18
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	12	0.18
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	12	0.18
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	12	0.18
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	19	0.18
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	19	0.18
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	19	0.18
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	19	0.18
(1,20)	1:A:31:SER:N	1:A:44:THR:O	9	0.18
(1,20)	1:A:31:SER:N	1:B:44:THR:O	9	0.18
(1,20)	1:B:31:SER:N	1:A:44:THR:O	9	0.18
(1,20)	1:B:31:SER:N	1:B:44:THR:O	9	0.18
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	13	0.18
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	13	0.18
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	13	0.18
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	13	0.18
(1,16)	1:A:19:ALA:N	1:A:28:VAL:O	1	0.18
(1,16)	1:A:19:ALA:N	1:B:28:VAL:O	1	0.18
(1,16)	1:B:19:ALA:N	1:A:28:VAL:O	1	0.18
(1,16)	1:B:19:ALA:N	1:B:28:VAL:O	1	0.18
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	18	0.18
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	18	0.18
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	18	0.18
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	18	0.18
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	7	0.17
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	7	0.17
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	7	0.17
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	7	0.17
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	7	0.17
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	7	0.17
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	7	0.17
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	7	0.17
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	7	0.17
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	7	0.17
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	7	0.17
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	11	0.17
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	11	0.17
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	11	0.17
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	11	0.17
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	11	0.17
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	11	0.17
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	11	0.17
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	11	0.17
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	11	0.17
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	11	0.17
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	11	0.17
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	11	0.17
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	13	0.17
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	13	0.17
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	13	0.17
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	13	0.17
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	13	0.17
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	13	0.17
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	13	0.17
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	13	0.17
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	13	0.17
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	13	0.17
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	13	0.17
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	13	0.17
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	8	0.17
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	8	0.17
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	8	0.17
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	8	0.17
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	8	0.17
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	8	0.17
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	8	0.17
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	8	0.17
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	8	0.17
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	8	0.17
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	8	0.17
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	8	0.17
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	16	0.17
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	16	0.17
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	16	0.17
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	16	0.17
(2,257)	1:A:42:GLU:H	1:A:42:GLU:HG2	10	0.17
(2,257)	1:A:42:GLU:H	1:B:42:GLU:HG2	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,257)	1:B:42:GLU:H	1:A:42:GLU:HG2	10	0.17
(2,257)	1:B:42:GLU:H	1:B:42:GLU:HG2	10	0.17
(2,257)	1:A:42:GLU:H	1:A:42:GLU:HG2	15	0.17
(2,257)	1:A:42:GLU:H	1:B:42:GLU:HG2	15	0.17
(2,257)	1:B:42:GLU:H	1:A:42:GLU:HG2	15	0.17
(2,257)	1:B:42:GLU:H	1:B:42:GLU:HG2	15	0.17
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	20	0.17
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	20	0.17
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	20	0.17
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	20	0.17
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	20	0.17
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	20	0.17
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	20	0.17
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	20	0.17
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	17	0.17
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	17	0.17
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	17	0.17
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	17	0.17
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	17	0.17
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	17	0.17
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	17	0.17
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	17	0.17
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	14	0.17
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	14	0.17
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	20	0.17
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	20	0.17
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	8	0.17
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	8	0.17
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	8	0.17
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	8	0.17
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	8	0.17
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	8	0.17
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	8	0.17
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	8	0.17
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	8	0.17
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	8	0.17
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	8	0.17
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	8	0.17
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	8	0.17
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	8	0.17
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	8	0.17
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	8	0.17
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	8	0.17
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	8	0.17
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	8	0.17
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	8	0.17
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	8	0.17
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	8	0.17
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	8	0.17
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	2	0.17
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	2	0.17
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	2	0.17
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	2	0.17
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	2	0.17
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	2	0.17
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	2	0.17
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	2	0.17
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	2	0.17
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	2	0.17
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	2	0.17
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	2	0.17
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	2	0.17
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	2	0.17
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	2	0.17
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	2	0.17
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	2	0.17
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	2	0.17
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	2	0.17
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	2	0.17
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	2	0.17
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	2	0.17
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	2	0.17
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	2	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	1	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	1	0.17
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	1	0.17
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	1	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	1	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	1	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	1	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	1	0.17
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	1	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	1	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	1	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	1	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	1	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	1	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	1	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	1	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	1	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	1	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	1	0.17
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	1	0.17
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	1	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	1	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	1	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	3	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	3	0.17
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	3	0.17
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	3	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	3	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	3	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	3	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	3	0.17
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	3	0.17
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	3	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	3	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	3	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	3	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	3	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	3	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	3	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	3	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	3	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	3	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	3	0.17
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	3	0.17
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	3	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	3	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	3	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	18	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	18	0.17
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	18	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	18	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	18	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	18	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	18	0.17
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	18	0.17
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	18	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	18	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	18	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	18	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	18	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	18	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	18	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	18	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	18	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	18	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	18	0.17
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	18	0.17
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	18	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	18	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	18	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	20	0.17
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	20	0.17
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	20	0.17
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	20	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	20	0.17
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	20	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	20	0.17
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	20	0.17
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	20	0.17
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	20	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	20	0.17
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	20	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	20	0.17
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	20	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	20	0.17
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	20	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	20	0.17
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	20	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	20	0.17
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	20	0.17
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	20	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	20	0.17
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	20	0.17
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	4	0.17
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	4	0.17
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	4	0.17
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	4	0.17
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	4	0.17
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	4	0.17
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	4	0.17
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	4	0.17
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	4	0.17
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	4	0.17
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	4	0.17
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	4	0.17
(2,1278)	1:A:130:ASN:HA	1:A:130:ASN:HD21	11	0.17
(2,1278)	1:A:130:ASN:HA	1:B:130:ASN:HD21	11	0.17
(2,1278)	1:B:130:ASN:HA	1:A:130:ASN:HD21	11	0.17
(2,1278)	1:B:130:ASN:HA	1:B:130:ASN:HD21	11	0.17
(2,1208)	1:A:107:ASP:HB3	1:A:110:ALA:H	10	0.17
(2,1208)	1:A:107:ASP:HB3	1:B:110:ALA:H	10	0.17
(2,1208)	1:B:107:ASP:HB3	1:A:110:ALA:H	10	0.17
(2,1208)	1:B:107:ASP:HB3	1:B:110:ALA:H	10	0.17
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	12	0.17
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	12	0.17
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	12	0.17
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	12	0.17
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	12	0.17
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	12	0.17
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	12	0.17
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	12	0.17
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	12	0.17
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	12	0.17
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	12	0.17
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	12	0.17
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	12	0.17
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	12	0.17
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	12	0.17
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	12	0.17
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	12	0.17
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	12	0.17
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	12	0.17
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	12	0.17
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	12	0.17
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	12	0.17
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	12	0.17
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	12	0.17
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	12	0.17
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	12	0.17
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	12	0.17
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	12	0.17
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	12	0.17
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	12	0.17
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	12	0.17
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	12	0.17
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	12	0.17
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	12	0.17
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	12	0.17
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	8	0.17
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	8	0.17
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	8	0.17
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	8	0.17
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	16	0.17
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	16	0.17
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	16	0.17
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	16	0.17
(1,9)	1:A:10:THR:H	1:A:20:THR:O	3	0.17
(1,9)	1:A:10:THR:H	1:B:20:THR:O	3	0.17
(1,9)	1:B:10:THR:H	1:A:20:THR:O	3	0.17
(1,9)	1:B:10:THR:H	1:B:20:THR:O	3	0.17
(1,9)	1:A:10:THR:H	1:A:20:THR:O	8	0.17
(1,9)	1:A:10:THR:H	1:B:20:THR:O	8	0.17
(1,9)	1:B:10:THR:H	1:A:20:THR:O	8	0.17
(1,9)	1:B:10:THR:H	1:B:20:THR:O	8	0.17
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	5	0.17
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	5	0.17
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	5	0.17
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	5	0.17
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	8	0.17
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	8	0.17
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	8	0.17
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	18	0.17
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	18	0.17
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	18	0.17
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	18	0.17
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	11	0.17
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	11	0.17
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	11	0.17
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	11	0.17
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	20	0.17
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	20	0.17
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	20	0.17
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	20	0.17
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	16	0.17
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	16	0.17
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	16	0.17
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	16	0.17
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	8	0.17
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	8	0.17
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	8	0.17
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	8	0.17
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	16	0.17
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	16	0.17
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	16	0.17
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	16	0.17
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	17	0.17
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	17	0.17
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	17	0.17
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	17	0.17
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	3	0.17
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	3	0.17
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	3	0.17
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	3	0.17
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	11	0.17
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	11	0.17
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	11	0.17
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	11	0.17
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	4	0.17
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	4	0.17
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	4	0.17
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	4	0.17
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	10	0.17
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	10	0.17
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	10	0.17
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	15	0.17
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	15	0.17
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	15	0.17
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	15	0.17
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	18	0.17
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	18	0.17
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	18	0.17
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	18	0.17
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	2	0.17
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	2	0.17
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	2	0.17
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	2	0.17
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	3	0.17
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	3	0.17
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	3	0.17
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	3	0.17
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	7	0.17
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	7	0.17
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	7	0.17
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	7	0.17
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	8	0.17
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	8	0.17
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	8	0.17
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	8	0.17
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	15	0.17
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	15	0.17
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	15	0.17
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	15	0.17
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	13	0.17
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	13	0.17
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	13	0.17
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	13	0.17
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	18	0.17
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	18	0.17
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	18	0.17
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	18	0.17
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	3	0.17
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	3	0.17
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	3	0.17
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	20	0.17
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	20	0.17
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	20	0.17
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	20	0.17
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	20	0.17
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	20	0.17
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	20	0.17
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	20	0.17
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	1	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	1	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	1	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	1	0.17
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	2	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	2	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	2	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	2	0.17
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	8	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	8	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	8	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	8	0.17
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	10	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	10	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	10	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	10	0.17
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	11	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	11	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	11	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	11	0.17
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	17	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	17	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	17	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	17	0.17
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	19	0.17
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	19	0.17
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	19	0.17
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	19	0.17
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	4	0.17
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	4	0.17
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	4	0.17
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	4	0.17
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	5	0.17
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	5	0.17
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	5	0.17
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	7	0.17
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	7	0.17
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	7	0.17
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	7	0.17
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	9	0.17
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	9	0.17
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	9	0.17
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	9	0.17
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	13	0.17
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	13	0.17
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	13	0.17
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	13	0.17
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	16	0.17
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	16	0.17
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	16	0.17
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	16	0.17
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	19	0.17
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	19	0.17
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	19	0.17
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	19	0.17
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	3	0.17
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	3	0.17
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	3	0.17
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	3	0.17
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	8	0.17
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	8	0.17
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	8	0.17
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	8	0.17
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	11	0.17
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	11	0.17
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	11	0.17
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	11	0.17
(1,38)	1:A:54:TYR:O	1:A:58:PHE:N	12	0.17
(1,38)	1:A:54:TYR:O	1:B:58:PHE:N	12	0.17
(1,38)	1:B:54:TYR:O	1:A:58:PHE:N	12	0.17
(1,38)	1:B:54:TYR:O	1:B:58:PHE:N	12	0.17
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	1	0.17
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	1	0.17
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	1	0.17
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	16	0.17
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	16	0.17
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	16	0.17
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	16	0.17
(1,34)	1:A:52:ALA:O	1:A:56:ALA:N	18	0.17
(1,34)	1:A:52:ALA:O	1:B:56:ALA:N	18	0.17
(1,34)	1:B:52:ALA:O	1:A:56:ALA:N	18	0.17
(1,34)	1:B:52:ALA:O	1:B:56:ALA:N	18	0.17
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	2	0.17
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	2	0.17
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	2	0.17
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	2	0.17
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	11	0.17
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	11	0.17
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	11	0.17
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	11	0.17
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	2	0.17
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	2	0.17
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	2	0.17
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	2	0.17
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	5	0.17
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	5	0.17
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	5	0.17
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	5	0.17
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	6	0.17
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	6	0.17
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	6	0.17
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	6	0.17
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	8	0.17
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	8	0.17
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	8	0.17
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	8	0.17
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	19	0.17
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	19	0.17
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	19	0.17
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	19	0.17
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	4	0.17
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	4	0.17
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	4	0.17
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	4	0.17
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	13	0.17
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	13	0.17
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	13	0.17
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	1	0.17
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	1	0.17
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	1	0.17
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	1	0.17
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	5	0.17
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	5	0.17
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	5	0.17
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	5	0.17
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	3	0.17
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	3	0.17
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	3	0.17
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	3	0.17
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	14	0.17
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	14	0.17
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	14	0.17
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	14	0.17
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	17	0.17
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	17	0.17
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	17	0.17
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	17	0.17
(1,20)	1:A:31:SER:N	1:A:44:THR:O	18	0.17
(1,20)	1:A:31:SER:N	1:B:44:THR:O	18	0.17
(1,20)	1:B:31:SER:N	1:A:44:THR:O	18	0.17
(1,20)	1:B:31:SER:N	1:B:44:THR:O	18	0.17
(1,2)	1:A:10:THR:O	1:A:20:THR:N	15	0.17
(1,2)	1:A:10:THR:O	1:B:20:THR:N	15	0.17
(1,2)	1:B:10:THR:O	1:A:20:THR:N	15	0.17
(1,2)	1:B:10:THR:O	1:B:20:THR:N	15	0.17
(1,2)	1:A:10:THR:O	1:A:20:THR:N	20	0.17
(1,2)	1:A:10:THR:O	1:B:20:THR:N	20	0.17
(1,2)	1:B:10:THR:O	1:A:20:THR:N	20	0.17
(1,2)	1:B:10:THR:O	1:B:20:THR:N	20	0.17
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	18	0.17
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	18	0.17
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	18	0.17
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	18	0.17
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	17	0.16
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	17	0.16
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	17	0.16
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	6	0.16
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	6	0.16
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	6	0.16
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	6	0.16
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	6	0.16
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	6	0.16
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	6	0.16
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	6	0.16
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	6	0.16
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	6	0.16
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	6	0.16
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	6	0.16
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	2	0.16
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	2	0.16
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	2	0.16
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	2	0.16
(2,257)	1:A:42:GLU:H	1:A:42:GLU:HG2	3	0.16
(2,257)	1:A:42:GLU:H	1:B:42:GLU:HG2	3	0.16
(2,257)	1:B:42:GLU:H	1:A:42:GLU:HG2	3	0.16
(2,257)	1:B:42:GLU:H	1:B:42:GLU:HG2	3	0.16
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD11	16	0.16
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD12	16	0.16
(2,217)	1:A:30:LEU:H	1:A:30:LEU:HD13	16	0.16
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD11	16	0.16
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD12	16	0.16
(2,217)	1:A:30:LEU:H	1:B:30:LEU:HD13	16	0.16
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD11	16	0.16
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD12	16	0.16
(2,217)	1:B:30:LEU:H	1:A:30:LEU:HD13	16	0.16
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD11	16	0.16
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD12	16	0.16
(2,217)	1:B:30:LEU:H	1:B:30:LEU:HD13	16	0.16
(2,162)	1:A:12:THR:HG21	1:A:13:GLY:H	14	0.16
(2,162)	1:A:12:THR:HG21	1:B:13:GLY:H	14	0.16
(2,162)	1:A:12:THR:HG22	1:A:13:GLY:H	14	0.16
(2,162)	1:A:12:THR:HG22	1:B:13:GLY:H	14	0.16
(2,162)	1:A:12:THR:HG23	1:A:13:GLY:H	14	0.16
(2,162)	1:A:12:THR:HG23	1:B:13:GLY:H	14	0.16
(2,162)	1:B:12:THR:HG21	1:A:13:GLY:H	14	0.16
(2,162)	1:B:12:THR:HG21	1:B:13:GLY:H	14	0.16
(2,162)	1:B:12:THR:HG22	1:A:13:GLY:H	14	0.16
(2,162)	1:B:12:THR:HG22	1:B:13:GLY:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:B:12:THR:HG23	1:A:13:GLY:H	14	0.16
(2,162)	1:B:12:THR:HG23	1:B:13:GLY:H	14	0.16
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	3	0.16
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	3	0.16
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG11	7	0.16
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG12	7	0.16
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG13	7	0.16
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG11	7	0.16
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG12	7	0.16
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG13	7	0.16
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG11	7	0.16
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG12	7	0.16
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG13	7	0.16
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG11	7	0.16
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG12	7	0.16
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG13	7	0.16
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG11	7	0.16
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG12	7	0.16
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG13	7	0.16
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG11	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG12	7	0.16
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG13	7	0.16
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG11	7	0.16
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG12	7	0.16
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG13	7	0.16
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG11	7	0.16
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG12	7	0.16
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG13	7	0.16
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	1	0.16
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	1	0.16
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	1	0.16
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	1	0.16
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	1	0.16
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	1	0.16
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	1	0.16
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	1	0.16
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	1	0.16
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	1	0.16
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	1	0.16
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	1	0.16
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	1	0.16
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	1	0.16
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	1	0.16
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	1	0.16
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	1	0.16
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	1	0.16
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	1	0.16
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	1	0.16
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	1	0.16
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	1	0.16
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	1	0.16
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	1	0.16
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	5	0.16
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	5	0.16
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	5	0.16
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	5	0.16
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	5	0.16
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	5	0.16
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	5	0.16
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	5	0.16
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	5	0.16
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	5	0.16
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	5	0.16
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	5	0.16
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	5	0.16
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	5	0.16
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	5	0.16
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	5	0.16
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	5	0.16
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	5	0.16
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	5	0.16
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	5	0.16
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	5	0.16
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	5	0.16
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	5	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD11	3	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD12	3	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD13	3	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD21	3	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD22	3	0.16
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD23	3	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD11	3	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD12	3	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD13	3	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD21	3	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD22	3	0.16
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD23	3	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD11	3	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD12	3	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD13	3	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD21	3	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD22	3	0.16
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD23	3	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD11	3	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD12	3	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD13	3	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD21	3	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD22	3	0.16
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD23	3	0.16
(2,1451)	1:A:32:ALA:HB1	1:A:38:GLY:HA2	7	0.16
(2,1451)	1:A:32:ALA:HB1	1:A:38:GLY:HA3	7	0.16
(2,1451)	1:A:32:ALA:HB1	1:B:38:GLY:HA2	7	0.16
(2,1451)	1:A:32:ALA:HB1	1:B:38:GLY:HA3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1451)	1:A:32:ALA:HB2	1:A:38:GLY:HA2	7	0.16
(2,1451)	1:A:32:ALA:HB2	1:A:38:GLY:HA3	7	0.16
(2,1451)	1:A:32:ALA:HB2	1:B:38:GLY:HA2	7	0.16
(2,1451)	1:A:32:ALA:HB2	1:B:38:GLY:HA3	7	0.16
(2,1451)	1:A:32:ALA:HB3	1:A:38:GLY:HA2	7	0.16
(2,1451)	1:A:32:ALA:HB3	1:A:38:GLY:HA3	7	0.16
(2,1451)	1:A:32:ALA:HB3	1:B:38:GLY:HA2	7	0.16
(2,1451)	1:A:32:ALA:HB3	1:B:38:GLY:HA3	7	0.16
(2,1451)	1:B:32:ALA:HB1	1:A:38:GLY:HA2	7	0.16
(2,1451)	1:B:32:ALA:HB1	1:A:38:GLY:HA3	7	0.16
(2,1451)	1:B:32:ALA:HB1	1:B:38:GLY:HA2	7	0.16
(2,1451)	1:B:32:ALA:HB1	1:B:38:GLY:HA3	7	0.16
(2,1451)	1:B:32:ALA:HB2	1:A:38:GLY:HA2	7	0.16
(2,1451)	1:B:32:ALA:HB2	1:A:38:GLY:HA3	7	0.16
(2,1451)	1:B:32:ALA:HB2	1:B:38:GLY:HA2	7	0.16
(2,1451)	1:B:32:ALA:HB2	1:B:38:GLY:HA3	7	0.16
(2,1451)	1:B:32:ALA:HB3	1:A:38:GLY:HA2	7	0.16
(2,1451)	1:B:32:ALA:HB3	1:A:38:GLY:HA3	7	0.16
(2,1451)	1:B:32:ALA:HB3	1:B:38:GLY:HA2	7	0.16
(2,1451)	1:B:32:ALA:HB3	1:B:38:GLY:HA3	7	0.16
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	17	0.16
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	17	0.16
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	17	0.16
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	17	0.16
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	17	0.16
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	17	0.16
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	17	0.16
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	17	0.16
(2,137)	1:A:3:ILE:HG21	1:A:6:LYS:HB2	10	0.16
(2,137)	1:A:3:ILE:HG21	1:B:6:LYS:HB2	10	0.16
(2,137)	1:A:3:ILE:HG22	1:A:6:LYS:HB2	10	0.16
(2,137)	1:A:3:ILE:HG22	1:B:6:LYS:HB2	10	0.16
(2,137)	1:A:3:ILE:HG23	1:A:6:LYS:HB2	10	0.16
(2,137)	1:A:3:ILE:HG23	1:B:6:LYS:HB2	10	0.16
(2,137)	1:B:3:ILE:HG21	1:A:6:LYS:HB2	10	0.16
(2,137)	1:B:3:ILE:HG21	1:B:6:LYS:HB2	10	0.16
(2,137)	1:B:3:ILE:HG22	1:A:6:LYS:HB2	10	0.16
(2,137)	1:B:3:ILE:HG22	1:B:6:LYS:HB2	10	0.16
(2,137)	1:B:3:ILE:HG23	1:A:6:LYS:HB2	10	0.16
(2,137)	1:B:3:ILE:HG23	1:B:6:LYS:HB2	10	0.16
(2,1245)	1:A:117:ARG:H	1:A:117:ARG:HG2	17	0.16
(2,1245)	1:A:117:ARG:H	1:B:117:ARG:HG2	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1245)	1:B:117:ARG:H	1:A:117:ARG:HG2	17	0.16
(2,1245)	1:B:117:ARG:H	1:B:117:ARG:HG2	17	0.16
(2,1208)	1:A:107:ASP:HB3	1:A:110:ALA:H	9	0.16
(2,1208)	1:A:107:ASP:HB3	1:B:110:ALA:H	9	0.16
(2,1208)	1:B:107:ASP:HB3	1:A:110:ALA:H	9	0.16
(2,1208)	1:B:107:ASP:HB3	1:B:110:ALA:H	9	0.16
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	5	0.16
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	5	0.16
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	5	0.16
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	5	0.16
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	5	0.16
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	5	0.16
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	5	0.16
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	5	0.16
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	5	0.16
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	5	0.16
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	5	0.16
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	5	0.16
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	5	0.16
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	5	0.16
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	5	0.16
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	5	0.16
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	5	0.16
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	5	0.16
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	5	0.16
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	5	0.16
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	5	0.16
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	5	0.16
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	5	0.16
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	5	0.16
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	5	0.16
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	5	0.16
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	5	0.16
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	5	0.16
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	5	0.16
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	5	0.16
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	5	0.16
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	5	0.16
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	5	0.16
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	5	0.16
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	5	0.16
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	19	0.16
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	19	0.16
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	19	0.16
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	19	0.16
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	19	0.16
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	19	0.16
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	19	0.16
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	19	0.16
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	19	0.16
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	19	0.16
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	19	0.16
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	19	0.16
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	19	0.16
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	19	0.16
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	19	0.16
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	19	0.16
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	19	0.16
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	19	0.16
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	19	0.16
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	19	0.16
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	19	0.16
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	19	0.16
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	19	0.16
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	19	0.16
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	19	0.16
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	19	0.16
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	19	0.16
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	19	0.16
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	19	0.16
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	19	0.16
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	19	0.16
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	19	0.16
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	19	0.16
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	19	0.16
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	19	0.16
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	19	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	11	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	11	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	11	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	11	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	11	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	11	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	11	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	11	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	11	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	11	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	11	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	12	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	12	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	12	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	12	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	12	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	12	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	12	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	12	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	12	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	12	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	12	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	12	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	15	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	15	0.16
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	15	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	15	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	15	0.16
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	15	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	15	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	15	0.16
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	15	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	15	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	15	0.16
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	15	0.16
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	9	0.16
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	9	0.16
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	9	0.16
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	9	0.16
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	15	0.16
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	15	0.16
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	15	0.16
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	15	0.16
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	9	0.16
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	9	0.16
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	9	0.16
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	11	0.16
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	11	0.16
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	11	0.16
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	11	0.16
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	12	0.16
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	12	0.16
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	12	0.16
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	12	0.16
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	14	0.16
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	14	0.16
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	14	0.16
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	14	0.16
(1,9)	1:A:10:THR:H	1:A:20:THR:O	11	0.16
(1,9)	1:A:10:THR:H	1:B:20:THR:O	11	0.16
(1,9)	1:B:10:THR:H	1:A:20:THR:O	11	0.16
(1,9)	1:B:10:THR:H	1:B:20:THR:O	11	0.16
(1,9)	1:A:10:THR:H	1:A:20:THR:O	14	0.16
(1,9)	1:A:10:THR:H	1:B:20:THR:O	14	0.16
(1,9)	1:B:10:THR:H	1:A:20:THR:O	14	0.16
(1,9)	1:B:10:THR:H	1:B:20:THR:O	14	0.16
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	6	0.16
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	6	0.16
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	6	0.16
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	6	0.16
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	12	0.16
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	12	0.16
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	12	0.16
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	12	0.16
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	13	0.16
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	13	0.16
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	13	0.16
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	13	0.16
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	16	0.16
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	16	0.16
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	16	0.16
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	16	0.16
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	6	0.16
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	6	0.16
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	6	0.16
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	6	0.16
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	12	0.16
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	12	0.16
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	12	0.16
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	5	0.16
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	5	0.16
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	5	0.16
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	5	0.16
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	18	0.16
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	18	0.16
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	18	0.16
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	18	0.16
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	5	0.16
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	5	0.16
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	5	0.16
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	5	0.16
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	4	0.16
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	4	0.16
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	4	0.16
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	4	0.16
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	6	0.16
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	6	0.16
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	6	0.16
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	6	0.16
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	4	0.16
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	4	0.16
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	4	0.16
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	4	0.16
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	13	0.16
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	13	0.16
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	13	0.16
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	13	0.16
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	17	0.16
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	17	0.16
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	17	0.16
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	17	0.16
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	16	0.16
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	16	0.16
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	16	0.16
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	16	0.16
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	20	0.16
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	20	0.16
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	20	0.16
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	6	0.16
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	6	0.16
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	6	0.16
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	6	0.16
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	9	0.16
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	9	0.16
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	9	0.16
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	9	0.16
(1,61)	1:A:82:GLU:H	1:A:98:GLU:O	19	0.16
(1,61)	1:A:82:GLU:H	1:B:98:GLU:O	19	0.16
(1,61)	1:B:82:GLU:H	1:A:98:GLU:O	19	0.16
(1,61)	1:B:82:GLU:H	1:B:98:GLU:O	19	0.16
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	6	0.16
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	6	0.16
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	6	0.16
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	6	0.16
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	15	0.16
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	15	0.16
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	15	0.16
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	15	0.16
(1,6)	1:A:17:GLY:O	1:A:30:LEU:N	9	0.16
(1,6)	1:A:17:GLY:O	1:B:30:LEU:N	9	0.16
(1,6)	1:B:17:GLY:O	1:A:30:LEU:N	9	0.16
(1,6)	1:B:17:GLY:O	1:B:30:LEU:N	9	0.16
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	8	0.16
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	8	0.16
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	8	0.16
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	8	0.16
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	9	0.16
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	9	0.16
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	9	0.16
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	9	0.16
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	11	0.16
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	11	0.16
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	11	0.16
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	11	0.16
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	13	0.16
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	13	0.16
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	13	0.16
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	13	0.16
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	2	0.16
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	2	0.16
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	2	0.16
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	6	0.16
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	6	0.16
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	6	0.16
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	6	0.16
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	9	0.16
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	9	0.16
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	9	0.16
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	9	0.16
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	19	0.16
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	19	0.16
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	19	0.16
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	19	0.16
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	17	0.16
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	17	0.16
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	17	0.16
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	17	0.16
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	19	0.16
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	19	0.16
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	19	0.16
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	19	0.16
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	8	0.16
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	8	0.16
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	8	0.16
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	8	0.16
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	4	0.16
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	4	0.16
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	4	0.16
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	4	0.16
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	6	0.16
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	6	0.16
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	6	0.16
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	6	0.16
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	16	0.16
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	16	0.16
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	16	0.16
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	16	0.16
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	14	0.16
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	14	0.16
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	14	0.16
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	2	0.16
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	2	0.16
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	2	0.16
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	2	0.16
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	13	0.16
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	13	0.16
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	13	0.16
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	13	0.16
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	1	0.16
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	1	0.16
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	1	0.16
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	1	0.16
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	10	0.16
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	10	0.16
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	10	0.16
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	10	0.16
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	4	0.16
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	4	0.16
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	4	0.16
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	4	0.16
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	8	0.16
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	8	0.16
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	8	0.16
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	8	0.16
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	8	0.16
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	8	0.16
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	8	0.16
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	8	0.16
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	16	0.16
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	16	0.16
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	16	0.16
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	16	0.16
(1,20)	1:A:31:SER:N	1:A:44:THR:O	2	0.16
(1,20)	1:A:31:SER:N	1:B:44:THR:O	2	0.16
(1,20)	1:B:31:SER:N	1:A:44:THR:O	2	0.16
(1,20)	1:B:31:SER:N	1:B:44:THR:O	2	0.16
(1,2)	1:A:10:THR:O	1:A:20:THR:N	2	0.16
(1,2)	1:A:10:THR:O	1:B:20:THR:N	2	0.16
(1,2)	1:B:10:THR:O	1:A:20:THR:N	2	0.16
(1,2)	1:B:10:THR:O	1:B:20:THR:N	2	0.16
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	4	0.16
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	4	0.16
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	4	0.16
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	7	0.16
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	7	0.16
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	7	0.16
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	7	0.16
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	9	0.16
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	9	0.16
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	9	0.16
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	9	0.16
(2,911)	1:A:39:ALA:H	1:A:40:GLY:H	8	0.15
(2,911)	1:A:39:ALA:H	1:B:40:GLY:H	8	0.15
(2,911)	1:B:39:ALA:H	1:A:40:GLY:H	8	0.15
(2,911)	1:B:39:ALA:H	1:B:40:GLY:H	8	0.15
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	8	0.15
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	8	0.15
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	8	0.15
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	8	0.15
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	8	0.15
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	8	0.15
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	8	0.15
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	8	0.15
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	8	0.15
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	8	0.15
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	8	0.15
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	8	0.15
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	9	0.15
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	9	0.15
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	9	0.15
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	9	0.15
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	9	0.15
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	9	0.15
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	9	0.15
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	9	0.15
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	9	0.15
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	9	0.15
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	9	0.15
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	9	0.15
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	1	0.15
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	1	0.15
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	1	0.15
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	1	0.15
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	1	0.15
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	1	0.15
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	1	0.15
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	1	0.15
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	1	0.15
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	1	0.15
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	1	0.15
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	5	0.15
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	5	0.15
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	5	0.15
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	5	0.15
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	5	0.15
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	5	0.15
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	5	0.15
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	5	0.15
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	5	0.15
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	5	0.15
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	5	0.15
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	5	0.15
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	3	0.15
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	3	0.15
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	3	0.15
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	3	0.15
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	19	0.15
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	19	0.15
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	19	0.15
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	19	0.15
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	2	0.15
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	2	0.15
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	2	0.15
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	2	0.15
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	2	0.15
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	2	0.15
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	2	0.15
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	2	0.15
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	5	0.15
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	5	0.15
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	5	0.15
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	5	0.15
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	5	0.15
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	5	0.15
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	5	0.15
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG11	13	0.15
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG12	13	0.15
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG13	13	0.15
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG11	13	0.15
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG12	13	0.15
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG13	13	0.15
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG11	13	0.15
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG12	13	0.15
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG13	13	0.15
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG11	13	0.15
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG12	13	0.15
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG13	13	0.15
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG11	13	0.15
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG12	13	0.15
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG13	13	0.15
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG11	13	0.15
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG12	13	0.15
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG13	13	0.15
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG11	13	0.15
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG12	13	0.15
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG13	13	0.15
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG11	13	0.15
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG12	13	0.15
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG13	13	0.15
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD11	18	0.15
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD12	18	0.15
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD13	18	0.15
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD21	18	0.15
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD22	18	0.15
(2,1518)	1:A:73:LEU:H	1:A:73:LEU:HD23	18	0.15
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD11	18	0.15
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD12	18	0.15
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD13	18	0.15
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD21	18	0.15
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD22	18	0.15
(2,1518)	1:A:73:LEU:H	1:B:73:LEU:HD23	18	0.15
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD11	18	0.15
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD12	18	0.15
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD13	18	0.15
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD21	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD22	18	0.15
(2,1518)	1:B:73:LEU:H	1:A:73:LEU:HD23	18	0.15
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD11	18	0.15
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD12	18	0.15
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD13	18	0.15
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD21	18	0.15
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD22	18	0.15
(2,1518)	1:B:73:LEU:H	1:B:73:LEU:HD23	18	0.15
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	15	0.15
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	15	0.15
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	15	0.15
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	15	0.15
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	15	0.15
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	15	0.15
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	15	0.15
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	15	0.15
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	15	0.15
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	15	0.15
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	15	0.15
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	15	0.15
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	15	0.15
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	15	0.15
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	15	0.15
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	15	0.15
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	15	0.15
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	15	0.15
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	15	0.15
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	15	0.15
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	15	0.15
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	15	0.15
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	15	0.15
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	15	0.15
(2,1208)	1:A:107:ASP:HB3	1:A:110:ALA:H	2	0.15
(2,1208)	1:A:107:ASP:HB3	1:B:110:ALA:H	2	0.15
(2,1208)	1:B:107:ASP:HB3	1:A:110:ALA:H	2	0.15
(2,1208)	1:B:107:ASP:HB3	1:B:110:ALA:H	2	0.15
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	1	0.15
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	1	0.15
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	1	0.15
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	1	0.15
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	10	0.15
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	10	0.15
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	10	0.15
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	15	0.15
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	15	0.15
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	15	0.15
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	15	0.15
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	19	0.15
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	19	0.15
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	19	0.15
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	19	0.15
(1,9)	1:A:10:THR:H	1:A:20:THR:O	18	0.15
(1,9)	1:A:10:THR:H	1:B:20:THR:O	18	0.15
(1,9)	1:B:10:THR:H	1:A:20:THR:O	18	0.15
(1,9)	1:B:10:THR:H	1:B:20:THR:O	18	0.15
(1,87)	1:A:117:ARG:O	1:A:121:VAL:H	20	0.15
(1,87)	1:A:117:ARG:O	1:B:121:VAL:H	20	0.15
(1,87)	1:B:117:ARG:O	1:A:121:VAL:H	20	0.15
(1,87)	1:B:117:ARG:O	1:B:121:VAL:H	20	0.15
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	6	0.15
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	6	0.15
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	6	0.15
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	6	0.15
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	7	0.15
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	7	0.15
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	7	0.15
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	7	0.15
(1,82)	1:A:113:THR:O	1:A:117:ARG:N	2	0.15
(1,82)	1:A:113:THR:O	1:B:117:ARG:N	2	0.15
(1,82)	1:B:113:THR:O	1:A:117:ARG:N	2	0.15
(1,82)	1:B:113:THR:O	1:B:117:ARG:N	2	0.15
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	15	0.15
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	15	0.15
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	15	0.15
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	15	0.15
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	4	0.15
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	4	0.15
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	4	0.15
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	4	0.15
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	9	0.15
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	9	0.15
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	9	0.15
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	13	0.15
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	13	0.15
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	13	0.15
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	13	0.15
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	7	0.15
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	7	0.15
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	7	0.15
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	7	0.15
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	12	0.15
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	12	0.15
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	12	0.15
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	12	0.15
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	18	0.15
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	18	0.15
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	18	0.15
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	18	0.15
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	14	0.15
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	14	0.15
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	14	0.15
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	14	0.15
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	2	0.15
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	2	0.15
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	2	0.15
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	2	0.15
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	8	0.15
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	8	0.15
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	8	0.15
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	8	0.15
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	10	0.15
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	10	0.15
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	10	0.15
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	10	0.15
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	12	0.15
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	12	0.15
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	12	0.15
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	12	0.15
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	14	0.15
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	14	0.15
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	14	0.15
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	14	0.15
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	20	0.15
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	20	0.15
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	20	0.15
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	3	0.15
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	3	0.15
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	3	0.15
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	3	0.15
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	9	0.15
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	9	0.15
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	9	0.15
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	9	0.15
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	14	0.15
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	14	0.15
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	14	0.15
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	14	0.15
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	16	0.15
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	16	0.15
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	16	0.15
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	16	0.15
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	18	0.15
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	18	0.15
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	18	0.15
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	18	0.15
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	20	0.15
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	20	0.15
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	20	0.15
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	20	0.15
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	3	0.15
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	3	0.15
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	3	0.15
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	3	0.15
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	7	0.15
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	7	0.15
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	7	0.15
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	7	0.15
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	8	0.15
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	8	0.15
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	8	0.15
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	8	0.15
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	11	0.15
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	11	0.15
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	11	0.15
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	1	0.15
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	1	0.15
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	1	0.15
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	1	0.15
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	13	0.15
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	13	0.15
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	13	0.15
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	13	0.15
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	14	0.15
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	14	0.15
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	14	0.15
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	14	0.15
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	5	0.15
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	5	0.15
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	5	0.15
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	5	0.15
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	11	0.15
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	11	0.15
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	11	0.15
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	11	0.15
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	4	0.15
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	4	0.15
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	4	0.15
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	4	0.15
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	1	0.15
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	1	0.15
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	1	0.15
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	1	0.15
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	12	0.15
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	12	0.15
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	12	0.15
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	12	0.15
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	18	0.15
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	18	0.15
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	18	0.15
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	18	0.15
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	20	0.15
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	20	0.15
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	20	0.15
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	20	0.15
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	5	0.15
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	5	0.15
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	5	0.15
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	1	0.15
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	1	0.15
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	1	0.15
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	1	0.15
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	6	0.15
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	6	0.15
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	6	0.15
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	6	0.15
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	17	0.15
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	17	0.15
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	17	0.15
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	17	0.15
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	8	0.15
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	8	0.15
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	8	0.15
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	8	0.15
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	6	0.15
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	6	0.15
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	6	0.15
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	6	0.15
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	9	0.15
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	9	0.15
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	9	0.15
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	9	0.15
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	20	0.15
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	20	0.15
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	20	0.15
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	20	0.15
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	2	0.15
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	2	0.15
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	2	0.15
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	2	0.15
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	3	0.15
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	3	0.15
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	3	0.15
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	3	0.15
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	11	0.15
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	11	0.15
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	11	0.15
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:A:60:SER:O	1:A:64:PHE:N	3	0.15
(1,42)	1:A:60:SER:O	1:B:64:PHE:N	3	0.15
(1,42)	1:B:60:SER:O	1:A:64:PHE:N	3	0.15
(1,42)	1:B:60:SER:O	1:B:64:PHE:N	3	0.15
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	17	0.15
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	17	0.15
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	17	0.15
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	17	0.15
(1,39)	1:A:58:PHE:O	1:A:62:MET:H	7	0.15
(1,39)	1:A:58:PHE:O	1:B:62:MET:H	7	0.15
(1,39)	1:B:58:PHE:O	1:A:62:MET:H	7	0.15
(1,39)	1:B:58:PHE:O	1:B:62:MET:H	7	0.15
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	7	0.15
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	7	0.15
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	7	0.15
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	7	0.15
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	20	0.15
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	20	0.15
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	20	0.15
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	20	0.15
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	3	0.15
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	3	0.15
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	3	0.15
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	3	0.15
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	8	0.15
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	8	0.15
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	8	0.15
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	8	0.15
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	17	0.15
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	17	0.15
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	17	0.15
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	17	0.15
(1,31)	1:A:51:ALA:O	1:A:55:SER:H	5	0.15
(1,31)	1:A:51:ALA:O	1:B:55:SER:H	5	0.15
(1,31)	1:B:51:ALA:O	1:A:55:SER:H	5	0.15
(1,31)	1:B:51:ALA:O	1:B:55:SER:H	5	0.15
(1,31)	1:A:51:ALA:O	1:A:55:SER:H	14	0.15
(1,31)	1:A:51:ALA:O	1:B:55:SER:H	14	0.15
(1,31)	1:B:51:ALA:O	1:A:55:SER:H	14	0.15
(1,31)	1:B:51:ALA:O	1:B:55:SER:H	14	0.15
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	14	0.15
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	14	0.15
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	14	0.15
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	1	0.15
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	1	0.15
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	1	0.15
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	1	0.15
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	3	0.15
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	3	0.15
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	3	0.15
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	3	0.15
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	12	0.15
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	12	0.15
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	12	0.15
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	12	0.15
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	18	0.15
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	18	0.15
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	18	0.15
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	18	0.15
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	11	0.15
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	11	0.15
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	11	0.15
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	11	0.15
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	15	0.15
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	15	0.15
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	15	0.15
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	15	0.15
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	19	0.15
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	19	0.15
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	19	0.15
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	19	0.15
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	14	0.15
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	14	0.15
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	14	0.15
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	14	0.15
(1,20)	1:A:31:SER:N	1:A:44:THR:O	3	0.15
(1,20)	1:A:31:SER:N	1:B:44:THR:O	3	0.15
(1,20)	1:B:31:SER:N	1:A:44:THR:O	3	0.15
(1,20)	1:B:31:SER:N	1:B:44:THR:O	3	0.15
(1,2)	1:A:10:THR:O	1:A:20:THR:N	17	0.15
(1,2)	1:A:10:THR:O	1:B:20:THR:N	17	0.15
(1,2)	1:B:10:THR:O	1:A:20:THR:N	17	0.15
(1,2)	1:B:10:THR:O	1:B:20:THR:N	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:A:10:THR:O	1:A:20:THR:N	18	0.15
(1,2)	1:A:10:THR:O	1:B:20:THR:N	18	0.15
(1,2)	1:B:10:THR:O	1:A:20:THR:N	18	0.15
(1,2)	1:B:10:THR:O	1:B:20:THR:N	18	0.15
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	1	0.15
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	1	0.15
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	1	0.15
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	1	0.15
(1,1)	1:A:10:THR:O	1:A:20:THR:H	6	0.15
(1,1)	1:A:10:THR:O	1:B:20:THR:H	6	0.15
(1,1)	1:B:10:THR:O	1:A:20:THR:H	6	0.15
(1,1)	1:B:10:THR:O	1:B:20:THR:H	6	0.15
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	7	0.14
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	7	0.14
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	7	0.14
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	7	0.14
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	20	0.14
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	20	0.14
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	20	0.14
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	20	0.14
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	10	0.14
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	10	0.14
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	10	0.14
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	10	0.14
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	10	0.14
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	10	0.14
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	10	0.14
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	10	0.14
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	10	0.14
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	10	0.14
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	10	0.14
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	10	0.14
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	14	0.14
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	14	0.14
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	14	0.14
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	14	0.14
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	14	0.14
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	14	0.14
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	14	0.14
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	14	0.14
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	14	0.14
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	14	0.14
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	14	0.14
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	8	0.14
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	8	0.14
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	8	0.14
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	8	0.14
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	12	0.14
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	12	0.14
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	12	0.14
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	12	0.14
(2,288)	1:A:66:ALA:HB1	1:A:71:GLN:HE21	16	0.14
(2,288)	1:A:66:ALA:HB1	1:B:71:GLN:HE21	16	0.14
(2,288)	1:A:66:ALA:HB2	1:A:71:GLN:HE21	16	0.14
(2,288)	1:A:66:ALA:HB2	1:B:71:GLN:HE21	16	0.14
(2,288)	1:A:66:ALA:HB3	1:A:71:GLN:HE21	16	0.14
(2,288)	1:A:66:ALA:HB3	1:B:71:GLN:HE21	16	0.14
(2,288)	1:B:66:ALA:HB1	1:A:71:GLN:HE21	16	0.14
(2,288)	1:B:66:ALA:HB1	1:B:71:GLN:HE21	16	0.14
(2,288)	1:B:66:ALA:HB2	1:A:71:GLN:HE21	16	0.14
(2,288)	1:B:66:ALA:HB2	1:B:71:GLN:HE21	16	0.14
(2,288)	1:B:66:ALA:HB3	1:A:71:GLN:HE21	16	0.14
(2,288)	1:B:66:ALA:HB3	1:B:71:GLN:HE21	16	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	4	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	4	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	4	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	4	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	4	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	4	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	4	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	4	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	4	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	4	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	4	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	4	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	4	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	4	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	4	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	4	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	4	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	4	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	4	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	4	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	4	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	4	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	4	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	4	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	4	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	4	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	4	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	4	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	4	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	4	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	4	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	4	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	4	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	4	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	4	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	15	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	15	0.14
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	15	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	15	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	15	0.14
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	15	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	15	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	15	0.14
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	15	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	15	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	15	0.14
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	15	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	15	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	15	0.14
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	15	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	15	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	15	0.14
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	15	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	15	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	15	0.14
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	15	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	15	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	15	0.14
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	15	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	15	0.14
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	15	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	15	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	15	0.14
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	15	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	15	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	15	0.14
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	15	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	15	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	15	0.14
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	15	0.14
(2,257)	1:A:42:GLU:H	1:A:42:GLU:HG2	11	0.14
(2,257)	1:A:42:GLU:H	1:B:42:GLU:HG2	11	0.14
(2,257)	1:B:42:GLU:H	1:A:42:GLU:HG2	11	0.14
(2,257)	1:B:42:GLU:H	1:B:42:GLU:HG2	11	0.14
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	16	0.14
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	16	0.14
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	16	0.14
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	16	0.14
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	16	0.14
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	16	0.14
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	16	0.14
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	16	0.14
(2,162)	1:A:12:THR:HG21	1:A:13:GLY:H	6	0.14
(2,162)	1:A:12:THR:HG21	1:B:13:GLY:H	6	0.14
(2,162)	1:A:12:THR:HG22	1:A:13:GLY:H	6	0.14
(2,162)	1:A:12:THR:HG22	1:B:13:GLY:H	6	0.14
(2,162)	1:A:12:THR:HG23	1:A:13:GLY:H	6	0.14
(2,162)	1:A:12:THR:HG23	1:B:13:GLY:H	6	0.14
(2,162)	1:B:12:THR:HG21	1:A:13:GLY:H	6	0.14
(2,162)	1:B:12:THR:HG21	1:B:13:GLY:H	6	0.14
(2,162)	1:B:12:THR:HG22	1:A:13:GLY:H	6	0.14
(2,162)	1:B:12:THR:HG22	1:B:13:GLY:H	6	0.14
(2,162)	1:B:12:THR:HG23	1:A:13:GLY:H	6	0.14
(2,162)	1:B:12:THR:HG23	1:B:13:GLY:H	6	0.14
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG2	9	0.14
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG3	9	0.14
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG2	9	0.14
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG3	9	0.14
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG2	9	0.14
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG3	9	0.14
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG2	9	0.14
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	7	0.14
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	7	0.14
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	7	0.14
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	7	0.14
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	7	0.14
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	7	0.14
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	7	0.14
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	7	0.14
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	7	0.14
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	7	0.14
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	7	0.14
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	7	0.14
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	7	0.14
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	7	0.14
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	7	0.14
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	7	0.14
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	7	0.14
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	7	0.14
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	7	0.14
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	7	0.14
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	7	0.14
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	7	0.14
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	7	0.14
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	7	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	6	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	6	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	6	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	6	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	6	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	6	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	6	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	6	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	6	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	6	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	6	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	6	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	6	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	6	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	6	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	6	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	6	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	6	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	6	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	6	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	6	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	6	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	6	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	20	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	20	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	20	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	20	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	20	0.14
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	20	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	20	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	20	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	20	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	20	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	20	0.14
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	20	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	20	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	20	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	20	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	20	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	20	0.14
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	20	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	20	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	20	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	20	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	20	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	20	0.14
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	20	0.14
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA2	9	0.14
(2,1492)	1:A:49:LEU:HD11	1:A:53:GLY:HA3	9	0.14
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA2	9	0.14
(2,1492)	1:A:49:LEU:HD11	1:B:53:GLY:HA3	9	0.14
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA2	9	0.14
(2,1492)	1:A:49:LEU:HD12	1:A:53:GLY:HA3	9	0.14
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA2	9	0.14
(2,1492)	1:A:49:LEU:HD12	1:B:53:GLY:HA3	9	0.14
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA2	9	0.14
(2,1492)	1:A:49:LEU:HD13	1:A:53:GLY:HA3	9	0.14
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA2	9	0.14
(2,1492)	1:A:49:LEU:HD13	1:B:53:GLY:HA3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA2	9	0.14
(2,1492)	1:B:49:LEU:HD11	1:A:53:GLY:HA3	9	0.14
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA2	9	0.14
(2,1492)	1:B:49:LEU:HD11	1:B:53:GLY:HA3	9	0.14
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA2	9	0.14
(2,1492)	1:B:49:LEU:HD12	1:A:53:GLY:HA3	9	0.14
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA2	9	0.14
(2,1492)	1:B:49:LEU:HD12	1:B:53:GLY:HA3	9	0.14
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA2	9	0.14
(2,1492)	1:B:49:LEU:HD13	1:A:53:GLY:HA3	9	0.14
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA2	9	0.14
(2,1492)	1:B:49:LEU:HD13	1:B:53:GLY:HA3	9	0.14
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE2	2	0.14
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE3	2	0.14
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE2	2	0.14
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE3	2	0.14
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE2	2	0.14
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE3	2	0.14
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE2	2	0.14
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE3	2	0.14
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE2	2	0.14
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE3	2	0.14
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE2	2	0.14
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE3	2	0.14
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE2	2	0.14
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE3	2	0.14
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE2	2	0.14
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE3	2	0.14
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	18	0.14
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	18	0.14
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	18	0.14
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	18	0.14
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	18	0.14
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	18	0.14
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	18	0.14
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	18	0.14
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	3	0.14
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	3	0.14
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	3	0.14
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	3	0.14
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	3	0.14
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	3	0.14
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	3	0.14
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	3	0.14
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	3	0.14
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	3	0.14
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	3	0.14
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	3	0.14
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	3	0.14
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	3	0.14
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	3	0.14
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	3	0.14
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	3	0.14
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	3	0.14
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	3	0.14
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	3	0.14
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	3	0.14
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	3	0.14
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	3	0.14
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	3	0.14
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	3	0.14
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	3	0.14
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	3	0.14
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	3	0.14
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	3	0.14
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	3	0.14
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	3	0.14
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	3	0.14
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	3	0.14
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	3	0.14
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	3	0.14
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	4	0.14
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	4	0.14
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	4	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	4	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	4	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	4	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	4	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	4	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	4	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	4	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	4	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	14	0.14
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	14	0.14
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	14	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	14	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	14	0.14
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	14	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	14	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	14	0.14
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	14	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	14	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	14	0.14
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	14	0.14
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	6	0.14
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	6	0.14
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	6	0.14
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	6	0.14
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	12	0.14
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	12	0.14
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	12	0.14
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	12	0.14
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	10	0.14
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	10	0.14
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	10	0.14
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	10	0.14
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	11	0.14
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	11	0.14
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	11	0.14
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	11	0.14
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	13	0.14
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	13	0.14
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	13	0.14
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	13	0.14
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	18	0.14
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	18	0.14
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	18	0.14
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	18	0.14
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	19	0.14
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	19	0.14
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	19	0.14
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	19	0.14
(1,93)	1:A:101:VAL:H	1:A:137:VAL:O	5	0.14
(1,93)	1:A:101:VAL:H	1:B:137:VAL:O	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:B:101:VAL:H	1:A:137:VAL:O	5	0.14
(1,93)	1:B:101:VAL:H	1:B:137:VAL:O	5	0.14
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	8	0.14
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	8	0.14
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	8	0.14
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	8	0.14
(1,9)	1:A:10:THR:H	1:A:20:THR:O	9	0.14
(1,9)	1:A:10:THR:H	1:B:20:THR:O	9	0.14
(1,9)	1:B:10:THR:H	1:A:20:THR:O	9	0.14
(1,9)	1:B:10:THR:H	1:B:20:THR:O	9	0.14
(1,9)	1:A:10:THR:H	1:A:20:THR:O	15	0.14
(1,9)	1:A:10:THR:H	1:B:20:THR:O	15	0.14
(1,9)	1:B:10:THR:H	1:A:20:THR:O	15	0.14
(1,9)	1:B:10:THR:H	1:B:20:THR:O	15	0.14
(1,87)	1:A:117:ARG:O	1:A:121:VAL:H	16	0.14
(1,87)	1:A:117:ARG:O	1:B:121:VAL:H	16	0.14
(1,87)	1:B:117:ARG:O	1:A:121:VAL:H	16	0.14
(1,87)	1:B:117:ARG:O	1:B:121:VAL:H	16	0.14
(1,84)	1:A:114:LEU:O	1:A:118:ALA:N	13	0.14
(1,84)	1:A:114:LEU:O	1:B:118:ALA:N	13	0.14
(1,84)	1:B:114:LEU:O	1:A:118:ALA:N	13	0.14
(1,84)	1:B:114:LEU:O	1:B:118:ALA:N	13	0.14
(1,82)	1:A:113:THR:O	1:A:117:ARG:N	12	0.14
(1,82)	1:A:113:THR:O	1:B:117:ARG:N	12	0.14
(1,82)	1:B:113:THR:O	1:A:117:ARG:N	12	0.14
(1,82)	1:B:113:THR:O	1:B:117:ARG:N	12	0.14
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	2	0.14
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	2	0.14
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	2	0.14
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	2	0.14
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	7	0.14
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	7	0.14
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	7	0.14
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	7	0.14
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	19	0.14
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	19	0.14
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	19	0.14
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	19	0.14
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	12	0.14
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	12	0.14
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	12	0.14
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	14	0.14
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	14	0.14
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	14	0.14
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	14	0.14
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	2	0.14
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	2	0.14
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	2	0.14
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	2	0.14
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	9	0.14
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	9	0.14
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	9	0.14
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	9	0.14
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	14	0.14
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	14	0.14
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	14	0.14
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	14	0.14
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	17	0.14
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	17	0.14
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	17	0.14
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	17	0.14
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	20	0.14
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	20	0.14
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	20	0.14
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	20	0.14
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	7	0.14
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	7	0.14
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	7	0.14
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	7	0.14
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	9	0.14
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	9	0.14
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	9	0.14
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	9	0.14
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	2	0.14
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	2	0.14
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	2	0.14
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	2	0.14
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	13	0.14
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	13	0.14
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	13	0.14
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	13	0.14
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	15	0.14
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	15	0.14
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	15	0.14
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	19	0.14
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	19	0.14
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	19	0.14
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	19	0.14
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	20	0.14
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	20	0.14
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	20	0.14
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	20	0.14
(1,70)	1:A:82:GLU:O	1:A:98:GLU:N	5	0.14
(1,70)	1:A:82:GLU:O	1:B:98:GLU:N	5	0.14
(1,70)	1:B:82:GLU:O	1:A:98:GLU:N	5	0.14
(1,70)	1:B:82:GLU:O	1:B:98:GLU:N	5	0.14
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	2	0.14
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	2	0.14
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	2	0.14
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	2	0.14
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	17	0.14
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	17	0.14
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	17	0.14
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	17	0.14
(1,65)	1:A:101:VAL:O	1:A:139:ALA:H	17	0.14
(1,65)	1:A:101:VAL:O	1:B:139:ALA:H	17	0.14
(1,65)	1:B:101:VAL:O	1:A:139:ALA:H	17	0.14
(1,65)	1:B:101:VAL:O	1:B:139:ALA:H	17	0.14
(1,64)	1:A:99:LEU:O	1:A:137:VAL:N	12	0.14
(1,64)	1:A:99:LEU:O	1:B:137:VAL:N	12	0.14
(1,64)	1:B:99:LEU:O	1:A:137:VAL:N	12	0.14
(1,64)	1:B:99:LEU:O	1:B:137:VAL:N	12	0.14
(1,64)	1:A:99:LEU:O	1:A:137:VAL:N	19	0.14
(1,64)	1:A:99:LEU:O	1:B:137:VAL:N	19	0.14
(1,64)	1:B:99:LEU:O	1:A:137:VAL:N	19	0.14
(1,64)	1:B:99:LEU:O	1:B:137:VAL:N	19	0.14
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	17	0.14
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	17	0.14
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	17	0.14
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	17	0.14
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	18	0.14
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	18	0.14
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	18	0.14
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	2	0.14
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	2	0.14
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	2	0.14
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	2	0.14
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	7	0.14
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	7	0.14
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	7	0.14
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	7	0.14
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	10	0.14
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	10	0.14
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	10	0.14
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	10	0.14
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	12	0.14
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	12	0.14
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	12	0.14
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	12	0.14
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	13	0.14
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	13	0.14
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	13	0.14
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	13	0.14
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	17	0.14
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	17	0.14
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	17	0.14
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	17	0.14
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	2	0.14
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	2	0.14
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	2	0.14
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	2	0.14
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	10	0.14
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	10	0.14
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	10	0.14
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	10	0.14
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	4	0.14
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	4	0.14
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	4	0.14
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	4	0.14
(1,52)	1:A:88:ASN:N	1:A:92:GLY:O	16	0.14
(1,52)	1:A:88:ASN:N	1:B:92:GLY:O	16	0.14
(1,52)	1:B:88:ASN:N	1:A:92:GLY:O	16	0.14
(1,52)	1:B:88:ASN:N	1:B:92:GLY:O	16	0.14
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	7	0.14
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	7	0.14
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	7	0.14
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	8	0.14
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	8	0.14
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	8	0.14
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	8	0.14
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	14	0.14
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	14	0.14
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	14	0.14
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	14	0.14
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	15	0.14
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	15	0.14
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	15	0.14
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	15	0.14
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	4	0.14
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	4	0.14
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	4	0.14
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	4	0.14
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	10	0.14
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	10	0.14
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	10	0.14
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	10	0.14
(1,46)	1:A:62:MET:O	1:A:66:ALA:N	14	0.14
(1,46)	1:A:62:MET:O	1:B:66:ALA:N	14	0.14
(1,46)	1:B:62:MET:O	1:A:66:ALA:N	14	0.14
(1,46)	1:B:62:MET:O	1:B:66:ALA:N	14	0.14
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	15	0.14
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	15	0.14
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	15	0.14
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	15	0.14
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	18	0.14
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	18	0.14
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	18	0.14
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	18	0.14
(1,43)	1:A:61:ALA:O	1:A:65:VAL:H	5	0.14
(1,43)	1:A:61:ALA:O	1:B:65:VAL:H	5	0.14
(1,43)	1:B:61:ALA:O	1:A:65:VAL:H	5	0.14
(1,43)	1:B:61:ALA:O	1:B:65:VAL:H	5	0.14
(1,42)	1:A:60:SER:O	1:A:64:PHE:N	15	0.14
(1,42)	1:A:60:SER:O	1:B:64:PHE:N	15	0.14
(1,42)	1:B:60:SER:O	1:A:64:PHE:N	15	0.14
(1,42)	1:B:60:SER:O	1:B:64:PHE:N	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	2	0.14
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	2	0.14
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	2	0.14
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	2	0.14
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	9	0.14
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	9	0.14
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	9	0.14
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	9	0.14
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	15	0.14
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	15	0.14
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	15	0.14
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	15	0.14
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	20	0.14
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	20	0.14
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	20	0.14
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	20	0.14
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	3	0.14
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	3	0.14
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	3	0.14
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	3	0.14
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	8	0.14
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	8	0.14
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	8	0.14
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	8	0.14
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	11	0.14
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	11	0.14
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	11	0.14
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	11	0.14
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	14	0.14
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	14	0.14
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	14	0.14
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	14	0.14
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	17	0.14
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	17	0.14
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	17	0.14
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	17	0.14
(1,34)	1:A:52:ALA:O	1:A:56:ALA:N	19	0.14
(1,34)	1:A:52:ALA:O	1:B:56:ALA:N	19	0.14
(1,34)	1:B:52:ALA:O	1:A:56:ALA:N	19	0.14
(1,34)	1:B:52:ALA:O	1:B:56:ALA:N	19	0.14
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	7	0.14
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	7	0.14
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	7	0.14
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	13	0.14
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	13	0.14
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	13	0.14
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	13	0.14
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	18	0.14
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	18	0.14
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	18	0.14
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	18	0.14
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	20	0.14
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	20	0.14
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	20	0.14
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	20	0.14
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	12	0.14
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	12	0.14
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	12	0.14
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	12	0.14
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	6	0.14
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	6	0.14
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	6	0.14
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	6	0.14
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	13	0.14
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	13	0.14
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	13	0.14
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	13	0.14
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	17	0.14
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	17	0.14
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	17	0.14
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	17	0.14
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	13	0.14
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	13	0.14
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	13	0.14
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	13	0.14
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	18	0.14
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	18	0.14
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	18	0.14
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	18	0.14
(1,20)	1:A:31:SER:N	1:A:44:THR:O	8	0.14
(1,20)	1:A:31:SER:N	1:B:44:THR:O	8	0.14
(1,20)	1:B:31:SER:N	1:A:44:THR:O	8	0.14
(1,20)	1:B:31:SER:N	1:B:44:THR:O	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:A:31:SER:N	1:A:44:THR:O	11	0.14
(1,20)	1:A:31:SER:N	1:B:44:THR:O	11	0.14
(1,20)	1:B:31:SER:N	1:A:44:THR:O	11	0.14
(1,20)	1:B:31:SER:N	1:B:44:THR:O	11	0.14
(1,20)	1:A:31:SER:N	1:A:44:THR:O	17	0.14
(1,20)	1:A:31:SER:N	1:B:44:THR:O	17	0.14
(1,20)	1:B:31:SER:N	1:A:44:THR:O	17	0.14
(1,20)	1:B:31:SER:N	1:B:44:THR:O	17	0.14
(1,18)	1:A:17:GLY:N	1:A:30:LEU:O	14	0.14
(1,18)	1:A:17:GLY:N	1:B:30:LEU:O	14	0.14
(1,18)	1:B:17:GLY:N	1:A:30:LEU:O	14	0.14
(1,18)	1:B:17:GLY:N	1:B:30:LEU:O	14	0.14
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	13	0.13
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	13	0.13
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	13	0.13
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	13	0.13
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	14	0.13
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	14	0.13
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	14	0.13
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	14	0.13
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	4	0.13
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	4	0.13
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	4	0.13
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	4	0.13
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	4	0.13
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	4	0.13
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	4	0.13
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	4	0.13
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	4	0.13
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	4	0.13
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	4	0.13
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	4	0.13
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	15	0.13
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	15	0.13
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	15	0.13
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	15	0.13
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	15	0.13
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	15	0.13
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	15	0.13
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	15	0.13
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	15	0.13
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	15	0.13
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	15	0.13
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB1	17	0.13
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB2	17	0.13
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB3	17	0.13
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB1	17	0.13
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB2	17	0.13
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB3	17	0.13
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB1	17	0.13
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB2	17	0.13
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB3	17	0.13
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB1	17	0.13
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB2	17	0.13
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB3	17	0.13
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB1	19	0.13
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB2	19	0.13
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB3	19	0.13
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB1	19	0.13
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB2	19	0.13
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB3	19	0.13
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB1	19	0.13
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB2	19	0.13
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB3	19	0.13
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB1	19	0.13
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB2	19	0.13
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB3	19	0.13
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	11	0.13
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	11	0.13
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	11	0.13
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	11	0.13
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	11	0.13
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	11	0.13
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	11	0.13
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	11	0.13
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	11	0.13
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	11	0.13
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	11	0.13
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	11	0.13
(2,53)	1:A:77:THR:HA	1:A:104:PRO:HD3	6	0.13
(2,53)	1:A:77:THR:HA	1:B:104:PRO:HD3	6	0.13
(2,53)	1:B:77:THR:HA	1:A:104:PRO:HD3	6	0.13
(2,53)	1:B:77:THR:HA	1:B:104:PRO:HD3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:A:77:THR:HA	1:A:104:PRO:HD3	11	0.13
(2,53)	1:A:77:THR:HA	1:B:104:PRO:HD3	11	0.13
(2,53)	1:B:77:THR:HA	1:A:104:PRO:HD3	11	0.13
(2,53)	1:B:77:THR:HA	1:B:104:PRO:HD3	11	0.13
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB1	8	0.13
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB2	8	0.13
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB3	8	0.13
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB1	8	0.13
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB2	8	0.13
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB3	8	0.13
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB1	8	0.13
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB2	8	0.13
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB3	8	0.13
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB1	8	0.13
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB2	8	0.13
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB3	8	0.13
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB1	8	0.13
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB2	8	0.13
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB3	8	0.13
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB1	8	0.13
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB2	8	0.13
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB3	8	0.13
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB1	8	0.13
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB2	8	0.13
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB3	8	0.13
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB1	8	0.13
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB2	8	0.13
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB3	8	0.13
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB1	8	0.13
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB2	8	0.13
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB3	8	0.13
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB1	8	0.13
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB2	8	0.13
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB3	8	0.13
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB1	8	0.13
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB2	8	0.13
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB3	8	0.13
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB1	8	0.13
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB2	8	0.13
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB3	8	0.13
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	7	0.13
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	7	0.13
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	7	0.13
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	7	0.13
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	7	0.13
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	7	0.13
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	7	0.13
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	7	0.13
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	7	0.13
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	7	0.13
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	7	0.13
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	5	0.13
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	5	0.13
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	5	0.13
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	5	0.13
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	7	0.13
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	7	0.13
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	7	0.13
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	7	0.13
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	6	0.13
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	6	0.13
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	6	0.13
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	6	0.13
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	6	0.13
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	6	0.13
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	6	0.13
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	6	0.13
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	6	0.13
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	6	0.13
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	6	0.13
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	6	0.13
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	6	0.13
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	6	0.13
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	6	0.13
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	6	0.13
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	6	0.13
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	6	0.13
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	6	0.13
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	6	0.13
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	6	0.13
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	6	0.13
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	6	0.13
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	6	0.13
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	6	0.13
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	6	0.13
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	6	0.13
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	6	0.13
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	6	0.13
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	6	0.13
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	6	0.13
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	6	0.13
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	6	0.13
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	6	0.13
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	6	0.13
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	17	0.13
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	17	0.13
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	17	0.13
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	17	0.13
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	17	0.13
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	17	0.13
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	17	0.13
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	17	0.13
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	17	0.13
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	17	0.13
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	17	0.13
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	17	0.13
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	17	0.13
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	17	0.13
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	17	0.13
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	17	0.13
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	17	0.13
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	17	0.13
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	17	0.13
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	17	0.13
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	17	0.13
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	17	0.13
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	17	0.13
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	17	0.13
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	17	0.13
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	17	0.13
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	17	0.13
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	17	0.13
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	17	0.13
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	17	0.13
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	17	0.13
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	17	0.13
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	17	0.13
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	17	0.13
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	17	0.13
(2,257)	1:A:42:GLU:H	1:A:42:GLU:HG2	8	0.13
(2,257)	1:A:42:GLU:H	1:B:42:GLU:HG2	8	0.13
(2,257)	1:B:42:GLU:H	1:A:42:GLU:HG2	8	0.13
(2,257)	1:B:42:GLU:H	1:B:42:GLU:HG2	8	0.13
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	9	0.13
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	9	0.13
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	9	0.13
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	9	0.13
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	9	0.13
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	9	0.13
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	9	0.13
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	9	0.13
(2,162)	1:A:12:THR:HG21	1:A:13:GLY:H	16	0.13
(2,162)	1:A:12:THR:HG21	1:B:13:GLY:H	16	0.13
(2,162)	1:A:12:THR:HG22	1:A:13:GLY:H	16	0.13
(2,162)	1:A:12:THR:HG22	1:B:13:GLY:H	16	0.13
(2,162)	1:A:12:THR:HG23	1:A:13:GLY:H	16	0.13
(2,162)	1:A:12:THR:HG23	1:B:13:GLY:H	16	0.13
(2,162)	1:B:12:THR:HG21	1:A:13:GLY:H	16	0.13
(2,162)	1:B:12:THR:HG21	1:B:13:GLY:H	16	0.13
(2,162)	1:B:12:THR:HG22	1:A:13:GLY:H	16	0.13
(2,162)	1:B:12:THR:HG22	1:B:13:GLY:H	16	0.13
(2,162)	1:B:12:THR:HG23	1:A:13:GLY:H	16	0.13
(2,162)	1:B:12:THR:HG23	1:B:13:GLY:H	16	0.13
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	6	0.13
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	6	0.13
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG21	2	0.13
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG22	2	0.13
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG23	2	0.13
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG21	2	0.13
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG22	2	0.13
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG23	2	0.13
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG21	2	0.13
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG22	2	0.13
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG23	2	0.13
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG21	2	0.13
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG22	2	0.13
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG23	2	0.13
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG21	2	0.13
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG22	2	0.13
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG23	2	0.13
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG21	2	0.13
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG22	2	0.13
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG23	2	0.13
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG21	2	0.13
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG22	2	0.13
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG23	2	0.13
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG21	2	0.13
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG22	2	0.13
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG23	2	0.13
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	9	0.13
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	9	0.13
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	9	0.13
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	9	0.13
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	9	0.13
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	9	0.13
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	9	0.13
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	9	0.13
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	9	0.13
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	9	0.13
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	9	0.13
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	9	0.13
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	9	0.13
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	9	0.13
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	9	0.13
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	9	0.13
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	9	0.13
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	9	0.13
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	9	0.13
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	9	0.13
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	9	0.13
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	9	0.13
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	9	0.13
(2,1531)	1:A:80:THR:HB	1:A:100:ARG:HB2	13	0.13
(2,1531)	1:A:80:THR:HB	1:A:100:ARG:HB3	13	0.13
(2,1531)	1:A:80:THR:HB	1:B:100:ARG:HB2	13	0.13
(2,1531)	1:A:80:THR:HB	1:B:100:ARG:HB3	13	0.13
(2,1531)	1:B:80:THR:HB	1:A:100:ARG:HB2	13	0.13
(2,1531)	1:B:80:THR:HB	1:A:100:ARG:HB3	13	0.13
(2,1531)	1:B:80:THR:HB	1:B:100:ARG:HB2	13	0.13
(2,1531)	1:B:80:THR:HB	1:B:100:ARG:HB3	13	0.13
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	9	0.13
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	9	0.13
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	9	0.13
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	9	0.13
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	9	0.13
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	9	0.13
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	9	0.13
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	9	0.13
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	9	0.13
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	9	0.13
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	9	0.13
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	9	0.13
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	9	0.13
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	9	0.13
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	9	0.13
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	9	0.13
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	9	0.13
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	9	0.13
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	9	0.13
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	9	0.13
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	9	0.13
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	9	0.13
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	9	0.13
(2,1471)	1:A:35:GLU:HB2	1:A:36:LEU:HD11	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:A:36:LEU:HD12	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:A:36:LEU:HD13	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:A:36:LEU:HD21	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:A:36:LEU:HD22	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:A:36:LEU:HD23	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:B:36:LEU:HD11	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:B:36:LEU:HD12	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:B:36:LEU:HD13	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:B:36:LEU:HD21	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:B:36:LEU:HD22	13	0.13
(2,1471)	1:A:35:GLU:HB2	1:B:36:LEU:HD23	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:A:36:LEU:HD11	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:A:36:LEU:HD12	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:A:36:LEU:HD13	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:A:36:LEU:HD21	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:A:36:LEU:HD22	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:A:36:LEU:HD23	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:B:36:LEU:HD11	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:B:36:LEU:HD12	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:B:36:LEU:HD13	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:B:36:LEU:HD21	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:B:36:LEU:HD22	13	0.13
(2,1471)	1:A:35:GLU:HB3	1:B:36:LEU:HD23	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:A:36:LEU:HD11	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:A:36:LEU:HD12	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:A:36:LEU:HD13	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:A:36:LEU:HD21	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:A:36:LEU:HD22	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:A:36:LEU:HD23	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:B:36:LEU:HD11	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:B:36:LEU:HD12	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:B:36:LEU:HD13	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:B:36:LEU:HD21	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1471)	1:B:35:GLU:HB2	1:B:36:LEU:HD22	13	0.13
(2,1471)	1:B:35:GLU:HB2	1:B:36:LEU:HD23	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:A:36:LEU:HD11	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:A:36:LEU:HD12	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:A:36:LEU:HD13	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:A:36:LEU:HD21	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:A:36:LEU:HD22	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:A:36:LEU:HD23	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:B:36:LEU:HD11	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:B:36:LEU:HD12	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:B:36:LEU:HD13	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:B:36:LEU:HD21	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:B:36:LEU:HD22	13	0.13
(2,1471)	1:B:35:GLU:HB3	1:B:36:LEU:HD23	13	0.13
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE2	3	0.13
(2,1422)	1:A:23:ASP:HB2	1:A:25:LYS:HE3	3	0.13
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE2	3	0.13
(2,1422)	1:A:23:ASP:HB2	1:B:25:LYS:HE3	3	0.13
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE2	3	0.13
(2,1422)	1:A:23:ASP:HB3	1:A:25:LYS:HE3	3	0.13
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE2	3	0.13
(2,1422)	1:A:23:ASP:HB3	1:B:25:LYS:HE3	3	0.13
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE2	3	0.13
(2,1422)	1:B:23:ASP:HB2	1:A:25:LYS:HE3	3	0.13
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE2	3	0.13
(2,1422)	1:B:23:ASP:HB2	1:B:25:LYS:HE3	3	0.13
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE2	3	0.13
(2,1422)	1:B:23:ASP:HB3	1:A:25:LYS:HE3	3	0.13
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE2	3	0.13
(2,1422)	1:B:23:ASP:HB3	1:B:25:LYS:HE3	3	0.13
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD21	8	0.13
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD22	8	0.13
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD23	8	0.13
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD21	8	0.13
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD22	8	0.13
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD23	8	0.13
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD21	8	0.13
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD22	8	0.13
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD23	8	0.13
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD21	8	0.13
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD22	8	0.13
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD23	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD21	8	0.13
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD22	8	0.13
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD23	8	0.13
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD21	8	0.13
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD22	8	0.13
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD23	8	0.13
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD21	8	0.13
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD22	8	0.13
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD23	8	0.13
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD21	8	0.13
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD22	8	0.13
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD23	8	0.13
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD21	9	0.13
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD22	9	0.13
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD23	9	0.13
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD21	9	0.13
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD22	9	0.13
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD23	9	0.13
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD21	9	0.13
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD22	9	0.13
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD23	9	0.13
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD21	9	0.13
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD22	9	0.13
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD23	9	0.13
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD21	9	0.13
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD22	9	0.13
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD23	9	0.13
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD21	9	0.13
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD22	9	0.13
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD23	9	0.13
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD21	9	0.13
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD22	9	0.13
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD23	9	0.13
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD21	9	0.13
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD22	9	0.13
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD23	9	0.13
(2,1276)	1:A:129:ARG:HG3	1:A:130:ASN:H	20	0.13
(2,1276)	1:A:129:ARG:HG3	1:B:130:ASN:H	20	0.13
(2,1276)	1:B:129:ARG:HG3	1:A:130:ASN:H	20	0.13
(2,1276)	1:B:129:ARG:HG3	1:B:130:ASN:H	20	0.13
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	1	0.13
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	1	0.13
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	1	0.13
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	1	0.13
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	1	0.13
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	1	0.13
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	1	0.13
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	1	0.13
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	1	0.13
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	1	0.13
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	1	0.13
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	1	0.13
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	1	0.13
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	1	0.13
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	1	0.13
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	1	0.13
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	1	0.13
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	1	0.13
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	1	0.13
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	1	0.13
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	1	0.13
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	1	0.13
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	1	0.13
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	1	0.13
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	1	0.13
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	1	0.13
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	1	0.13
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	1	0.13
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	1	0.13
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	1	0.13
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	1	0.13
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	1	0.13
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	1	0.13
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	1	0.13
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	1	0.13
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	3	0.13
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	3	0.13
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	3	0.13
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	3	0.13
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	3	0.13
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	3	0.13
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	3	0.13
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	3	0.13
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	3	0.13
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	3	0.13
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	3	0.13
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	9	0.13
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	9	0.13
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	9	0.13
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	9	0.13
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	9	0.13
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	9	0.13
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	9	0.13
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	9	0.13
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	9	0.13
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	9	0.13
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	9	0.13
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	9	0.13
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	3	0.13
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	3	0.13
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	3	0.13
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	3	0.13
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	20	0.13
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	20	0.13
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	20	0.13
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	20	0.13
(1,93)	1:A:101:VAL:H	1:A:137:VAL:O	6	0.13
(1,93)	1:A:101:VAL:H	1:B:137:VAL:O	6	0.13
(1,93)	1:B:101:VAL:H	1:A:137:VAL:O	6	0.13
(1,93)	1:B:101:VAL:H	1:B:137:VAL:O	6	0.13
(1,93)	1:A:101:VAL:H	1:A:137:VAL:O	12	0.13
(1,93)	1:A:101:VAL:H	1:B:137:VAL:O	12	0.13
(1,93)	1:B:101:VAL:H	1:A:137:VAL:O	12	0.13
(1,93)	1:B:101:VAL:H	1:B:137:VAL:O	12	0.13
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	20	0.13
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	20	0.13
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	20	0.13
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	20	0.13
(1,91)	1:A:99:LEU:H	1:A:135:ARG:O	6	0.13
(1,91)	1:A:99:LEU:H	1:B:135:ARG:O	6	0.13
(1,91)	1:B:99:LEU:H	1:A:135:ARG:O	6	0.13
(1,91)	1:B:99:LEU:H	1:B:135:ARG:O	6	0.13
(1,9)	1:A:10:THR:H	1:A:20:THR:O	1	0.13
(1,9)	1:A:10:THR:H	1:B:20:THR:O	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:B:10:THR:H	1:A:20:THR:O	1	0.13
(1,9)	1:B:10:THR:H	1:B:20:THR:O	1	0.13
(1,9)	1:A:10:THR:H	1:A:20:THR:O	16	0.13
(1,9)	1:A:10:THR:H	1:B:20:THR:O	16	0.13
(1,9)	1:B:10:THR:H	1:A:20:THR:O	16	0.13
(1,9)	1:B:10:THR:H	1:B:20:THR:O	16	0.13
(1,9)	1:A:10:THR:H	1:A:20:THR:O	17	0.13
(1,9)	1:A:10:THR:H	1:B:20:THR:O	17	0.13
(1,9)	1:B:10:THR:H	1:A:20:THR:O	17	0.13
(1,9)	1:B:10:THR:H	1:B:20:THR:O	17	0.13
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	20	0.13
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	20	0.13
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	20	0.13
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	20	0.13
(1,85)	1:A:115:VAL:O	1:A:119:HIS:H	11	0.13
(1,85)	1:A:115:VAL:O	1:B:119:HIS:H	11	0.13
(1,85)	1:B:115:VAL:O	1:A:119:HIS:H	11	0.13
(1,85)	1:B:115:VAL:O	1:B:119:HIS:H	11	0.13
(1,84)	1:A:114:LEU:O	1:A:118:ALA:N	5	0.13
(1,84)	1:A:114:LEU:O	1:B:118:ALA:N	5	0.13
(1,84)	1:B:114:LEU:O	1:A:118:ALA:N	5	0.13
(1,84)	1:B:114:LEU:O	1:B:118:ALA:N	5	0.13
(1,84)	1:A:114:LEU:O	1:A:118:ALA:N	10	0.13
(1,84)	1:A:114:LEU:O	1:B:118:ALA:N	10	0.13
(1,84)	1:B:114:LEU:O	1:A:118:ALA:N	10	0.13
(1,84)	1:B:114:LEU:O	1:B:118:ALA:N	10	0.13
(1,82)	1:A:113:THR:O	1:A:117:ARG:N	17	0.13
(1,82)	1:A:113:THR:O	1:B:117:ARG:N	17	0.13
(1,82)	1:B:113:THR:O	1:A:117:ARG:N	17	0.13
(1,82)	1:B:113:THR:O	1:B:117:ARG:N	17	0.13
(1,81)	1:A:113:THR:O	1:A:117:ARG:H	2	0.13
(1,81)	1:A:113:THR:O	1:B:117:ARG:H	2	0.13
(1,81)	1:B:113:THR:O	1:A:117:ARG:H	2	0.13
(1,81)	1:B:113:THR:O	1:B:117:ARG:H	2	0.13
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	3	0.13
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	3	0.13
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	3	0.13
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	3	0.13
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	7	0.13
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	7	0.13
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	7	0.13
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	10	0.13
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	10	0.13
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	10	0.13
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	10	0.13
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	15	0.13
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	15	0.13
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	15	0.13
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	15	0.13
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	16	0.13
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	16	0.13
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	16	0.13
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	16	0.13
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	4	0.13
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	4	0.13
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	4	0.13
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	4	0.13
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	8	0.13
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	8	0.13
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	8	0.13
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	8	0.13
(1,76)	1:A:107:ASP:O	1:A:111:ALA:N	10	0.13
(1,76)	1:A:107:ASP:O	1:B:111:ALA:N	10	0.13
(1,76)	1:B:107:ASP:O	1:A:111:ALA:N	10	0.13
(1,76)	1:B:107:ASP:O	1:B:111:ALA:N	10	0.13
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	3	0.13
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	3	0.13
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	3	0.13
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	3	0.13
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	19	0.13
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	19	0.13
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	19	0.13
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	19	0.13
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	1	0.13
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	1	0.13
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	1	0.13
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	1	0.13
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	12	0.13
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	12	0.13
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	12	0.13
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	12	0.13
(1,72)	1:A:80:THR:N	1:A:100:ARG:O	6	0.13
(1,72)	1:A:80:THR:N	1:B:100:ARG:O	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:B:80:THR:N	1:A:100:ARG:O	6	0.13
(1,72)	1:B:80:THR:N	1:B:100:ARG:O	6	0.13
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	1	0.13
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	1	0.13
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	1	0.13
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	1	0.13
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	9	0.13
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	9	0.13
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	9	0.13
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	9	0.13
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	16	0.13
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	16	0.13
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	16	0.13
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	16	0.13
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	18	0.13
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	18	0.13
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	18	0.13
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	18	0.13
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	5	0.13
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	5	0.13
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	5	0.13
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	5	0.13
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	6	0.13
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	6	0.13
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	6	0.13
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	6	0.13
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	8	0.13
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	8	0.13
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	8	0.13
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	8	0.13
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	12	0.13
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	12	0.13
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	12	0.13
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	12	0.13
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	15	0.13
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	15	0.13
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	15	0.13
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	15	0.13
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	1	0.13
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	1	0.13
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	1	0.13
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	9	0.13
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	9	0.13
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	9	0.13
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	9	0.13
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	19	0.13
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	19	0.13
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	19	0.13
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	19	0.13
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	7	0.13
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	7	0.13
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	7	0.13
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	7	0.13
(1,60)	1:A:84:GLY:O	1:A:96:ASP:N	3	0.13
(1,60)	1:A:84:GLY:O	1:B:96:ASP:N	3	0.13
(1,60)	1:B:84:GLY:O	1:A:96:ASP:N	3	0.13
(1,60)	1:B:84:GLY:O	1:B:96:ASP:N	3	0.13
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	14	0.13
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	14	0.13
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	14	0.13
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	14	0.13
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	16	0.13
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	16	0.13
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	16	0.13
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	16	0.13
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	3	0.13
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	3	0.13
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	3	0.13
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	3	0.13
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	10	0.13
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	10	0.13
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	10	0.13
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	10	0.13
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	11	0.13
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	11	0.13
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	11	0.13
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	11	0.13
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	17	0.13
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	17	0.13
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	17	0.13
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	17	0.13
(1,5)	1:A:17:GLY:O	1:A:30:LEU:H	8	0.13
(1,5)	1:A:17:GLY:O	1:B:30:LEU:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:B:17:GLY:O	1:A:30:LEU:H	8	0.13
(1,5)	1:B:17:GLY:O	1:B:30:LEU:H	8	0.13
(1,5)	1:A:17:GLY:O	1:A:30:LEU:H	10	0.13
(1,5)	1:A:17:GLY:O	1:B:30:LEU:H	10	0.13
(1,5)	1:B:17:GLY:O	1:A:30:LEU:H	10	0.13
(1,5)	1:B:17:GLY:O	1:B:30:LEU:H	10	0.13
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	1	0.13
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	1	0.13
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	1	0.13
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	1	0.13
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	2	0.13
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	2	0.13
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	2	0.13
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	2	0.13
(1,44)	1:A:61:ALA:O	1:A:65:VAL:N	18	0.13
(1,44)	1:A:61:ALA:O	1:B:65:VAL:N	18	0.13
(1,44)	1:B:61:ALA:O	1:A:65:VAL:N	18	0.13
(1,44)	1:B:61:ALA:O	1:B:65:VAL:N	18	0.13
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	12	0.13
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	12	0.13
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	12	0.13
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	12	0.13
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	8	0.13
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	8	0.13
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	8	0.13
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	8	0.13
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	5	0.13
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	5	0.13
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	5	0.13
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	5	0.13
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	6	0.13
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	6	0.13
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	6	0.13
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	6	0.13
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	9	0.13
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	9	0.13
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	9	0.13
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	9	0.13
(1,34)	1:A:52:ALA:O	1:A:56:ALA:N	13	0.13
(1,34)	1:A:52:ALA:O	1:B:56:ALA:N	13	0.13
(1,34)	1:B:52:ALA:O	1:A:56:ALA:N	13	0.13
(1,34)	1:B:52:ALA:O	1:B:56:ALA:N	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:A:51:ALA:O	1:A:55:SER:H	6	0.13
(1,31)	1:A:51:ALA:O	1:B:55:SER:H	6	0.13
(1,31)	1:B:51:ALA:O	1:A:55:SER:H	6	0.13
(1,31)	1:B:51:ALA:O	1:B:55:SER:H	6	0.13
(1,31)	1:A:51:ALA:O	1:A:55:SER:H	12	0.13
(1,31)	1:A:51:ALA:O	1:B:55:SER:H	12	0.13
(1,31)	1:B:51:ALA:O	1:A:55:SER:H	12	0.13
(1,31)	1:B:51:ALA:O	1:B:55:SER:H	12	0.13
(1,29)	1:A:50:PHE:O	1:A:54:TYR:H	18	0.13
(1,29)	1:A:50:PHE:O	1:B:54:TYR:H	18	0.13
(1,29)	1:B:50:PHE:O	1:A:54:TYR:H	18	0.13
(1,29)	1:B:50:PHE:O	1:B:54:TYR:H	18	0.13
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	11	0.13
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	11	0.13
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	11	0.13
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	11	0.13
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	15	0.13
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	15	0.13
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	15	0.13
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	15	0.13
(1,20)	1:A:31:SER:N	1:A:44:THR:O	12	0.13
(1,20)	1:A:31:SER:N	1:B:44:THR:O	12	0.13
(1,20)	1:B:31:SER:N	1:A:44:THR:O	12	0.13
(1,20)	1:B:31:SER:N	1:B:44:THR:O	12	0.13
(1,20)	1:A:31:SER:N	1:A:44:THR:O	19	0.13
(1,20)	1:A:31:SER:N	1:B:44:THR:O	19	0.13
(1,20)	1:B:31:SER:N	1:A:44:THR:O	19	0.13
(1,20)	1:B:31:SER:N	1:B:44:THR:O	19	0.13
(1,19)	1:A:31:SER:H	1:A:44:THR:O	5	0.13
(1,19)	1:A:31:SER:H	1:B:44:THR:O	5	0.13
(1,19)	1:B:31:SER:H	1:A:44:THR:O	5	0.13
(1,19)	1:B:31:SER:H	1:B:44:THR:O	5	0.13
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	3	0.13
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	3	0.13
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	3	0.13
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	3	0.13
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	15	0.13
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	15	0.13
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	15	0.13
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	15	0.13
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	15	0.12
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	15	0.12
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	15	0.12
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	5	0.12
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	5	0.12
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	5	0.12
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	5	0.12
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	5	0.12
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	5	0.12
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	5	0.12
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	5	0.12
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	5	0.12
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	5	0.12
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	5	0.12
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	5	0.12
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	9	0.12
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	9	0.12
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	9	0.12
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	9	0.12
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	9	0.12
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	9	0.12
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	9	0.12
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	9	0.12
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	9	0.12
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	9	0.12
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	9	0.12
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	9	0.12
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	12	0.12
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	12	0.12
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	12	0.12
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	12	0.12
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	12	0.12
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	12	0.12
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	12	0.12
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	12	0.12
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	12	0.12
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	12	0.12
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	12	0.12
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	12	0.12
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	19	0.12
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	19	0.12
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	19	0.12
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	19	0.12
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	19	0.12
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	19	0.12
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	19	0.12
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	19	0.12
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	19	0.12
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	19	0.12
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	19	0.12
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	8	0.12
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	8	0.12
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	8	0.12
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	8	0.12
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	8	0.12
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	8	0.12
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	8	0.12
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	8	0.12
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	8	0.12
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	8	0.12
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	8	0.12
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	8	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB1	11	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB2	11	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB3	11	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB1	11	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB2	11	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB3	11	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB1	11	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB2	11	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB3	11	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB1	11	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB2	11	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB3	11	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB1	15	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB2	15	0.12
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB3	15	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB1	15	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB2	15	0.12
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB3	15	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB1	15	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB2	15	0.12
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB3	15	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB1	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB2	15	0.12
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB3	15	0.12
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	3	0.12
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	3	0.12
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	3	0.12
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	3	0.12
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	3	0.12
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	3	0.12
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	3	0.12
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	3	0.12
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	3	0.12
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	3	0.12
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	3	0.12
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	3	0.12
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	14	0.12
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	14	0.12
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	14	0.12
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	14	0.12
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	14	0.12
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	14	0.12
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	14	0.12
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	14	0.12
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	14	0.12
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	14	0.12
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	14	0.12
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	14	0.12
(2,53)	1:A:77:THR:HA	1:A:104:PRO:HD3	20	0.12
(2,53)	1:A:77:THR:HA	1:B:104:PRO:HD3	20	0.12
(2,53)	1:B:77:THR:HA	1:A:104:PRO:HD3	20	0.12
(2,53)	1:B:77:THR:HA	1:B:104:PRO:HD3	20	0.12
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	9	0.12
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	9	0.12
(2,427)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	9	0.12
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	9	0.12
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	9	0.12
(2,427)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	9	0.12
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	9	0.12
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	9	0.12
(2,427)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	9	0.12
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	9	0.12
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	9	0.12
(2,427)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,383)	1:A:80:THR:HB	1:A:100:ARG:HB2	13	0.12
(2,383)	1:A:80:THR:HB	1:B:100:ARG:HB2	13	0.12
(2,383)	1:B:80:THR:HB	1:A:100:ARG:HB2	13	0.12
(2,383)	1:B:80:THR:HB	1:B:100:ARG:HB2	13	0.12
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	4	0.12
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	4	0.12
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	4	0.12
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	4	0.12
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	20	0.12
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	20	0.12
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	20	0.12
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	20	0.12
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB1	2	0.12
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB2	2	0.12
(2,270)	1:A:51:ALA:HB1	1:A:81:ALA:HB3	2	0.12
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB1	2	0.12
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB2	2	0.12
(2,270)	1:A:51:ALA:HB1	1:B:81:ALA:HB3	2	0.12
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB1	2	0.12
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB2	2	0.12
(2,270)	1:A:51:ALA:HB2	1:A:81:ALA:HB3	2	0.12
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB1	2	0.12
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB2	2	0.12
(2,270)	1:A:51:ALA:HB2	1:B:81:ALA:HB3	2	0.12
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB1	2	0.12
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB2	2	0.12
(2,270)	1:A:51:ALA:HB3	1:A:81:ALA:HB3	2	0.12
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB1	2	0.12
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB2	2	0.12
(2,270)	1:A:51:ALA:HB3	1:B:81:ALA:HB3	2	0.12
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB1	2	0.12
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB2	2	0.12
(2,270)	1:B:51:ALA:HB1	1:A:81:ALA:HB3	2	0.12
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB1	2	0.12
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB2	2	0.12
(2,270)	1:B:51:ALA:HB1	1:B:81:ALA:HB3	2	0.12
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB1	2	0.12
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB2	2	0.12
(2,270)	1:B:51:ALA:HB2	1:A:81:ALA:HB3	2	0.12
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB1	2	0.12
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB2	2	0.12
(2,270)	1:B:51:ALA:HB2	1:B:81:ALA:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB1	2	0.12
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB2	2	0.12
(2,270)	1:B:51:ALA:HB3	1:A:81:ALA:HB3	2	0.12
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB1	2	0.12
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB2	2	0.12
(2,270)	1:B:51:ALA:HB3	1:B:81:ALA:HB3	2	0.12
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	3	0.12
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	3	0.12
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	3	0.12
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	3	0.12
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	3	0.12
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	3	0.12
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	3	0.12
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	3	0.12
(2,1644)	1:A:129:ARG:HG2	1:A:130:ASN:H	18	0.12
(2,1644)	1:A:129:ARG:HG2	1:B:130:ASN:H	18	0.12
(2,1644)	1:A:129:ARG:HG3	1:A:130:ASN:H	18	0.12
(2,1644)	1:A:129:ARG:HG3	1:B:130:ASN:H	18	0.12
(2,1644)	1:B:129:ARG:HG2	1:A:130:ASN:H	18	0.12
(2,1644)	1:B:129:ARG:HG2	1:B:130:ASN:H	18	0.12
(2,1644)	1:B:129:ARG:HG3	1:A:130:ASN:H	18	0.12
(2,1644)	1:B:129:ARG:HG3	1:B:130:ASN:H	18	0.12
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG11	17	0.12
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG12	17	0.12
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG13	17	0.12
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG21	17	0.12
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG22	17	0.12
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG23	17	0.12
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG11	17	0.12
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG12	17	0.12
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG13	17	0.12
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG21	17	0.12
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG22	17	0.12
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG23	17	0.12
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG11	17	0.12
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG12	17	0.12
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG13	17	0.12
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG21	17	0.12
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG22	17	0.12
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG23	17	0.12
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG11	17	0.12
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG12	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG13	17	0.12
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG21	17	0.12
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG22	17	0.12
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG23	17	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	9	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	9	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	9	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	9	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	9	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	9	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	9	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	9	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	10	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	10	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	10	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	10	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	10	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	10	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	10	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	10	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	11	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	11	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	11	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	11	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	11	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	11	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	11	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	11	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	13	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	13	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	13	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	13	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	13	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	13	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	13	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	13	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	20	0.12
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	20	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	20	0.12
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	20	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	20	0.12
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	20	0.12
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	20	0.12
(2,1594)	1:A:103:LEU:HD11	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD11	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD12	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD12	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD13	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD13	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD21	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD21	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD22	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD22	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD23	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:A:103:LEU:HD23	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD11	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD11	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD12	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD12	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD13	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD13	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD21	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD21	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD22	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD22	1:B:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD23	1:A:104:PRO:HD2	5	0.12
(2,1594)	1:B:103:LEU:HD23	1:B:104:PRO:HD2	5	0.12
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG2	12	0.12
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG3	12	0.12
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG2	12	0.12
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG3	12	0.12
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG2	12	0.12
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG3	12	0.12
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG2	12	0.12
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG3	12	0.12
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	15	0.12
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	15	0.12
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	15	0.12
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	15	0.12
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	15	0.12
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	15	0.12
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	15	0.12
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	15	0.12
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	15	0.12
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	15	0.12
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	15	0.12
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	15	0.12
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	15	0.12
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	15	0.12
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	15	0.12
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	15	0.12
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	15	0.12
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	15	0.12
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	15	0.12
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	15	0.12
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	15	0.12
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	15	0.12
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	15	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	1	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	1	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	1	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	1	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	1	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	1	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	1	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	1	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	1	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	1	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	1	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	1	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	1	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	1	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	1	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	1	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	1	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	1	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	1	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	1	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	1	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	1	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	1	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	1	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	7	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	7	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	7	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	7	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	7	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	7	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	7	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	7	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	7	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	7	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	7	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	7	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	7	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	7	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	7	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	7	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	7	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	7	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	7	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	7	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	7	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	7	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	7	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	12	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	12	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	12	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	12	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	12	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	12	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	12	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	12	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	12	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	12	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	12	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	12	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	12	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	12	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	12	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	12	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	12	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	12	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	12	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	12	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	12	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	12	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	12	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD11	18	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD12	18	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD13	18	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD21	18	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD22	18	0.12
(2,1524)	1:A:77:THR:HB	1:A:103:LEU:HD23	18	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD11	18	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD12	18	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD13	18	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD21	18	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD22	18	0.12
(2,1524)	1:A:77:THR:HB	1:B:103:LEU:HD23	18	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD11	18	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD12	18	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD13	18	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD21	18	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD22	18	0.12
(2,1524)	1:B:77:THR:HB	1:A:103:LEU:HD23	18	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD11	18	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD12	18	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD13	18	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD21	18	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD22	18	0.12
(2,1524)	1:B:77:THR:HB	1:B:103:LEU:HD23	18	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD11	17	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD12	17	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD13	17	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD21	17	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD22	17	0.12
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD23	17	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD11	17	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD12	17	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD13	17	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD21	17	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD22	17	0.12
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD23	17	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD11	17	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD12	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD13	17	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD21	17	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD22	17	0.12
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD23	17	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD11	17	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD12	17	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD13	17	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD21	17	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD22	17	0.12
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD23	17	0.12
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	8	0.12
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	8	0.12
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	8	0.12
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	8	0.12
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	8	0.12
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	8	0.12
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	8	0.12
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	8	0.12
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD21	4	0.12
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD22	4	0.12
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD23	4	0.12
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD21	4	0.12
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD22	4	0.12
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD23	4	0.12
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD21	4	0.12
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD22	4	0.12
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD23	4	0.12
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD21	4	0.12
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD22	4	0.12
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD23	4	0.12
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD21	4	0.12
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD22	4	0.12
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD23	4	0.12
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD21	4	0.12
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD22	4	0.12
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD23	4	0.12
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD21	4	0.12
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD22	4	0.12
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD23	4	0.12
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD21	4	0.12
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD22	4	0.12
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD23	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1276)	1:A:129:ARG:HG3	1:A:130:ASN:H	14	0.12
(2,1276)	1:A:129:ARG:HG3	1:B:130:ASN:H	14	0.12
(2,1276)	1:B:129:ARG:HG3	1:A:130:ASN:H	14	0.12
(2,1276)	1:B:129:ARG:HG3	1:B:130:ASN:H	14	0.12
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	8	0.12
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	8	0.12
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	8	0.12
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	8	0.12
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	8	0.12
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	8	0.12
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	8	0.12
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	8	0.12
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	8	0.12
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	8	0.12
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	8	0.12
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	8	0.12
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	10	0.12
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	10	0.12
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	10	0.12
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	10	0.12
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	7	0.12
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	7	0.12
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	7	0.12
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	7	0.12
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	14	0.12
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	14	0.12
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	14	0.12
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	14	0.12
(1,94)	1:A:101:VAL:N	1:A:137:VAL:O	17	0.12
(1,94)	1:A:101:VAL:N	1:B:137:VAL:O	17	0.12
(1,94)	1:B:101:VAL:N	1:A:137:VAL:O	17	0.12
(1,94)	1:B:101:VAL:N	1:B:137:VAL:O	17	0.12
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	2	0.12
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	2	0.12
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	2	0.12
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	2	0.12
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	4	0.12
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	4	0.12
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	4	0.12
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	4	0.12
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	17	0.12
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	17	0.12
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	17	0.12
(1,9)	1:A:10:THR:H	1:A:20:THR:O	12	0.12
(1,9)	1:A:10:THR:H	1:B:20:THR:O	12	0.12
(1,9)	1:B:10:THR:H	1:A:20:THR:O	12	0.12
(1,9)	1:B:10:THR:H	1:B:20:THR:O	12	0.12
(1,9)	1:A:10:THR:H	1:A:20:THR:O	19	0.12
(1,9)	1:A:10:THR:H	1:B:20:THR:O	19	0.12
(1,9)	1:B:10:THR:H	1:A:20:THR:O	19	0.12
(1,9)	1:B:10:THR:H	1:B:20:THR:O	19	0.12
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	4	0.12
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	4	0.12
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	4	0.12
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	4	0.12
(1,85)	1:A:115:VAL:O	1:A:119:HIS:H	1	0.12
(1,85)	1:A:115:VAL:O	1:B:119:HIS:H	1	0.12
(1,85)	1:B:115:VAL:O	1:A:119:HIS:H	1	0.12
(1,85)	1:B:115:VAL:O	1:B:119:HIS:H	1	0.12
(1,85)	1:A:115:VAL:O	1:A:119:HIS:H	17	0.12
(1,85)	1:A:115:VAL:O	1:B:119:HIS:H	17	0.12
(1,85)	1:B:115:VAL:O	1:A:119:HIS:H	17	0.12
(1,85)	1:B:115:VAL:O	1:B:119:HIS:H	17	0.12
(1,84)	1:A:114:LEU:O	1:A:118:ALA:N	19	0.12
(1,84)	1:A:114:LEU:O	1:B:118:ALA:N	19	0.12
(1,84)	1:B:114:LEU:O	1:A:118:ALA:N	19	0.12
(1,84)	1:B:114:LEU:O	1:B:118:ALA:N	19	0.12
(1,82)	1:A:113:THR:O	1:A:117:ARG:N	8	0.12
(1,82)	1:A:113:THR:O	1:B:117:ARG:N	8	0.12
(1,82)	1:B:113:THR:O	1:A:117:ARG:N	8	0.12
(1,82)	1:B:113:THR:O	1:B:117:ARG:N	8	0.12
(1,81)	1:A:113:THR:O	1:A:117:ARG:H	12	0.12
(1,81)	1:A:113:THR:O	1:B:117:ARG:H	12	0.12
(1,81)	1:B:113:THR:O	1:A:117:ARG:H	12	0.12
(1,81)	1:B:113:THR:O	1:B:117:ARG:H	12	0.12
(1,8)	1:A:19:ALA:O	1:A:28:VAL:N	1	0.12
(1,8)	1:A:19:ALA:O	1:B:28:VAL:N	1	0.12
(1,8)	1:B:19:ALA:O	1:A:28:VAL:N	1	0.12
(1,8)	1:B:19:ALA:O	1:B:28:VAL:N	1	0.12
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	5	0.12
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	5	0.12
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	5	0.12
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	6	0.12
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	6	0.12
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	6	0.12
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	6	0.12
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	4	0.12
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	4	0.12
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	4	0.12
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	4	0.12
(1,74)	1:A:80:THR:O	1:A:100:ARG:N	6	0.12
(1,74)	1:A:80:THR:O	1:B:100:ARG:N	6	0.12
(1,74)	1:B:80:THR:O	1:A:100:ARG:N	6	0.12
(1,74)	1:B:80:THR:O	1:B:100:ARG:N	6	0.12
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	20	0.12
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	20	0.12
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	20	0.12
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	20	0.12
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	7	0.12
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	7	0.12
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	7	0.12
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	7	0.12
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	17	0.12
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	17	0.12
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	17	0.12
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	17	0.12
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	6	0.12
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	6	0.12
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	6	0.12
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	6	0.12
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	10	0.12
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	10	0.12
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	10	0.12
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	10	0.12
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	13	0.12
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	13	0.12
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	13	0.12
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	13	0.12
(1,64)	1:A:99:LEU:O	1:A:137:VAL:N	15	0.12
(1,64)	1:A:99:LEU:O	1:B:137:VAL:N	15	0.12
(1,64)	1:B:99:LEU:O	1:A:137:VAL:N	15	0.12
(1,64)	1:B:99:LEU:O	1:B:137:VAL:N	15	0.12
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	2	0.12
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	2	0.12
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	2	0.12
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	8	0.12
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	8	0.12
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	8	0.12
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	8	0.12
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	10	0.12
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	10	0.12
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	10	0.12
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	10	0.12
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	20	0.12
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	20	0.12
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	20	0.12
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	20	0.12
(1,61)	1:A:82:GLU:H	1:A:98:GLU:O	9	0.12
(1,61)	1:A:82:GLU:H	1:B:98:GLU:O	9	0.12
(1,61)	1:B:82:GLU:H	1:A:98:GLU:O	9	0.12
(1,61)	1:B:82:GLU:H	1:B:98:GLU:O	9	0.12
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	15	0.12
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	15	0.12
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	15	0.12
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	15	0.12
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	18	0.12
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	18	0.12
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	18	0.12
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	18	0.12
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	5	0.12
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	5	0.12
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	5	0.12
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	5	0.12
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	9	0.12
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	9	0.12
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	9	0.12
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	9	0.12
(1,54)	1:A:86:GLY:N	1:A:94:ALA:O	17	0.12
(1,54)	1:A:86:GLY:N	1:B:94:ALA:O	17	0.12
(1,54)	1:B:86:GLY:N	1:A:94:ALA:O	17	0.12
(1,54)	1:B:86:GLY:N	1:B:94:ALA:O	17	0.12
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	12	0.12
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	12	0.12
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	12	0.12
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:A:17:GLY:O	1:A:30:LEU:H	12	0.12
(1,5)	1:A:17:GLY:O	1:B:30:LEU:H	12	0.12
(1,5)	1:B:17:GLY:O	1:A:30:LEU:H	12	0.12
(1,5)	1:B:17:GLY:O	1:B:30:LEU:H	12	0.12
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	7	0.12
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	7	0.12
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	7	0.12
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	7	0.12
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	12	0.12
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	12	0.12
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	12	0.12
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	12	0.12
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	16	0.12
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	16	0.12
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	16	0.12
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	16	0.12
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	7	0.12
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	7	0.12
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	7	0.12
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	7	0.12
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	10	0.12
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	10	0.12
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	10	0.12
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	10	0.12
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	11	0.12
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	11	0.12
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	11	0.12
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	11	0.12
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	16	0.12
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	16	0.12
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	16	0.12
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	16	0.12
(1,42)	1:A:60:SER:O	1:A:64:PHE:N	5	0.12
(1,42)	1:A:60:SER:O	1:B:64:PHE:N	5	0.12
(1,42)	1:B:60:SER:O	1:A:64:PHE:N	5	0.12
(1,42)	1:B:60:SER:O	1:B:64:PHE:N	5	0.12
(1,42)	1:A:60:SER:O	1:A:64:PHE:N	7	0.12
(1,42)	1:A:60:SER:O	1:B:64:PHE:N	7	0.12
(1,42)	1:B:60:SER:O	1:A:64:PHE:N	7	0.12
(1,42)	1:B:60:SER:O	1:B:64:PHE:N	7	0.12
(1,42)	1:A:60:SER:O	1:A:64:PHE:N	20	0.12
(1,42)	1:A:60:SER:O	1:B:64:PHE:N	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:B:60:SER:O	1:A:64:PHE:N	20	0.12
(1,42)	1:B:60:SER:O	1:B:64:PHE:N	20	0.12
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	5	0.12
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	5	0.12
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	5	0.12
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	5	0.12
(1,40)	1:A:58:PHE:O	1:A:62:MET:N	14	0.12
(1,40)	1:A:58:PHE:O	1:B:62:MET:N	14	0.12
(1,40)	1:B:58:PHE:O	1:A:62:MET:N	14	0.12
(1,40)	1:B:58:PHE:O	1:B:62:MET:N	14	0.12
(1,39)	1:A:58:PHE:O	1:A:62:MET:H	1	0.12
(1,39)	1:A:58:PHE:O	1:B:62:MET:H	1	0.12
(1,39)	1:B:58:PHE:O	1:A:62:MET:H	1	0.12
(1,39)	1:B:58:PHE:O	1:B:62:MET:H	1	0.12
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	7	0.12
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	7	0.12
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	7	0.12
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	7	0.12
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	9	0.12
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	9	0.12
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	9	0.12
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	9	0.12
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	15	0.12
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	15	0.12
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	15	0.12
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	15	0.12
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	17	0.12
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	17	0.12
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	17	0.12
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	17	0.12
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	12	0.12
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	12	0.12
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	12	0.12
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	12	0.12
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	15	0.12
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	15	0.12
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	15	0.12
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	15	0.12
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	18	0.12
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	18	0.12
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	18	0.12
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:A:52:ALA:O	1:A:56:ALA:N	3	0.12
(1,34)	1:A:52:ALA:O	1:B:56:ALA:N	3	0.12
(1,34)	1:B:52:ALA:O	1:A:56:ALA:N	3	0.12
(1,34)	1:B:52:ALA:O	1:B:56:ALA:N	3	0.12
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	4	0.12
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	4	0.12
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	4	0.12
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	4	0.12
(1,32)	1:A:51:ALA:O	1:A:55:SER:N	15	0.12
(1,32)	1:A:51:ALA:O	1:B:55:SER:N	15	0.12
(1,32)	1:B:51:ALA:O	1:A:55:SER:N	15	0.12
(1,32)	1:B:51:ALA:O	1:B:55:SER:N	15	0.12
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	7	0.12
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	7	0.12
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	7	0.12
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	7	0.12
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	20	0.12
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	20	0.12
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	20	0.12
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	20	0.12
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	13	0.12
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	13	0.12
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	13	0.12
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	13	0.12
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	1	0.12
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	1	0.12
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	1	0.12
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	1	0.12
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	4	0.12
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	4	0.12
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	4	0.12
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	4	0.12
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	5	0.12
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	5	0.12
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	5	0.12
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	5	0.12
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	16	0.12
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	16	0.12
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	16	0.12
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	16	0.12
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	6	0.12
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	6	0.12
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	6	0.12
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	7	0.12
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	7	0.12
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	7	0.12
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	7	0.12
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	9	0.12
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	9	0.12
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	9	0.12
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	9	0.12
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	14	0.12
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	14	0.12
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	14	0.12
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	14	0.12
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	17	0.12
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	17	0.12
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	17	0.12
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	17	0.12
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	20	0.12
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	20	0.12
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	20	0.12
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	20	0.12
(1,22)	1:A:46:PRO:O	1:A:50:PHE:N	11	0.12
(1,22)	1:A:46:PRO:O	1:B:50:PHE:N	11	0.12
(1,22)	1:B:46:PRO:O	1:A:50:PHE:N	11	0.12
(1,22)	1:B:46:PRO:O	1:B:50:PHE:N	11	0.12
(1,20)	1:A:31:SER:N	1:A:44:THR:O	14	0.12
(1,20)	1:A:31:SER:N	1:B:44:THR:O	14	0.12
(1,20)	1:B:31:SER:N	1:A:44:THR:O	14	0.12
(1,20)	1:B:31:SER:N	1:B:44:THR:O	14	0.12
(1,20)	1:A:31:SER:N	1:A:44:THR:O	16	0.12
(1,20)	1:A:31:SER:N	1:B:44:THR:O	16	0.12
(1,20)	1:B:31:SER:N	1:A:44:THR:O	16	0.12
(1,20)	1:B:31:SER:N	1:B:44:THR:O	16	0.12
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	10	0.12
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	10	0.12
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	10	0.12
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	10	0.12
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	13	0.12
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	13	0.12
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	13	0.12
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	16	0.12
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	16	0.12
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	16	0.12
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	16	0.12
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	17	0.12
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	17	0.12
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	17	0.12
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	17	0.12
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	20	0.12
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	20	0.12
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	20	0.12
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	20	0.12
(1,1)	1:A:10:THR:O	1:A:20:THR:H	1	0.12
(1,1)	1:A:10:THR:O	1:B:20:THR:H	1	0.12
(1,1)	1:B:10:THR:O	1:A:20:THR:H	1	0.12
(1,1)	1:B:10:THR:O	1:B:20:THR:H	1	0.12
(2,898)	1:A:34:ARG:HA	1:A:38:GLY:H	3	0.11
(2,898)	1:A:34:ARG:HA	1:B:38:GLY:H	3	0.11
(2,898)	1:B:34:ARG:HA	1:A:38:GLY:H	3	0.11
(2,898)	1:B:34:ARG:HA	1:B:38:GLY:H	3	0.11
(2,894)	1:A:36:LEU:H	1:A:36:LEU:HD21	17	0.11
(2,894)	1:A:36:LEU:H	1:A:36:LEU:HD22	17	0.11
(2,894)	1:A:36:LEU:H	1:A:36:LEU:HD23	17	0.11
(2,894)	1:A:36:LEU:H	1:B:36:LEU:HD21	17	0.11
(2,894)	1:A:36:LEU:H	1:B:36:LEU:HD22	17	0.11
(2,894)	1:A:36:LEU:H	1:B:36:LEU:HD23	17	0.11
(2,894)	1:B:36:LEU:H	1:A:36:LEU:HD21	17	0.11
(2,894)	1:B:36:LEU:H	1:A:36:LEU:HD22	17	0.11
(2,894)	1:B:36:LEU:H	1:A:36:LEU:HD23	17	0.11
(2,894)	1:B:36:LEU:H	1:B:36:LEU:HD21	17	0.11
(2,894)	1:B:36:LEU:H	1:B:36:LEU:HD22	17	0.11
(2,894)	1:B:36:LEU:H	1:B:36:LEU:HD23	17	0.11
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	2	0.11
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	2	0.11
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	2	0.11
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	2	0.11
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	2	0.11
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	2	0.11
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	2	0.11
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	2	0.11
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	2	0.11
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	2	0.11
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	2	0.11
(2,860)	1:A:26:LEU:HD11	1:A:27:ASP:H	16	0.11
(2,860)	1:A:26:LEU:HD11	1:B:27:ASP:H	16	0.11
(2,860)	1:A:26:LEU:HD12	1:A:27:ASP:H	16	0.11
(2,860)	1:A:26:LEU:HD12	1:B:27:ASP:H	16	0.11
(2,860)	1:A:26:LEU:HD13	1:A:27:ASP:H	16	0.11
(2,860)	1:A:26:LEU:HD13	1:B:27:ASP:H	16	0.11
(2,860)	1:B:26:LEU:HD11	1:A:27:ASP:H	16	0.11
(2,860)	1:B:26:LEU:HD11	1:B:27:ASP:H	16	0.11
(2,860)	1:B:26:LEU:HD12	1:A:27:ASP:H	16	0.11
(2,860)	1:B:26:LEU:HD12	1:B:27:ASP:H	16	0.11
(2,860)	1:B:26:LEU:HD13	1:A:27:ASP:H	16	0.11
(2,860)	1:B:26:LEU:HD13	1:B:27:ASP:H	16	0.11
(2,693)	1:A:106:LEU:HD21	1:A:111:ALA:HA	17	0.11
(2,693)	1:A:106:LEU:HD21	1:B:111:ALA:HA	17	0.11
(2,693)	1:A:106:LEU:HD22	1:A:111:ALA:HA	17	0.11
(2,693)	1:A:106:LEU:HD22	1:B:111:ALA:HA	17	0.11
(2,693)	1:A:106:LEU:HD23	1:A:111:ALA:HA	17	0.11
(2,693)	1:A:106:LEU:HD23	1:B:111:ALA:HA	17	0.11
(2,693)	1:B:106:LEU:HD21	1:A:111:ALA:HA	17	0.11
(2,693)	1:B:106:LEU:HD21	1:B:111:ALA:HA	17	0.11
(2,693)	1:B:106:LEU:HD22	1:A:111:ALA:HA	17	0.11
(2,693)	1:B:106:LEU:HD22	1:B:111:ALA:HA	17	0.11
(2,693)	1:B:106:LEU:HD23	1:A:111:ALA:HA	17	0.11
(2,693)	1:B:106:LEU:HD23	1:B:111:ALA:HA	17	0.11
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB1	3	0.11
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB2	3	0.11
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB3	3	0.11
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB1	3	0.11
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB2	3	0.11
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB3	3	0.11
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB1	3	0.11
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB2	3	0.11
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB3	3	0.11
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB1	3	0.11
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB2	3	0.11
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB3	3	0.11
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB1	14	0.11
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB2	14	0.11
(2,669)	1:A:102:ALA:HA	1:A:139:ALA:HB3	14	0.11
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB1	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB2	14	0.11
(2,669)	1:A:102:ALA:HA	1:B:139:ALA:HB3	14	0.11
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB1	14	0.11
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB2	14	0.11
(2,669)	1:B:102:ALA:HA	1:A:139:ALA:HB3	14	0.11
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB1	14	0.11
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB2	14	0.11
(2,669)	1:B:102:ALA:HA	1:B:139:ALA:HB3	14	0.11
(2,643)	1:A:137:VAL:H	1:A:137:VAL:HG11	11	0.11
(2,643)	1:A:137:VAL:H	1:A:137:VAL:HG12	11	0.11
(2,643)	1:A:137:VAL:H	1:A:137:VAL:HG13	11	0.11
(2,643)	1:A:137:VAL:H	1:B:137:VAL:HG11	11	0.11
(2,643)	1:A:137:VAL:H	1:B:137:VAL:HG12	11	0.11
(2,643)	1:A:137:VAL:H	1:B:137:VAL:HG13	11	0.11
(2,643)	1:B:137:VAL:H	1:A:137:VAL:HG11	11	0.11
(2,643)	1:B:137:VAL:H	1:A:137:VAL:HG12	11	0.11
(2,643)	1:B:137:VAL:H	1:A:137:VAL:HG13	11	0.11
(2,643)	1:B:137:VAL:H	1:B:137:VAL:HG11	11	0.11
(2,643)	1:B:137:VAL:H	1:B:137:VAL:HG12	11	0.11
(2,643)	1:B:137:VAL:H	1:B:137:VAL:HG13	11	0.11
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG11	5	0.11
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG12	5	0.11
(2,642)	1:A:100:ARG:HA	1:A:137:VAL:HG13	5	0.11
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG11	5	0.11
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG12	5	0.11
(2,642)	1:A:100:ARG:HA	1:B:137:VAL:HG13	5	0.11
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG11	5	0.11
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG12	5	0.11
(2,642)	1:B:100:ARG:HA	1:A:137:VAL:HG13	5	0.11
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG11	5	0.11
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG12	5	0.11
(2,642)	1:B:100:ARG:HA	1:B:137:VAL:HG13	5	0.11
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB1	4	0.11
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB2	4	0.11
(2,491)	1:A:106:LEU:HD11	1:A:110:ALA:HB3	4	0.11
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB1	4	0.11
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB2	4	0.11
(2,491)	1:A:106:LEU:HD11	1:B:110:ALA:HB3	4	0.11
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB1	4	0.11
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB2	4	0.11
(2,491)	1:A:106:LEU:HD12	1:A:110:ALA:HB3	4	0.11
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB1	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB2	4	0.11
(2,491)	1:A:106:LEU:HD12	1:B:110:ALA:HB3	4	0.11
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB1	4	0.11
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB2	4	0.11
(2,491)	1:A:106:LEU:HD13	1:A:110:ALA:HB3	4	0.11
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB1	4	0.11
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB2	4	0.11
(2,491)	1:A:106:LEU:HD13	1:B:110:ALA:HB3	4	0.11
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB1	4	0.11
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB2	4	0.11
(2,491)	1:B:106:LEU:HD11	1:A:110:ALA:HB3	4	0.11
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB1	4	0.11
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB2	4	0.11
(2,491)	1:B:106:LEU:HD11	1:B:110:ALA:HB3	4	0.11
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB1	4	0.11
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB2	4	0.11
(2,491)	1:B:106:LEU:HD12	1:A:110:ALA:HB3	4	0.11
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB1	4	0.11
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB2	4	0.11
(2,491)	1:B:106:LEU:HD12	1:B:110:ALA:HB3	4	0.11
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB1	4	0.11
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB2	4	0.11
(2,491)	1:B:106:LEU:HD13	1:A:110:ALA:HB3	4	0.11
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB1	4	0.11
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB2	4	0.11
(2,491)	1:B:106:LEU:HD13	1:B:110:ALA:HB3	4	0.11
(2,444)	1:A:99:LEU:HA	1:A:99:LEU:HD11	1	0.11
(2,444)	1:A:99:LEU:HA	1:A:99:LEU:HD12	1	0.11
(2,444)	1:A:99:LEU:HA	1:A:99:LEU:HD13	1	0.11
(2,444)	1:A:99:LEU:HA	1:B:99:LEU:HD11	1	0.11
(2,444)	1:A:99:LEU:HA	1:B:99:LEU:HD12	1	0.11
(2,444)	1:A:99:LEU:HA	1:B:99:LEU:HD13	1	0.11
(2,444)	1:B:99:LEU:HA	1:A:99:LEU:HD11	1	0.11
(2,444)	1:B:99:LEU:HA	1:A:99:LEU:HD12	1	0.11
(2,444)	1:B:99:LEU:HA	1:A:99:LEU:HD13	1	0.11
(2,444)	1:B:99:LEU:HA	1:B:99:LEU:HD11	1	0.11
(2,444)	1:B:99:LEU:HA	1:B:99:LEU:HD12	1	0.11
(2,444)	1:B:99:LEU:HA	1:B:99:LEU:HD13	1	0.11
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	15	0.11
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	15	0.11
(2,426)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	15	0.11
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	15	0.11
(2,426)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	15	0.11
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	15	0.11
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	15	0.11
(2,426)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	15	0.11
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	15	0.11
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	15	0.11
(2,426)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	15	0.11
(2,383)	1:A:80:THR:HB	1:A:100:ARG:HB2	15	0.11
(2,383)	1:A:80:THR:HB	1:B:100:ARG:HB2	15	0.11
(2,383)	1:B:80:THR:HB	1:A:100:ARG:HB2	15	0.11
(2,383)	1:B:80:THR:HB	1:B:100:ARG:HB2	15	0.11
(2,31)	1:A:16:ASP:HB3	1:A:31:SER:HA	1	0.11
(2,31)	1:A:16:ASP:HB3	1:B:31:SER:HA	1	0.11
(2,31)	1:B:16:ASP:HB3	1:A:31:SER:HA	1	0.11
(2,31)	1:B:16:ASP:HB3	1:B:31:SER:HA	1	0.11
(2,257)	1:A:42:GLU:H	1:A:42:GLU:HG2	18	0.11
(2,257)	1:A:42:GLU:H	1:B:42:GLU:HG2	18	0.11
(2,257)	1:B:42:GLU:H	1:A:42:GLU:HG2	18	0.11
(2,257)	1:B:42:GLU:H	1:B:42:GLU:HG2	18	0.11
(2,1646)	1:A:129:ARG:HG2	1:A:130:ASN:HD21	13	0.11
(2,1646)	1:A:129:ARG:HG2	1:A:130:ASN:HD22	13	0.11
(2,1646)	1:A:129:ARG:HG2	1:B:130:ASN:HD21	13	0.11
(2,1646)	1:A:129:ARG:HG2	1:B:130:ASN:HD22	13	0.11
(2,1646)	1:A:129:ARG:HG3	1:A:130:ASN:HD21	13	0.11
(2,1646)	1:A:129:ARG:HG3	1:A:130:ASN:HD22	13	0.11
(2,1646)	1:A:129:ARG:HG3	1:B:130:ASN:HD21	13	0.11
(2,1646)	1:A:129:ARG:HG3	1:B:130:ASN:HD22	13	0.11
(2,1646)	1:B:129:ARG:HG2	1:A:130:ASN:HD21	13	0.11
(2,1646)	1:B:129:ARG:HG2	1:A:130:ASN:HD22	13	0.11
(2,1646)	1:B:129:ARG:HG2	1:B:130:ASN:HD21	13	0.11
(2,1646)	1:B:129:ARG:HG2	1:B:130:ASN:HD22	13	0.11
(2,1646)	1:B:129:ARG:HG3	1:A:130:ASN:HD21	13	0.11
(2,1646)	1:B:129:ARG:HG3	1:A:130:ASN:HD22	13	0.11
(2,1646)	1:B:129:ARG:HG3	1:B:130:ASN:HD21	13	0.11
(2,1646)	1:B:129:ARG:HG3	1:B:130:ASN:HD22	13	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG11	4	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG12	4	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG13	4	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG21	4	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG22	4	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG23	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG11	4	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG12	4	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG13	4	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG21	4	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG22	4	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG23	4	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG11	4	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG12	4	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG13	4	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG21	4	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG22	4	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG23	4	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG11	4	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG12	4	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG13	4	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG21	4	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG22	4	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG23	4	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG11	9	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG12	9	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG13	9	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG21	9	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG22	9	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG23	9	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG11	9	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG12	9	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG13	9	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG21	9	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG22	9	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG23	9	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG11	9	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG12	9	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG13	9	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG21	9	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG22	9	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG23	9	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG11	9	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG12	9	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG13	9	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG21	9	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG22	9	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG23	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG11	11	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG12	11	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG13	11	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG21	11	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG22	11	0.11
(2,1629)	1:A:121:VAL:H	1:A:121:VAL:HG23	11	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG11	11	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG12	11	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG13	11	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG21	11	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG22	11	0.11
(2,1629)	1:A:121:VAL:H	1:B:121:VAL:HG23	11	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG11	11	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG12	11	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG13	11	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG21	11	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG22	11	0.11
(2,1629)	1:B:121:VAL:H	1:A:121:VAL:HG23	11	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG11	11	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG12	11	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG13	11	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG21	11	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG22	11	0.11
(2,1629)	1:B:121:VAL:H	1:B:121:VAL:HG23	11	0.11
(2,162)	1:A:12:THR:HG21	1:A:13:GLY:H	4	0.11
(2,162)	1:A:12:THR:HG21	1:B:13:GLY:H	4	0.11
(2,162)	1:A:12:THR:HG22	1:A:13:GLY:H	4	0.11
(2,162)	1:A:12:THR:HG22	1:B:13:GLY:H	4	0.11
(2,162)	1:A:12:THR:HG23	1:A:13:GLY:H	4	0.11
(2,162)	1:A:12:THR:HG23	1:B:13:GLY:H	4	0.11
(2,162)	1:B:12:THR:HG21	1:A:13:GLY:H	4	0.11
(2,162)	1:B:12:THR:HG21	1:B:13:GLY:H	4	0.11
(2,162)	1:B:12:THR:HG22	1:A:13:GLY:H	4	0.11
(2,162)	1:B:12:THR:HG22	1:B:13:GLY:H	4	0.11
(2,162)	1:B:12:THR:HG23	1:A:13:GLY:H	4	0.11
(2,162)	1:B:12:THR:HG23	1:B:13:GLY:H	4	0.11
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	1	0.11
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	1	0.11
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	1	0.11
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	1	0.11
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	1	0.11
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	1	0.11
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	1	0.11
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG2	14	0.11
(2,1614)	1:A:117:ARG:H	1:A:117:ARG:HG3	14	0.11
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG2	14	0.11
(2,1614)	1:A:117:ARG:H	1:B:117:ARG:HG3	14	0.11
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG2	14	0.11
(2,1614)	1:B:117:ARG:H	1:A:117:ARG:HG3	14	0.11
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG2	14	0.11
(2,1614)	1:B:117:ARG:H	1:B:117:ARG:HG3	14	0.11
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG21	6	0.11
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG22	6	0.11
(2,1582)	1:A:100:ARG:HG2	1:A:137:VAL:HG23	6	0.11
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG21	6	0.11
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG22	6	0.11
(2,1582)	1:A:100:ARG:HG2	1:B:137:VAL:HG23	6	0.11
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG21	6	0.11
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG22	6	0.11
(2,1582)	1:A:100:ARG:HG3	1:A:137:VAL:HG23	6	0.11
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG21	6	0.11
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG22	6	0.11
(2,1582)	1:A:100:ARG:HG3	1:B:137:VAL:HG23	6	0.11
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG21	6	0.11
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG22	6	0.11
(2,1582)	1:B:100:ARG:HG2	1:A:137:VAL:HG23	6	0.11
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG21	6	0.11
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG22	6	0.11
(2,1582)	1:B:100:ARG:HG2	1:B:137:VAL:HG23	6	0.11
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG21	6	0.11
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG22	6	0.11
(2,1582)	1:B:100:ARG:HG3	1:A:137:VAL:HG23	6	0.11
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG21	6	0.11
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG22	6	0.11
(2,1582)	1:B:100:ARG:HG3	1:B:137:VAL:HG23	6	0.11
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG11	15	0.11
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG12	15	0.11
(2,1581)	1:A:100:ARG:HG2	1:A:137:VAL:HG13	15	0.11
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG11	15	0.11
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG12	15	0.11
(2,1581)	1:A:100:ARG:HG2	1:B:137:VAL:HG13	15	0.11
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG11	15	0.11
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG12	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1581)	1:A:100:ARG:HG3	1:A:137:VAL:HG13	15	0.11
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG11	15	0.11
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG12	15	0.11
(2,1581)	1:A:100:ARG:HG3	1:B:137:VAL:HG13	15	0.11
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG11	15	0.11
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG12	15	0.11
(2,1581)	1:B:100:ARG:HG2	1:A:137:VAL:HG13	15	0.11
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG11	15	0.11
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG12	15	0.11
(2,1581)	1:B:100:ARG:HG2	1:B:137:VAL:HG13	15	0.11
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG11	15	0.11
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG12	15	0.11
(2,1581)	1:B:100:ARG:HG3	1:A:137:VAL:HG13	15	0.11
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG11	15	0.11
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG12	15	0.11
(2,1581)	1:B:100:ARG:HG3	1:B:137:VAL:HG13	15	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD11	1	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD12	1	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD13	1	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD21	1	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD22	1	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD23	1	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD11	1	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD12	1	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD13	1	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD21	1	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD22	1	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD23	1	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD11	1	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD12	1	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD13	1	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD21	1	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD22	1	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD23	1	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD11	1	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD12	1	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD13	1	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD21	1	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD22	1	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD23	1	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD11	7	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD12	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD13	7	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD21	7	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD22	7	0.11
(2,1562)	1:A:99:LEU:HA	1:A:99:LEU:HD23	7	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD11	7	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD12	7	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD13	7	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD21	7	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD22	7	0.11
(2,1562)	1:A:99:LEU:HA	1:B:99:LEU:HD23	7	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD11	7	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD12	7	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD13	7	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD21	7	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD22	7	0.11
(2,1562)	1:B:99:LEU:HA	1:A:99:LEU:HD23	7	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD11	7	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD12	7	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD13	7	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD21	7	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD22	7	0.11
(2,1562)	1:B:99:LEU:HA	1:B:99:LEU:HD23	7	0.11
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG2	4	0.11
(2,1551)	1:A:89:GLU:H	1:A:89:GLU:HG3	4	0.11
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG2	4	0.11
(2,1551)	1:A:89:GLU:H	1:B:89:GLU:HG3	4	0.11
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG2	4	0.11
(2,1551)	1:B:89:GLU:H	1:A:89:GLU:HG3	4	0.11
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG2	4	0.11
(2,1551)	1:B:89:GLU:H	1:B:89:GLU:HG3	4	0.11
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB1	4	0.11
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB2	4	0.11
(2,1550)	1:A:88:ASN:HB2	1:A:94:ALA:HB3	4	0.11
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB1	4	0.11
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB2	4	0.11
(2,1550)	1:A:88:ASN:HB2	1:B:94:ALA:HB3	4	0.11
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB1	4	0.11
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB2	4	0.11
(2,1550)	1:A:88:ASN:HB3	1:A:94:ALA:HB3	4	0.11
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB1	4	0.11
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB2	4	0.11
(2,1550)	1:A:88:ASN:HB3	1:B:94:ALA:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB1	4	0.11
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB2	4	0.11
(2,1550)	1:B:88:ASN:HB2	1:A:94:ALA:HB3	4	0.11
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB1	4	0.11
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB2	4	0.11
(2,1550)	1:B:88:ASN:HB2	1:B:94:ALA:HB3	4	0.11
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB1	4	0.11
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB2	4	0.11
(2,1550)	1:B:88:ASN:HB3	1:A:94:ALA:HB3	4	0.11
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB1	4	0.11
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB2	4	0.11
(2,1550)	1:B:88:ASN:HB3	1:B:94:ALA:HB3	4	0.11
(2,1531)	1:A:80:THR:HB	1:A:100:ARG:HB2	15	0.11
(2,1531)	1:A:80:THR:HB	1:A:100:ARG:HB3	15	0.11
(2,1531)	1:A:80:THR:HB	1:B:100:ARG:HB2	15	0.11
(2,1531)	1:A:80:THR:HB	1:B:100:ARG:HB3	15	0.11
(2,1531)	1:B:80:THR:HB	1:A:100:ARG:HB2	15	0.11
(2,1531)	1:B:80:THR:HB	1:A:100:ARG:HB3	15	0.11
(2,1531)	1:B:80:THR:HB	1:B:100:ARG:HB2	15	0.11
(2,1531)	1:B:80:THR:HB	1:B:100:ARG:HB3	15	0.11
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD11	14	0.11
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD12	14	0.11
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD13	14	0.11
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD21	14	0.11
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD22	14	0.11
(2,1474)	1:A:36:LEU:H	1:A:36:LEU:HD23	14	0.11
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD11	14	0.11
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD12	14	0.11
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD13	14	0.11
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD21	14	0.11
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD22	14	0.11
(2,1474)	1:A:36:LEU:H	1:B:36:LEU:HD23	14	0.11
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD11	14	0.11
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD12	14	0.11
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD13	14	0.11
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD21	14	0.11
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD22	14	0.11
(2,1474)	1:B:36:LEU:H	1:A:36:LEU:HD23	14	0.11
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD11	14	0.11
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD12	14	0.11
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD13	14	0.11
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD21	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD22	14	0.11
(2,1474)	1:B:36:LEU:H	1:B:36:LEU:HD23	14	0.11
(2,1448)	1:A:31:SER:HB2	1:A:41:ALA:HB1	1	0.11
(2,1448)	1:A:31:SER:HB2	1:A:41:ALA:HB2	1	0.11
(2,1448)	1:A:31:SER:HB2	1:A:41:ALA:HB3	1	0.11
(2,1448)	1:A:31:SER:HB2	1:B:41:ALA:HB1	1	0.11
(2,1448)	1:A:31:SER:HB2	1:B:41:ALA:HB2	1	0.11
(2,1448)	1:A:31:SER:HB2	1:B:41:ALA:HB3	1	0.11
(2,1448)	1:A:31:SER:HB3	1:A:41:ALA:HB1	1	0.11
(2,1448)	1:A:31:SER:HB3	1:A:41:ALA:HB2	1	0.11
(2,1448)	1:A:31:SER:HB3	1:A:41:ALA:HB3	1	0.11
(2,1448)	1:A:31:SER:HB3	1:B:41:ALA:HB1	1	0.11
(2,1448)	1:A:31:SER:HB3	1:B:41:ALA:HB2	1	0.11
(2,1448)	1:A:31:SER:HB3	1:B:41:ALA:HB3	1	0.11
(2,1448)	1:B:31:SER:HB2	1:A:41:ALA:HB1	1	0.11
(2,1448)	1:B:31:SER:HB2	1:A:41:ALA:HB2	1	0.11
(2,1448)	1:B:31:SER:HB2	1:A:41:ALA:HB3	1	0.11
(2,1448)	1:B:31:SER:HB2	1:B:41:ALA:HB1	1	0.11
(2,1448)	1:B:31:SER:HB2	1:B:41:ALA:HB2	1	0.11
(2,1448)	1:B:31:SER:HB2	1:B:41:ALA:HB3	1	0.11
(2,1448)	1:B:31:SER:HB3	1:A:41:ALA:HB1	1	0.11
(2,1448)	1:B:31:SER:HB3	1:A:41:ALA:HB2	1	0.11
(2,1448)	1:B:31:SER:HB3	1:A:41:ALA:HB3	1	0.11
(2,1448)	1:B:31:SER:HB3	1:B:41:ALA:HB1	1	0.11
(2,1448)	1:B:31:SER:HB3	1:B:41:ALA:HB2	1	0.11
(2,1448)	1:B:31:SER:HB3	1:B:41:ALA:HB3	1	0.11
(2,1417)	1:A:21:SER:HB2	1:A:26:LEU:H	20	0.11
(2,1417)	1:A:21:SER:HB2	1:B:26:LEU:H	20	0.11
(2,1417)	1:A:21:SER:HB3	1:A:26:LEU:H	20	0.11
(2,1417)	1:A:21:SER:HB3	1:B:26:LEU:H	20	0.11
(2,1417)	1:B:21:SER:HB2	1:A:26:LEU:H	20	0.11
(2,1417)	1:B:21:SER:HB2	1:B:26:LEU:H	20	0.11
(2,1417)	1:B:21:SER:HB3	1:A:26:LEU:H	20	0.11
(2,1417)	1:B:21:SER:HB3	1:B:26:LEU:H	20	0.11
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD21	5	0.11
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD22	5	0.11
(2,1401)	1:A:17:GLY:HA2	1:A:30:LEU:HD23	5	0.11
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD21	5	0.11
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD22	5	0.11
(2,1401)	1:A:17:GLY:HA2	1:B:30:LEU:HD23	5	0.11
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD21	5	0.11
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD22	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1401)	1:A:17:GLY:HA3	1:A:30:LEU:HD23	5	0.11
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD21	5	0.11
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD22	5	0.11
(2,1401)	1:A:17:GLY:HA3	1:B:30:LEU:HD23	5	0.11
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD21	5	0.11
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD22	5	0.11
(2,1401)	1:B:17:GLY:HA2	1:A:30:LEU:HD23	5	0.11
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD21	5	0.11
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD22	5	0.11
(2,1401)	1:B:17:GLY:HA2	1:B:30:LEU:HD23	5	0.11
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD21	5	0.11
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD22	5	0.11
(2,1401)	1:B:17:GLY:HA3	1:A:30:LEU:HD23	5	0.11
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD21	5	0.11
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD22	5	0.11
(2,1401)	1:B:17:GLY:HA3	1:B:30:LEU:HD23	5	0.11
(2,1245)	1:A:117:ARG:H	1:A:117:ARG:HG2	10	0.11
(2,1245)	1:A:117:ARG:H	1:B:117:ARG:HG2	10	0.11
(2,1245)	1:B:117:ARG:H	1:A:117:ARG:HG2	10	0.11
(2,1245)	1:B:117:ARG:H	1:B:117:ARG:HG2	10	0.11
(2,1245)	1:A:117:ARG:H	1:A:117:ARG:HG2	11	0.11
(2,1245)	1:A:117:ARG:H	1:B:117:ARG:HG2	11	0.11
(2,1245)	1:B:117:ARG:H	1:A:117:ARG:HG2	11	0.11
(2,1245)	1:B:117:ARG:H	1:B:117:ARG:HG2	11	0.11
(2,1245)	1:A:117:ARG:H	1:A:117:ARG:HG2	13	0.11
(2,1245)	1:A:117:ARG:H	1:B:117:ARG:HG2	13	0.11
(2,1245)	1:B:117:ARG:H	1:A:117:ARG:HG2	13	0.11
(2,1245)	1:B:117:ARG:H	1:B:117:ARG:HG2	13	0.11
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD11	11	0.11
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD12	11	0.11
(2,110)	1:A:1:MET:HE1	1:A:3:ILE:HD13	11	0.11
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD11	11	0.11
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD12	11	0.11
(2,110)	1:A:1:MET:HE1	1:B:3:ILE:HD13	11	0.11
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD11	11	0.11
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD12	11	0.11
(2,110)	1:A:1:MET:HE2	1:A:3:ILE:HD13	11	0.11
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD11	11	0.11
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD12	11	0.11
(2,110)	1:A:1:MET:HE2	1:B:3:ILE:HD13	11	0.11
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD11	11	0.11
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD12	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:1:MET:HE3	1:A:3:ILE:HD13	11	0.11
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD11	11	0.11
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD12	11	0.11
(2,110)	1:A:1:MET:HE3	1:B:3:ILE:HD13	11	0.11
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD11	11	0.11
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD12	11	0.11
(2,110)	1:B:1:MET:HE1	1:A:3:ILE:HD13	11	0.11
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD11	11	0.11
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD12	11	0.11
(2,110)	1:B:1:MET:HE1	1:B:3:ILE:HD13	11	0.11
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD11	11	0.11
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD12	11	0.11
(2,110)	1:B:1:MET:HE2	1:A:3:ILE:HD13	11	0.11
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD11	11	0.11
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD12	11	0.11
(2,110)	1:B:1:MET:HE2	1:B:3:ILE:HD13	11	0.11
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD11	11	0.11
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD12	11	0.11
(2,110)	1:B:1:MET:HE3	1:A:3:ILE:HD13	11	0.11
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD11	11	0.11
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD12	11	0.11
(2,110)	1:B:1:MET:HE3	1:B:3:ILE:HD13	11	0.11
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	17	0.11
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	17	0.11
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	17	0.11
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	17	0.11
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	17	0.11
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	17	0.11
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	17	0.11
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	17	0.11
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	17	0.11
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	17	0.11
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	17	0.11
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	17	0.11
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG21	18	0.11
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG22	18	0.11
(2,1076)	1:A:77:THR:H	1:A:77:THR:HG23	18	0.11
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG21	18	0.11
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG22	18	0.11
(2,1076)	1:A:77:THR:H	1:B:77:THR:HG23	18	0.11
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG21	18	0.11
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG22	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1076)	1:B:77:THR:H	1:A:77:THR:HG23	18	0.11
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG21	18	0.11
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG22	18	0.11
(2,1076)	1:B:77:THR:H	1:B:77:THR:HG23	18	0.11
(2,1011)	1:A:68:GLN:HG3	1:A:69:ASN:HD21	19	0.11
(2,1011)	1:A:68:GLN:HG3	1:B:69:ASN:HD21	19	0.11
(2,1011)	1:B:68:GLN:HG3	1:A:69:ASN:HD21	19	0.11
(2,1011)	1:B:68:GLN:HG3	1:B:69:ASN:HD21	19	0.11
(1,93)	1:A:101:VAL:H	1:A:137:VAL:O	4	0.11
(1,93)	1:A:101:VAL:H	1:B:137:VAL:O	4	0.11
(1,93)	1:B:101:VAL:H	1:A:137:VAL:O	4	0.11
(1,93)	1:B:101:VAL:H	1:B:137:VAL:O	4	0.11
(1,92)	1:A:99:LEU:N	1:A:135:ARG:O	7	0.11
(1,92)	1:A:99:LEU:N	1:B:135:ARG:O	7	0.11
(1,92)	1:B:99:LEU:N	1:A:135:ARG:O	7	0.11
(1,92)	1:B:99:LEU:N	1:B:135:ARG:O	7	0.11
(1,90)	1:A:97:VAL:N	1:A:133:ALA:O	16	0.11
(1,90)	1:A:97:VAL:N	1:B:133:ALA:O	16	0.11
(1,90)	1:B:97:VAL:N	1:A:133:ALA:O	16	0.11
(1,90)	1:B:97:VAL:N	1:B:133:ALA:O	16	0.11
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	1	0.11
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	1	0.11
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	1	0.11
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	1	0.11
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	2	0.11
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	2	0.11
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	2	0.11
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	2	0.11
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	3	0.11
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	3	0.11
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	3	0.11
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	3	0.11
(1,88)	1:A:117:ARG:O	1:A:121:VAL:N	15	0.11
(1,88)	1:A:117:ARG:O	1:B:121:VAL:N	15	0.11
(1,88)	1:B:117:ARG:O	1:A:121:VAL:N	15	0.11
(1,88)	1:B:117:ARG:O	1:B:121:VAL:N	15	0.11
(1,87)	1:A:117:ARG:O	1:A:121:VAL:H	11	0.11
(1,87)	1:A:117:ARG:O	1:B:121:VAL:H	11	0.11
(1,87)	1:B:117:ARG:O	1:A:121:VAL:H	11	0.11
(1,87)	1:B:117:ARG:O	1:B:121:VAL:H	11	0.11
(1,86)	1:A:115:VAL:O	1:A:119:HIS:N	10	0.11
(1,86)	1:A:115:VAL:O	1:B:119:HIS:N	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:B:115:VAL:O	1:A:119:HIS:N	10	0.11
(1,86)	1:B:115:VAL:O	1:B:119:HIS:N	10	0.11
(1,84)	1:A:114:LEU:O	1:A:118:ALA:N	4	0.11
(1,84)	1:A:114:LEU:O	1:B:118:ALA:N	4	0.11
(1,84)	1:B:114:LEU:O	1:A:118:ALA:N	4	0.11
(1,84)	1:B:114:LEU:O	1:B:118:ALA:N	4	0.11
(1,84)	1:A:114:LEU:O	1:A:118:ALA:N	18	0.11
(1,84)	1:A:114:LEU:O	1:B:118:ALA:N	18	0.11
(1,84)	1:B:114:LEU:O	1:A:118:ALA:N	18	0.11
(1,84)	1:B:114:LEU:O	1:B:118:ALA:N	18	0.11
(1,82)	1:A:113:THR:O	1:A:117:ARG:N	1	0.11
(1,82)	1:A:113:THR:O	1:B:117:ARG:N	1	0.11
(1,82)	1:B:113:THR:O	1:A:117:ARG:N	1	0.11
(1,82)	1:B:113:THR:O	1:B:117:ARG:N	1	0.11
(1,82)	1:A:113:THR:O	1:A:117:ARG:N	18	0.11
(1,82)	1:A:113:THR:O	1:B:117:ARG:N	18	0.11
(1,82)	1:B:113:THR:O	1:A:117:ARG:N	18	0.11
(1,82)	1:B:113:THR:O	1:B:117:ARG:N	18	0.11
(1,81)	1:A:113:THR:O	1:A:117:ARG:H	17	0.11
(1,81)	1:A:113:THR:O	1:B:117:ARG:H	17	0.11
(1,81)	1:B:113:THR:O	1:A:117:ARG:H	17	0.11
(1,81)	1:B:113:THR:O	1:B:117:ARG:H	17	0.11
(1,80)	1:A:110:ALA:O	1:A:114:LEU:N	2	0.11
(1,80)	1:A:110:ALA:O	1:B:114:LEU:N	2	0.11
(1,80)	1:B:110:ALA:O	1:A:114:LEU:N	2	0.11
(1,80)	1:B:110:ALA:O	1:B:114:LEU:N	2	0.11
(1,80)	1:A:110:ALA:O	1:A:114:LEU:N	4	0.11
(1,80)	1:A:110:ALA:O	1:B:114:LEU:N	4	0.11
(1,80)	1:B:110:ALA:O	1:A:114:LEU:N	4	0.11
(1,80)	1:B:110:ALA:O	1:B:114:LEU:N	4	0.11
(1,80)	1:A:110:ALA:O	1:A:114:LEU:N	10	0.11
(1,80)	1:A:110:ALA:O	1:B:114:LEU:N	10	0.11
(1,80)	1:B:110:ALA:O	1:A:114:LEU:N	10	0.11
(1,80)	1:B:110:ALA:O	1:B:114:LEU:N	10	0.11
(1,78)	1:A:108:ALA:O	1:A:112:LYS:N	18	0.11
(1,78)	1:A:108:ALA:O	1:B:112:LYS:N	18	0.11
(1,78)	1:B:108:ALA:O	1:A:112:LYS:N	18	0.11
(1,78)	1:B:108:ALA:O	1:B:112:LYS:N	18	0.11
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	3	0.11
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	3	0.11
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	3	0.11
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:A:107:ASP:O	1:A:111:ALA:H	19	0.11
(1,75)	1:A:107:ASP:O	1:B:111:ALA:H	19	0.11
(1,75)	1:B:107:ASP:O	1:A:111:ALA:H	19	0.11
(1,75)	1:B:107:ASP:O	1:B:111:ALA:H	19	0.11
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	10	0.11
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	10	0.11
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	10	0.11
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	10	0.11
(1,73)	1:A:80:THR:O	1:A:100:ARG:H	16	0.11
(1,73)	1:A:80:THR:O	1:B:100:ARG:H	16	0.11
(1,73)	1:B:80:THR:O	1:A:100:ARG:H	16	0.11
(1,73)	1:B:80:THR:O	1:B:100:ARG:H	16	0.11
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	3	0.11
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	3	0.11
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	3	0.11
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	3	0.11
(1,71)	1:A:80:THR:H	1:A:100:ARG:O	13	0.11
(1,71)	1:A:80:THR:H	1:B:100:ARG:O	13	0.11
(1,71)	1:B:80:THR:H	1:A:100:ARG:O	13	0.11
(1,71)	1:B:80:THR:H	1:B:100:ARG:O	13	0.11
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	2	0.11
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	2	0.11
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	2	0.11
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	2	0.11
(1,7)	1:A:19:ALA:O	1:A:28:VAL:H	19	0.11
(1,7)	1:A:19:ALA:O	1:B:28:VAL:H	19	0.11
(1,7)	1:B:19:ALA:O	1:A:28:VAL:H	19	0.11
(1,7)	1:B:19:ALA:O	1:B:28:VAL:H	19	0.11
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	4	0.11
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	4	0.11
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	4	0.11
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	4	0.11
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	12	0.11
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	12	0.11
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	12	0.11
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	12	0.11
(1,69)	1:A:82:GLU:O	1:A:98:GLU:H	20	0.11
(1,69)	1:A:82:GLU:O	1:B:98:GLU:H	20	0.11
(1,69)	1:B:82:GLU:O	1:A:98:GLU:H	20	0.11
(1,69)	1:B:82:GLU:O	1:B:98:GLU:H	20	0.11
(1,64)	1:A:99:LEU:O	1:A:137:VAL:N	1	0.11
(1,64)	1:A:99:LEU:O	1:B:137:VAL:N	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:B:99:LEU:O	1:A:137:VAL:N	1	0.11
(1,64)	1:B:99:LEU:O	1:B:137:VAL:N	1	0.11
(1,64)	1:A:99:LEU:O	1:A:137:VAL:N	6	0.11
(1,64)	1:A:99:LEU:O	1:B:137:VAL:N	6	0.11
(1,64)	1:B:99:LEU:O	1:A:137:VAL:N	6	0.11
(1,64)	1:B:99:LEU:O	1:B:137:VAL:N	6	0.11
(1,64)	1:A:99:LEU:O	1:A:137:VAL:N	11	0.11
(1,64)	1:A:99:LEU:O	1:B:137:VAL:N	11	0.11
(1,64)	1:B:99:LEU:O	1:A:137:VAL:N	11	0.11
(1,64)	1:B:99:LEU:O	1:B:137:VAL:N	11	0.11
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	13	0.11
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	13	0.11
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	13	0.11
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	13	0.11
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	15	0.11
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	15	0.11
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	15	0.11
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	15	0.11
(1,62)	1:A:82:GLU:N	1:A:98:GLU:O	16	0.11
(1,62)	1:A:82:GLU:N	1:B:98:GLU:O	16	0.11
(1,62)	1:B:82:GLU:N	1:A:98:GLU:O	16	0.11
(1,62)	1:B:82:GLU:N	1:B:98:GLU:O	16	0.11
(1,59)	1:A:84:GLY:O	1:A:96:ASP:H	6	0.11
(1,59)	1:A:84:GLY:O	1:B:96:ASP:H	6	0.11
(1,59)	1:B:84:GLY:O	1:A:96:ASP:H	6	0.11
(1,59)	1:B:84:GLY:O	1:B:96:ASP:H	6	0.11
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	8	0.11
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	8	0.11
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	8	0.11
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	8	0.11
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	11	0.11
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	11	0.11
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	11	0.11
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	11	0.11
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	13	0.11
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	13	0.11
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	13	0.11
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	13	0.11
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	16	0.11
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	16	0.11
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	16	0.11
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:A:97:VAL:O	1:A:135:ARG:H	18	0.11
(1,57)	1:A:97:VAL:O	1:B:135:ARG:H	18	0.11
(1,57)	1:B:97:VAL:O	1:A:135:ARG:H	18	0.11
(1,57)	1:B:97:VAL:O	1:B:135:ARG:H	18	0.11
(1,55)	1:A:84:GLY:H	1:A:96:ASP:O	14	0.11
(1,55)	1:A:84:GLY:H	1:B:96:ASP:O	14	0.11
(1,55)	1:B:84:GLY:H	1:A:96:ASP:O	14	0.11
(1,55)	1:B:84:GLY:H	1:B:96:ASP:O	14	0.11
(1,51)	1:A:88:ASN:H	1:A:92:GLY:O	6	0.11
(1,51)	1:A:88:ASN:H	1:B:92:GLY:O	6	0.11
(1,51)	1:B:88:ASN:H	1:A:92:GLY:O	6	0.11
(1,51)	1:B:88:ASN:H	1:B:92:GLY:O	6	0.11
(1,5)	1:A:17:GLY:O	1:A:30:LEU:H	15	0.11
(1,5)	1:A:17:GLY:O	1:B:30:LEU:H	15	0.11
(1,5)	1:B:17:GLY:O	1:A:30:LEU:H	15	0.11
(1,5)	1:B:17:GLY:O	1:B:30:LEU:H	15	0.11
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	2	0.11
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	2	0.11
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	2	0.11
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	2	0.11
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	13	0.11
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	13	0.11
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	13	0.11
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	13	0.11
(1,49)	1:A:86:GLY:O	1:A:94:ALA:H	19	0.11
(1,49)	1:A:86:GLY:O	1:B:94:ALA:H	19	0.11
(1,49)	1:B:86:GLY:O	1:A:94:ALA:H	19	0.11
(1,49)	1:B:86:GLY:O	1:B:94:ALA:H	19	0.11
(1,45)	1:A:62:MET:O	1:A:66:ALA:H	4	0.11
(1,45)	1:A:62:MET:O	1:B:66:ALA:H	4	0.11
(1,45)	1:B:62:MET:O	1:A:66:ALA:H	4	0.11
(1,45)	1:B:62:MET:O	1:B:66:ALA:H	4	0.11
(1,39)	1:A:58:PHE:O	1:A:62:MET:H	8	0.11
(1,39)	1:A:58:PHE:O	1:B:62:MET:H	8	0.11
(1,39)	1:B:58:PHE:O	1:A:62:MET:H	8	0.11
(1,39)	1:B:58:PHE:O	1:B:62:MET:H	8	0.11
(1,39)	1:A:58:PHE:O	1:A:62:MET:H	10	0.11
(1,39)	1:A:58:PHE:O	1:B:62:MET:H	10	0.11
(1,39)	1:B:58:PHE:O	1:A:62:MET:H	10	0.11
(1,39)	1:B:58:PHE:O	1:B:62:MET:H	10	0.11
(1,39)	1:A:58:PHE:O	1:A:62:MET:H	19	0.11
(1,39)	1:A:58:PHE:O	1:B:62:MET:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:B:58:PHE:O	1:A:62:MET:H	19	0.11
(1,39)	1:B:58:PHE:O	1:B:62:MET:H	19	0.11
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	1	0.11
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	1	0.11
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	1	0.11
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	1	0.11
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	2	0.11
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	2	0.11
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	2	0.11
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	2	0.11
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	4	0.11
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	4	0.11
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	4	0.11
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	4	0.11
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	5	0.11
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	5	0.11
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	5	0.11
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	5	0.11
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	11	0.11
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	11	0.11
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	11	0.11
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	11	0.11
(1,37)	1:A:54:TYR:O	1:A:58:PHE:H	16	0.11
(1,37)	1:A:54:TYR:O	1:B:58:PHE:H	16	0.11
(1,37)	1:B:54:TYR:O	1:A:58:PHE:H	16	0.11
(1,37)	1:B:54:TYR:O	1:B:58:PHE:H	16	0.11
(1,35)	1:A:53:GLY:O	1:A:57:CYS:H	4	0.11
(1,35)	1:A:53:GLY:O	1:B:57:CYS:H	4	0.11
(1,35)	1:B:53:GLY:O	1:A:57:CYS:H	4	0.11
(1,35)	1:B:53:GLY:O	1:B:57:CYS:H	4	0.11
(1,34)	1:A:52:ALA:O	1:A:56:ALA:N	1	0.11
(1,34)	1:A:52:ALA:O	1:B:56:ALA:N	1	0.11
(1,34)	1:B:52:ALA:O	1:A:56:ALA:N	1	0.11
(1,34)	1:B:52:ALA:O	1:B:56:ALA:N	1	0.11
(1,34)	1:A:52:ALA:O	1:A:56:ALA:N	8	0.11
(1,34)	1:A:52:ALA:O	1:B:56:ALA:N	8	0.11
(1,34)	1:B:52:ALA:O	1:A:56:ALA:N	8	0.11
(1,34)	1:B:52:ALA:O	1:B:56:ALA:N	8	0.11
(1,31)	1:A:51:ALA:O	1:A:55:SER:H	3	0.11
(1,31)	1:A:51:ALA:O	1:B:55:SER:H	3	0.11
(1,31)	1:B:51:ALA:O	1:A:55:SER:H	3	0.11
(1,31)	1:B:51:ALA:O	1:B:55:SER:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:A:51:ALA:O	1:A:55:SER:H	9	0.11
(1,31)	1:A:51:ALA:O	1:B:55:SER:H	9	0.11
(1,31)	1:B:51:ALA:O	1:A:55:SER:H	9	0.11
(1,31)	1:B:51:ALA:O	1:B:55:SER:H	9	0.11
(1,3)	1:A:12:THR:O	1:A:18:ARG:H	14	0.11
(1,3)	1:A:12:THR:O	1:B:18:ARG:H	14	0.11
(1,3)	1:B:12:THR:O	1:A:18:ARG:H	14	0.11
(1,3)	1:B:12:THR:O	1:B:18:ARG:H	14	0.11
(1,28)	1:A:49:LEU:O	1:A:53:GLY:N	2	0.11
(1,28)	1:A:49:LEU:O	1:B:53:GLY:N	2	0.11
(1,28)	1:B:49:LEU:O	1:A:53:GLY:N	2	0.11
(1,28)	1:B:49:LEU:O	1:B:53:GLY:N	2	0.11
(1,27)	1:A:49:LEU:O	1:A:53:GLY:H	4	0.11
(1,27)	1:A:49:LEU:O	1:B:53:GLY:H	4	0.11
(1,27)	1:B:49:LEU:O	1:A:53:GLY:H	4	0.11
(1,27)	1:B:49:LEU:O	1:B:53:GLY:H	4	0.11
(1,26)	1:A:48:GLN:O	1:A:52:ALA:N	10	0.11
(1,26)	1:A:48:GLN:O	1:B:52:ALA:N	10	0.11
(1,26)	1:B:48:GLN:O	1:A:52:ALA:N	10	0.11
(1,26)	1:B:48:GLN:O	1:B:52:ALA:N	10	0.11
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	4	0.11
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	4	0.11
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	4	0.11
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	4	0.11
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	11	0.11
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	11	0.11
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	11	0.11
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	11	0.11
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	15	0.11
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	15	0.11
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	15	0.11
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	15	0.11
(1,25)	1:A:48:GLN:O	1:A:52:ALA:H	17	0.11
(1,25)	1:A:48:GLN:O	1:B:52:ALA:H	17	0.11
(1,25)	1:B:48:GLN:O	1:A:52:ALA:H	17	0.11
(1,25)	1:B:48:GLN:O	1:B:52:ALA:H	17	0.11
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	10	0.11
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	10	0.11
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	10	0.11
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	10	0.11
(1,24)	1:A:47:GLU:O	1:A:51:ALA:N	12	0.11
(1,24)	1:A:47:GLU:O	1:B:51:ALA:N	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:B:47:GLU:O	1:A:51:ALA:N	12	0.11
(1,24)	1:B:47:GLU:O	1:B:51:ALA:N	12	0.11
(1,23)	1:A:47:GLU:O	1:A:51:ALA:H	19	0.11
(1,23)	1:A:47:GLU:O	1:B:51:ALA:H	19	0.11
(1,23)	1:B:47:GLU:O	1:A:51:ALA:H	19	0.11
(1,23)	1:B:47:GLU:O	1:B:51:ALA:H	19	0.11
(1,20)	1:A:31:SER:N	1:A:44:THR:O	4	0.11
(1,20)	1:A:31:SER:N	1:B:44:THR:O	4	0.11
(1,20)	1:B:31:SER:N	1:A:44:THR:O	4	0.11
(1,20)	1:B:31:SER:N	1:B:44:THR:O	4	0.11
(1,20)	1:A:31:SER:N	1:A:44:THR:O	6	0.11
(1,20)	1:A:31:SER:N	1:B:44:THR:O	6	0.11
(1,20)	1:B:31:SER:N	1:A:44:THR:O	6	0.11
(1,20)	1:B:31:SER:N	1:B:44:THR:O	6	0.11
(1,20)	1:A:31:SER:N	1:A:44:THR:O	7	0.11
(1,20)	1:A:31:SER:N	1:B:44:THR:O	7	0.11
(1,20)	1:B:31:SER:N	1:A:44:THR:O	7	0.11
(1,20)	1:B:31:SER:N	1:B:44:THR:O	7	0.11
(1,20)	1:A:31:SER:N	1:A:44:THR:O	10	0.11
(1,20)	1:A:31:SER:N	1:B:44:THR:O	10	0.11
(1,20)	1:B:31:SER:N	1:A:44:THR:O	10	0.11
(1,20)	1:B:31:SER:N	1:B:44:THR:O	10	0.11
(1,15)	1:A:19:ALA:H	1:A:28:VAL:O	5	0.11
(1,15)	1:A:19:ALA:H	1:B:28:VAL:O	5	0.11
(1,15)	1:B:19:ALA:H	1:A:28:VAL:O	5	0.11
(1,15)	1:B:19:ALA:H	1:B:28:VAL:O	5	0.11

10 Dihedral-angle violation analysis

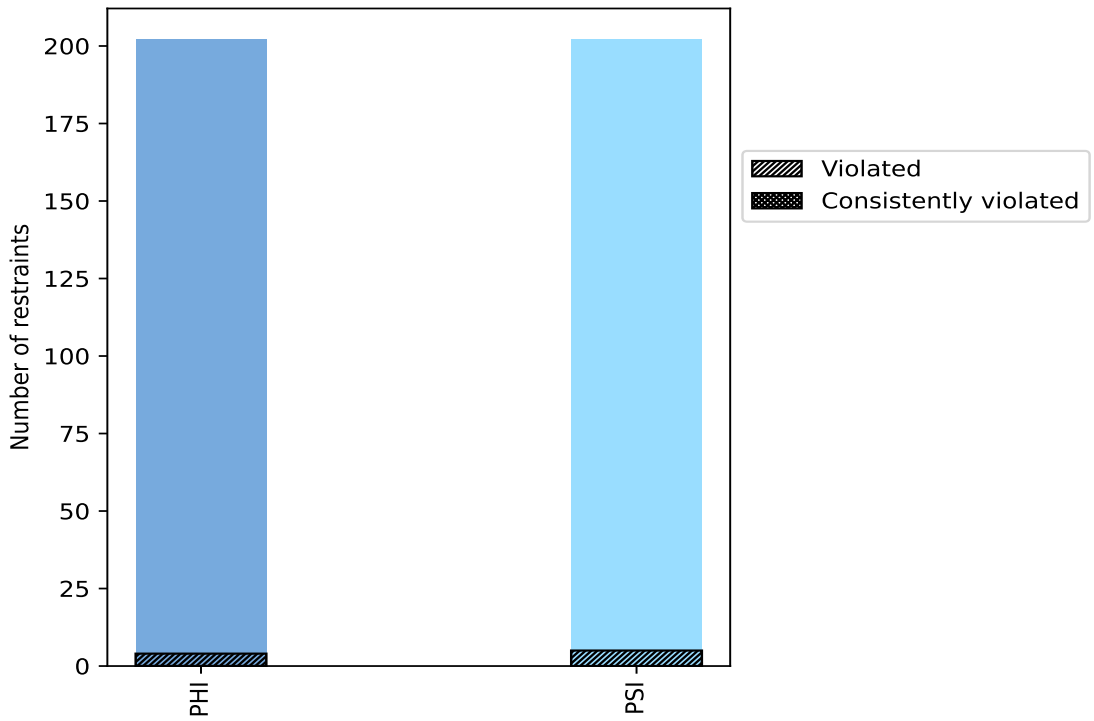
10.1 Summary of dihedral-angle violations

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	202	50.0	4	2.0	1.0	0	0.0	0.0
PSI	202	50.0	5	2.5	1.2	0	0.0	0.0
Total	404	100.0	9	2.2	2.2	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



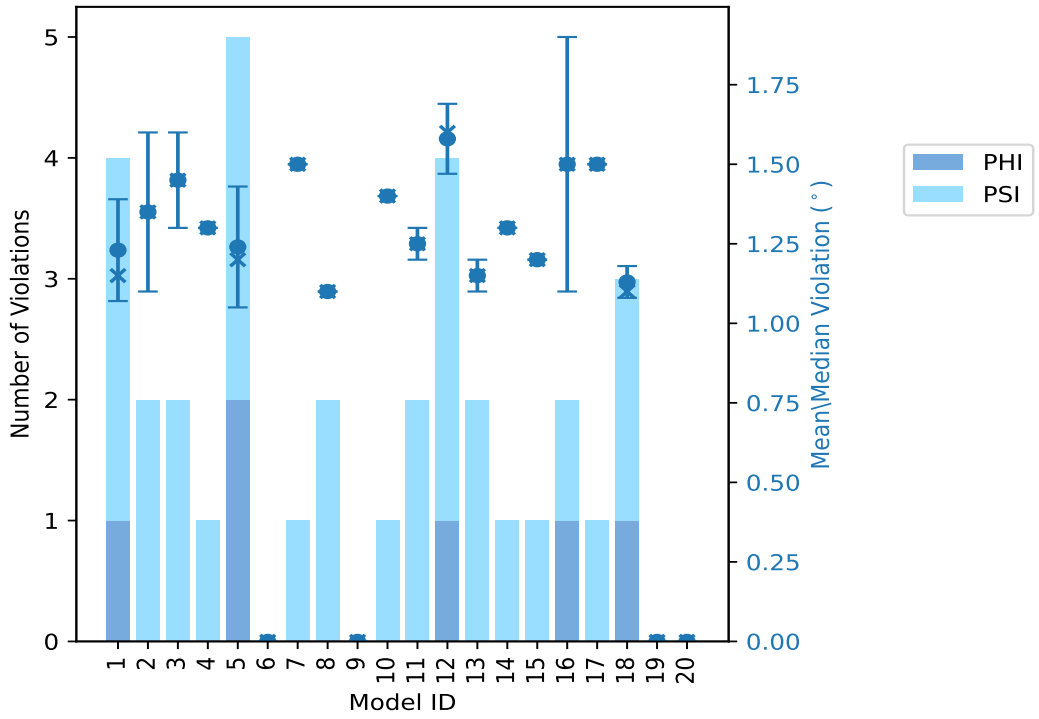
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	3	4	1.23	1.5	0.16	1.15
2	0	2	2	1.35	1.6	0.25	1.35
3	0	2	2	1.45	1.6	0.15	1.45
4	0	1	1	1.3	1.3	0.0	1.3
5	2	3	5	1.24	1.6	0.19	1.2
6	0	0	0	0.0	0.0	0.0	0.0
7	0	1	1	1.5	1.5	0.0	1.5
8	0	2	2	1.1	1.1	0.0	1.1
9	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	1.4	1.4	0.0	1.4
11	0	2	2	1.25	1.3	0.05	1.25
12	1	3	4	1.58	1.7	0.11	1.6
13	0	2	2	1.15	1.2	0.05	1.15
14	0	1	1	1.3	1.3	0.0	1.3
15	0	1	1	1.2	1.2	0.0	1.2
16	1	1	2	1.5	1.9	0.4	1.5
17	0	1	1	1.5	1.5	0.0	1.5
18	1	2	3	1.13	1.2	0.05	1.1
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
2	2	4	1	5.0
2	0	2	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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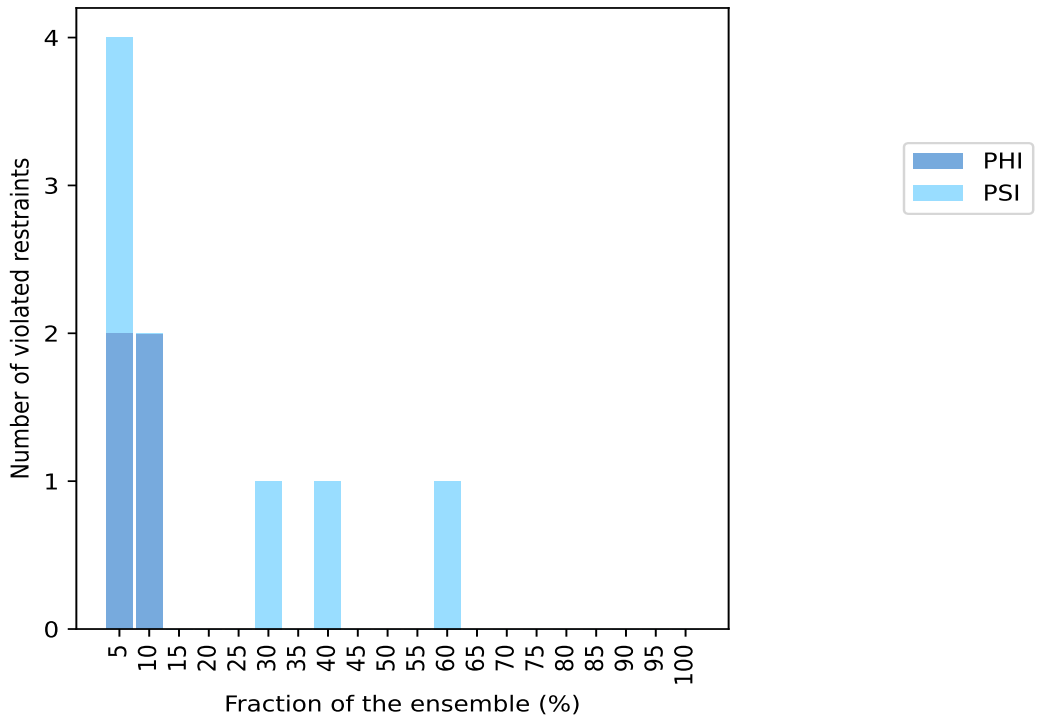
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	1	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

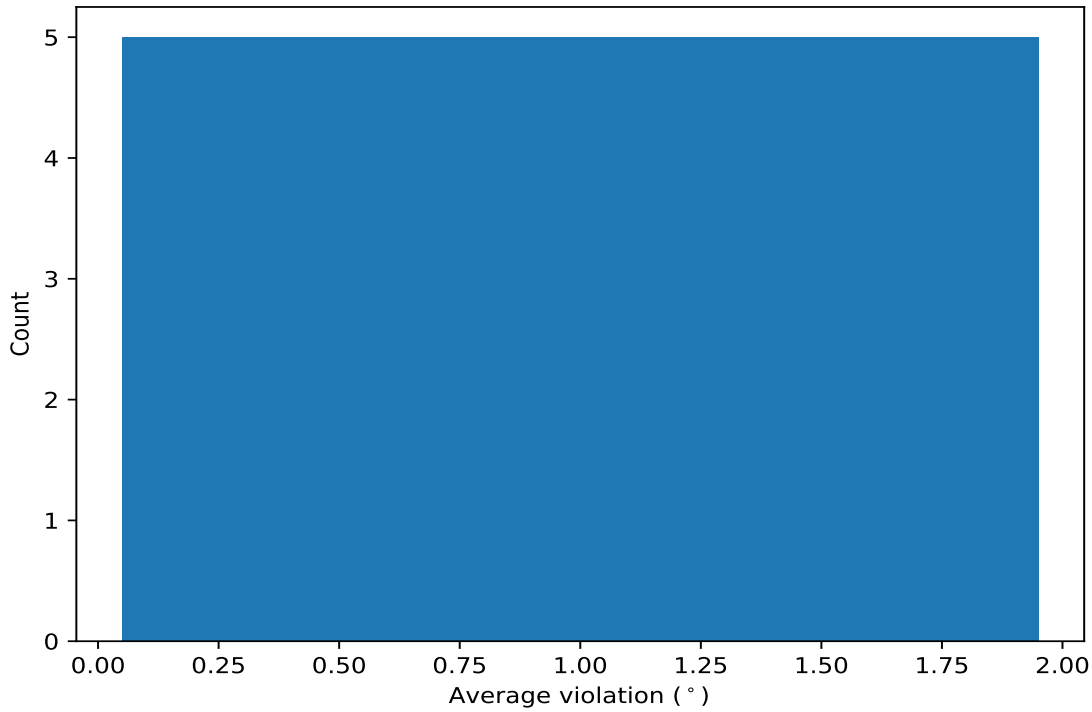


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation 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.

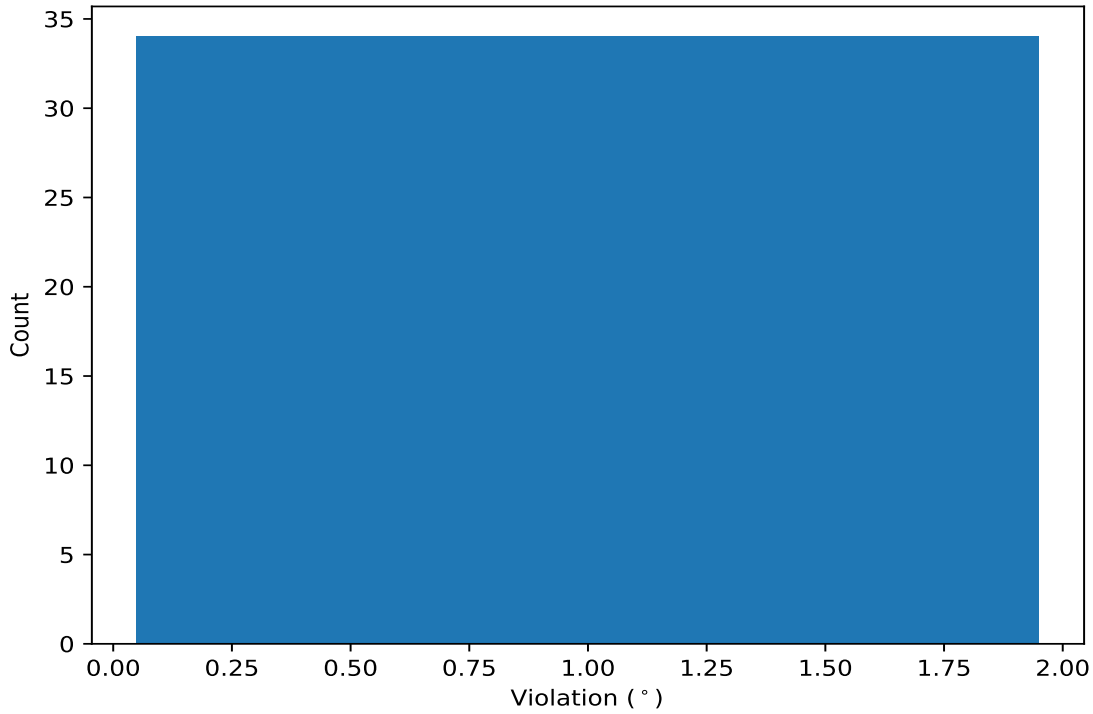
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	12	1.42	0.23	1.45
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	8	1.19	0.08	1.2
(1,47)	1:A:16:ASP:N	1:A:16:ASP:CA	1:A:16:ASP:C	1:A:17:GLY:N	6	1.38	0.23	1.35
(1,46)	1:B:15:ARG:C	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	2	1.35	0.25	1.35
(1,374)	1:B:129:ARG:C	1:B:130:ASN:N	1:B:130:ASN:CA	1:B:130:ASN:C	2	1.15	0.05	1.15

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints (i)

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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	16	1.9
(1,47)	1:A:16:ASP:N	1:A:16:ASP:CA	1:A:16:ASP:C	1:A:17:GLY:N	12	1.7
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	2	1.6
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	5	1.6
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	12	1.6
(1,47)	1:A:16:ASP:N	1:A:16:ASP:CA	1:A:16:ASP:C	1:A:17:GLY:N	3	1.6
(1,46)	1:B:15:ARG:C	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	12	1.6
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	7	1.5
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	17	1.5
(1,47)	1:A:16:ASP:N	1:A:16:ASP:CA	1:A:16:ASP:C	1:A:17:GLY:N	1	1.5
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	10	1.4
(1,44)	1:B:15:ARG:N	1:B:15:ARG:CA	1:B:15:ARG:C	1:B:16:ASP:N	12	1.4
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	11	1.3
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	14	1.3
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	3	1.3
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	4	1.3
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	13	1.2
(1,47)	1:A:16:ASP:N	1:A:16:ASP:CA	1:A:16:ASP:C	1:A:17:GLY:N	5	1.2
(1,47)	1:A:16:ASP:N	1:A:16:ASP:CA	1:A:16:ASP:C	1:A:17:GLY:N	18	1.2
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	1	1.2
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	11	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	15	1.2
(1,374)	1:B:129:ARG:C	1:B:130:ASN:N	1:B:130:ASN:CA	1:B:130:ASN:C	5	1.2
(1,69)	1:A:22:HIS:C	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	18	1.1
(1,55)	1:A:19:ALA:N	1:A:19:ALA:CA	1:A:19:ALA:C	1:A:20:THR:N	13	1.1
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	1	1.1
(1,48)	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	1:B:17:GLY:N	8	1.1
(1,47)	1:A:16:ASP:N	1:A:16:ASP:CA	1:A:16:ASP:C	1:A:17:GLY:N	8	1.1
(1,46)	1:B:15:ARG:C	1:B:16:ASP:N	1:B:16:ASP:CA	1:B:16:ASP:C	16	1.1
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	2	1.1
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	5	1.1
(1,403)	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1:A:139:ALA:N	18	1.1
(1,374)	1:B:129:ARG:C	1:B:130:ASN:N	1:B:130:ASN:CA	1:B:130:ASN:C	1	1.1
(1,373)	1:A:129:ARG:C	1:A:130:ASN:N	1:A:130:ASN:CA	1:A:130:ASN:C	5	1.1