Full wwPDB NMR Structure Validation Report (i)

Oct 12, 2023 – 01:21 pm BST

PDB ID	:	8A4F
BMRB ID	:	34736
Title	:	Human Interleukin-4 mutant - C3T-IL4
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Deposited on	:	2022-06-11

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

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

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

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

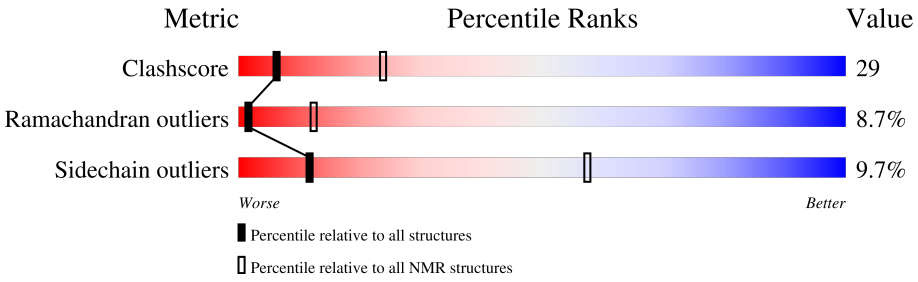
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 45%.

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	129	67% 22% 10%

2 Ensemble composition and analysis (i)

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2121 atoms, of which 1072 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interleukin-4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	129	2121	654	1072	192	197	6	0

There is a discrepancy between the modelled and reference sequences:

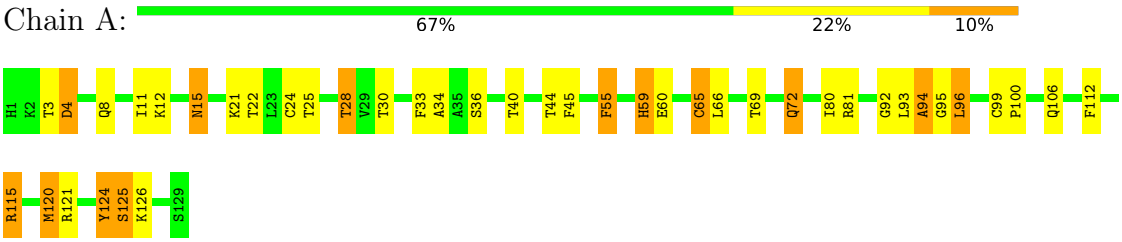
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	THR	CYS	engineered mutation	UNP P05112

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: Interleukin-4

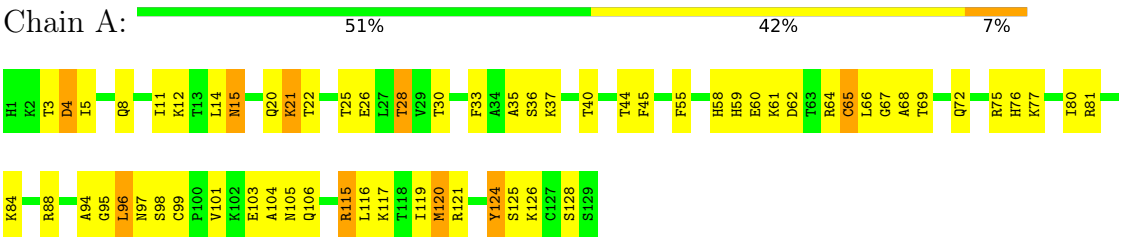


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

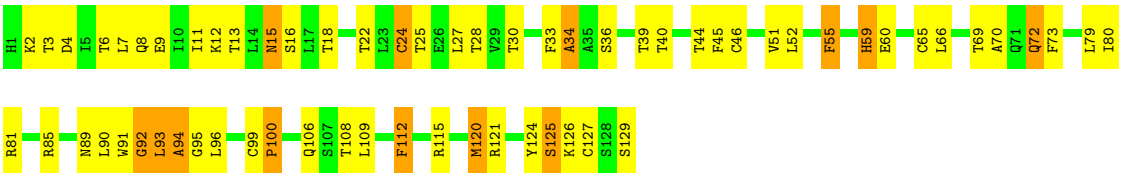
4.2.1 Score per residue for model 1

• Molecule 1: Interleukin-4



4.2.2 Score per residue for model 2

• Molecule 1: Interleukin-4


H1 K2 T3 D4 I5 T6 L7 Q8 E9 I10 I11 K12 T13 L14 N15 S16 L17 T18 T22 L23 C24 T25 E26 L27 T28 V29 T30 F33 A34 A35 S36 T39 T40 T44 F45 C46 V51 L52 F55 H59 E60 C65 L66 T69 A70 Q71 Q72 F73 L79 I80
R81 R85 N89 L90 W91 G92 L93 A94 G95 L96 C99 P100 Q106 S107 T108 L109 F112 R115 M120 R121 Y124 S125 K126 C127 S128 S129

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 200 calculated structures, 2 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	

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	835
Number of shifts mapped to atoms	835
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

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	1049	1072	1067	61±5
All	All	2098	2144	2134	122

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ASN:ND2	1:A:16:SER:H	0.66	1.88	2	1
1:A:15:ASN:ND2	1:A:16:SER:N	0.64	2.44	2	1
1:A:69:THR:H	1:A:72:GLN:HE21	0.63	1.35	1	1
1:A:12:LYS:O	1:A:15:ASN:ND2	0.63	2.32	2	1
1:A:8:GLN:NE2	1:A:124:TYR:CD1	0.62	2.68	2	1
1:A:81:ARG:NH1	1:A:85:ARG:NH1	0.61	2.48	2	1
1:A:120:MET:SD	1:A:120:MET:N	0.61	2.74	2	2
1:A:69:THR:H	1:A:72:GLN:NE2	0.60	1.95	1	1
1:A:39:THR:OG1	1:A:44:THR:N	0.60	2.35	2	1
1:A:27:LEU:O	1:A:109:LEU:N	0.59	2.35	2	1
1:A:9:GLU:O	1:A:13:THR:HG23	0.58	1.99	2	1
1:A:59:HIS:CD2	1:A:60:GLU:H	0.58	2.17	2	1
1:A:59:HIS:CD2	1:A:60:GLU:N	0.57	2.73	2	1
1:A:66:LEU:N	1:A:66:LEU:HD12	0.57	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:HIS:CG	1:A:60:GLU:N	0.56	2.70	2	1
1:A:33:PHE:O	1:A:34:ALA:O	0.55	2.24	2	1
1:A:92:GLY:O	1:A:94:ALA:N	0.55	2.38	2	1
1:A:106:GLN:H	1:A:106:GLN:CD	0.55	2.04	2	1
1:A:93:LEU:O	1:A:95:GLY:N	0.55	2.40	2	1
1:A:69:THR:N	1:A:72:GLN:HE21	0.54	2.00	1	1
1:A:62:ASP:OD1	1:A:65:CYS:N	0.54	2.40	1	1
1:A:89:ASN:C	1:A:91:TRP:H	0.54	2.06	2	1
1:A:7:LEU:N	1:A:7:LEU:HD22	0.54	2.18	2	1
1:A:124:TYR:O	1:A:126:LYS:N	0.54	2.40	2	2
1:A:117:LYS:NZ	1:A:121:ARG:NH1	0.53	2.55	1	1
1:A:72:GLN:N	1:A:72:GLN:OE1	0.53	2.41	2	1
1:A:59:HIS:O	1:A:59:HIS:CG	0.53	2.61	1	1
1:A:72:GLN:OE1	1:A:73:PHE:N	0.53	2.42	2	1
1:A:69:THR:O	1:A:72:GLN:OE1	0.53	2.27	2	1
1:A:24:CYS:N	1:A:65:CYS:SG	0.52	2.82	2	1
1:A:40:THR:O	1:A:44:THR:OG1	0.52	2.27	1	2
1:A:92:GLY:C	1:A:94:ALA:N	0.52	2.62	2	1
1:A:117:LYS:NZ	1:A:121:ARG:HH11	0.52	2.02	1	1
1:A:7:LEU:N	1:A:7:LEU:CD2	0.52	2.72	2	1
1:A:124:TYR:C	1:A:126:LYS:H	0.52	2.07	1	2
1:A:66:LEU:C	1:A:66:LEU:HD23	0.51	2.25	1	1
1:A:94:ALA:O	1:A:96:LEU:N	0.51	2.43	1	1
1:A:103:GLU:C	1:A:105:ASN:H	0.51	2.08	1	1
1:A:124:TYR:C	1:A:126:LYS:N	0.51	2.64	2	2
1:A:75:ARG:O	1:A:77:LYS:N	0.51	2.44	1	1
1:A:24:CYS:O	1:A:65:CYS:SG	0.51	2.69	2	1
1:A:2:LYS:NZ	1:A:4:ASP:OD2	0.50	2.43	2	1
1:A:46:CYS:O	1:A:99:CYS:SG	0.50	2.69	2	1
1:A:88:ARG:HH11	1:A:94:ALA:CB	0.50	2.19	1	1
1:A:15:ASN:CG	1:A:16:SER:N	0.50	2.64	2	1
1:A:94:ALA:C	1:A:96:LEU:N	0.50	2.65	1	1
1:A:66:LEU:N	1:A:66:LEU:CD1	0.50	2.75	2	1
1:A:72:GLN:O	1:A:75:ARG:N	0.49	2.46	1	1
1:A:67:GLY:O	1:A:68:ALA:HB3	0.49	2.08	1	1
1:A:89:ASN:C	1:A:91:TRP:N	0.49	2.66	2	1
1:A:96:LEU:N	1:A:96:LEU:HD12	0.49	2.23	2	1
1:A:116:LEU:O	1:A:120:MET:SD	0.48	2.71	1	1
1:A:124:TYR:C	1:A:124:TYR:CD1	0.48	2.87	1	1
1:A:66:LEU:HD23	1:A:67:GLY:N	0.48	2.23	1	1
1:A:15:ASN:HD22	1:A:15:ASN:N	0.48	2.06	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ARG:C	1:A:77:LYS:N	0.48	2.65	1	1
1:A:112:PHE:CD1	1:A:112:PHE:C	0.48	2.87	2	1
1:A:59:HIS:CG	1:A:60:GLU:H	0.48	2.27	2	1
1:A:93:LEU:C	1:A:95:GLY:N	0.48	2.65	2	1
1:A:55:PHE:CD2	1:A:55:PHE:C	0.48	2.84	2	1
1:A:5:ILE:O	1:A:5:ILE:HG22	0.47	2.10	1	1
1:A:92:GLY:C	1:A:94:ALA:H	0.47	2.13	2	1
1:A:103:GLU:C	1:A:105:ASN:N	0.47	2.67	1	1
1:A:89:ASN:O	1:A:91:TRP:N	0.47	2.48	2	1
1:A:96:LEU:N	1:A:96:LEU:CD1	0.47	2.77	2	1
1:A:11:ILE:HD12	1:A:12:LYS:N	0.46	2.26	2	1
1:A:22:THR:O	1:A:64:ARG:O	0.46	2.34	1	1
1:A:40:THR:O	1:A:44:THR:CB	0.46	2.63	1	2
1:A:105:ASN:O	1:A:106:GLN:NE2	0.46	2.49	1	1
1:A:8:GLN:O	1:A:12:LYS:CB	0.46	2.63	2	1
1:A:55:PHE:CD2	1:A:55:PHE:O	0.45	2.69	2	1
1:A:66:LEU:HD12	1:A:66:LEU:H	0.45	1.70	2	1
1:A:79:LEU:O	1:A:80:ILE:C	0.45	2.55	2	1
1:A:103:GLU:O	1:A:105:ASN:N	0.45	2.49	1	1
1:A:11:ILE:HG22	1:A:12:LYS:N	0.45	2.27	1	1
1:A:69:THR:HG22	1:A:72:GLN:NE2	0.45	2.27	1	1
1:A:96:LEU:CD2	1:A:97:ASN:H	0.45	2.24	1	1
1:A:3:THR:CB	1:A:6:THR:HG1	0.45	2.25	2	1
1:A:4:ASP:OD2	1:A:124:TYR:OH	0.45	2.35	2	1
1:A:99:CYS:N	1:A:100:PRO:CD	0.44	2.81	2	1
1:A:58:HIS:N	1:A:58:HIS:ND1	0.44	2.64	1	1
1:A:33:PHE:O	1:A:35:ALA:N	0.44	2.47	1	1
1:A:40:THR:N	1:A:44:THR:OG1	0.44	2.50	1	1
1:A:55:PHE:C	1:A:55:PHE:CD1	0.44	2.90	1	1
1:A:62:ASP:OD2	1:A:66:LEU:O	0.44	2.36	1	1
1:A:80:ILE:HG13	1:A:81:ARG:N	0.44	2.28	1	1
1:A:9:GLU:O	1:A:13:THR:CG2	0.44	2.65	2	1
1:A:36:SER:O	1:A:36:SER:OG	0.44	2.34	2	1
1:A:3:THR:OG1	1:A:6:THR:OG1	0.43	2.34	2	1
1:A:51:VAL:HG23	1:A:52:LEU:N	0.43	2.28	2	1
1:A:81:ARG:NH1	1:A:85:ARG:CZ	0.43	2.81	2	1
1:A:101:VAL:O	1:A:101:VAL:HG23	0.43	2.14	1	1
1:A:8:GLN:NE2	1:A:128:SER:OG	0.43	2.51	1	1
1:A:39:THR:OG1	1:A:40:THR:N	0.43	2.52	2	1
1:A:121:ARG:O	1:A:125:SER:CB	0.43	2.67	2	1
1:A:35:ALA:C	1:A:37:LYS:H	0.43	2.17	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ASN:O	1:A:117:LYS:NZ	0.43	2.52	1	1
1:A:127:CYS:C	1:A:129:SER:H	0.43	2.17	2	1
1:A:20:GLN:O	1:A:21:LYS:O	0.42	2.38	1	1
1:A:103:GLU:CD	1:A:106:GLN:HE22	0.42	2.17	1	1
1:A:72:GLN:OE1	1:A:72:GLN:C	0.42	2.58	2	1
1:A:69:THR:OG1	1:A:70:ALA:N	0.42	2.51	2	1
1:A:94:ALA:C	1:A:96:LEU:H	0.42	2.16	1	1
1:A:3:THR:O	1:A:4:ASP:OD2	0.42	2.37	1	1
1:A:14:LEU:N	1:A:14:LEU:HD12	0.42	2.30	1	1
1:A:81:ARG:HH11	1:A:85:ARG:NH1	0.42	2.10	2	1
1:A:121:ARG:O	1:A:125:SER:OG	0.42	2.37	2	1
1:A:28:THR:OG1	1:A:106:GLN:OE1	0.42	2.38	1	1
1:A:66:LEU:C	1:A:66:LEU:CD2	0.41	2.89	1	1
1:A:14:LEU:N	1:A:14:LEU:CD1	0.41	2.83	1	1
1:A:121:ARG:O	1:A:125:SER:N	0.41	2.52	2	1
1:A:127:CYS:C	1:A:129:SER:N	0.41	2.74	2	1
1:A:117:LYS:O	1:A:121:ARG:CB	0.41	2.69	1	1
1:A:11:ILE:O	1:A:15:ASN:ND2	0.41	2.53	1	1
1:A:119:ILE:N	1:A:119:ILE:CD1	0.40	2.83	1	1
1:A:115:ARG:CA	1:A:115:ARG:HE	0.40	2.29	1	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	127/129 (98%)	94±2 (74±1%)	22±0 (17±0%)	11±1 (9±1%)	1	12
All	All	254/258 (98%)	189 (74%)	43 (17%)	22 (9%)	1	12

All 21 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	125	SER	2
1	A	4	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	21	LYS	1
1	A	26	GLU	1
1	A	36	SER	1
1	A	60	GLU	1
1	A	61	LYS	1
1	A	65	CYS	1
1	A	76	HIS	1
1	A	95	GLY	1
1	A	98	SER	1
1	A	104	ALA	1
1	A	18	THR	1
1	A	25	THR	1
1	A	34	ALA	1
1	A	59	HIS	1
1	A	90	LEU	1
1	A	92	GLY	1
1	A	93	LEU	1
1	A	94	ALA	1
1	A	100	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	118/118 (100%)	106±0 (90±0%)	12±0 (10±0%)	12 57
All	All	236/236 (100%)	213 (90%)	23 (10%)	12 57

All 17 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	15	ASN	2
1	A	28	THR	2
1	A	30	THR	2
1	A	45	PHE	2
1	A	115	ARG	2
1	A	120	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	A	25	THR	1
1	A	84	LYS	1
1	A	96	LEU	1
1	A	99	CYS	1
1	A	124	TYR	1
1	A	22	THR	1
1	A	24	CYS	1
1	A	55	PHE	1
1	A	72	GLN	1
1	A	108	THR	1
1	A	112	PHE	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 45% for the well-defined parts and 45% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ChemicalShifts_c3tIL4_pH5_BMRB-STAR.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	835
Number of shifts mapped to atoms	835
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
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	124	-1.09 ± 0.35	Should be applied

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 45%, i.e. 820 atoms were assigned a chemical shift out of a possible 1836. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	375/646 (58%)	251/260 (97%)	0/258 (0%)	124/128 (97%)
Sidechain	443/1060 (42%)	443/683 (65%)	0/325 (0%)	0/52 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/130 (2%)	2/64 (3%)	0/55 (0%)	0/11 (0%)
Overall	820/1836 (45%)	696/1007 (69%)	0/638 (0%)	124/191 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 45%, i.e. 820 atoms were assigned a chemical shift out of a possible 1836. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	375/646 (58%)	251/260 (97%)	0/258 (0%)	124/128 (97%)
Sidechain	443/1060 (42%)	443/683 (65%)	0/325 (0%)	0/52 (0%)
Aromatic	2/130 (2%)	2/64 (3%)	0/55 (0%)	0/11 (0%)
Overall	820/1836 (45%)	696/1007 (69%)	0/638 (0%)	124/191 (65%)

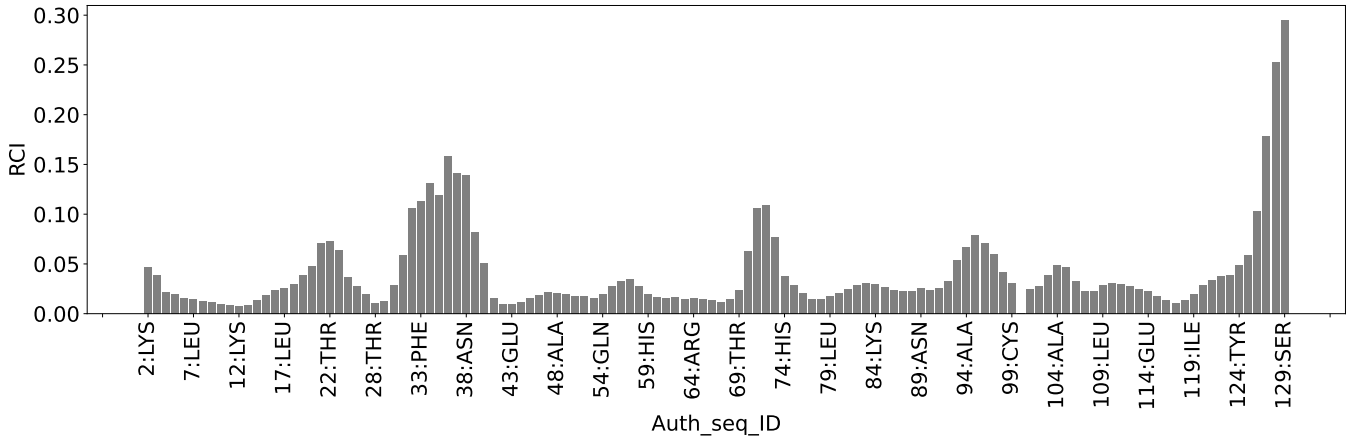
7.1.4 Statistically unusual chemical shifts (i)

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	1488
Intra-residue (|i-j|=0)	447
Sequential (|i-j|=1)	540
Medium range (|i-j|>1 and |i-j|<5)	357
Long range (|i-j|≥5)	56
Inter-chain	0
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	102
Number of unmapped restraints	0
Number of restraints per residue	12.3
Number of long range restraints per residue[1]	0.5

[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)	74.0	0.2
0.2-0.5 (Medium)	170.5	0.5
>0.5 (Large)	1032.0	8.27

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)	4.5	8.54
10.0-20.0 (Medium)	4.0	19.29
>20.0 (Large)	4.5	132.53

9 Distance violation analysis (i)

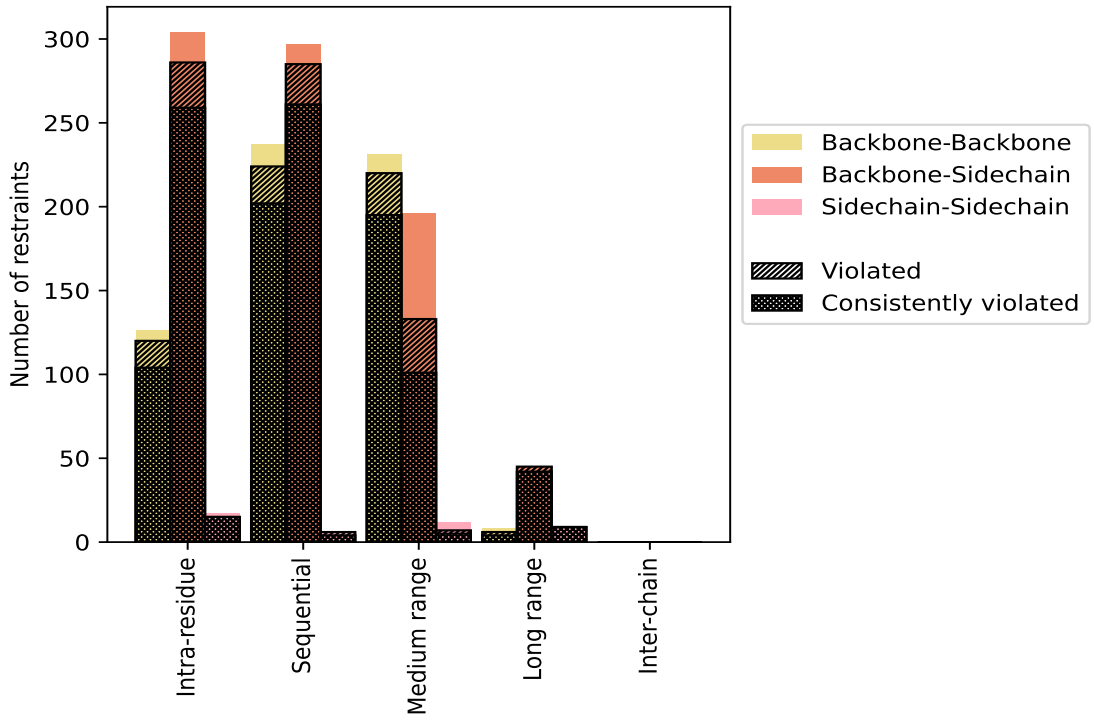
9.1 Summary of distance violations (i)

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)	447	30.0	421	94.2	28.3	378	84.6	25.4
Backbone-Backbone	126	8.5	120	95.2	8.1	104	82.5	7.0
Backbone-Sidechain	304	20.4	286	94.1	19.2	259	85.2	17.4
Sidechain-Sidechain	17	1.1	15	88.2	1.0	15	88.2	1.0
Sequential (|i-j|=1)	540	36.3	515	95.4	34.6	467	86.5	31.4
Backbone-Backbone	237	15.9	224	94.5	15.1	202	85.2	13.6
Backbone-Sidechain	297	20.0	285	96.0	19.2	261	87.9	17.5
Sidechain-Sidechain	6	0.4	6	100.0	0.4	4	66.7	0.3
Medium range (|i-j|>1 & |i-j|<5)	357	24.0	331	92.7	22.2	297	83.2	20.0
Backbone-Backbone	231	15.5	220	95.2	14.8	195	84.4	13.1
Backbone-Sidechain	114	7.7	104	91.2	7.0	97	85.1	6.5
Sidechain-Sidechain	12	0.8	7	58.3	0.5	5	41.7	0.3
Long range (|i-j|≥5)	56	3.8	54	96.4	3.6	52	92.9	3.5
Backbone-Backbone	8	0.5	6	75.0	0.4	4	50.0	0.3
Backbone-Sidechain	39	2.6	39	100.0	2.6	39	100.0	2.6
Sidechain-Sidechain	9	0.6	9	100.0	0.6	9	100.0	0.6
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	88	5.9	35	39.8	2.4	7	8.0	0.5
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1488	100.0	1356	91.1	91.1	1201	80.7	80.7
Backbone-Backbone	602	40.5	570	94.7	38.3	505	83.9	33.9
Backbone-Sidechain	842	56.6	749	89.0	50.3	663	78.7	44.6
Sidechain-Sidechain	44	3.0	37	84.1	2.5	33	75.0	2.2

[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

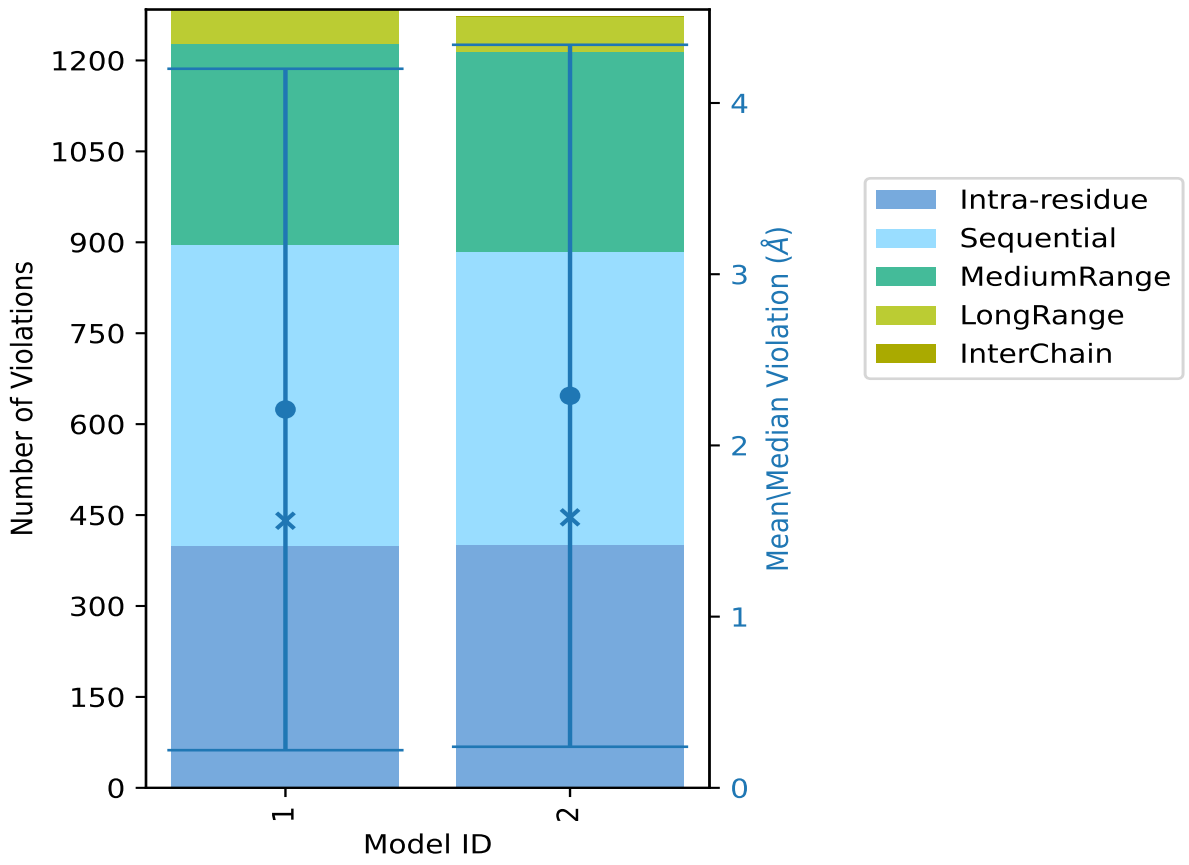
9.2 Distance violation statistics for each model

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	399	497	331	57	0	1284	2.21	8.19	1.99	1.56
2	400	485	330	58	0	1273	2.29	8.27	2.05	1.58

[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

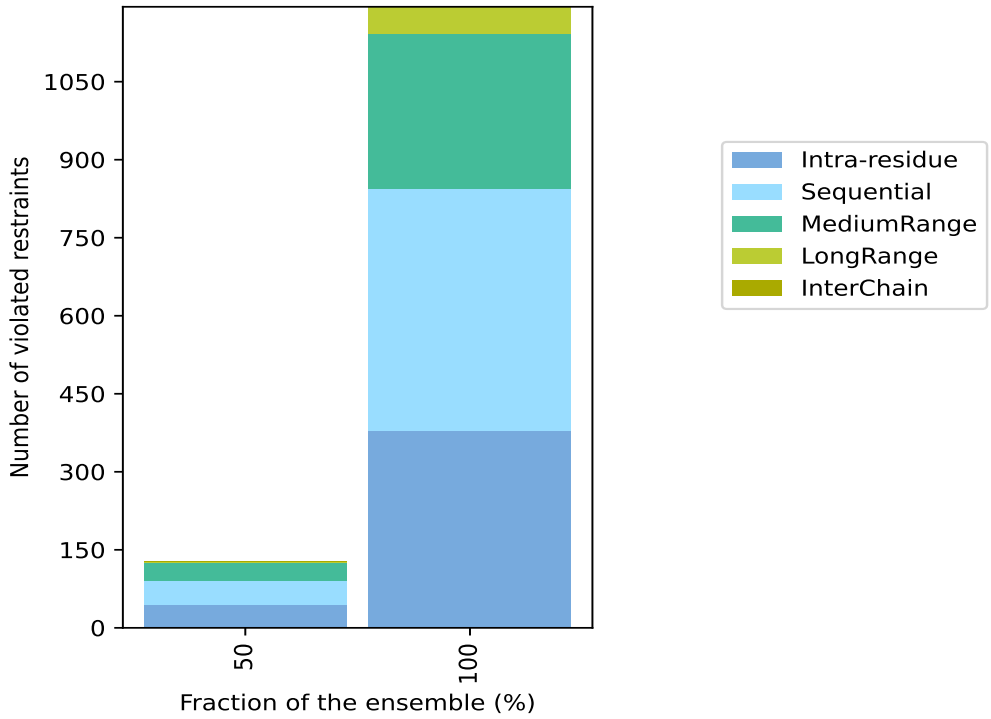
9.3 Distance violation statistics for the ensemble

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, 79(IR:26, SQ:25, MR:26, LR:2, 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]	%
43	48	34	2	0	127	1	50.0
378	467	297	52	0	1194	2	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

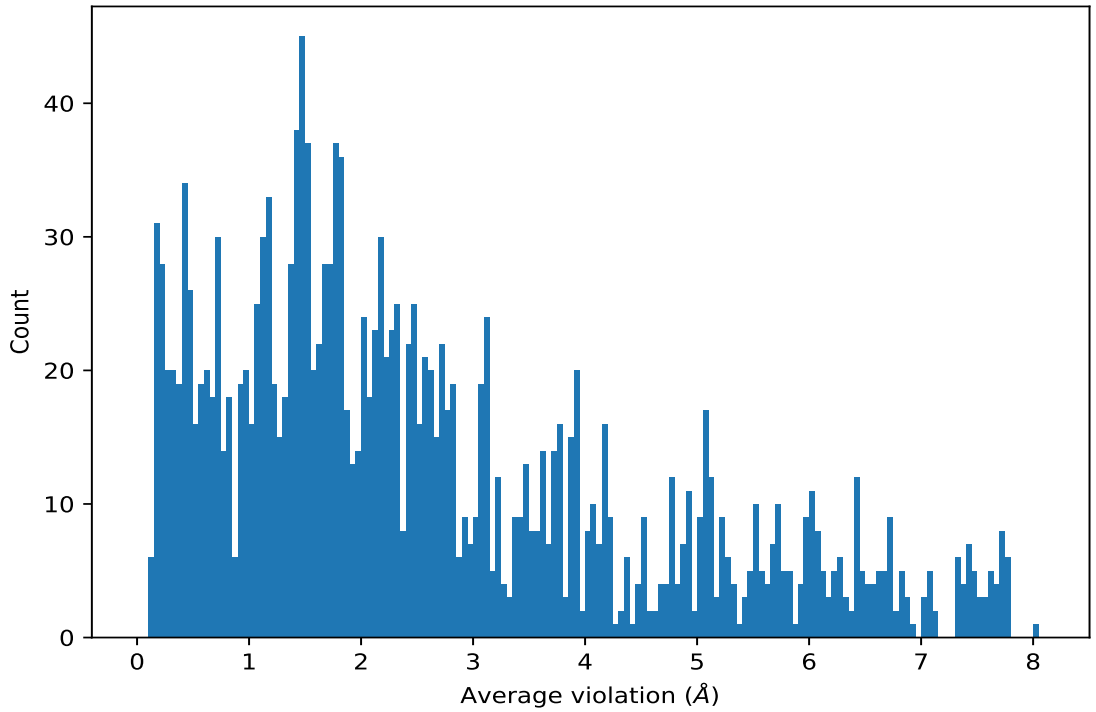
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(7,331)	1:93:A:LEU:HG	1:93:A:LEU:H	2	8.04	0.22	8.04
(7,170)	1:49:A:ALA:HB1	1:49:A:ALA:H	2	7.77	0.03	7.77
(7,170)	1:49:A:ALA:HB2	1:49:A:ALA:H	2	7.77	0.03	7.77
(7,170)	1:49:A:ALA:HB3	1:49:A:ALA:H	2	7.77	0.03	7.77
(7,21)	1:7:A:LEU:HD21	1:7:A:LEU:H	2	7.76	0.39	7.76
(7,21)	1:7:A:LEU:HD22	1:7:A:LEU:H	2	7.76	0.39	7.76
(7,21)	1:7:A:LEU:HD23	1:7:A:LEU:H	2	7.76	0.39	7.76
(7,42)	1:12:A:LYS:H	1:12:A:LYS:HB2	2	7.74	0.0	7.74
(7,42)	1:12:A:LYS:H	1:12:A:LYS:HB3	2	7.74	0.0	7.74
(7,398)	1:113:A:LEU:HB2	1:113:A:LEU:H	2	7.74	0.0	7.74
(7,398)	1:113:A:LEU:HB3	1:113:A:LEU:H	2	7.74	0.0	7.74
(7,74)	1:19:A:GLU:H	1:19:A:GLU:HG2	2	7.73	0.28	7.73
(7,150)	1:42:A:LYS:HB2	1:42:A:LYS:H	2	7.72	0.02	7.72
(7,47)	1:14:A:LEU:H	1:14:A:LEU:HB2	2	7.72	0.02	7.72
(6,184)	1:42:A:LYS:HB2	1:43:A:GLU:H	2	7.71	0.01	7.71
(7,30)	1:9:A:GLU:H	1:9:A:GLU:HB2	2	7.67	0.03	7.67

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,438)	1:126:A:LYS:HB2	1:126:A:LYS:H	2	7.67	0.0	7.67
(7,180)	1:52:A:LEU:HB2	1:52:A:LEU:H	2	7.66	0.05	7.66
(7,314)	1:90:A:LEU:HG	1:90:A:LEU:H	2	7.65	0.61	7.65
(7,26)	1:8:A:GLN:HB2	1:8:A:GLN:H	2	7.64	0.08	7.64
(7,289)	1:85:A:ARG:HB2	1:85:A:ARG:H	2	7.63	0.12	7.63
(7,289)	1:85:A:ARG:HB3	1:85:A:ARG:H	2	7.63	0.12	7.63
(7,301)	1:88:A:ARG:HB2	1:88:A:ARG:H	2	7.63	0.11	7.63
(7,301)	1:88:A:ARG:HB3	1:88:A:ARG:H	2	7.63	0.11	7.63
(6,354)	1:85:A:ARG:HB2	1:86:A:LEU:H	2	7.58	0.0	7.58
(6,354)	1:85:A:ARG:HB3	1:86:A:LEU:H	2	7.58	0.0	7.58
(7,282)	1:83:A:LEU:HB2	1:83:A:LEU:H	2	7.58	0.14	7.58
(7,237)	1:71:A:GLN:HB2	1:71:A:GLN:H	2	7.52	0.02	7.52
(7,313)	1:90:A:LEU:HB2	1:90:A:LEU:H	2	7.5	0.3	7.5
(7,386)	1:110:A:GLU:HB2	1:110:A:GLU:H	2	7.5	0.01	7.5
(7,408)	1:117:A:LYS:HB2	1:117:A:LYS:H	2	7.49	0.01	7.49
(6,496)	1:117:A:LYS:HB3	1:118:A:THR:H	2	7.47	0.01	7.47
(6,213)	1:48:A:ALA:HB1	1:49:A:ALA:H	2	7.46	0.02	7.46
(6,213)	1:48:A:ALA:HB2	1:49:A:ALA:H	2	7.46	0.02	7.46
(6,213)	1:48:A:ALA:HB3	1:49:A:ALA:H	2	7.46	0.02	7.46
(6,420)	1:100:A:PRO:HB2	1:101:A:VAL:H	2	7.44	0.58	7.44
(7,428)	1:123:A:LYS:HB3	1:123:A:LYS:H	2	7.44	0.0	7.44
(6,215)	1:49:A:ALA:HB1	1:50:A:THR:H	2	7.44	0.06	7.44
(6,215)	1:49:A:ALA:HB2	1:50:A:THR:H	2	7.44	0.06	7.44
(6,215)	1:49:A:ALA:HB3	1:50:A:THR:H	2	7.44	0.06	7.44
(7,407)	1:117:A:LYS:HB3	1:117:A:LYS:H	2	7.43	0.01	7.43
(6,540)	1:129:A:SER:H	1:128:A:SER:H	2	7.4	0.16	7.4
(7,429)	1:123:A:LYS:HB2	1:123:A:LYS:H	2	7.39	0.08	7.39
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD11	2	7.36	0.84	7.36
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD12	2	7.36	0.84	7.36
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD13	2	7.36	0.84	7.36
(6,486)	1:113:A:LEU:H	1:114:A:GLU:H	2	7.34	0.0	7.34
(7,433)	1:124:A:TYR:HB2	1:124:A:TYR:H	2	7.34	0.28	7.34
(6,371)	1:88:A:ARG:HB2	1:89:A:ASN:H	2	7.32	0.08	7.32
(6,371)	1:88:A:ARG:HB3	1:89:A:ASN:H	2	7.32	0.08	7.32
(6,513)	1:120:A:MET:HB2	1:121:A:ARG:H	2	7.32	0.01	7.32
(7,330)	1:93:A:LEU:HB2	1:93:A:LEU:H	2	7.32	0.19	7.32
(6,183)	1:42:A:LYS:HB3	1:43:A:GLU:H	2	7.14	0.08	7.14
(7,18)	1:7:A:LEU:HB2	1:7:A:LEU:H	2	7.12	0.64	7.12
(7,151)	1:42:A:LYS:HG3	1:42:A:LYS:H	2	7.08	0.0	7.08
(7,19)	1:7:A:LEU:HG	1:7:A:LEU:H	2	7.07	0.83	7.07
(7,333)	1:93:A:LEU:HD21	1:93:A:LEU:H	2	7.06	0.76	7.06
(7,333)	1:93:A:LEU:HD22	1:93:A:LEU:H	2	7.06	0.76	7.06

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,333)	1:93:A:LEU:HD23	1:93:A:LEU:H	2	7.06	0.76	7.06
(6,427)	1:102:A:LYS:HG2	1:103:A:GLU:H	2	7.01	0.9	7.01
(6,427)	1:102:A:LYS:HG3	1:103:A:GLU:H	2	7.01	0.9	7.01
(7,17)	1:7:A:LEU:HB3	1:7:A:LEU:H	2	7.0	0.52	7.0
(7,355)	1:102:A:LYS:HB2	1:102:A:LYS:H	2	6.91	0.32	6.91
(7,316)	1:90:A:LEU:HD21	1:90:A:LEU:H	2	6.86	0.88	6.86
(7,316)	1:90:A:LEU:HD22	1:90:A:LEU:H	2	6.86	0.88	6.86
(7,316)	1:90:A:LEU:HD23	1:90:A:LEU:H	2	6.86	0.88	6.86
(6,527)	1:124:A:TYR:HB2	1:125:A:SER:H	2	6.84	0.87	6.84
(4,30)	1:9:A:GLU:HA	1:13:A:THR:H	2	6.83	0.07	6.83
(7,437)	1:126:A:LYS:HB3	1:126:A:LYS:H	2	6.83	0.39	6.83
(6,345)	1:83:A:LEU:HB2	1:84:A:LYS:H	2	6.82	0.62	6.82
(6,381)	1:90:A:LEU:HB2	1:91:A:TRP:H	2	6.8	0.42	6.8
(7,48)	1:14:A:LEU:H	1:14:A:LEU:HG	2	6.78	0.58	6.78
(6,392)	1:93:A:LEU:HG	1:92:A:GLY:H	2	6.77	0.52	6.77
(7,265)	1:79:A:LEU:HG	1:79:A:LEU:H	2	6.74	1.08	6.74
(4,99)	1:35:A:ALA:HB1	1:37:A:LYS:H	2	6.74	0.65	6.74
(4,99)	1:35:A:ALA:HB2	1:37:A:LYS:H	2	6.74	0.65	6.74
(4,99)	1:35:A:ALA:HB3	1:37:A:LYS:H	2	6.74	0.65	6.74
(6,298)	1:72:A:GLN:HA	1:73:A:PHE:H	2	6.72	0.15	6.72
(7,332)	1:93:A:LEU:HD11	1:93:A:LEU:H	2	6.7	0.2	6.7
(7,332)	1:93:A:LEU:HD12	1:93:A:LEU:H	2	6.7	0.2	6.7
(7,332)	1:93:A:LEU:HD13	1:93:A:LEU:H	2	6.7	0.2	6.7
(7,302)	1:88:A:ARG:HG3	1:88:A:ARG:H	2	6.7	1.12	6.7
(4,164)	1:55:A:PHE:HA	1:58:A:HIS:H	2	6.68	0.04	6.68
(7,291)	1:85:A:ARG:HG2	1:85:A:ARG:H	2	6.67	1.34	6.67
(4,84)	1:31:A:ASP:HB3	1:33:A:PHE:H	2	6.66	0.56	6.66
(4,348)	1:124:A:TYR:HA	1:126:A:LYS:H	2	6.66	0.12	6.66
(4,142)	1:47:A:ARG:HA	1:50:A:THR:H	2	6.66	0.04	6.66
(7,84)	1:21:A:LYS:HG2	1:21:A:LYS:H	2	6.64	0.77	6.64
(7,84)	1:21:A:LYS:HG3	1:21:A:LYS:H	2	6.64	0.77	6.64
(6,512)	1:120:A:MET:HB3	1:121:A:ARG:H	2	6.63	0.01	6.63
(4,274)	1:92:A:GLY:HA2	1:94:A:ALA:H	2	6.62	0.5	6.62
(7,439)	1:126:A:LYS:HG3	1:126:A:LYS:H	2	6.6	0.88	6.6
(7,83)	1:21:A:LYS:HB2	1:21:A:LYS:H	2	6.58	0.05	6.58
(7,181)	1:52:A:LEU:HD11	1:52:A:LEU:H	2	6.57	0.07	6.57
(7,181)	1:52:A:LEU:HD12	1:52:A:LEU:H	2	6.57	0.07	6.57
(7,181)	1:52:A:LEU:HD13	1:52:A:LEU:H	2	6.57	0.07	6.57
(6,289)	1:71:A:GLN:HB2	1:72:A:GLN:H	2	6.52	0.06	6.52
(4,180)	1:62:A:ASP:HB3	1:64:A:ARG:H	2	6.52	0.24	6.52
(7,78)	1:20:A:GLN:H	1:20:A:GLN:HG2	2	6.51	0.48	6.51
(7,78)	1:20:A:GLN:H	1:20:A:GLN:HG3	2	6.51	0.48	6.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,312)	1:90:A:LEU:HB3	1:90:A:LEU:H	2	6.48	0.01	6.48
(4,275)	1:93:A:LEU:HA	1:95:A:GLY:H	2	6.48	0.42	6.48
(6,419)	1:100:A:PRO:HB3	1:101:A:VAL:H	2	6.45	0.14	6.45
(7,82)	1:21:A:LYS:HB3	1:21:A:LYS:H	2	6.45	0.48	6.45
(7,149)	1:42:A:LYS:HB3	1:42:A:LYS:H	2	6.45	0.02	6.45
(7,46)	1:14:A:LEU:H	1:14:A:LEU:HB3	2	6.44	0.01	6.44
(7,179)	1:52:A:LEU:HB3	1:52:A:LEU:H	2	6.44	0.01	6.44
(6,217)	1:50:A:THR:HA	1:51:A:VAL:H	2	6.43	0.0	6.43
(7,329)	1:93:A:LEU:HB3	1:93:A:LEU:H	2	6.43	0.02	6.43
(6,500)	1:118:A:THR:HA	1:119:A:ILE:H	2	6.42	0.0	6.42
(6,15)	1:7:A:LEU:H	1:6:A:THR:HA	2	6.42	0.02	6.42
(6,282)	1:69:A:THR:HB	1:70:A:ALA:H	2	6.41	0.07	6.41
(7,244)	1:72:A:GLN:HE21	1:72:A:GLN:H	2	6.41	0.19	6.41
(7,244)	1:72:A:GLN:HE22	1:72:A:GLN:H	2	6.41	0.19	6.41
(7,315)	1:90:A:LEU:HD11	1:90:A:LEU:H	2	6.4	0.12	6.4
(7,315)	1:90:A:LEU:HD12	1:90:A:LEU:H	2	6.4	0.12	6.4
(7,315)	1:90:A:LEU:HD13	1:90:A:LEU:H	2	6.4	0.12	6.4
(7,356)	1:102:A:LYS:HG2	1:102:A:LYS:H	2	6.36	0.51	6.36
(7,356)	1:102:A:LYS:HG3	1:102:A:LYS:H	2	6.36	0.51	6.36
(7,182)	1:52:A:LEU:HD21	1:52:A:LEU:H	2	6.31	0.07	6.31
(7,182)	1:52:A:LEU:HD22	1:52:A:LEU:H	2	6.31	0.07	6.31
(7,182)	1:52:A:LEU:HD23	1:52:A:LEU:H	2	6.31	0.07	6.31
(7,20)	1:7:A:LEU:HD11	1:7:A:LEU:H	2	6.26	0.05	6.26
(7,20)	1:7:A:LEU:HD12	1:7:A:LEU:H	2	6.26	0.05	6.26
(7,20)	1:7:A:LEU:HD13	1:7:A:LEU:H	2	6.26	0.05	6.26
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD21	2	6.26	0.12	6.26
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD22	2	6.26	0.12	6.26
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD23	2	6.26	0.12	6.26
(6,322)	1:79:A:LEU:HG	1:80:A:ILE:H	2	6.24	0.33	6.24
(6,444)	1:106:A:GLN:H	1:105:A:ASN:H	2	6.22	0.62	6.22
(4,100)	1:35:A:ALA:HB1	1:38:A:ASN:H	2	6.2	1.13	6.2
(4,100)	1:35:A:ALA:HB2	1:38:A:ASN:H	2	6.2	1.13	6.2
(4,100)	1:35:A:ALA:HB3	1:38:A:ASN:H	2	6.2	1.13	6.2
(6,506)	1:119:A:ILE:HG22	1:120:A:MET:H	2	6.18	0.31	6.18
(6,497)	1:117:A:LYS:HB2	1:118:A:THR:H	2	6.16	0.01	6.16
(6,380)	1:90:A:LEU:HB3	1:91:A:TRP:H	2	6.16	0.61	6.16
(7,290)	1:85:A:ARG:HG3	1:85:A:ARG:H	2	6.14	0.59	6.14
(4,349)	1:124:A:TYR:H	1:126:A:LYS:H	2	6.12	0.16	6.12
(6,332)	1:80:A:ILE:HD11	1:81:A:ARG:H	2	6.12	0.31	6.12
(6,332)	1:80:A:ILE:HD12	1:81:A:ARG:H	2	6.12	0.31	6.12
(6,332)	1:80:A:ILE:HD13	1:81:A:ARG:H	2	6.12	0.31	6.12
(6,534)	1:126:A:LYS:HB2	1:127:A:CYS:H	2	6.09	0.39	6.09

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,303)	1:88:A:ARG:HG2	1:88:A:ARG:H	2	6.08	0.57	6.08
(6,395)	1:93:A:LEU:HD11	1:94:A:ALA:H	2	6.05	0.09	6.05
(6,395)	1:93:A:LEU:HD12	1:94:A:ALA:H	2	6.05	0.09	6.05
(6,395)	1:93:A:LEU:HD13	1:94:A:ALA:H	2	6.05	0.09	6.05
(6,395)	1:93:A:LEU:HD21	1:94:A:ALA:H	2	6.05	0.09	6.05
(6,395)	1:93:A:LEU:HD22	1:94:A:ALA:H	2	6.05	0.09	6.05
(6,395)	1:93:A:LEU:HD23	1:94:A:ALA:H	2	6.05	0.09	6.05
(6,95)	1:21:A:LYS:HB3	1:22:A:THR:H	2	6.04	0.01	6.04
(4,161)	1:55:A:PHE:HE1	1:59:A:HIS:H	2	6.04	0.25	6.04
(4,161)	1:55:A:PHE:HE2	1:59:A:HIS:H	2	6.04	0.25	6.04
(7,288)	1:85:A:ARG:HD2	1:85:A:ARG:H	2	6.04	0.32	6.04
(7,288)	1:85:A:ARG:HD3	1:85:A:ARG:H	2	6.04	0.32	6.04
(6,533)	1:126:A:LYS:HB3	1:127:A:CYS:H	2	6.04	0.21	6.04
(4,134)	1:45:A:PHE:HA	1:49:A:ALA:H	2	6.02	0.0	6.02
(6,3)	1:3:A:THR:HG21	1:4:A:ASP:H	2	6.02	0.0	6.02
(6,3)	1:3:A:THR:HG22	1:4:A:ASP:H	2	6.02	0.0	6.02
(6,3)	1:3:A:THR:HG23	1:4:A:ASP:H	2	6.02	0.0	6.02
(7,253)	1:75:A:ARG:HD2	1:75:A:ARG:H	2	6.01	0.53	6.01
(4,157)	1:55:A:PHE:HD1	1:58:A:HIS:H	2	5.98	0.3	5.98
(4,157)	1:55:A:PHE:HD2	1:58:A:HIS:H	2	5.98	0.3	5.98
(4,152)	1:51:A:VAL:HA	1:55:A:PHE:H	2	5.97	0.11	5.97
(7,400)	1:113:A:LEU:HD11	1:113:A:LEU:H	2	5.97	0.02	5.97
(7,400)	1:113:A:LEU:HD12	1:113:A:LEU:H	2	5.97	0.02	5.97
(7,400)	1:113:A:LEU:HD13	1:113:A:LEU:H	2	5.97	0.02	5.97
(4,344)	1:122:A:GLU:HA	1:125:A:SER:H	2	5.97	0.0	5.97
(6,426)	1:102:A:LYS:HB2	1:103:A:GLU:H	2	5.96	0.04	5.96
(7,152)	1:42:A:LYS:HG2	1:42:A:LYS:H	2	5.96	0.03	5.96
(4,272)	1:92:A:GLY:HA2	1:95:A:GLY:H	2	5.94	0.82	5.94
(7,210)	1:60:A:GLU:HG2	1:60:A:GLU:H	2	5.94	0.58	5.94
(4,354)	1:127:A:CYS:H	1:129:A:SER:H	2	5.9	0.94	5.9
(7,24)	1:8:A:GLN:HG2	1:8:A:GLN:H	2	5.9	0.35	5.9
(7,440)	1:126:A:LYS:HG2	1:126:A:LYS:H	2	5.88	0.44	5.88
(6,297)	1:72:A:GLN:HB2	1:73:A:PHE:H	2	5.84	0.08	5.84
(6,394)	1:93:A:LEU:HG	1:94:A:ALA:H	2	5.83	0.08	5.83
(4,59)	1:17:A:LEU:HA	1:20:A:GLN:H	2	5.82	0.71	5.82
(7,273)	1:81:A:ARG:HD3	1:81:A:ARG:H	2	5.81	0.28	5.81
(6,413)	1:98:A:SER:H	1:99:A:CYS:H	2	5.8	0.07	5.8
(6,485)	1:113:A:LEU:HD21	1:114:A:GLU:H	2	5.78	0.02	5.78
(6,485)	1:113:A:LEU:HD22	1:114:A:GLU:H	2	5.78	0.02	5.78
(6,485)	1:113:A:LEU:HD23	1:114:A:GLU:H	2	5.78	0.02	5.78
(4,258)	1:86:A:LEU:HA	1:90:A:LEU:H	2	5.77	0.05	5.77
(6,378)	1:90:A:LEU:HG	1:89:A:ASN:H	2	5.76	0.45	5.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,206)	1:72:A:GLN:HB2	1:75:A:ARG:H	2	5.72	0.08	5.72
(7,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	2	5.72	0.0	5.72
(7,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	2	5.72	0.0	5.72
(7,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	2	5.72	0.0	5.72
(4,14)	1:8:A:GLN:H	1:6:A:THR:HA	2	5.7	0.1	5.7
(6,296)	1:72:A:GLN:HB3	1:73:A:PHE:H	2	5.7	0.31	5.7
(6,356)	1:85:A:ARG:HG2	1:86:A:LEU:H	2	5.7	0.12	5.7
(4,191)	1:69:A:THR:H	1:71:A:GLN:H	2	5.7	0.09	5.7
(6,96)	1:21:A:LYS:HB2	1:22:A:THR:H	2	5.7	0.23	5.7
(6,355)	1:85:A:ARG:HG3	1:86:A:LEU:H	2	5.7	0.32	5.7
(4,331)	1:118:A:THR:H	1:120:A:MET:H	2	5.68	0.15	5.68
(4,18)	1:7:A:LEU:HA	1:9:A:GLU:H	2	5.68	0.01	5.68
(4,32)	1:13:A:THR:H	1:9:A:GLU:HB3	2	5.66	0.09	5.66
(4,111)	1:40:A:THR:HG21	1:44:A:THR:H	2	5.66	0.15	5.66
(4,111)	1:40:A:THR:HG22	1:44:A:THR:H	2	5.66	0.15	5.66
(4,111)	1:40:A:THR:HG23	1:44:A:THR:H	2	5.66	0.15	5.66
(4,257)	1:86:A:LEU:H	1:88:A:ARG:H	2	5.66	0.04	5.66
(4,102)	1:36:A:SER:H	1:38:A:ASN:H	2	5.64	0.75	5.64
(4,268)	1:91:A:TRP:H	1:93:A:LEU:H	2	5.64	0.1	5.64
(4,129)	1:44:A:THR:HA	1:48:A:ALA:H	2	5.62	0.08	5.62
(4,181)	1:62:A:ASP:HB2	1:64:A:ARG:H	2	5.62	0.42	5.62
(7,274)	1:81:A:ARG:HD2	1:81:A:ARG:H	2	5.58	0.24	5.58
(4,85)	1:31:A:ASP:HB2	1:33:A:PHE:H	2	5.57	0.3	5.57
(7,252)	1:75:A:ARG:HD3	1:75:A:ARG:H	2	5.56	0.16	5.56
(4,98)	1:35:A:ALA:H	1:37:A:LYS:H	2	5.56	0.25	5.56
(7,399)	1:113:A:LEU:HG	1:113:A:LEU:H	2	5.56	0.0	5.56
(4,219)	1:74:A:HIS:H	1:76:A:HIS:H	2	5.52	0.4	5.52
(4,97)	1:34:A:ALA:H	1:36:A:SER:H	2	5.52	0.75	5.52
(6,284)	1:69:A:THR:H	1:70:A:ALA:H	2	5.51	0.07	5.51
(6,391)	1:93:A:LEU:HD11	1:92:A:GLY:H	2	5.51	0.68	5.51
(6,391)	1:93:A:LEU:HD12	1:92:A:GLY:H	2	5.51	0.68	5.51
(6,391)	1:93:A:LEU:HD13	1:92:A:GLY:H	2	5.51	0.68	5.51
(6,391)	1:93:A:LEU:HD21	1:92:A:GLY:H	2	5.51	0.68	5.51
(6,391)	1:93:A:LEU:HD22	1:92:A:GLY:H	2	5.51	0.68	5.51
(6,391)	1:93:A:LEU:HD23	1:92:A:GLY:H	2	5.51	0.68	5.51
(7,417)	1:119:A:ILE:HG22	1:119:A:ILE:H	2	5.5	0.11	5.5
(6,163)	1:37:A:LYS:HB2	1:36:A:SER:H	2	5.48	0.28	5.48
(6,163)	1:37:A:LYS:HB3	1:36:A:SER:H	2	5.48	0.28	5.48
(6,484)	1:113:A:LEU:HD11	1:114:A:GLU:H	2	5.45	0.0	5.45
(6,484)	1:113:A:LEU:HD12	1:114:A:GLU:H	2	5.45	0.0	5.45
(6,484)	1:113:A:LEU:HD13	1:114:A:GLU:H	2	5.45	0.0	5.45
(7,27)	1:8:A:GLN:HE21	1:8:A:GLN:H	2	5.44	0.15	5.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,27)	1:8:A:GLN:HE22	1:8:A:GLN:H	2	5.44	0.15	5.44
(4,150)	1:50:A:THR:HA	1:52:A:LEU:H	2	5.41	0.01	5.41
(4,309)	1:111:A:ASN:HA	1:113:A:LEU:H	2	5.38	0.14	5.38
(4,147)	1:49:A:ALA:HB1	1:52:A:LEU:H	2	5.32	0.02	5.32
(4,147)	1:49:A:ALA:HB2	1:52:A:LEU:H	2	5.32	0.02	5.32
(4,147)	1:49:A:ALA:HB3	1:52:A:LEU:H	2	5.32	0.02	5.32
(6,87)	1:20:A:GLN:HB2	1:19:A:GLU:H	2	5.3	0.34	5.3
(4,312)	1:111:A:ASN:H	1:114:A:GLU:H	2	5.28	0.02	5.28
(4,141)	1:47:A:ARG:H	1:50:A:THR:H	2	5.28	0.12	5.28
(4,156)	1:55:A:PHE:HD1	1:57:A:SER:H	2	5.28	0.07	5.28
(4,156)	1:55:A:PHE:HD2	1:57:A:SER:H	2	5.28	0.07	5.28
(4,254)	1:85:A:ARG:HB2	1:87:A:ASP:H	2	5.27	0.02	5.27
(4,254)	1:85:A:ARG:HB3	1:87:A:ASP:H	2	5.27	0.02	5.27
(4,95)	1:34:A:ALA:HB1	1:38:A:ASN:H	2	5.24	0.04	5.24
(4,95)	1:34:A:ALA:HB2	1:38:A:ASN:H	2	5.24	0.04	5.24
(4,95)	1:34:A:ALA:HB3	1:38:A:ASN:H	2	5.24	0.04	5.24
(6,295)	1:73:A:PHE:HB2	1:72:A:GLN:H	2	5.24	0.1	5.24
(4,220)	1:74:A:HIS:H	1:77:A:LYS:H	2	5.23	0.13	5.23
(4,343)	1:122:A:GLU:HA	1:124:A:TYR:H	2	5.22	0.23	5.22
(4,264)	1:88:A:ARG:HB2	1:90:A:LEU:H	2	5.22	0.19	5.22
(4,264)	1:88:A:ARG:HB3	1:90:A:LEU:H	2	5.22	0.19	5.22
(4,167)	1:55:A:PHE:HB3	1:57:A:SER:H	2	5.22	0.0	5.22
(4,65)	1:21:A:LYS:HA	1:23:A:LEU:H	2	5.16	1.05	5.16
(4,34)	1:13:A:THR:H	1:9:A:GLU:HG2	2	5.15	0.01	5.15
(4,34)	1:13:A:THR:H	1:9:A:GLU:HG3	2	5.15	0.01	5.15
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG21	2	5.14	0.22	5.14
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG22	2	5.14	0.22	5.14
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG23	2	5.14	0.22	5.14
(4,165)	1:55:A:PHE:HA	1:59:A:HIS:H	2	5.12	0.23	5.12
(6,273)	1:66:A:LEU:HB2	1:67:A:GLY:H	2	5.12	1.08	5.12
(6,273)	1:66:A:LEU:HB3	1:67:A:GLY:H	2	5.12	1.08	5.12
(6,405)	1:96:A:LEU:HD11	1:97:A:ASN:H	2	5.11	1.19	5.11
(6,405)	1:96:A:LEU:HD12	1:97:A:ASN:H	2	5.11	1.19	5.11
(6,405)	1:96:A:LEU:HD13	1:97:A:ASN:H	2	5.11	1.19	5.11
(6,405)	1:96:A:LEU:HD21	1:97:A:ASN:H	2	5.11	1.19	5.11
(6,405)	1:96:A:LEU:HD22	1:97:A:ASN:H	2	5.11	1.19	5.11
(6,405)	1:96:A:LEU:HD23	1:97:A:ASN:H	2	5.11	1.19	5.11
(4,108)	1:40:A:THR:HA	1:43:A:GLU:H	2	5.08	0.07	5.08
(4,198)	1:69:A:THR:HG21	1:72:A:GLN:HE21	2	5.07	0.48	5.07
(4,198)	1:69:A:THR:HG21	1:72:A:GLN:HE22	2	5.07	0.48	5.07
(4,198)	1:69:A:THR:HG22	1:72:A:GLN:HE21	2	5.07	0.48	5.07
(4,198)	1:69:A:THR:HG22	1:72:A:GLN:HE22	2	5.07	0.48	5.07

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,198)	1:69:A:THR:HG23	1:72:A:GLN:HE21	2	5.07	0.48	5.07
(4,198)	1:69:A:THR:HG23	1:72:A:GLN:HE22	2	5.07	0.48	5.07
(4,199)	1:69:A:THR:HG21	1:72:A:GLN:HE21	2	5.07	0.48	5.07
(4,199)	1:69:A:THR:HG21	1:72:A:GLN:HE22	2	5.07	0.48	5.07
(4,199)	1:69:A:THR:HG22	1:72:A:GLN:HE21	2	5.07	0.48	5.07
(4,199)	1:69:A:THR:HG22	1:72:A:GLN:HE22	2	5.07	0.48	5.07
(4,199)	1:69:A:THR:HG23	1:72:A:GLN:HE21	2	5.07	0.48	5.07
(4,199)	1:69:A:THR:HG23	1:72:A:GLN:HE22	2	5.07	0.48	5.07
(4,112)	1:43:A:GLU:HA	1:40:A:THR:H	2	5.07	0.08	5.07
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG21	2	5.06	0.02	5.06
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG22	2	5.06	0.02	5.06
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG23	2	5.06	0.02	5.06
(6,353)	1:85:A:ARG:HD2	1:86:A:LEU:H	2	5.04	0.09	5.04
(6,353)	1:85:A:ARG:HD3	1:86:A:LEU:H	2	5.04	0.09	5.04
(6,272)	1:66:A:LEU:HD11	1:67:A:GLY:H	2	5.03	0.49	5.03
(6,272)	1:66:A:LEU:HD12	1:67:A:GLY:H	2	5.03	0.49	5.03
(6,272)	1:66:A:LEU:HD13	1:67:A:GLY:H	2	5.03	0.49	5.03
(6,272)	1:66:A:LEU:HD21	1:67:A:GLY:H	2	5.03	0.49	5.03
(6,272)	1:66:A:LEU:HD22	1:67:A:GLY:H	2	5.03	0.49	5.03
(6,272)	1:66:A:LEU:HD23	1:67:A:GLY:H	2	5.03	0.49	5.03
(4,205)	1:72:A:GLN:HB3	1:75:A:ARG:H	2	5.01	0.03	5.01
(6,515)	1:120:A:MET:HG2	1:121:A:ARG:H	2	4.97	0.03	4.97
(6,514)	1:120:A:MET:HG3	1:121:A:ARG:H	2	4.96	0.03	4.96
(6,522)	1:124:A:TYR:HD1	1:123:A:LYS:H	2	4.94	0.36	4.94
(6,522)	1:124:A:TYR:HD2	1:123:A:LYS:H	2	4.94	0.36	4.94
(4,73)	1:25:A:THR:H	1:27:A:LEU:H	2	4.94	0.01	4.94
(4,177)	1:58:A:HIS:HA	1:60:A:GLU:H	2	4.92	1.44	4.92
(4,269)	1:91:A:TRP:HA	1:93:A:LEU:H	2	4.92	0.13	4.92
(7,341)	1:96:A:LEU:HD11	1:96:A:LEU:H	2	4.91	0.8	4.91
(7,341)	1:96:A:LEU:HD12	1:96:A:LEU:H	2	4.91	0.8	4.91
(7,341)	1:96:A:LEU:HD13	1:96:A:LEU:H	2	4.91	0.8	4.91
(7,341)	1:96:A:LEU:HD21	1:96:A:LEU:H	2	4.91	0.8	4.91
(7,341)	1:96:A:LEU:HD22	1:96:A:LEU:H	2	4.91	0.8	4.91
(7,341)	1:96:A:LEU:HD23	1:96:A:LEU:H	2	4.91	0.8	4.91
(4,160)	1:55:A:PHE:HE1	1:58:A:HIS:H	2	4.88	0.16	4.88
(4,160)	1:55:A:PHE:HE2	1:58:A:HIS:H	2	4.88	0.16	4.88
(4,175)	1:57:A:SER:HB2	1:59:A:HIS:H	2	4.88	0.08	4.88
(4,175)	1:57:A:SER:HB3	1:59:A:HIS:H	2	4.88	0.08	4.88
(6,249)	1:59:A:HIS:HD2	1:60:A:GLU:H	2	4.86	1.0	4.86
(6,249)	1:59:A:HIS:HD1	1:60:A:GLU:H	2	4.86	1.0	4.86
(4,266)	1:89:A:ASN:HA	1:93:A:LEU:H	2	4.86	0.01	4.86
(6,456)	1:109:A:LEU:HA	1:108:A:THR:H	2	4.81	0.57	4.81

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,418)	1:119:A:ILE:HD11	1:119:A:ILE:H	2	4.8	0.72	4.8
(7,418)	1:119:A:ILE:HD12	1:119:A:ILE:H	2	4.8	0.72	4.8
(7,418)	1:119:A:ILE:HD13	1:119:A:ILE:H	2	4.8	0.72	4.8
(2,31)	1:23:A:LEU:HD11	1:68:A:ALA:H	2	4.78	0.68	4.78
(2,31)	1:23:A:LEU:HD12	1:68:A:ALA:H	2	4.78	0.68	4.78
(2,31)	1:23:A:LEU:HD13	1:68:A:ALA:H	2	4.78	0.68	4.78
(2,31)	1:23:A:LEU:HD21	1:68:A:ALA:H	2	4.78	0.68	4.78
(2,31)	1:23:A:LEU:HD22	1:68:A:ALA:H	2	4.78	0.68	4.78
(2,31)	1:23:A:LEU:HD23	1:68:A:ALA:H	2	4.78	0.68	4.78
(7,80)	1:20:A:GLN:HE21	1:20:A:GLN:HG2	2	4.77	0.04	4.77
(7,80)	1:20:A:GLN:HE21	1:20:A:GLN:HG3	2	4.77	0.04	4.77
(7,80)	1:20:A:GLN:HE22	1:20:A:GLN:HG2	2	4.77	0.04	4.77
(7,80)	1:20:A:GLN:HE22	1:20:A:GLN:HG3	2	4.77	0.04	4.77
(6,525)	1:124:A:TYR:HD1	1:125:A:SER:H	2	4.76	0.87	4.76
(6,525)	1:124:A:TYR:HD2	1:125:A:SER:H	2	4.76	0.87	4.76
(4,63)	1:18:A:THR:HG1	1:20:A:GLN:H	2	4.72	0.15	4.72
(4,168)	1:55:A:PHE:HB3	1:58:A:HIS:H	2	4.72	0.09	4.72
(6,17)	1:6:A:THR:H	1:7:A:LEU:HA	2	4.72	0.04	4.72
(4,33)	1:13:A:THR:H	1:9:A:GLU:HB2	2	4.7	0.0	4.7
(6,86)	1:20:A:GLN:HB3	1:19:A:GLU:H	2	4.69	0.44	4.69
(6,116)	1:27:A:LEU:HD11	1:28:A:THR:H	2	4.68	0.06	4.68
(6,116)	1:27:A:LEU:HD12	1:28:A:THR:H	2	4.68	0.06	4.68
(6,116)	1:27:A:LEU:HD13	1:28:A:THR:H	2	4.68	0.06	4.68
(2,6)	1:31:A:ASP:H	1:105:A:ASN:HB2	2	4.6	0.46	4.6
(2,6)	1:31:A:ASP:H	1:105:A:ASN:HB3	2	4.6	0.46	4.6
(4,260)	1:87:A:ASP:HB3	1:90:A:LEU:H	2	4.59	0.36	4.59
(6,167)	1:39:A:THR:HB	1:38:A:ASN:H	2	4.56	0.25	4.56
(6,168)	1:39:A:THR:HG1	1:38:A:ASN:H	2	4.54	1.38	4.54
(4,197)	1:69:A:THR:HG21	1:72:A:GLN:H	2	4.51	0.14	4.51
(4,197)	1:69:A:THR:HG22	1:72:A:GLN:H	2	4.51	0.14	4.51
(4,197)	1:69:A:THR:HG23	1:72:A:GLN:H	2	4.51	0.14	4.51
(4,261)	1:87:A:ASP:HB2	1:90:A:LEU:H	2	4.5	0.25	4.5
(7,310)	1:89:A:ASN:HB2	1:89:A:ASN:HD21	2	4.5	0.33	4.5
(7,310)	1:89:A:ASN:HB2	1:89:A:ASN:HD22	2	4.5	0.33	4.5
(7,310)	1:89:A:ASN:HB3	1:89:A:ASN:HD21	2	4.5	0.33	4.5
(7,310)	1:89:A:ASN:HB3	1:89:A:ASN:HD22	2	4.5	0.33	4.5
(4,196)	1:69:A:THR:HG21	1:71:A:GLN:H	2	4.46	0.2	4.46
(4,196)	1:69:A:THR:HG22	1:71:A:GLN:H	2	4.46	0.2	4.46
(4,196)	1:69:A:THR:HG23	1:71:A:GLN:H	2	4.46	0.2	4.46
(6,415)	1:100:A:PRO:HG2	1:99:A:CYS:H	2	4.45	0.79	4.45
(6,414)	1:100:A:PRO:HG3	1:99:A:CYS:H	2	4.44	1.33	4.44
(6,403)	1:96:A:LEU:HD11	1:95:A:GLY:H	2	4.36	1.14	4.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,403)	1:96:A:LEU:HD12	1:95:A:GLY:H	2	4.36	1.14	4.36
(6,403)	1:96:A:LEU:HD13	1:95:A:GLY:H	2	4.36	1.14	4.36
(6,403)	1:96:A:LEU:HD21	1:95:A:GLY:H	2	4.36	1.14	4.36
(6,403)	1:96:A:LEU:HD22	1:95:A:GLY:H	2	4.36	1.14	4.36
(6,403)	1:96:A:LEU:HD23	1:95:A:GLY:H	2	4.36	1.14	4.36
(3,85)	1:30:A:THR:H	1:106:A:GLN:O	2	4.34	0.08	4.34
(4,49)	1:14:A:LEU:HA	1:18:A:THR:H	2	4.33	0.12	4.33
(4,211)	1:72:A:GLN:H	1:76:A:HIS:H	2	4.28	0.12	4.28
(6,357)	1:86:A:LEU:HD11	1:85:A:ARG:H	2	4.22	0.52	4.22
(6,357)	1:86:A:LEU:HD12	1:85:A:ARG:H	2	4.22	0.52	4.22
(6,357)	1:86:A:LEU:HD13	1:85:A:ARG:H	2	4.22	0.52	4.22
(2,26)	1:96:A:LEU:HD11	1:46:A:CYS:H	2	4.2	0.34	4.2
(2,26)	1:96:A:LEU:HD12	1:46:A:CYS:H	2	4.2	0.34	4.2
(2,26)	1:96:A:LEU:HD13	1:46:A:CYS:H	2	4.2	0.34	4.2
(2,26)	1:96:A:LEU:HD21	1:46:A:CYS:H	2	4.2	0.34	4.2
(2,26)	1:96:A:LEU:HD22	1:46:A:CYS:H	2	4.2	0.34	4.2
(2,26)	1:96:A:LEU:HD23	1:46:A:CYS:H	2	4.2	0.34	4.2
(2,22)	1:96:A:LEU:HD11	1:43:A:GLU:H	2	4.19	0.27	4.19
(2,22)	1:96:A:LEU:HD12	1:43:A:GLU:H	2	4.19	0.27	4.19
(2,22)	1:96:A:LEU:HD13	1:43:A:GLU:H	2	4.19	0.27	4.19
(2,22)	1:96:A:LEU:HD21	1:43:A:GLU:H	2	4.19	0.27	4.19
(2,22)	1:96:A:LEU:HD22	1:43:A:GLU:H	2	4.19	0.27	4.19
(2,22)	1:96:A:LEU:HD23	1:43:A:GLU:H	2	4.19	0.27	4.19
(4,315)	1:112:A:PHE:HD1	1:116:A:LEU:H	2	4.18	0.2	4.18
(4,315)	1:112:A:PHE:HD2	1:116:A:LEU:H	2	4.18	0.2	4.18
(7,79)	1:20:A:GLN:H	1:20:A:GLN:HE21	2	4.18	0.16	4.18
(7,79)	1:20:A:GLN:H	1:20:A:GLN:HE22	2	4.18	0.16	4.18
(6,324)	1:79:A:LEU:HD11	1:80:A:ILE:H	2	4.16	0.03	4.16
(6,324)	1:79:A:LEU:HD12	1:80:A:ILE:H	2	4.16	0.03	4.16
(6,324)	1:79:A:LEU:HD13	1:80:A:ILE:H	2	4.16	0.03	4.16
(6,324)	1:79:A:LEU:HD21	1:80:A:ILE:H	2	4.16	0.03	4.16
(6,324)	1:79:A:LEU:HD22	1:80:A:ILE:H	2	4.16	0.03	4.16
(6,324)	1:79:A:LEU:HD23	1:80:A:ILE:H	2	4.16	0.03	4.16
(4,276)	1:93:A:LEU:HA	1:96:A:LEU:H	2	4.14	0.69	4.14
(6,61)	1:16:A:SER:H	1:15:A:ASN:HD21	2	4.14	1.28	4.14
(6,61)	1:16:A:SER:H	1:15:A:ASN:HD22	2	4.14	1.28	4.14
(6,62)	1:16:A:SER:H	1:15:A:ASN:HD21	2	4.14	1.28	4.14
(6,62)	1:16:A:SER:H	1:15:A:ASN:HD22	2	4.14	1.28	4.14
(6,339)	1:82:A:PHE:HD1	1:83:A:LEU:H	2	4.12	0.47	4.12
(6,339)	1:82:A:PHE:HD2	1:83:A:LEU:H	2	4.12	0.47	4.12
(6,27)	1:8:A:GLN:HB3	1:9:A:GLU:H	2	4.08	0.45	4.08
(6,358)	1:86:A:LEU:HD21	1:85:A:ARG:H	2	4.06	0.4	4.06

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,358)	1:86:A:LEU:HD22	1:85:A:ARG:H	2	4.06	0.4	4.06
(6,358)	1:86:A:LEU:HD23	1:85:A:ARG:H	2	4.06	0.4	4.06
(7,226)	1:66:A:LEU:HD11	1:66:A:LEU:H	2	4.05	1.04	4.05
(7,226)	1:66:A:LEU:HD12	1:66:A:LEU:H	2	4.05	1.04	4.05
(7,226)	1:66:A:LEU:HD13	1:66:A:LEU:H	2	4.05	1.04	4.05
(7,226)	1:66:A:LEU:HD21	1:66:A:LEU:H	2	4.05	1.04	4.05
(7,226)	1:66:A:LEU:HD22	1:66:A:LEU:H	2	4.05	1.04	4.05
(7,226)	1:66:A:LEU:HD23	1:66:A:LEU:H	2	4.05	1.04	4.05
(7,108)	1:29:A:VAL:HG21	1:29:A:VAL:H	2	4.03	0.42	4.03
(7,108)	1:29:A:VAL:HG22	1:29:A:VAL:H	2	4.03	0.42	4.03
(7,108)	1:29:A:VAL:HG23	1:29:A:VAL:H	2	4.03	0.42	4.03
(7,277)	1:82:A:PHE:HD1	1:82:A:PHE:H	2	4.01	1.19	4.01
(7,277)	1:82:A:PHE:HD2	1:82:A:PHE:H	2	4.01	1.19	4.01
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD11	2	4.0	0.5	4.0
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD12	2	4.0	0.5	4.0
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD13	2	4.0	0.5	4.0
(4,22)	1:7:A:LEU:H	1:11:A:ILE:H	2	3.98	0.06	3.98
(4,79)	1:28:A:THR:HA	1:30:A:THR:H	2	3.97	0.17	3.97
(6,510)	1:120:A:MET:HB3	1:119:A:ILE:H	2	3.94	0.05	3.94
(2,24)	1:96:A:LEU:HD11	1:45:A:PHE:H	2	3.94	0.31	3.94
(2,24)	1:96:A:LEU:HD12	1:45:A:PHE:H	2	3.94	0.31	3.94
(2,24)	1:96:A:LEU:HD13	1:45:A:PHE:H	2	3.94	0.31	3.94
(2,24)	1:96:A:LEU:HD21	1:45:A:PHE:H	2	3.94	0.31	3.94
(2,24)	1:96:A:LEU:HD22	1:45:A:PHE:H	2	3.94	0.31	3.94
(2,24)	1:96:A:LEU:HD23	1:45:A:PHE:H	2	3.94	0.31	3.94
(4,280)	1:96:A:LEU:HD11	1:98:A:SER:H	2	3.93	0.12	3.93
(4,280)	1:96:A:LEU:HD12	1:98:A:SER:H	2	3.93	0.12	3.93
(4,280)	1:96:A:LEU:HD13	1:98:A:SER:H	2	3.93	0.12	3.93
(4,280)	1:96:A:LEU:HD21	1:98:A:SER:H	2	3.93	0.12	3.93
(4,280)	1:96:A:LEU:HD22	1:98:A:SER:H	2	3.93	0.12	3.93
(4,280)	1:96:A:LEU:HD23	1:98:A:SER:H	2	3.93	0.12	3.93
(2,32)	1:23:A:LEU:HD11	1:72:A:GLN:HE21	2	3.9	1.1	3.9
(2,32)	1:23:A:LEU:HD12	1:72:A:GLN:HE21	2	3.9	1.1	3.9
(2,32)	1:23:A:LEU:HD13	1:72:A:GLN:HE21	2	3.9	1.1	3.9
(2,32)	1:23:A:LEU:HD21	1:72:A:GLN:HE21	2	3.9	1.1	3.9
(2,32)	1:23:A:LEU:HD22	1:72:A:GLN:HE21	2	3.9	1.1	3.9
(2,32)	1:23:A:LEU:HD23	1:72:A:GLN:HE21	2	3.9	1.1	3.9
(4,151)	1:51:A:VAL:H	1:55:A:PHE:H	2	3.9	0.09	3.9
(7,359)	1:103:A:GLU:HG2	1:103:A:GLU:H	2	3.88	0.34	3.88
(7,359)	1:103:A:GLU:HG3	1:103:A:GLU:H	2	3.88	0.34	3.88
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD11	2	3.87	0.64	3.87
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD12	2	3.87	0.64	3.87

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD13	2	3.87	0.64	3.87
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD21	2	3.87	0.64	3.87
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD22	2	3.87	0.64	3.87
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD23	2	3.87	0.64	3.87
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD11	2	3.86	0.44	3.86
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD12	2	3.86	0.44	3.86
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD13	2	3.86	0.44	3.86
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD21	2	3.86	0.44	3.86
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD22	2	3.86	0.44	3.86
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD23	2	3.86	0.44	3.86
(4,267)	1:90:A:LEU:H	1:93:A:LEU:H	2	3.85	0.08	3.85
(6,28)	1:8:A:GLN:HB2	1:9:A:GLU:H	2	3.82	0.57	3.82
(7,190)	1:56:A:TYR:HD1	1:56:A:TYR:H	2	3.82	0.08	3.82
(7,190)	1:56:A:TYR:HD2	1:56:A:TYR:H	2	3.82	0.08	3.82
(7,372)	1:106:A:GLN:HG2	1:106:A:GLN:HE21	2	3.79	0.01	3.79
(7,372)	1:106:A:GLN:HG2	1:106:A:GLN:HE22	2	3.79	0.01	3.79
(7,372)	1:106:A:GLN:HG3	1:106:A:GLN:HE21	2	3.79	0.01	3.79
(7,372)	1:106:A:GLN:HG3	1:106:A:GLN:HE22	2	3.79	0.01	3.79
(6,144)	1:32:A:ILE:HD11	1:33:A:PHE:HE1	2	3.78	1.62	3.78
(6,144)	1:32:A:ILE:HD11	1:33:A:PHE:HE2	2	3.78	1.62	3.78
(6,144)	1:32:A:ILE:HD12	1:33:A:PHE:HE1	2	3.78	1.62	3.78
(6,144)	1:32:A:ILE:HD12	1:33:A:PHE:HE2	2	3.78	1.62	3.78
(6,144)	1:32:A:ILE:HD13	1:33:A:PHE:HE1	2	3.78	1.62	3.78
(6,144)	1:32:A:ILE:HD13	1:33:A:PHE:HE2	2	3.78	1.62	3.78
(4,293)	1:108:A:THR:HG21	1:111:A:ASN:HD21	2	3.76	0.12	3.76
(4,293)	1:108:A:THR:HG21	1:111:A:ASN:HD22	2	3.76	0.12	3.76
(4,293)	1:108:A:THR:HG22	1:111:A:ASN:HD21	2	3.76	0.12	3.76
(4,293)	1:108:A:THR:HG22	1:111:A:ASN:HD22	2	3.76	0.12	3.76
(4,293)	1:108:A:THR:HG23	1:111:A:ASN:HD21	2	3.76	0.12	3.76
(4,293)	1:108:A:THR:HG23	1:111:A:ASN:HD22	2	3.76	0.12	3.76
(6,93)	1:20:A:GLN:HG2	1:21:A:LYS:H	2	3.74	0.78	3.74
(6,93)	1:20:A:GLN:HG3	1:21:A:LYS:H	2	3.74	0.78	3.74
(4,159)	1:55:A:PHE:HE1	1:57:A:SER:H	2	3.72	0.08	3.72
(4,159)	1:55:A:PHE:HE2	1:57:A:SER:H	2	3.72	0.08	3.72
(6,256)	1:61:A:LYS:H	1:62:A:ASP:H	2	3.72	0.83	3.72
(2,23)	1:96:A:LEU:HD11	1:44:A:THR:H	2	3.72	0.38	3.72
(2,23)	1:96:A:LEU:HD12	1:44:A:THR:H	2	3.72	0.38	3.72
(2,23)	1:96:A:LEU:HD13	1:44:A:THR:H	2	3.72	0.38	3.72
(2,23)	1:96:A:LEU:HD21	1:44:A:THR:H	2	3.72	0.38	3.72
(2,23)	1:96:A:LEU:HD22	1:44:A:THR:H	2	3.72	0.38	3.72
(2,23)	1:96:A:LEU:HD23	1:44:A:THR:H	2	3.72	0.38	3.72
(7,111)	1:30:A:THR:HG21	1:30:A:THR:H	2	3.72	0.04	3.72

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,111)	1:30:A:THR:HG22	1:30:A:THR:H	2	3.72	0.04	3.72
(7,111)	1:30:A:THR:HG23	1:30:A:THR:H	2	3.72	0.04	3.72
(6,232)	1:56:A:TYR:HD1	1:55:A:PHE:H	2	3.68	0.12	3.68
(6,232)	1:56:A:TYR:HD2	1:55:A:PHE:H	2	3.68	0.12	3.68
(7,365)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	2	3.67	0.05	3.67
(7,365)	1:105:A:ASN:HB3	1:105:A:ASN:HD22	2	3.67	0.05	3.67
(2,34)	1:69:A:THR:HG21	1:75:A:ARG:H	2	3.66	0.13	3.66
(2,34)	1:69:A:THR:HG22	1:75:A:ARG:H	2	3.66	0.13	3.66
(2,34)	1:69:A:THR:HG23	1:75:A:ARG:H	2	3.66	0.13	3.66
(6,302)	1:73:A:PHE:HD1	1:74:A:HIS:H	2	3.64	0.08	3.64
(6,302)	1:73:A:PHE:HD2	1:74:A:HIS:H	2	3.64	0.08	3.64
(4,135)	1:48:A:ALA:H	1:45:A:PHE:HE1	2	3.64	0.12	3.64
(4,135)	1:48:A:ALA:H	1:45:A:PHE:HE2	2	3.64	0.12	3.64
(4,281)	1:96:A:LEU:HD11	1:99:A:CYS:H	2	3.62	0.68	3.62
(4,281)	1:96:A:LEU:HD12	1:99:A:CYS:H	2	3.62	0.68	3.62
(4,281)	1:96:A:LEU:HD13	1:99:A:CYS:H	2	3.62	0.68	3.62
(4,281)	1:96:A:LEU:HD21	1:99:A:CYS:H	2	3.62	0.68	3.62
(4,281)	1:96:A:LEU:HD22	1:99:A:CYS:H	2	3.62	0.68	3.62
(4,281)	1:96:A:LEU:HD23	1:99:A:CYS:H	2	3.62	0.68	3.62
(4,55)	1:16:A:SER:HB2	1:19:A:GLU:H	2	3.6	0.52	3.6
(4,55)	1:16:A:SER:HB3	1:19:A:GLU:H	2	3.6	0.52	3.6
(6,31)	1:10:A:ILE:H	1:9:A:GLU:HB2	2	3.6	0.15	3.6
(6,31)	1:10:A:ILE:H	1:9:A:GLU:HB3	2	3.6	0.15	3.6
(7,139)	1:38:A:ASN:HB2	1:38:A:ASN:HD21	2	3.59	0.17	3.59
(7,139)	1:38:A:ASN:HB2	1:38:A:ASN:HD22	2	3.59	0.17	3.59
(2,40)	1:45:A:PHE:HD1	1:94:A:ALA:H	2	3.57	0.08	3.57
(2,40)	1:45:A:PHE:HD2	1:94:A:ALA:H	2	3.57	0.08	3.57
(6,478)	1:112:A:PHE:HD1	1:113:A:LEU:H	2	3.57	0.01	3.57
(6,478)	1:112:A:PHE:HD2	1:113:A:LEU:H	2	3.57	0.01	3.57
(7,431)	1:124:A:TYR:HD1	1:124:A:TYR:H	2	3.57	0.43	3.57
(7,431)	1:124:A:TYR:HD2	1:124:A:TYR:H	2	3.57	0.43	3.57
(7,232)	1:69:A:THR:HG21	1:69:A:THR:H	2	3.53	0.07	3.53
(7,232)	1:69:A:THR:HG22	1:69:A:THR:H	2	3.53	0.07	3.53
(7,232)	1:69:A:THR:HG23	1:69:A:THR:H	2	3.53	0.07	3.53
(4,292)	1:108:A:THR:HG21	1:111:A:ASN:H	2	3.52	0.27	3.52
(4,292)	1:108:A:THR:HG22	1:111:A:ASN:H	2	3.52	0.27	3.52
(4,292)	1:108:A:THR:HG23	1:111:A:ASN:H	2	3.52	0.27	3.52
(6,445)	1:106:A:GLN:HB2	1:107:A:SER:H	2	3.5	0.16	3.5
(6,445)	1:106:A:GLN:HB3	1:107:A:SER:H	2	3.5	0.16	3.5
(2,33)	1:23:A:LEU:HD11	1:72:A:GLN:HE22	2	3.49	0.64	3.49
(2,33)	1:23:A:LEU:HD12	1:72:A:GLN:HE22	2	3.49	0.64	3.49
(2,33)	1:23:A:LEU:HD13	1:72:A:GLN:HE22	2	3.49	0.64	3.49

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,33)	1:23:A:LEU:HD21	1:72:A:GLN:HE22	2	3.49	0.64	3.49
(2,33)	1:23:A:LEU:HD22	1:72:A:GLN:HE22	2	3.49	0.64	3.49
(2,33)	1:23:A:LEU:HD23	1:72:A:GLN:HE22	2	3.49	0.64	3.49
(7,191)	1:56:A:TYR:HE1	1:56:A:TYR:H	2	3.49	0.05	3.49
(7,191)	1:56:A:TYR:HE2	1:56:A:TYR:H	2	3.49	0.05	3.49
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD11	2	3.48	1.27	3.48
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD12	2	3.48	1.27	3.48
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD13	2	3.48	1.27	3.48
(6,287)	1:70:A:ALA:H	1:71:A:GLN:H	2	3.48	0.08	3.48
(6,115)	1:27:A:LEU:HG	1:28:A:THR:H	2	3.46	0.02	3.46
(4,149)	1:50:A:THR:H	1:52:A:LEU:H	2	3.44	0.04	3.44
(6,201)	1:46:A:CYS:H	1:45:A:PHE:HD1	2	3.44	0.04	3.44
(6,201)	1:46:A:CYS:H	1:45:A:PHE:HD2	2	3.44	0.04	3.44
(7,404)	1:115:A:ARG:H	1:115:A:ARG:HE	2	3.44	0.6	3.44
(6,461)	1:109:A:LEU:HD21	1:110:A:GLU:H	2	3.4	0.18	3.4
(6,461)	1:109:A:LEU:HD22	1:110:A:GLU:H	2	3.4	0.18	3.4
(6,461)	1:109:A:LEU:HD23	1:110:A:GLU:H	2	3.4	0.18	3.4
(6,404)	1:96:A:LEU:HB2	1:97:A:ASN:H	2	3.4	0.64	3.4
(6,404)	1:96:A:LEU:HB3	1:97:A:ASN:H	2	3.4	0.64	3.4
(6,432)	1:103:A:GLU:HG2	1:104:A:ALA:H	2	3.38	0.53	3.38
(6,432)	1:103:A:GLU:HG3	1:104:A:ALA:H	2	3.38	0.53	3.38
(4,184)	1:66:A:LEU:HD11	1:63:A:THR:H	2	3.36	0.09	3.36
(4,184)	1:66:A:LEU:HD12	1:63:A:THR:H	2	3.36	0.09	3.36
(4,184)	1:66:A:LEU:HD13	1:63:A:THR:H	2	3.36	0.09	3.36
(4,184)	1:66:A:LEU:HD21	1:63:A:THR:H	2	3.36	0.09	3.36
(4,184)	1:66:A:LEU:HD22	1:63:A:THR:H	2	3.36	0.09	3.36
(4,184)	1:66:A:LEU:HD23	1:63:A:THR:H	2	3.36	0.09	3.36
(4,296)	1:108:A:THR:HB	1:111:A:ASN:H	2	3.35	0.6	3.35
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD11	2	3.3	0.88	3.3
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD12	2	3.3	0.88	3.3
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD13	2	3.3	0.88	3.3
(7,351)	1:101:A:VAL:HG11	1:101:A:VAL:H	2	3.28	0.14	3.28
(7,351)	1:101:A:VAL:HG12	1:101:A:VAL:H	2	3.28	0.14	3.28
(7,351)	1:101:A:VAL:HG13	1:101:A:VAL:H	2	3.28	0.14	3.28
(6,441)	1:105:A:ASN:HB3	1:106:A:GLN:H	2	3.28	0.68	3.28
(6,423)	1:101:A:VAL:HG21	1:102:A:LYS:H	2	3.24	0.66	3.24
(6,423)	1:101:A:VAL:HG22	1:102:A:LYS:H	2	3.24	0.66	3.24
(6,423)	1:101:A:VAL:HG23	1:102:A:LYS:H	2	3.24	0.66	3.24
(7,371)	1:106:A:GLN:HG2	1:106:A:GLN:H	2	3.24	0.34	3.24
(7,371)	1:106:A:GLN:HG3	1:106:A:GLN:H	2	3.24	0.34	3.24
(6,440)	1:106:A:GLN:HE21	1:105:A:ASN:H	2	3.24	0.24	3.24
(6,440)	1:106:A:GLN:HE22	1:105:A:ASN:H	2	3.24	0.24	3.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,447)	1:129:A:SER:HB2	1:129:A:SER:H	2	3.23	0.51	3.23
(7,447)	1:129:A:SER:HB3	1:129:A:SER:H	2	3.23	0.51	3.23
(7,370)	1:106:A:GLN:HB2	1:106:A:GLN:H	2	3.23	0.02	3.23
(7,370)	1:106:A:GLN:HB3	1:106:A:GLN:H	2	3.23	0.02	3.23
(6,483)	1:113:A:LEU:HG	1:114:A:GLU:H	2	3.22	0.01	3.22
(6,250)	1:59:A:HIS:HB2	1:60:A:GLU:H	2	3.17	1.01	3.17
(6,250)	1:59:A:HIS:HB3	1:60:A:GLU:H	2	3.17	1.01	3.17
(6,283)	1:69:A:THR:HG21	1:70:A:ALA:H	2	3.16	0.18	3.16
(6,283)	1:69:A:THR:HG22	1:70:A:ALA:H	2	3.16	0.18	3.16
(6,283)	1:69:A:THR:HG23	1:70:A:ALA:H	2	3.16	0.18	3.16
(2,13)	1:30:A:THR:HG21	1:103:A:GLU:H	2	3.14	0.04	3.14
(2,13)	1:30:A:THR:HG22	1:103:A:GLU:H	2	3.14	0.04	3.14
(2,13)	1:30:A:THR:HG23	1:103:A:GLU:H	2	3.14	0.04	3.14
(2,46)	1:33:A:PHE:HE1	1:116:A:LEU:H	2	3.14	0.54	3.14
(2,46)	1:33:A:PHE:HE2	1:116:A:LEU:H	2	3.14	0.54	3.14
(4,270)	1:91:A:TRP:HE3	1:93:A:LEU:H	2	3.14	0.11	3.14
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD21	2	3.14	0.03	3.14
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD22	2	3.14	0.03	3.14
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD23	2	3.14	0.03	3.14
(7,107)	1:29:A:VAL:HG11	1:29:A:VAL:H	2	3.14	0.43	3.14
(7,107)	1:29:A:VAL:HG12	1:29:A:VAL:H	2	3.14	0.43	3.14
(7,107)	1:29:A:VAL:HG13	1:29:A:VAL:H	2	3.14	0.43	3.14
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD11	2	3.13	0.03	3.13
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD12	2	3.13	0.03	3.13
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD13	2	3.13	0.03	3.13
(6,499)	1:118:A:THR:HG1	1:119:A:ILE:H	2	3.12	0.43	3.12
(6,499)	1:118:A:THR:HG21	1:119:A:ILE:H	2	3.12	0.43	3.12
(6,499)	1:118:A:THR:HG22	1:119:A:ILE:H	2	3.12	0.43	3.12
(6,499)	1:118:A:THR:HG23	1:119:A:ILE:H	2	3.12	0.43	3.12
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD21	2	3.1	0.1	3.1
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD22	2	3.1	0.1	3.1
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD23	2	3.1	0.1	3.1
(7,389)	1:111:A:ASN:HA	1:111:A:ASN:HD21	2	3.1	0.15	3.1
(7,389)	1:111:A:ASN:HA	1:111:A:ASN:HD22	2	3.1	0.15	3.1
(4,283)	1:101:A:VAL:HG11	1:103:A:GLU:H	2	3.09	0.27	3.09
(4,283)	1:101:A:VAL:HG12	1:103:A:GLU:H	2	3.09	0.27	3.09
(4,283)	1:101:A:VAL:HG13	1:103:A:GLU:H	2	3.09	0.27	3.09
(4,283)	1:101:A:VAL:HG21	1:103:A:GLU:H	2	3.09	0.27	3.09
(4,283)	1:101:A:VAL:HG22	1:103:A:GLU:H	2	3.09	0.27	3.09
(4,283)	1:101:A:VAL:HG23	1:103:A:GLU:H	2	3.09	0.27	3.09
(4,314)	1:112:A:PHE:HD1	1:115:A:ARG:H	2	3.08	0.07	3.08
(4,314)	1:112:A:PHE:HD2	1:115:A:ARG:H	2	3.08	0.07	3.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,366)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	2	3.08	0.06	3.08
(7,366)	1:105:A:ASN:HB2	1:105:A:ASN:HD22	2	3.08	0.06	3.08
(7,368)	1:106:A:GLN:HA	1:106:A:GLN:H	2	3.08	0.01	3.08
(2,44)	1:28:A:THR:HG21	1:108:A:THR:H	2	3.07	0.28	3.07
(2,44)	1:28:A:THR:HG22	1:108:A:THR:H	2	3.07	0.28	3.07
(2,44)	1:28:A:THR:HG23	1:108:A:THR:H	2	3.07	0.28	3.07
(2,44)	1:28:A:THR:HG1	1:108:A:THR:H	2	3.07	0.28	3.07
(7,138)	1:38:A:ASN:HB3	1:38:A:ASN:HD21	2	3.07	0.31	3.07
(7,138)	1:38:A:ASN:HB3	1:38:A:ASN:HD22	2	3.07	0.31	3.07
(7,309)	1:89:A:ASN:HA	1:89:A:ASN:HD21	2	3.07	1.11	3.07
(7,309)	1:89:A:ASN:HA	1:89:A:ASN:HD22	2	3.07	1.11	3.07
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG21	2	3.03	0.36	3.03
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG22	2	3.03	0.36	3.03
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG23	2	3.03	0.36	3.03
(6,288)	1:71:A:GLN:HB3	1:72:A:GLN:H	2	3.03	0.16	3.03
(6,152)	1:33:A:PHE:HD1	1:34:A:ALA:H	2	3.02	0.34	3.02
(6,152)	1:33:A:PHE:HD2	1:34:A:ALA:H	2	3.02	0.34	3.02
(7,124)	1:33:A:PHE:HD1	1:33:A:PHE:H	2	3.01	0.08	3.01
(7,124)	1:33:A:PHE:HD2	1:33:A:PHE:H	2	3.01	0.08	3.01
(6,526)	1:124:A:TYR:HB3	1:125:A:SER:H	2	3.0	0.27	3.0
(2,28)	1:29:A:VAL:HG11	1:55:A:PHE:H	2	2.96	0.23	2.96
(2,28)	1:29:A:VAL:HG12	1:55:A:PHE:H	2	2.96	0.23	2.96
(2,28)	1:29:A:VAL:HG13	1:55:A:PHE:H	2	2.96	0.23	2.96
(6,292)	1:72:A:GLN:HG2	1:71:A:GLN:H	2	2.96	0.18	2.96
(6,292)	1:72:A:GLN:HG3	1:71:A:GLN:H	2	2.96	0.18	2.96
(7,369)	1:106:A:GLN:HA	1:106:A:GLN:HE21	2	2.96	0.66	2.96
(7,369)	1:106:A:GLN:HA	1:106:A:GLN:HE22	2	2.96	0.66	2.96
(6,453)	1:108:A:THR:HG21	1:109:A:LEU:H	2	2.94	0.39	2.94
(6,453)	1:108:A:THR:HG22	1:109:A:LEU:H	2	2.94	0.39	2.94
(6,453)	1:108:A:THR:HG23	1:109:A:LEU:H	2	2.94	0.39	2.94
(6,143)	1:32:A:ILE:HD11	1:33:A:PHE:H	2	2.94	0.48	2.94
(6,143)	1:32:A:ILE:HD12	1:33:A:PHE:H	2	2.94	0.48	2.94
(6,143)	1:32:A:ILE:HD13	1:33:A:PHE:H	2	2.94	0.48	2.94
(6,384)	1:91:A:TRP:HE3	1:92:A:GLY:H	2	2.94	0.5	2.94
(7,125)	1:33:A:PHE:HE1	1:33:A:PHE:H	2	2.92	0.05	2.92
(7,125)	1:33:A:PHE:HE2	1:33:A:PHE:H	2	2.92	0.05	2.92
(4,351)	1:125:A:SER:HA	1:127:A:CYS:H	2	2.88	0.01	2.88
(7,396)	1:112:A:PHE:HD1	1:112:A:PHE:H	2	2.88	0.04	2.88
(7,396)	1:112:A:PHE:HD2	1:112:A:PHE:H	2	2.88	0.04	2.88
(6,72)	1:17:A:LEU:HG	1:16:A:SER:H	2	2.86	0.03	2.86
(2,18)	1:8:A:GLN:H	1:124:A:TYR:HE1	2	2.86	0.93	2.86
(2,18)	1:8:A:GLN:H	1:124:A:TYR:HE2	2	2.86	0.93	2.86

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,44)	1:12:A:LYS:H	1:11:A:ILE:HG13	2	2.84	1.28	2.84
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD11	2	2.84	0.02	2.84
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD12	2	2.84	0.02	2.84
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD13	2	2.84	0.02	2.84
(4,285)	1:103:A:GLU:HB2	1:105:A:ASN:H	2	2.83	0.13	2.83
(4,285)	1:103:A:GLU:HB3	1:105:A:ASN:H	2	2.83	0.13	2.83
(7,248)	1:73:A:PHE:HD1	1:73:A:PHE:H	2	2.83	0.0	2.83
(7,248)	1:73:A:PHE:HD2	1:73:A:PHE:H	2	2.83	0.0	2.83
(6,140)	1:32:A:ILE:HG13	1:33:A:PHE:H	2	2.82	0.17	2.82
(6,279)	1:69:A:THR:HG21	1:68:A:ALA:H	2	2.82	0.06	2.82
(6,279)	1:69:A:THR:HG22	1:68:A:ALA:H	2	2.82	0.06	2.82
(6,279)	1:69:A:THR:HG23	1:68:A:ALA:H	2	2.82	0.06	2.82
(6,431)	1:103:A:GLU:HB2	1:104:A:ALA:H	2	2.82	0.77	2.82
(6,431)	1:103:A:GLU:HB3	1:104:A:ALA:H	2	2.82	0.77	2.82
(2,39)	1:56:A:TYR:HE1	1:88:A:ARG:H	2	2.8	0.05	2.8
(2,39)	1:56:A:TYR:HE2	1:88:A:ARG:H	2	2.8	0.05	2.8
(4,80)	1:28:A:THR:HB	1:30:A:THR:H	2	2.8	0.38	2.8
(7,276)	1:82:A:PHE:HE1	1:82:A:PHE:H	2	2.8	1.02	2.8
(7,276)	1:82:A:PHE:HE2	1:82:A:PHE:H	2	2.8	1.02	2.8
(6,185)	1:43:A:GLU:HG2	1:42:A:LYS:H	2	2.79	0.25	2.79
(6,185)	1:43:A:GLU:HG3	1:42:A:LYS:H	2	2.79	0.25	2.79
(6,416)	1:99:A:CYS:HA	1:100:A:PRO:HD2	2	2.78	0.09	2.78
(6,416)	1:99:A:CYS:HA	1:100:A:PRO:HD3	2	2.78	0.09	2.78
(3,86)	1:30:A:THR:N	1:106:A:GLN:O	2	2.77	0.15	2.77
(2,43)	1:30:A:THR:HG21	1:106:A:GLN:HE21	2	2.76	1.01	2.76
(2,43)	1:30:A:THR:HG21	1:106:A:GLN:HE22	2	2.76	1.01	2.76
(2,43)	1:30:A:THR:HG22	1:106:A:GLN:HE21	2	2.76	1.01	2.76
(2,43)	1:30:A:THR:HG22	1:106:A:GLN:HE22	2	2.76	1.01	2.76
(2,43)	1:30:A:THR:HG23	1:106:A:GLN:HE21	2	2.76	1.01	2.76
(2,43)	1:30:A:THR:HG23	1:106:A:GLN:HE22	2	2.76	1.01	2.76
(7,104)	1:28:A:THR:HG21	1:28:A:THR:H	2	2.76	0.01	2.76
(7,104)	1:28:A:THR:HG22	1:28:A:THR:H	2	2.76	0.01	2.76
(7,104)	1:28:A:THR:HG23	1:28:A:THR:H	2	2.76	0.01	2.76
(7,295)	1:86:A:LEU:HD11	1:86:A:LEU:H	2	2.75	0.27	2.75
(7,295)	1:86:A:LEU:HD12	1:86:A:LEU:H	2	2.75	0.27	2.75
(7,295)	1:86:A:LEU:HD13	1:86:A:LEU:H	2	2.75	0.27	2.75
(7,51)	1:15:A:ASN:H	1:15:A:ASN:HD21	2	2.74	0.34	2.74
(6,24)	1:7:A:LEU:HD11	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,24)	1:7:A:LEU:HD12	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,24)	1:7:A:LEU:HD13	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,24)	1:7:A:LEU:HD21	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,24)	1:7:A:LEU:HD22	1:8:A:GLN:H	2	2.74	0.42	2.74

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,24)	1:7:A:LEU:HD23	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,25)	1:7:A:LEU:HD11	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,25)	1:7:A:LEU:HD12	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,25)	1:7:A:LEU:HD13	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,25)	1:7:A:LEU:HD21	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,25)	1:7:A:LEU:HD22	1:8:A:GLN:H	2	2.74	0.42	2.74
(6,25)	1:7:A:LEU:HD23	1:8:A:GLN:H	2	2.74	0.42	2.74
(7,325)	1:91:A:TRP:HB2	1:91:A:TRP:H	2	2.72	0.02	2.72
(7,325)	1:91:A:TRP:HB3	1:91:A:TRP:H	2	2.72	0.02	2.72
(4,299)	1:108:A:THR:H	1:111:A:ASN:HD21	2	2.71	0.37	2.71
(4,299)	1:108:A:THR:H	1:111:A:ASN:HD22	2	2.71	0.37	2.71
(6,460)	1:109:A:LEU:HD11	1:110:A:GLU:H	2	2.71	0.08	2.71
(6,460)	1:109:A:LEU:HD12	1:110:A:GLU:H	2	2.71	0.08	2.71
(6,460)	1:109:A:LEU:HD13	1:110:A:GLU:H	2	2.71	0.08	2.71
(6,233)	1:55:A:PHE:HD1	1:56:A:TYR:H	2	2.7	0.3	2.7
(6,233)	1:55:A:PHE:HD2	1:56:A:TYR:H	2	2.7	0.3	2.7
(6,262)	1:63:A:THR:HG21	1:64:A:ARG:H	2	2.68	0.19	2.68
(6,262)	1:63:A:THR:HG22	1:64:A:ARG:H	2	2.68	0.19	2.68
(6,262)	1:63:A:THR:HG23	1:64:A:ARG:H	2	2.68	0.19	2.68
(4,271)	1:92:A:GLY:HA3	1:95:A:GLY:H	2	2.68	0.4	2.68
(2,12)	1:30:A:THR:HG21	1:104:A:ALA:H	2	2.68	0.29	2.68
(2,12)	1:30:A:THR:HG22	1:104:A:ALA:H	2	2.68	0.29	2.68
(2,12)	1:30:A:THR:HG23	1:104:A:ALA:H	2	2.68	0.29	2.68
(6,452)	1:107:A:SER:H	1:108:A:THR:H	2	2.68	0.72	2.68
(2,38)	1:56:A:TYR:HE1	1:87:A:ASP:H	2	2.66	0.76	2.66
(2,38)	1:56:A:TYR:HE2	1:87:A:ASP:H	2	2.66	0.76	2.66
(6,385)	1:91:A:TRP:HB2	1:92:A:GLY:H	2	2.66	0.06	2.66
(6,385)	1:91:A:TRP:HB3	1:92:A:GLY:H	2	2.66	0.06	2.66
(7,352)	1:101:A:VAL:HG21	1:101:A:VAL:H	2	2.66	1.0	2.66
(7,352)	1:101:A:VAL:HG22	1:101:A:VAL:H	2	2.66	1.0	2.66
(7,352)	1:101:A:VAL:HG23	1:101:A:VAL:H	2	2.66	1.0	2.66
(6,446)	1:106:A:GLN:HG2	1:107:A:SER:H	2	2.64	0.29	2.64
(6,446)	1:106:A:GLN:HG3	1:107:A:SER:H	2	2.64	0.29	2.64
(4,259)	1:87:A:ASP:HA	1:90:A:LEU:H	2	2.64	0.05	2.64
(4,328)	1:117:A:LYS:HA	1:121:A:ARG:H	2	2.64	0.05	2.64
(7,296)	1:86:A:LEU:HD21	1:86:A:LEU:H	2	2.64	0.41	2.64
(7,296)	1:86:A:LEU:HD22	1:86:A:LEU:H	2	2.64	0.41	2.64
(7,296)	1:86:A:LEU:HD23	1:86:A:LEU:H	2	2.64	0.41	2.64
(4,110)	1:40:A:THR:HG21	1:43:A:GLU:H	2	2.64	0.01	2.64
(4,110)	1:40:A:THR:HG22	1:43:A:GLU:H	2	2.64	0.01	2.64
(4,110)	1:40:A:THR:HG23	1:43:A:GLU:H	2	2.64	0.01	2.64
(6,179)	1:40:A:THR:HG21	1:41:A:GLU:H	2	2.64	0.01	2.64

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,179)	1:40:A:THR:HG22	1:41:A:GLU:H	2	2.64	0.01	2.64
(6,179)	1:40:A:THR:HG23	1:41:A:GLU:H	2	2.64	0.01	2.64
(2,41)	1:30:A:THR:HA	1:105:A:ASN:H	2	2.62	0.37	2.62
(4,350)	1:125:A:SER:HB2	1:127:A:CYS:H	2	2.61	0.05	2.61
(4,350)	1:125:A:SER:HB3	1:127:A:CYS:H	2	2.61	0.05	2.61
(6,379)	1:90:A:LEU:HA	1:91:A:TRP:H	2	2.61	0.14	2.61
(6,425)	1:102:A:LYS:HB3	1:103:A:GLU:H	2	2.6	0.4	2.6
(6,360)	1:86:A:LEU:HB2	1:87:A:ASP:H	2	2.6	0.03	2.6
(6,360)	1:86:A:LEU:HB3	1:87:A:ASP:H	2	2.6	0.03	2.6
(6,335)	1:82:A:PHE:HD1	1:81:A:ARG:H	2	2.59	1.03	2.59
(6,335)	1:82:A:PHE:HD2	1:81:A:ARG:H	2	2.59	1.03	2.59
(6,397)	1:94:A:ALA:HB1	1:95:A:GLY:H	2	2.58	0.02	2.58
(6,397)	1:94:A:ALA:HB2	1:95:A:GLY:H	2	2.58	0.02	2.58
(6,397)	1:94:A:ALA:HB3	1:95:A:GLY:H	2	2.58	0.02	2.58
(6,246)	1:58:A:HIS:HB2	1:59:A:HIS:H	2	2.58	0.17	2.58
(6,246)	1:58:A:HIS:HB3	1:59:A:HIS:H	2	2.58	0.17	2.58
(7,382)	1:109:A:LEU:HD11	1:109:A:LEU:H	2	2.58	0.07	2.58
(7,382)	1:109:A:LEU:HD12	1:109:A:LEU:H	2	2.58	0.07	2.58
(7,382)	1:109:A:LEU:HD13	1:109:A:LEU:H	2	2.58	0.07	2.58
(2,29)	1:29:A:VAL:HG21	1:55:A:PHE:H	2	2.58	0.2	2.58
(2,29)	1:29:A:VAL:HG22	1:55:A:PHE:H	2	2.58	0.2	2.58
(2,29)	1:29:A:VAL:HG23	1:55:A:PHE:H	2	2.58	0.2	2.58
(6,402)	1:96:A:LEU:HB2	1:95:A:GLY:H	2	2.58	0.17	2.58
(6,402)	1:96:A:LEU:HB3	1:95:A:GLY:H	2	2.58	0.17	2.58
(4,62)	1:18:A:THR:H	1:20:A:GLN:H	2	2.56	0.08	2.56
(6,142)	1:32:A:ILE:HG21	1:33:A:PHE:H	2	2.56	0.12	2.56
(6,142)	1:32:A:ILE:HG22	1:33:A:PHE:H	2	2.56	0.12	2.56
(6,142)	1:32:A:ILE:HG23	1:33:A:PHE:H	2	2.56	0.12	2.56
(7,347)	1:99:A:CYS:HB3	1:99:A:CYS:H	2	2.56	0.22	2.56
(7,354)	1:102:A:LYS:HB3	1:102:A:LYS:H	2	2.55	0.4	2.55
(6,132)	1:31:A:ASP:HB3	1:32:A:ILE:H	2	2.54	0.68	2.54
(4,93)	1:32:A:ILE:HG21	1:34:A:ALA:H	2	2.54	0.01	2.54
(4,93)	1:32:A:ILE:HG22	1:34:A:ALA:H	2	2.54	0.01	2.54
(4,93)	1:32:A:ILE:HG23	1:34:A:ALA:H	2	2.54	0.01	2.54
(6,327)	1:80:A:ILE:HG21	1:79:A:LEU:H	2	2.51	0.78	2.51
(6,327)	1:80:A:ILE:HG22	1:79:A:LEU:H	2	2.51	0.78	2.51
(6,327)	1:80:A:ILE:HG23	1:79:A:LEU:H	2	2.51	0.78	2.51
(7,203)	1:59:A:HIS:HB3	1:59:A:HIS:H	2	2.51	0.02	2.51
(6,411)	1:98:A:SER:HB2	1:99:A:CYS:H	2	2.5	0.18	2.5
(6,411)	1:98:A:SER:HB3	1:99:A:CYS:H	2	2.5	0.18	2.5
(6,463)	1:110:A:GLU:HB3	1:111:A:ASN:H	2	2.5	0.04	2.5
(6,277)	1:68:A:ALA:HA	1:69:A:THR:H	2	2.5	0.21	2.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,491)	1:116:A:LEU:H	1:115:A:ARG:HE	2	2.5	0.07	2.5
(7,270)	1:80:A:ILE:HG21	1:80:A:ILE:H	2	2.5	0.8	2.5
(7,270)	1:80:A:ILE:HG22	1:80:A:ILE:H	2	2.5	0.8	2.5
(7,270)	1:80:A:ILE:HG23	1:80:A:ILE:H	2	2.5	0.8	2.5
(6,158)	1:35:A:ALA:H	1:36:A:SER:H	2	2.49	0.05	2.49
(7,411)	1:118:A:THR:HG21	1:118:A:THR:H	2	2.48	0.72	2.48
(7,411)	1:118:A:THR:HG22	1:118:A:THR:H	2	2.48	0.72	2.48
(7,411)	1:118:A:THR:HG23	1:118:A:THR:H	2	2.48	0.72	2.48
(4,213)	1:73:A:PHE:HB2	1:75:A:ARG:H	2	2.47	0.12	2.47
(4,213)	1:73:A:PHE:HB3	1:75:A:ARG:H	2	2.47	0.12	2.47
(6,300)	1:73:A:PHE:HB3	1:74:A:HIS:H	2	2.47	0.07	2.47
(6,157)	1:35:A:ALA:HB1	1:36:A:SER:H	2	2.46	0.06	2.46
(6,157)	1:35:A:ALA:HB2	1:36:A:SER:H	2	2.46	0.06	2.46
(6,157)	1:35:A:ALA:HB3	1:36:A:SER:H	2	2.46	0.06	2.46
(2,14)	1:30:A:THR:HG21	1:105:A:ASN:H	2	2.46	0.12	2.46
(2,14)	1:30:A:THR:HG22	1:105:A:ASN:H	2	2.46	0.12	2.46
(2,14)	1:30:A:THR:HG23	1:105:A:ASN:H	2	2.46	0.12	2.46
(2,37)	1:56:A:TYR:HD1	1:84:A:LYS:H	2	2.46	0.95	2.46
(2,37)	1:56:A:TYR:HD2	1:84:A:LYS:H	2	2.46	0.95	2.46
(6,422)	1:101:A:VAL:HG11	1:102:A:LYS:H	2	2.46	0.0	2.46
(6,422)	1:101:A:VAL:HG12	1:102:A:LYS:H	2	2.46	0.0	2.46
(6,422)	1:101:A:VAL:HG13	1:102:A:LYS:H	2	2.46	0.0	2.46
(7,348)	1:99:A:CYS:HB2	1:99:A:CYS:H	2	2.46	0.19	2.46
(7,385)	1:110:A:GLU:HB3	1:110:A:GLU:H	2	2.46	0.0	2.46
(6,117)	1:27:A:LEU:HD21	1:28:A:THR:H	2	2.45	0.01	2.45
(6,117)	1:27:A:LEU:HD22	1:28:A:THR:H	2	2.45	0.01	2.45
(6,117)	1:27:A:LEU:HD23	1:28:A:THR:H	2	2.45	0.01	2.45
(7,159)	1:45:A:PHE:H	1:45:A:PHE:HD1	2	2.45	0.01	2.45
(7,159)	1:45:A:PHE:H	1:45:A:PHE:HD2	2	2.45	0.01	2.45
(6,465)	1:110:A:GLU:HG2	1:111:A:ASN:H	2	2.44	0.02	2.44
(6,465)	1:110:A:GLU:HG3	1:111:A:ASN:H	2	2.44	0.02	2.44
(7,177)	1:51:A:VAL:HG21	1:51:A:VAL:H	2	2.43	0.18	2.43
(7,177)	1:51:A:VAL:HG22	1:51:A:VAL:H	2	2.43	0.18	2.43
(7,177)	1:51:A:VAL:HG23	1:51:A:VAL:H	2	2.43	0.18	2.43
(4,109)	1:40:A:THR:HG21	1:42:A:LYS:H	2	2.42	0.09	2.42
(4,109)	1:40:A:THR:HG22	1:42:A:LYS:H	2	2.42	0.09	2.42
(4,109)	1:40:A:THR:HG23	1:42:A:LYS:H	2	2.42	0.09	2.42
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG21	2	2.42	0.84	2.42
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG22	2	2.42	0.84	2.42
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG23	2	2.42	0.84	2.42
(6,328)	1:80:A:ILE:HD11	1:79:A:LEU:H	2	2.41	0.12	2.41
(6,328)	1:80:A:ILE:HD12	1:79:A:LEU:H	2	2.41	0.12	2.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,328)	1:80:A:ILE:HD13	1:79:A:LEU:H	2	2.41	0.12	2.41
(6,476)	1:112:A:PHE:HB3	1:113:A:LEU:H	2	2.41	0.04	2.41
(7,243)	1:72:A:GLN:HE21	1:72:A:GLN:H	2	2.41	0.19	2.41
(7,243)	1:72:A:GLN:HE22	1:72:A:GLN:H	2	2.41	0.19	2.41
(4,148)	1:50:A:THR:HG21	1:52:A:LEU:H	2	2.41	0.03	2.41
(4,148)	1:50:A:THR:HG22	1:52:A:LEU:H	2	2.41	0.03	2.41
(4,148)	1:50:A:THR:HG23	1:52:A:LEU:H	2	2.41	0.03	2.41
(6,539)	1:128:A:SER:H	1:129:A:SER:H	2	2.4	0.16	2.4
(7,443)	1:128:A:SER:HA	1:128:A:SER:H	2	2.4	0.3	2.4
(6,457)	1:109:A:LEU:HB3	1:110:A:GLU:H	2	2.39	0.17	2.39
(6,375)	1:89:A:ASN:HB2	1:90:A:LEU:H	2	2.38	0.46	2.38
(7,140)	1:38:A:ASN:HD21	1:38:A:ASN:H	2	2.38	0.58	2.38
(7,140)	1:38:A:ASN:HD22	1:38:A:ASN:H	2	2.38	0.58	2.38
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG21	2	2.37	0.92	2.37
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG22	2	2.37	0.92	2.37
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG23	2	2.37	0.92	2.37
(7,376)	1:108:A:THR:HB	1:108:A:THR:H	2	2.37	0.05	2.37
(7,204)	1:59:A:HIS:HB2	1:59:A:HIS:H	2	2.33	0.02	2.33
(4,96)	1:34:A:ALA:HA	1:36:A:SER:H	2	2.33	0.64	2.33
(4,303)	1:112:A:PHE:HB2	1:110:A:GLU:H	2	2.33	0.05	2.33
(4,303)	1:112:A:PHE:HB3	1:110:A:GLU:H	2	2.33	0.05	2.33
(7,77)	1:20:A:GLN:H	1:20:A:GLN:HB2	2	2.33	0.01	2.33
(4,288)	1:104:A:ALA:HB1	1:106:A:GLN:HE21	2	2.32	0.35	2.32
(4,288)	1:104:A:ALA:HB1	1:106:A:GLN:HE22	2	2.32	0.35	2.32
(4,288)	1:104:A:ALA:HB2	1:106:A:GLN:HE21	2	2.32	0.35	2.32
(4,288)	1:104:A:ALA:HB2	1:106:A:GLN:HE22	2	2.32	0.35	2.32
(4,288)	1:104:A:ALA:HB3	1:106:A:GLN:HE21	2	2.32	0.35	2.32
(4,288)	1:104:A:ALA:HB3	1:106:A:GLN:HE22	2	2.32	0.35	2.32
(6,439)	1:106:A:GLN:HG2	1:105:A:ASN:H	2	2.32	0.43	2.32
(6,439)	1:106:A:GLN:HG3	1:105:A:ASN:H	2	2.32	0.43	2.32
(6,507)	1:119:A:ILE:HD11	1:120:A:MET:H	2	2.3	0.22	2.3
(6,507)	1:119:A:ILE:HD12	1:120:A:MET:H	2	2.3	0.22	2.3
(6,507)	1:119:A:ILE:HD13	1:120:A:MET:H	2	2.3	0.22	2.3
(6,126)	1:29:A:VAL:HG11	1:30:A:THR:H	2	2.3	0.58	2.3
(6,126)	1:29:A:VAL:HG12	1:30:A:THR:H	2	2.3	0.58	2.3
(6,126)	1:29:A:VAL:HG13	1:30:A:THR:H	2	2.3	0.58	2.3
(6,181)	1:41:A:GLU:H	1:42:A:LYS:H	2	2.3	0.03	2.3
(2,19)	1:112:A:PHE:HD1	1:32:A:ILE:H	2	2.3	0.04	2.3
(2,19)	1:112:A:PHE:HD2	1:32:A:ILE:H	2	2.3	0.04	2.3
(6,91)	1:20:A:GLN:HB3	1:21:A:LYS:H	2	2.3	0.38	2.3
(6,449)	1:107:A:SER:HB2	1:108:A:THR:H	2	2.3	0.68	2.3
(6,449)	1:107:A:SER:HB3	1:108:A:THR:H	2	2.3	0.68	2.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1)	1:29:A:VAL:H	1:107:A:SER:H	2	2.29	0.01	2.29
(6,147)	1:34:A:ALA:HB1	1:33:A:PHE:H	2	2.29	0.02	2.29
(6,147)	1:34:A:ALA:HB2	1:33:A:PHE:H	2	2.29	0.02	2.29
(6,147)	1:34:A:ALA:HB3	1:33:A:PHE:H	2	2.29	0.02	2.29
(4,1)	1:4:A:ASP:HA	1:7:A:LEU:H	2	2.28	0.05	2.28
(7,129)	1:35:A:ALA:HB1	1:35:A:ALA:H	2	2.28	0.01	2.28
(7,129)	1:35:A:ALA:HB2	1:35:A:ALA:H	2	2.28	0.01	2.28
(7,129)	1:35:A:ALA:HB3	1:35:A:ALA:H	2	2.28	0.01	2.28
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG21	2	2.27	0.14	2.27
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG22	2	2.27	0.14	2.27
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG23	2	2.27	0.14	2.27
(7,335)	1:94:A:ALA:HB1	1:94:A:ALA:H	2	2.27	0.02	2.27
(7,335)	1:94:A:ALA:HB2	1:94:A:ALA:H	2	2.27	0.02	2.27
(7,335)	1:94:A:ALA:HB3	1:94:A:ALA:H	2	2.27	0.02	2.27
(7,374)	1:107:A:SER:HB2	1:107:A:SER:H	2	2.27	0.04	2.27
(7,374)	1:107:A:SER:HB3	1:107:A:SER:H	2	2.27	0.04	2.27
(6,387)	1:91:A:TRP:H	1:92:A:GLY:H	2	2.26	0.34	2.26
(7,416)	1:119:A:ILE:HG21	1:119:A:ILE:H	2	2.26	0.14	2.26
(7,234)	1:70:A:ALA:HB1	1:70:A:ALA:H	2	2.26	0.01	2.26
(7,234)	1:70:A:ALA:HB2	1:70:A:ALA:H	2	2.26	0.01	2.26
(7,234)	1:70:A:ALA:HB3	1:70:A:ALA:H	2	2.26	0.01	2.26
(7,343)	1:97:A:ASN:HB2	1:97:A:ASN:H	2	2.26	0.03	2.26
(7,343)	1:97:A:ASN:HB3	1:97:A:ASN:H	2	2.26	0.03	2.26
(4,170)	1:56:A:TYR:HA	1:58:A:HIS:H	2	2.23	0.07	2.23
(6,530)	1:125:A:SER:HB2	1:126:A:LYS:H	2	2.22	0.08	2.22
(6,530)	1:125:A:SER:HB3	1:126:A:LYS:H	2	2.22	0.08	2.22
(7,345)	1:98:A:SER:HB2	1:98:A:SER:H	2	2.22	0.18	2.22
(7,345)	1:98:A:SER:HB3	1:98:A:SER:H	2	2.22	0.18	2.22
(7,442)	1:127:A:CYS:HB2	1:127:A:CYS:H	2	2.22	0.09	2.22
(7,442)	1:127:A:CYS:HB3	1:127:A:CYS:H	2	2.22	0.09	2.22
(6,410)	1:97:A:ASN:H	1:98:A:SER:H	2	2.22	0.43	2.22
(6,443)	1:105:A:ASN:H	1:106:A:GLN:H	2	2.22	0.62	2.22
(6,470)	1:111:A:ASN:HB3	1:112:A:PHE:H	2	2.22	0.1	2.22
(7,119)	1:32:A:ILE:HG21	1:32:A:ILE:H	2	2.22	0.34	2.22
(7,119)	1:32:A:ILE:HG22	1:32:A:ILE:H	2	2.22	0.34	2.22
(7,119)	1:32:A:ILE:HG23	1:32:A:ILE:H	2	2.22	0.34	2.22
(6,194)	1:44:A:THR:H	1:45:A:PHE:HD1	2	2.21	0.05	2.21
(6,194)	1:44:A:THR:H	1:45:A:PHE:HD2	2	2.21	0.05	2.21
(7,136)	1:38:A:ASN:HB3	1:38:A:ASN:H	2	2.21	0.26	2.21
(6,537)	1:127:A:CYS:HB2	1:128:A:SER:H	2	2.2	0.25	2.2
(6,537)	1:127:A:CYS:HB3	1:128:A:SER:H	2	2.2	0.25	2.2
(6,346)	1:83:A:LEU:HD11	1:84:A:LYS:H	2	2.2	0.05	2.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,346)	1:83:A:LEU:HD12	1:84:A:LYS:H	2	2.2	0.05	2.2
(6,346)	1:83:A:LEU:HD13	1:84:A:LYS:H	2	2.2	0.05	2.2
(7,317)	1:91:A:TRP:HA	1:91:A:TRP:H	2	2.19	0.12	2.19
(6,362)	1:86:A:LEU:HD11	1:87:A:ASP:H	2	2.18	0.02	2.18
(6,362)	1:86:A:LEU:HD12	1:87:A:ASP:H	2	2.18	0.02	2.18
(6,362)	1:86:A:LEU:HD13	1:87:A:ASP:H	2	2.18	0.02	2.18
(7,86)	1:22:A:THR:H	1:22:A:THR:HG21	2	2.18	0.23	2.18
(7,86)	1:22:A:THR:H	1:22:A:THR:HG22	2	2.18	0.23	2.18
(7,86)	1:22:A:THR:H	1:22:A:THR:HG23	2	2.18	0.23	2.18
(7,384)	1:110:A:GLU:HA	1:110:A:GLU:H	2	2.18	0.0	2.18
(2,48)	1:12:A:LYS:HB2	1:125:A:SER:H	2	2.18	0.08	2.18
(2,48)	1:12:A:LYS:HB3	1:125:A:SER:H	2	2.18	0.08	2.18
(6,121)	1:28:A:THR:HG21	1:29:A:VAL:H	2	2.18	0.03	2.18
(6,121)	1:28:A:THR:HG22	1:29:A:VAL:H	2	2.18	0.03	2.18
(6,121)	1:28:A:THR:HG23	1:29:A:VAL:H	2	2.18	0.03	2.18
(2,45)	1:33:A:PHE:HD1	1:115:A:ARG:H	2	2.17	0.02	2.17
(2,45)	1:33:A:PHE:HD2	1:115:A:ARG:H	2	2.17	0.02	2.17
(7,360)	1:104:A:ALA:HA	1:104:A:ALA:H	2	2.17	0.04	2.17
(4,341)	1:121:A:ARG:H	1:123:A:LYS:H	2	2.16	0.09	2.16
(4,229)	1:77:A:LYS:H	1:79:A:LEU:H	2	2.16	0.03	2.16
(7,383)	1:109:A:LEU:HD21	1:109:A:LEU:H	2	2.16	0.04	2.16
(7,383)	1:109:A:LEU:HD22	1:109:A:LEU:H	2	2.16	0.04	2.16
(7,383)	1:109:A:LEU:HD23	1:109:A:LEU:H	2	2.16	0.04	2.16
(6,305)	1:74:A:HIS:HB2	1:75:A:ARG:H	2	2.16	0.26	2.16
(6,305)	1:74:A:HIS:HB3	1:75:A:ARG:H	2	2.16	0.26	2.16
(6,331)	1:80:A:ILE:HG21	1:81:A:ARG:H	2	2.16	0.49	2.16
(6,331)	1:80:A:ILE:HG22	1:81:A:ARG:H	2	2.16	0.49	2.16
(6,331)	1:80:A:ILE:HG23	1:81:A:ARG:H	2	2.16	0.49	2.16
(6,71)	1:17:A:LEU:HB2	1:16:A:SER:H	2	2.15	0.03	2.15
(6,408)	1:97:A:ASN:HB2	1:98:A:SER:H	2	2.15	0.03	2.15
(6,408)	1:97:A:ASN:HB3	1:98:A:SER:H	2	2.15	0.03	2.15
(6,344)	1:83:A:LEU:HB3	1:84:A:LYS:H	2	2.15	0.45	2.15
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD11	2	2.14	0.23	2.14
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD12	2	2.14	0.23	2.14
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD13	2	2.14	0.23	2.14
(7,221)	1:65:A:CYS:HB2	1:65:A:CYS:H	2	2.14	0.56	2.14
(7,412)	1:119:A:ILE:HA	1:119:A:ILE:H	2	2.14	0.02	2.14
(7,95)	1:25:A:THR:H	1:25:A:THR:HG21	2	2.14	0.16	2.14
(7,95)	1:25:A:THR:H	1:25:A:THR:HG22	2	2.14	0.16	2.14
(7,95)	1:25:A:THR:H	1:25:A:THR:HG23	2	2.14	0.16	2.14
(7,444)	1:128:A:SER:HB3	1:128:A:SER:H	2	2.14	0.2	2.14
(4,238)	1:80:A:ILE:HA	1:84:A:LYS:H	2	2.13	0.51	2.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,409)	1:97:A:ASN:HA	1:98:A:SER:H	2	2.13	0.45	2.13
(7,211)	1:61:A:LYS:HA	1:61:A:LYS:H	2	2.13	0.04	2.13
(7,219)	1:65:A:CYS:HA	1:65:A:CYS:H	2	2.13	0.03	2.13
(7,233)	1:70:A:ALA:HA	1:70:A:ALA:H	2	2.13	0.03	2.13
(6,219)	1:50:A:THR:HG21	1:51:A:VAL:H	2	2.12	0.06	2.12
(6,219)	1:50:A:THR:HG22	1:51:A:VAL:H	2	2.12	0.06	2.12
(6,219)	1:50:A:THR:HG23	1:51:A:VAL:H	2	2.12	0.06	2.12
(6,98)	1:22:A:THR:H	1:23:A:LEU:H	2	2.12	1.15	2.12
(7,346)	1:99:A:CYS:HA	1:99:A:CYS:H	2	2.12	0.03	2.12
(7,202)	1:59:A:HIS:HA	1:59:A:HIS:H	2	2.11	0.0	2.11
(6,347)	1:83:A:LEU:HD21	1:84:A:LYS:H	2	2.1	0.28	2.1
(6,347)	1:83:A:LEU:HD22	1:84:A:LYS:H	2	2.1	0.28	2.1
(6,347)	1:83:A:LEU:HD23	1:84:A:LYS:H	2	2.1	0.28	2.1
(6,363)	1:86:A:LEU:HD21	1:87:A:ASP:H	2	2.09	0.2	2.09
(6,363)	1:86:A:LEU:HD22	1:87:A:ASP:H	2	2.09	0.2	2.09
(6,363)	1:86:A:LEU:HD23	1:87:A:ASP:H	2	2.09	0.2	2.09
(7,353)	1:102:A:LYS:HA	1:102:A:LYS:H	2	2.09	0.03	2.09
(6,434)	1:103:A:GLU:H	1:104:A:ALA:H	2	2.09	0.43	2.09
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD11	2	2.09	0.01	2.09
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD12	2	2.09	0.01	2.09
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD13	2	2.09	0.01	2.09
(7,342)	1:97:A:ASN:HA	1:97:A:ASN:H	2	2.08	0.01	2.08
(6,505)	1:119:A:ILE:HG21	1:120:A:MET:H	2	2.07	0.71	2.07
(7,55)	1:15:A:ASN:HB3	1:15:A:ASN:HD21	2	2.07	0.39	2.07
(7,55)	1:15:A:ASN:HB3	1:15:A:ASN:HD22	2	2.07	0.39	2.07
(7,56)	1:15:A:ASN:HB3	1:15:A:ASN:HD21	2	2.07	0.39	2.07
(7,56)	1:15:A:ASN:HB3	1:15:A:ASN:HD22	2	2.07	0.39	2.07
(4,297)	1:108:A:THR:HA	1:110:A:GLU:H	2	2.06	0.2	2.06
(4,306)	1:110:A:GLU:H	1:112:A:PHE:H	2	2.06	0.05	2.06
(7,387)	1:110:A:GLU:HG2	1:110:A:GLU:H	2	2.05	0.0	2.05
(7,387)	1:110:A:GLU:HG3	1:110:A:GLU:H	2	2.05	0.0	2.05
(6,330)	1:80:A:ILE:HG12	1:81:A:ARG:H	2	2.04	1.14	2.04
(6,330)	1:80:A:ILE:HG13	1:81:A:ARG:H	2	2.04	1.14	2.04
(7,338)	1:96:A:LEU:HA	1:96:A:LEU:H	2	2.04	0.0	2.04
(4,279)	1:96:A:LEU:HB2	1:98:A:SER:H	2	2.04	0.44	2.04
(4,279)	1:96:A:LEU:HB3	1:98:A:SER:H	2	2.04	0.44	2.04
(6,498)	1:118:A:THR:HB	1:119:A:ILE:H	2	2.04	0.5	2.04
(7,103)	1:28:A:THR:HB	1:28:A:THR:H	2	2.03	0.01	2.03
(7,361)	1:104:A:ALA:HB1	1:104:A:ALA:H	2	2.03	0.24	2.03
(7,361)	1:104:A:ALA:HB2	1:104:A:ALA:H	2	2.03	0.24	2.03
(7,361)	1:104:A:ALA:HB3	1:104:A:ALA:H	2	2.03	0.24	2.03
(2,27)	1:96:A:LEU:HB2	1:46:A:CYS:H	2	2.02	0.12	2.02

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,27)	1:96:A:LEU:HB3	1:46:A:CYS:H	2	2.02	0.12	2.02
(4,317)	1:112:A:PHE:H	1:114:A:GLU:H	2	2.02	0.05	2.02
(7,271)	1:80:A:ILE:HD11	1:80:A:ILE:H	2	2.02	0.13	2.02
(7,271)	1:80:A:ILE:HD12	1:80:A:ILE:H	2	2.02	0.13	2.02
(7,271)	1:80:A:ILE:HD13	1:80:A:ILE:H	2	2.02	0.13	2.02
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG21	2	2.01	0.12	2.01
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG22	2	2.01	0.12	2.01
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG23	2	2.01	0.12	2.01
(6,6)	1:5:A:ILE:H	1:4:A:ASP:HB3	2	2.0	0.71	2.0
(4,339)	1:121:A:ARG:HA	1:123:A:LYS:H	2	2.0	0.21	2.0
(6,190)	1:44:A:THR:HG21	1:45:A:PHE:H	2	2.0	0.03	2.0
(6,190)	1:44:A:THR:HG22	1:45:A:PHE:H	2	2.0	0.03	2.0
(6,190)	1:44:A:THR:HG23	1:45:A:PHE:H	2	2.0	0.03	2.0
(4,104)	1:37:A:LYS:H	1:39:A:THR:H	2	1.99	0.64	1.99
(6,38)	1:11:A:ILE:H	1:10:A:ILE:HG12	2	1.98	0.04	1.98
(6,38)	1:11:A:ILE:H	1:10:A:ILE:HG13	2	1.98	0.04	1.98
(4,202)	1:70:A:ALA:HB1	1:74:A:HIS:H	2	1.98	0.3	1.98
(4,202)	1:70:A:ALA:HB2	1:74:A:HIS:H	2	1.98	0.3	1.98
(4,202)	1:70:A:ALA:HB3	1:74:A:HIS:H	2	1.98	0.3	1.98
(4,234)	1:82:A:PHE:HD1	1:79:A:LEU:H	2	1.97	0.77	1.97
(4,234)	1:82:A:PHE:HD2	1:79:A:LEU:H	2	1.97	0.77	1.97
(6,390)	1:92:A:GLY:H	1:93:A:LEU:H	2	1.96	0.39	1.96
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD11	2	1.96	0.02	1.96
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD12	2	1.96	0.02	1.96
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD13	2	1.96	0.02	1.96
(6,239)	1:56:A:TYR:HB2	1:57:A:SER:H	2	1.95	0.07	1.95
(4,335)	1:119:A:ILE:H	1:121:A:ARG:H	2	1.95	0.06	1.95
(4,325)	1:115:A:ARG:H	1:117:A:LYS:H	2	1.94	0.01	1.94
(4,313)	1:112:A:PHE:HB2	1:115:A:ARG:H	2	1.94	0.01	1.94
(4,313)	1:112:A:PHE:HB3	1:115:A:ARG:H	2	1.94	0.01	1.94
(7,305)	1:89:A:ASN:HD21	1:89:A:ASN:H	2	1.94	0.19	1.94
(4,289)	1:106:A:GLN:HB2	1:108:A:THR:H	2	1.94	0.01	1.94
(4,289)	1:106:A:GLN:HB3	1:108:A:THR:H	2	1.94	0.01	1.94
(4,173)	1:56:A:TYR:H	1:58:A:HIS:H	2	1.92	0.04	1.92
(6,260)	1:62:A:ASP:H	1:63:A:THR:H	2	1.91	0.14	1.91
(6,263)	1:63:A:THR:HA	1:64:A:ARG:H	2	1.91	0.45	1.91
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD11	2	1.9	0.12	1.9
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD12	2	1.9	0.12	1.9
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD13	2	1.9	0.12	1.9
(4,140)	1:47:A:ARG:H	1:49:A:ALA:H	2	1.9	0.06	1.9
(6,45)	1:12:A:LYS:H	1:11:A:ILE:HG12	2	1.89	0.6	1.89
(4,133)	1:45:A:PHE:HA	1:48:A:ALA:H	2	1.88	0.09	1.88

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,2)	1:4:A:ASP:H	1:3:A:THR:HB	2	1.88	0.45	1.88
(6,401)	1:95:A:GLY:HA2	1:96:A:LEU:H	2	1.88	0.01	1.88
(7,9)	1:5:A:ILE:H	1:5:A:ILE:HG13	2	1.88	0.06	1.88
(7,284)	1:83:A:LEU:HD11	1:83:A:LEU:H	2	1.87	0.39	1.87
(7,284)	1:83:A:LEU:HD12	1:83:A:LEU:H	2	1.87	0.39	1.87
(7,284)	1:83:A:LEU:HD13	1:83:A:LEU:H	2	1.87	0.39	1.87
(6,89)	1:20:A:GLN:HA	1:21:A:LYS:H	2	1.86	0.01	1.86
(2,20)	1:105:A:ASN:HB2	1:34:A:ALA:H	2	1.86	0.17	1.86
(2,20)	1:105:A:ASN:HB3	1:34:A:ALA:H	2	1.86	0.17	1.86
(6,251)	1:59:A:HIS:HA	1:60:A:GLU:H	2	1.86	0.19	1.86
(7,189)	1:55:A:PHE:HD1	1:55:A:PHE:H	2	1.86	0.02	1.86
(7,189)	1:55:A:PHE:HD2	1:55:A:PHE:H	2	1.86	0.02	1.86
(7,414)	1:119:A:ILE:HG13	1:119:A:ILE:H	2	1.86	0.86	1.86
(4,262)	1:87:A:ASP:H	1:89:A:ASN:H	2	1.85	0.23	1.85
(6,438)	1:104:A:ALA:H	1:105:A:ASN:H	2	1.85	0.63	1.85
(6,7)	1:5:A:ILE:H	1:4:A:ASP:HB2	2	1.84	0.36	1.84
(6,472)	1:112:A:PHE:HD1	1:111:A:ASN:H	2	1.84	0.05	1.84
(6,472)	1:112:A:PHE:HD2	1:111:A:ASN:H	2	1.84	0.05	1.84
(6,133)	1:31:A:ASP:HB2	1:32:A:ILE:H	2	1.83	0.24	1.83
(6,447)	1:106:A:GLN:HA	1:107:A:SER:H	2	1.83	0.02	1.83
(7,3)	1:3:A:THR:H	1:3:A:THR:HG21	2	1.83	0.18	1.83
(7,3)	1:3:A:THR:H	1:3:A:THR:HG22	2	1.83	0.18	1.83
(7,3)	1:3:A:THR:H	1:3:A:THR:HG23	2	1.83	0.18	1.83
(6,81)	1:18:A:THR:H	1:19:A:GLU:HB2	2	1.83	0.61	1.83
(6,81)	1:18:A:THR:H	1:19:A:GLU:HB3	2	1.83	0.61	1.83
(6,280)	1:68:A:ALA:HB1	1:69:A:THR:H	2	1.82	0.05	1.82
(6,280)	1:68:A:ALA:HB2	1:69:A:THR:H	2	1.82	0.05	1.82
(6,280)	1:68:A:ALA:HB3	1:69:A:THR:H	2	1.82	0.05	1.82
(7,57)	1:15:A:ASN:HB2	1:15:A:ASN:HD21	2	1.82	0.22	1.82
(7,57)	1:15:A:ASN:HB2	1:15:A:ASN:HD22	2	1.82	0.22	1.82
(7,58)	1:15:A:ASN:HB2	1:15:A:ASN:HD21	2	1.82	0.22	1.82
(7,58)	1:15:A:ASN:HB2	1:15:A:ASN:HD22	2	1.82	0.22	1.82
(6,92)	1:20:A:GLN:HB2	1:21:A:LYS:H	2	1.82	0.06	1.82
(4,326)	1:116:A:LEU:H	1:118:A:THR:H	2	1.82	0.03	1.82
(7,69)	1:18:A:THR:H	1:18:A:THR:HG21	2	1.81	0.07	1.81
(7,69)	1:18:A:THR:H	1:18:A:THR:HG22	2	1.81	0.07	1.81
(7,69)	1:18:A:THR:H	1:18:A:THR:HG23	2	1.81	0.07	1.81
(7,106)	1:29:A:VAL:HB	1:29:A:VAL:H	2	1.81	0.65	1.81
(2,8)	1:28:A:THR:HG21	1:108:A:THR:H	2	1.8	0.15	1.8
(2,8)	1:28:A:THR:HG22	1:108:A:THR:H	2	1.8	0.15	1.8
(2,8)	1:28:A:THR:HG23	1:108:A:THR:H	2	1.8	0.15	1.8
(4,224)	1:76:A:HIS:HB2	1:78:A:GLN:H	2	1.8	0.15	1.8

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,224)	1:76:A:HIS:HB3	1:78:A:GLN:H	2	1.8	0.15	1.8
(6,154)	1:34:A:ALA:HB1	1:35:A:ALA:H	2	1.8	1.01	1.8
(6,154)	1:34:A:ALA:HB2	1:35:A:ALA:H	2	1.8	1.01	1.8
(6,154)	1:34:A:ALA:HB3	1:35:A:ALA:H	2	1.8	1.01	1.8
(7,168)	1:48:A:ALA:HB1	1:48:A:ALA:H	2	1.8	0.03	1.8
(7,168)	1:48:A:ALA:HB2	1:48:A:ALA:H	2	1.8	0.03	1.8
(7,168)	1:48:A:ALA:HB3	1:48:A:ALA:H	2	1.8	0.03	1.8
(4,277)	1:94:A:ALA:HA	1:96:A:LEU:H	2	1.8	0.41	1.8
(4,86)	1:31:A:ASP:HB3	1:34:A:ALA:H	2	1.8	0.07	1.8
(4,201)	1:70:A:ALA:HB1	1:73:A:PHE:H	2	1.79	0.03	1.79
(4,201)	1:70:A:ALA:HB2	1:73:A:PHE:H	2	1.79	0.03	1.79
(4,201)	1:70:A:ALA:HB3	1:73:A:PHE:H	2	1.79	0.03	1.79
(4,278)	1:94:A:ALA:H	1:96:A:LEU:H	2	1.78	0.03	1.78
(6,101)	1:23:A:LEU:HA	1:24:A:CYS:H	2	1.78	0.03	1.78
(7,158)	1:44:A:THR:HG21	1:44:A:THR:H	2	1.78	0.01	1.78
(7,158)	1:44:A:THR:HG22	1:44:A:THR:H	2	1.78	0.01	1.78
(7,158)	1:44:A:THR:HG23	1:44:A:THR:H	2	1.78	0.01	1.78
(2,15)	1:120:A:MET:H	1:11:A:ILE:HG12	2	1.78	0.02	1.78
(2,15)	1:120:A:MET:H	1:11:A:ILE:HG13	2	1.78	0.02	1.78
(6,16)	1:7:A:LEU:H	1:6:A:THR:HB	2	1.78	0.27	1.78
(7,120)	1:32:A:ILE:HD11	1:32:A:ILE:H	2	1.78	0.1	1.78
(7,120)	1:32:A:ILE:HD12	1:32:A:ILE:H	2	1.78	0.1	1.78
(7,120)	1:32:A:ILE:HD13	1:32:A:ILE:H	2	1.78	0.1	1.78
(4,320)	1:113:A:LEU:H	1:115:A:ARG:H	2	1.77	0.03	1.77
(6,110)	1:24:A:CYS:HA	1:25:A:THR:H	2	1.77	0.0	1.77
(6,321)	1:79:A:LEU:HB2	1:80:A:ILE:H	2	1.77	0.25	1.77
(6,321)	1:79:A:LEU:HB3	1:80:A:ILE:H	2	1.77	0.25	1.77
(6,535)	1:126:A:LYS:HA	1:127:A:CYS:H	2	1.77	0.07	1.77
(7,127)	1:34:A:ALA:HB1	1:34:A:ALA:H	2	1.77	0.01	1.77
(7,127)	1:34:A:ALA:HB2	1:34:A:ALA:H	2	1.77	0.01	1.77
(7,127)	1:34:A:ALA:HB3	1:34:A:ALA:H	2	1.77	0.01	1.77
(4,304)	1:110:A:GLU:HA	1:112:A:PHE:H	2	1.76	0.05	1.76
(6,195)	1:44:A:THR:HG21	1:45:A:PHE:HD1	2	1.76	0.06	1.76
(6,195)	1:44:A:THR:HG21	1:45:A:PHE:HD2	2	1.76	0.06	1.76
(6,195)	1:44:A:THR:HG22	1:45:A:PHE:HD1	2	1.76	0.06	1.76
(6,195)	1:44:A:THR:HG22	1:45:A:PHE:HD2	2	1.76	0.06	1.76
(6,195)	1:44:A:THR:HG23	1:45:A:PHE:HD1	2	1.76	0.06	1.76
(6,195)	1:44:A:THR:HG23	1:45:A:PHE:HD2	2	1.76	0.06	1.76
(7,194)	1:56:A:TYR:HB2	1:56:A:TYR:H	2	1.76	0.0	1.76
(7,173)	1:50:A:THR:HG21	1:50:A:THR:H	2	1.76	0.01	1.76
(7,173)	1:50:A:THR:HG22	1:50:A:THR:H	2	1.76	0.01	1.76
(7,173)	1:50:A:THR:HG23	1:50:A:THR:H	2	1.76	0.01	1.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,10)	1:28:A:THR:HA	1:109:A:LEU:H	2	1.75	0.08	1.75
(4,300)	1:109:A:LEU:HD11	1:113:A:LEU:H	2	1.75	0.12	1.75
(4,300)	1:109:A:LEU:HD12	1:113:A:LEU:H	2	1.75	0.12	1.75
(4,300)	1:109:A:LEU:HD13	1:113:A:LEU:H	2	1.75	0.12	1.75
(4,227)	1:77:A:LYS:HA	1:79:A:LEU:H	2	1.74	0.04	1.74
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG21	2	1.74	0.08	1.74
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG22	2	1.74	0.08	1.74
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG23	2	1.74	0.08	1.74
(4,94)	1:34:A:ALA:HB1	1:37:A:LYS:H	2	1.74	0.03	1.74
(4,94)	1:34:A:ALA:HB2	1:37:A:LYS:H	2	1.74	0.03	1.74
(4,94)	1:34:A:ALA:HB3	1:37:A:LYS:H	2	1.74	0.03	1.74
(6,127)	1:29:A:VAL:HG21	1:30:A:THR:H	2	1.74	0.16	1.74
(6,127)	1:29:A:VAL:HG22	1:30:A:THR:H	2	1.74	0.16	1.74
(6,127)	1:29:A:VAL:HG23	1:30:A:THR:H	2	1.74	0.16	1.74
(6,450)	1:107:A:SER:HB2	1:108:A:THR:H	2	1.74	1.17	1.74
(7,339)	1:96:A:LEU:HB2	1:96:A:LEU:H	2	1.74	0.02	1.74
(7,339)	1:96:A:LEU:HB3	1:96:A:LEU:H	2	1.74	0.02	1.74
(2,30)	1:29:A:VAL:HG11	1:56:A:TYR:H	2	1.73	0.1	1.73
(2,30)	1:29:A:VAL:HG12	1:56:A:TYR:H	2	1.73	0.1	1.73
(2,30)	1:29:A:VAL:HG13	1:56:A:TYR:H	2	1.73	0.1	1.73
(2,30)	1:29:A:VAL:HG21	1:56:A:TYR:H	2	1.73	0.1	1.73
(2,30)	1:29:A:VAL:HG22	1:56:A:TYR:H	2	1.73	0.1	1.73
(2,30)	1:29:A:VAL:HG23	1:56:A:TYR:H	2	1.73	0.1	1.73
(4,106)	1:40:A:THR:H	1:43:A:GLU:H	2	1.72	0.34	1.72
(4,131)	1:45:A:PHE:H	1:47:A:ARG:H	2	1.72	0.18	1.72
(7,229)	1:68:A:ALA:HA	1:68:A:ALA:H	2	1.72	0.01	1.72
(7,413)	1:119:A:ILE:HB	1:119:A:ILE:H	2	1.72	0.09	1.72
(7,421)	1:120:A:MET:HB2	1:120:A:MET:H	2	1.71	0.02	1.71
(7,426)	1:122:A:GLU:HB2	1:122:A:GLU:H	2	1.7	0.06	1.7
(7,426)	1:122:A:GLU:HB3	1:122:A:GLU:H	2	1.7	0.06	1.7
(7,147)	1:41:A:GLU:HB2	1:41:A:GLU:H	2	1.7	0.09	1.7
(7,147)	1:41:A:GLU:HB3	1:41:A:GLU:H	2	1.7	0.09	1.7
(4,329)	1:117:A:LYS:H	1:119:A:ILE:H	2	1.69	0.07	1.69
(7,143)	1:39:A:THR:HG21	1:39:A:THR:H	2	1.68	0.6	1.68
(7,143)	1:39:A:THR:HG22	1:39:A:THR:H	2	1.68	0.6	1.68
(7,143)	1:39:A:THR:HG23	1:39:A:THR:H	2	1.68	0.6	1.68
(6,428)	1:103:A:GLU:HG2	1:102:A:LYS:H	2	1.68	0.04	1.68
(6,428)	1:103:A:GLU:HG3	1:102:A:LYS:H	2	1.68	0.04	1.68
(4,332)	1:119:A:ILE:HD11	1:121:A:ARG:H	2	1.68	0.6	1.68
(4,332)	1:119:A:ILE:HD12	1:121:A:ARG:H	2	1.68	0.6	1.68
(4,332)	1:119:A:ILE:HD13	1:121:A:ARG:H	2	1.68	0.6	1.68
(7,293)	1:86:A:LEU:HB2	1:86:A:LEU:H	2	1.67	0.1	1.67

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,293)	1:86:A:LEU:HB3	1:86:A:LEU:H	2	1.67	0.1	1.67
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD11	2	1.66	0.08	1.66
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD12	2	1.66	0.08	1.66
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD13	2	1.66	0.08	1.66
(6,229)	1:54:A:GLN:HB2	1:55:A:PHE:H	2	1.66	0.01	1.66
(6,229)	1:54:A:GLN:HB3	1:55:A:PHE:H	2	1.66	0.01	1.66
(4,214)	1:73:A:PHE:HA	1:75:A:ARG:H	2	1.66	0.17	1.66
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD11	2	1.66	0.14	1.66
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD12	2	1.66	0.14	1.66
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD13	2	1.66	0.14	1.66
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD21	2	1.66	0.14	1.66
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD22	2	1.66	0.14	1.66
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD23	2	1.66	0.14	1.66
(6,531)	1:125:A:SER:HA	1:126:A:LYS:H	2	1.66	0.06	1.66
(7,185)	1:54:A:GLN:HB2	1:54:A:GLN:H	2	1.66	0.08	1.66
(7,185)	1:54:A:GLN:HB3	1:54:A:GLN:H	2	1.66	0.08	1.66
(4,263)	1:88:A:ARG:H	1:90:A:LEU:H	2	1.65	0.39	1.65
(4,302)	1:109:A:LEU:HA	1:112:A:PHE:H	2	1.65	0.0	1.65
(4,336)	1:120:A:MET:HA	1:123:A:LYS:H	2	1.64	0.06	1.64
(4,347)	1:124:A:TYR:HA	1:127:A:CYS:H	2	1.64	0.01	1.64
(6,286)	1:70:A:ALA:HA	1:71:A:GLN:H	2	1.64	0.02	1.64
(4,273)	1:92:A:GLY:HA3	1:94:A:ALA:H	2	1.62	0.65	1.62
(7,380)	1:109:A:LEU:HB2	1:109:A:LEU:H	2	1.62	0.04	1.62
(4,287)	1:103:A:GLU:HA	1:105:A:ASN:H	2	1.62	0.43	1.62
(7,220)	1:65:A:CYS:HB3	1:65:A:CYS:H	2	1.62	0.19	1.62
(6,35)	1:10:A:ILE:H	1:11:A:ILE:HG12	2	1.61	0.64	1.61
(6,35)	1:10:A:ILE:H	1:11:A:ILE:HG13	2	1.61	0.64	1.61
(6,125)	1:29:A:VAL:H	1:30:A:THR:H	2	1.61	0.03	1.61
(6,314)	1:76:A:HIS:HA	1:77:A:LYS:H	2	1.6	0.01	1.6
(6,400)	1:95:A:GLY:HA3	1:96:A:LEU:H	2	1.6	0.02	1.6
(6,448)	1:106:A:GLN:H	1:107:A:SER:H	2	1.6	0.17	1.6
(7,230)	1:68:A:ALA:HB1	1:68:A:ALA:H	2	1.6	0.01	1.6
(7,230)	1:68:A:ALA:HB2	1:68:A:ALA:H	2	1.6	0.01	1.6
(7,230)	1:68:A:ALA:HB3	1:68:A:ALA:H	2	1.6	0.01	1.6
(2,36)	1:56:A:TYR:HD1	1:83:A:LEU:H	2	1.6	0.66	1.6
(2,36)	1:56:A:TYR:HD2	1:83:A:LEU:H	2	1.6	0.66	1.6
(6,236)	1:56:A:TYR:HD1	1:57:A:SER:H	2	1.6	0.02	1.6
(6,236)	1:56:A:TYR:HD2	1:57:A:SER:H	2	1.6	0.02	1.6
(6,244)	1:57:A:SER:HA	1:58:A:HIS:H	2	1.6	0.04	1.6
(6,407)	1:96:A:LEU:H	1:97:A:ASN:H	2	1.6	0.06	1.6
(6,13)	1:5:A:ILE:HD11	1:6:A:THR:H	2	1.59	0.11	1.59
(6,13)	1:5:A:ILE:HD12	1:6:A:THR:H	2	1.59	0.11	1.59

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,13)	1:5:A:ILE:HD13	1:6:A:THR:H	2	1.59	0.11	1.59
(7,308)	1:89:A:ASN:HB2	1:89:A:ASN:H	2	1.59	0.12	1.59
(6,73)	1:17:A:LEU:HA	1:18:A:THR:H	2	1.58	0.03	1.58
(6,141)	1:32:A:ILE:HG12	1:33:A:PHE:H	2	1.58	0.32	1.58
(6,205)	1:46:A:CYS:HB3	1:47:A:ARG:H	2	1.58	0.24	1.58
(7,435)	1:125:A:SER:HB2	1:125:A:SER:H	2	1.58	0.04	1.58
(7,435)	1:125:A:SER:HB3	1:125:A:SER:H	2	1.58	0.04	1.58
(6,261)	1:63:A:THR:HB	1:64:A:ARG:H	2	1.57	0.89	1.57
(7,31)	1:9:A:GLU:H	1:9:A:GLU:HG2	2	1.57	0.05	1.57
(7,31)	1:9:A:GLU:H	1:9:A:GLU:HG3	2	1.57	0.05	1.57
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD21	2	1.57	0.33	1.57
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD22	2	1.57	0.33	1.57
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD23	2	1.57	0.33	1.57
(7,137)	1:38:A:ASN:HB2	1:38:A:ASN:H	2	1.57	0.17	1.57
(7,228)	1:67:A:GLY:HA2	1:67:A:GLY:H	2	1.56	0.11	1.56
(4,158)	1:55:A:PHE:HE1	1:59:A:HIS:HD2	2	1.55	1.39	1.55
(4,158)	1:55:A:PHE:HE2	1:59:A:HIS:HD2	2	1.55	1.39	1.55
(7,70)	1:18:A:THR:H	1:18:A:THR:HB	2	1.55	0.13	1.55
(2,9)	1:29:A:VAL:H	1:109:A:LEU:H	2	1.54	0.36	1.54
(4,337)	1:120:A:MET:HA	1:122:A:GLU:H	2	1.54	0.12	1.54
(6,240)	1:56:A:TYR:HA	1:57:A:SER:H	2	1.54	0.01	1.54
(6,308)	1:74:A:HIS:H	1:75:A:ARG:H	2	1.54	0.17	1.54
(6,398)	1:94:A:ALA:HA	1:95:A:GLY:H	2	1.54	0.0	1.54
(7,381)	1:109:A:LEU:HG	1:109:A:LEU:H	2	1.54	0.01	1.54
(7,176)	1:51:A:VAL:HG11	1:51:A:VAL:H	2	1.53	0.75	1.53
(7,176)	1:51:A:VAL:HG12	1:51:A:VAL:H	2	1.53	0.75	1.53
(7,176)	1:51:A:VAL:HG13	1:51:A:VAL:H	2	1.53	0.75	1.53
(2,50)	1:93:A:LEU:HD11	1:6:A:THR:H	2	1.52	0.72	1.52
(2,50)	1:93:A:LEU:HD12	1:6:A:THR:H	2	1.52	0.72	1.52
(2,50)	1:93:A:LEU:HD13	1:6:A:THR:H	2	1.52	0.72	1.52
(2,50)	1:93:A:LEU:HD21	1:6:A:THR:H	2	1.52	0.72	1.52
(2,50)	1:93:A:LEU:HD22	1:6:A:THR:H	2	1.52	0.72	1.52
(2,50)	1:93:A:LEU:HD23	1:6:A:THR:H	2	1.52	0.72	1.52
(4,282)	1:96:A:LEU:HA	1:98:A:SER:H	2	1.52	1.02	1.52
(7,97)	1:27:A:LEU:HB3	1:27:A:LEU:H	2	1.52	0.01	1.52
(4,10)	1:5:A:ILE:H	1:8:A:GLN:HB2	2	1.52	0.04	1.52
(4,10)	1:5:A:ILE:H	1:8:A:GLN:HB3	2	1.52	0.04	1.52
(4,90)	1:32:A:ILE:HA	1:34:A:ALA:H	2	1.52	0.02	1.52
(6,442)	1:105:A:ASN:HA	1:106:A:GLN:H	2	1.52	0.07	1.52
(4,195)	1:72:A:GLN:HG2	1:69:A:THR:H	2	1.51	0.19	1.51
(4,342)	1:122:A:GLU:H	1:124:A:TYR:H	2	1.51	0.2	1.51
(6,406)	1:96:A:LEU:HA	1:97:A:ASN:H	2	1.51	0.35	1.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,310)	1:111:A:ASN:HA	1:114:A:GLU:H	2	1.5	0.1	1.5
(7,154)	1:43:A:GLU:HB2	1:43:A:GLU:H	2	1.5	0.08	1.5
(7,154)	1:43:A:GLU:HB3	1:43:A:GLU:H	2	1.5	0.08	1.5
(7,164)	1:46:A:CYS:HB3	1:46:A:CYS:H	2	1.5	0.08	1.5
(4,319)	1:113:A:LEU:HA	1:117:A:LYS:H	2	1.5	0.19	1.5
(6,57)	1:15:A:ASN:HD21	1:14:A:LEU:HA	2	1.5	0.15	1.5
(6,57)	1:15:A:ASN:HD22	1:14:A:LEU:HA	2	1.5	0.15	1.5
(6,58)	1:15:A:ASN:HD21	1:14:A:LEU:HA	2	1.5	0.15	1.5
(6,58)	1:15:A:ASN:HD22	1:14:A:LEU:HA	2	1.5	0.15	1.5
(7,145)	1:40:A:THR:HG21	1:40:A:THR:H	2	1.5	0.06	1.5
(7,145)	1:40:A:THR:HG22	1:40:A:THR:H	2	1.5	0.06	1.5
(7,145)	1:40:A:THR:HG23	1:40:A:THR:H	2	1.5	0.06	1.5
(7,327)	1:92:A:GLY:HA2	1:92:A:GLY:H	2	1.5	0.17	1.5
(6,281)	1:69:A:THR:HA	1:70:A:ALA:H	2	1.49	0.07	1.49
(7,155)	1:43:A:GLU:HG2	1:43:A:GLU:H	2	1.49	0.14	1.49
(7,155)	1:43:A:GLU:HG3	1:43:A:GLU:H	2	1.49	0.14	1.49
(2,47)	1:33:A:PHE:HZ	1:116:A:LEU:H	2	1.48	0.7	1.48
(6,136)	1:32:A:ILE:HG12	1:31:A:ASP:H	2	1.48	0.16	1.48
(6,136)	1:32:A:ILE:HG13	1:31:A:ASP:H	2	1.48	0.16	1.48
(6,376)	1:89:A:ASN:HA	1:90:A:LEU:H	2	1.48	0.09	1.48
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD11	2	1.48	0.04	1.48
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD12	2	1.48	0.04	1.48
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD13	2	1.48	0.04	1.48
(6,468)	1:110:A:GLU:HA	1:111:A:ASN:H	2	1.48	0.01	1.48
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG21	2	1.48	0.68	1.48
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG22	2	1.48	0.68	1.48
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG23	2	1.48	0.68	1.48
(4,250)	1:84:A:LYS:HA	1:86:A:LEU:H	2	1.47	0.06	1.47
(6,211)	1:48:A:ALA:HA	1:49:A:ALA:H	2	1.47	0.01	1.47
(6,214)	1:49:A:ALA:HA	1:50:A:THR:H	2	1.47	0.01	1.47
(6,325)	1:79:A:LEU:HA	1:80:A:ILE:H	2	1.47	0.0	1.47
(6,348)	1:83:A:LEU:HA	1:84:A:LYS:H	2	1.47	0.02	1.47
(4,144)	1:48:A:ALA:HA	1:51:A:VAL:H	2	1.46	0.22	1.46
(6,32)	1:10:A:ILE:HA	1:11:A:ILE:H	2	1.46	0.01	1.46
(6,493)	1:116:A:LEU:HA	1:117:A:LYS:H	2	1.46	0.01	1.46
(6,502)	1:119:A:ILE:HB	1:120:A:MET:H	2	1.46	0.02	1.46
(4,294)	1:111:A:ASN:HB3	1:108:A:THR:H	2	1.46	0.16	1.46
(6,118)	1:27:A:LEU:H	1:28:A:THR:H	2	1.46	0.05	1.46
(6,207)	1:46:A:CYS:HA	1:47:A:ARG:H	2	1.46	0.0	1.46
(6,234)	1:55:A:PHE:HA	1:56:A:TYR:H	2	1.46	0.01	1.46
(6,333)	1:80:A:ILE:HA	1:81:A:ARG:H	2	1.46	0.03	1.46
(6,481)	1:113:A:LEU:HA	1:114:A:GLU:H	2	1.46	0.01	1.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,495)	1:117:A:LYS:HA	1:118:A:THR:H	2	1.46	0.01	1.46
(6,511)	1:120:A:MET:HA	1:121:A:ARG:H	2	1.46	0.01	1.46
(6,186)	1:43:A:GLU:HB2	1:44:A:THR:H	2	1.46	0.08	1.46
(6,186)	1:43:A:GLU:HB3	1:44:A:THR:H	2	1.46	0.08	1.46
(6,336)	1:82:A:PHE:HB2	1:81:A:ARG:H	2	1.46	0.03	1.46
(6,336)	1:82:A:PHE:HB3	1:81:A:ARG:H	2	1.46	0.03	1.46
(6,166)	1:37:A:LYS:HB2	1:38:A:ASN:H	2	1.45	0.65	1.45
(6,166)	1:37:A:LYS:HB3	1:38:A:ASN:H	2	1.45	0.65	1.45
(4,316)	1:112:A:PHE:HA	1:115:A:ARG:H	2	1.45	0.07	1.45
(6,319)	1:79:A:LEU:HB2	1:78:A:GLN:H	2	1.45	0.27	1.45
(6,319)	1:79:A:LEU:HB3	1:78:A:GLN:H	2	1.45	0.27	1.45
(6,368)	1:87:A:ASP:HA	1:88:A:ARG:H	2	1.45	0.01	1.45
(6,482)	1:113:A:LEU:HB2	1:114:A:GLU:H	2	1.45	0.03	1.45
(6,482)	1:113:A:LEU:HB3	1:114:A:GLU:H	2	1.45	0.03	1.45
(6,508)	1:119:A:ILE:HA	1:120:A:MET:H	2	1.45	0.01	1.45
(7,73)	1:19:A:GLU:H	1:19:A:GLU:HG3	2	1.45	0.27	1.45
(4,243)	1:82:A:PHE:HD1	1:85:A:ARG:H	2	1.44	0.15	1.44
(4,243)	1:82:A:PHE:HD2	1:85:A:ARG:H	2	1.44	0.15	1.44
(4,322)	1:114:A:GLU:H	1:117:A:LYS:H	2	1.44	0.01	1.44
(6,59)	1:15:A:ASN:HA	1:16:A:SER:H	2	1.44	0.01	1.44
(6,247)	1:58:A:HIS:HA	1:59:A:HIS:H	2	1.44	0.02	1.44
(6,265)	1:64:A:ARG:HA	1:65:A:CYS:H	2	1.44	0.02	1.44
(6,352)	1:85:A:ARG:HA	1:86:A:LEU:H	2	1.44	0.03	1.44
(6,516)	1:121:A:ARG:HA	1:122:A:GLU:H	2	1.44	0.01	1.44
(6,528)	1:124:A:TYR:HA	1:125:A:SER:H	2	1.44	0.01	1.44
(4,119)	1:42:A:LYS:H	1:44:A:THR:H	2	1.44	0.07	1.44
(6,200)	1:45:A:PHE:HA	1:46:A:CYS:H	2	1.44	0.01	1.44
(6,230)	1:55:A:PHE:HB3	1:56:A:TYR:H	2	1.44	0.07	1.44
(6,306)	1:74:A:HIS:HB2	1:75:A:ARG:H	2	1.44	0.33	1.44
(6,316)	1:77:A:LYS:HA	1:78:A:GLN:H	2	1.44	0.0	1.44
(6,479)	1:112:A:PHE:HA	1:113:A:LEU:H	2	1.44	0.02	1.44
(6,489)	1:115:A:ARG:HA	1:116:A:LEU:H	2	1.44	0.0	1.44
(6,523)	1:123:A:LYS:HA	1:124:A:TYR:H	2	1.44	0.01	1.44
(7,130)	1:36:A:SER:HA	1:36:A:SER:H	2	1.44	0.26	1.44
(6,342)	1:82:A:PHE:HA	1:83:A:LEU:H	2	1.44	0.03	1.44
(6,386)	1:91:A:TRP:HA	1:92:A:GLY:H	2	1.44	0.01	1.44
(7,165)	1:46:A:CYS:HB2	1:46:A:CYS:H	2	1.43	0.09	1.43
(4,52)	1:15:A:ASN:HA	1:17:A:LEU:H	2	1.43	0.02	1.43
(6,487)	1:114:A:GLU:HA	1:115:A:ARG:H	2	1.43	0.0	1.43
(6,524)	1:123:A:LYS:H	1:124:A:TYR:H	2	1.43	0.05	1.43
(4,298)	1:108:A:THR:H	1:111:A:ASN:H	2	1.42	0.08	1.42
(6,238)	1:56:A:TYR:HB3	1:57:A:SER:H	2	1.42	0.12	1.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,473)	1:112:A:PHE:HB3	1:111:A:ASN:H	2	1.42	0.08	1.42
(6,253)	1:60:A:GLU:H	1:61:A:LYS:H	2	1.42	0.99	1.42
(4,11)	1:6:A:THR:H	1:8:A:GLN:H	2	1.42	0.21	1.42
(4,193)	1:69:A:THR:H	1:73:A:PHE:H	2	1.42	0.01	1.42
(6,290)	1:71:A:GLN:HA	1:72:A:GLN:H	2	1.42	0.01	1.42
(6,529)	1:124:A:TYR:H	1:125:A:SER:H	2	1.41	0.04	1.41
(7,285)	1:83:A:LEU:HD21	1:83:A:LEU:H	2	1.41	0.18	1.41
(7,285)	1:83:A:LEU:HD22	1:83:A:LEU:H	2	1.41	0.18	1.41
(7,285)	1:83:A:LEU:HD23	1:83:A:LEU:H	2	1.41	0.18	1.41
(7,323)	1:91:A:TRP:HD1	1:91:A:TRP:HB2	2	1.41	0.06	1.41
(6,102)	1:23:A:LEU:H	1:24:A:CYS:H	2	1.4	0.02	1.4
(4,318)	1:113:A:LEU:HA	1:116:A:LEU:H	2	1.4	0.05	1.4
(6,374)	1:89:A:ASN:HB3	1:90:A:LEU:H	2	1.39	0.26	1.39
(4,171)	1:56:A:TYR:HA	1:59:A:HIS:H	2	1.38	0.14	1.38
(7,236)	1:71:A:GLN:HB3	1:71:A:GLN:H	2	1.38	0.01	1.38
(6,285)	1:70:A:ALA:HB1	1:71:A:GLN:H	2	1.38	0.04	1.38
(6,285)	1:70:A:ALA:HB2	1:71:A:GLN:H	2	1.38	0.04	1.38
(6,285)	1:70:A:ALA:HB3	1:71:A:GLN:H	2	1.38	0.04	1.38
(7,222)	1:66:A:LEU:HA	1:66:A:LEU:H	2	1.38	0.3	1.38
(7,390)	1:111:A:ASN:HD21	1:111:A:ASN:H	2	1.38	0.0	1.38
(7,390)	1:111:A:ASN:HD22	1:111:A:ASN:H	2	1.38	0.0	1.38
(4,2)	1:4:A:ASP:HA	1:6:A:THR:H	2	1.38	0.34	1.38
(4,126)	1:44:A:THR:HA	1:46:A:CYS:H	2	1.37	0.04	1.37
(4,333)	1:119:A:ILE:HA	1:122:A:GLU:H	2	1.36	0.22	1.36
(6,503)	1:119:A:ILE:HG13	1:120:A:MET:H	2	1.36	0.29	1.36
(6,509)	1:119:A:ILE:H	1:120:A:MET:H	2	1.36	0.01	1.36
(7,441)	1:127:A:CYS:HA	1:127:A:CYS:H	2	1.36	0.32	1.36
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD11	2	1.36	0.95	1.36
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD12	2	1.36	0.95	1.36
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD13	2	1.36	0.95	1.36
(4,209)	1:72:A:GLN:HA	1:76:A:HIS:H	2	1.36	0.41	1.36
(4,245)	1:82:A:PHE:HA	1:85:A:ARG:H	2	1.36	0.21	1.36
(7,100)	1:27:A:LEU:HD11	1:27:A:LEU:H	2	1.36	0.08	1.36
(7,100)	1:27:A:LEU:HD12	1:27:A:LEU:H	2	1.36	0.08	1.36
(7,100)	1:27:A:LEU:HD13	1:27:A:LEU:H	2	1.36	0.08	1.36
(7,344)	1:98:A:SER:HA	1:98:A:SER:H	2	1.36	0.34	1.36
(4,42)	1:12:A:LYS:H	1:15:A:ASN:HB2	2	1.35	0.4	1.35
(4,42)	1:12:A:LYS:H	1:15:A:ASN:HB3	2	1.35	0.4	1.35
(4,185)	1:64:A:ARG:H	1:66:A:LEU:H	2	1.35	0.43	1.35
(6,5)	1:4:A:ASP:H	1:5:A:ILE:H	2	1.35	0.88	1.35
(4,244)	1:82:A:PHE:HA	1:84:A:LYS:H	2	1.34	0.14	1.34
(6,82)	1:19:A:GLU:H	1:18:A:THR:HB	2	1.34	0.68	1.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,129)	1:30:A:THR:HB	1:31:A:ASP:H	2	1.34	0.03	1.34
(6,536)	1:126:A:LYS:H	1:127:A:CYS:H	2	1.34	0.09	1.34
(4,301)	1:109:A:LEU:HD21	1:113:A:LEU:H	2	1.34	0.08	1.34
(4,301)	1:109:A:LEU:HD22	1:113:A:LEU:H	2	1.34	0.08	1.34
(4,301)	1:109:A:LEU:HD23	1:113:A:LEU:H	2	1.34	0.08	1.34
(6,480)	1:112:A:PHE:H	1:113:A:LEU:H	2	1.34	0.01	1.34
(6,469)	1:110:A:GLU:H	1:111:A:ASN:H	2	1.33	0.01	1.33
(7,216)	1:63:A:THR:HB	1:63:A:THR:H	2	1.33	0.02	1.33
(2,42)	1:30:A:THR:HA	1:106:A:GLN:HE21	2	1.32	0.58	1.32
(2,42)	1:30:A:THR:HA	1:106:A:GLN:HE22	2	1.32	0.58	1.32
(4,154)	1:52:A:LEU:HA	1:56:A:TYR:H	2	1.32	0.06	1.32
(7,134)	1:37:A:LYS:HB2	1:37:A:LYS:H	2	1.32	0.01	1.32
(7,134)	1:37:A:LYS:HB3	1:37:A:LYS:H	2	1.32	0.01	1.32
(6,365)	1:86:A:LEU:H	1:87:A:ASP:H	2	1.3	0.06	1.3
(5,3)	1:10:A:ILE:HA	1:14:A:LEU:H	2	1.3	0.26	1.3
(7,379)	1:109:A:LEU:HB3	1:109:A:LEU:H	2	1.3	0.08	1.3
(2,11)	1:28:A:THR:HG21	1:109:A:LEU:H	2	1.29	0.01	1.29
(2,11)	1:28:A:THR:HG22	1:109:A:LEU:H	2	1.29	0.01	1.29
(2,11)	1:28:A:THR:HG23	1:109:A:LEU:H	2	1.29	0.01	1.29
(6,399)	1:94:A:ALA:H	1:95:A:GLY:H	2	1.28	0.15	1.28
(6,109)	1:25:A:THR:H	1:24:A:CYS:HB2	2	1.28	0.62	1.28
(4,12)	1:6:A:THR:H	1:9:A:GLU:H	2	1.27	0.06	1.27
(4,235)	1:82:A:PHE:HB2	1:79:A:LEU:H	2	1.27	0.14	1.27
(4,235)	1:82:A:PHE:HB3	1:79:A:LEU:H	2	1.27	0.14	1.27
(6,382)	1:90:A:LEU:H	1:91:A:TRP:H	2	1.27	0.12	1.27
(4,117)	1:42:A:LYS:HA	1:44:A:THR:H	2	1.27	0.06	1.27
(6,421)	1:101:A:VAL:HB	1:102:A:LYS:H	2	1.26	0.42	1.26
(7,434)	1:125:A:SER:HA	1:125:A:SER:H	2	1.26	0.02	1.26
(4,327)	1:117:A:LYS:HA	1:120:A:MET:H	2	1.25	0.08	1.25
(7,319)	1:91:A:TRP:HE3	1:91:A:TRP:HB3	2	1.25	0.14	1.25
(7,415)	1:119:A:ILE:HG12	1:119:A:ILE:H	2	1.25	0.12	1.25
(6,18)	1:6:A:THR:H	1:7:A:LEU:HB2	2	1.24	0.28	1.24
(6,18)	1:6:A:THR:H	1:7:A:LEU:HB3	2	1.24	0.28	1.24
(4,44)	1:13:A:THR:H	1:15:A:ASN:HB2	2	1.23	0.17	1.23
(4,44)	1:13:A:THR:H	1:15:A:ASN:HB3	2	1.23	0.17	1.23
(7,98)	1:27:A:LEU:HB2	1:27:A:LEU:H	2	1.23	0.16	1.23
(7,378)	1:109:A:LEU:HA	1:109:A:LEU:H	2	1.23	0.04	1.23
(7,423)	1:120:A:MET:HG2	1:120:A:MET:H	2	1.23	0.01	1.23
(7,445)	1:128:A:SER:HB2	1:128:A:SER:H	2	1.23	0.15	1.23
(4,233)	1:79:A:LEU:HA	1:83:A:LEU:H	2	1.22	0.15	1.22
(7,266)	1:80:A:ILE:HA	1:80:A:ILE:H	2	1.22	0.09	1.22
(7,192)	1:56:A:TYR:HA	1:56:A:TYR:H	2	1.21	0.02	1.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,375)	1:108:A:THR:HA	1:108:A:THR:H	2	1.21	0.08	1.21
(6,462)	1:109:A:LEU:H	1:110:A:GLU:H	2	1.2	0.07	1.2
(7,52)	1:15:A:ASN:H	1:15:A:ASN:HD22	2	1.2	0.42	1.2
(7,446)	1:129:A:SER:HA	1:129:A:SER:H	2	1.2	0.06	1.2
(4,221)	1:75:A:ARG:HA	1:77:A:LYS:H	2	1.2	0.14	1.2
(6,464)	1:110:A:GLU:HB2	1:111:A:ASN:H	2	1.2	0.03	1.2
(4,128)	1:44:A:THR:HA	1:47:A:ARG:H	2	1.2	0.15	1.2
(7,254)	1:76:A:HIS:HA	1:76:A:HIS:H	2	1.2	0.08	1.2
(4,122)	1:43:A:GLU:HB2	1:45:A:PHE:H	2	1.19	0.01	1.19
(4,122)	1:43:A:GLU:HB3	1:45:A:PHE:H	2	1.19	0.01	1.19
(7,280)	1:83:A:LEU:HA	1:83:A:LEU:H	2	1.19	0.01	1.19
(7,405)	1:116:A:LEU:HA	1:116:A:LEU:H	2	1.19	0.01	1.19
(6,396)	1:93:A:LEU:H	1:94:A:ALA:H	2	1.19	0.06	1.19
(6,458)	1:109:A:LEU:HB2	1:110:A:GLU:H	2	1.19	0.07	1.19
(7,311)	1:90:A:LEU:HA	1:90:A:LEU:H	2	1.19	0.04	1.19
(7,16)	1:7:A:LEU:HA	1:7:A:LEU:H	2	1.18	0.04	1.18
(7,167)	1:48:A:ALA:HA	1:48:A:ALA:H	2	1.18	0.03	1.18
(7,397)	1:113:A:LEU:HA	1:113:A:LEU:H	2	1.18	0.01	1.18
(7,419)	1:120:A:MET:HA	1:120:A:MET:H	2	1.18	0.05	1.18
(4,340)	1:121:A:ARG:HA	1:124:A:TYR:H	2	1.18	0.3	1.18
(7,166)	1:47:A:ARG:HA	1:47:A:ARG:H	2	1.18	0.04	1.18
(7,424)	1:121:A:ARG:HA	1:121:A:ARG:H	2	1.18	0.0	1.18
(4,353)	1:126:A:LYS:HA	1:128:A:SER:H	2	1.18	0.94	1.18
(4,61)	1:18:A:THR:HA	1:20:A:GLN:H	2	1.17	0.48	1.17
(6,366)	1:87:A:ASP:HB3	1:88:A:ARG:H	2	1.17	0.44	1.17
(6,257)	1:62:A:ASP:HB3	1:63:A:THR:H	2	1.16	0.05	1.16
(7,402)	1:114:A:GLU:HA	1:114:A:GLU:H	2	1.16	0.01	1.16
(7,422)	1:120:A:MET:HG3	1:120:A:MET:H	2	1.16	0.14	1.16
(6,108)	1:25:A:THR:H	1:24:A:CYS:HB3	2	1.16	0.17	1.16
(7,101)	1:27:A:LEU:HD21	1:27:A:LEU:H	2	1.16	0.05	1.16
(7,101)	1:27:A:LEU:HD22	1:27:A:LEU:H	2	1.16	0.05	1.16
(7,101)	1:27:A:LEU:HD23	1:27:A:LEU:H	2	1.16	0.05	1.16
(7,227)	1:67:A:GLY:HA3	1:67:A:GLY:H	2	1.16	0.13	1.16
(4,200)	1:70:A:ALA:HB1	1:72:A:GLN:H	2	1.16	0.12	1.16
(4,200)	1:70:A:ALA:HB2	1:72:A:GLN:H	2	1.16	0.12	1.16
(4,200)	1:70:A:ALA:HB3	1:72:A:GLN:H	2	1.16	0.12	1.16
(6,304)	1:73:A:PHE:H	1:74:A:HIS:H	2	1.16	0.08	1.16
(6,301)	1:73:A:PHE:HB2	1:74:A:HIS:H	2	1.15	0.02	1.15
(7,377)	1:108:A:THR:HG21	1:108:A:THR:H	2	1.15	0.91	1.15
(7,377)	1:108:A:THR:HG22	1:108:A:THR:H	2	1.15	0.91	1.15
(7,377)	1:108:A:THR:HG23	1:108:A:THR:H	2	1.15	0.91	1.15
(4,130)	1:44:A:THR:H	1:47:A:ARG:H	2	1.14	0.03	1.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,230)	1:78:A:GLN:HA	1:80:A:ILE:H	2	1.14	0.4	1.14
(7,436)	1:126:A:LYS:HA	1:126:A:LYS:H	2	1.14	0.01	1.14
(4,20)	1:7:A:LEU:HA	1:11:A:ILE:H	2	1.14	0.13	1.14
(6,369)	1:87:A:ASP:H	1:88:A:ARG:H	2	1.14	0.12	1.14
(6,418)	1:100:A:PRO:HD2	1:99:A:CYS:H	2	1.14	0.84	1.14
(6,532)	1:125:A:SER:H	1:126:A:LYS:H	2	1.13	0.01	1.13
(7,215)	1:63:A:THR:HA	1:63:A:THR:H	2	1.13	0.05	1.13
(4,137)	1:46:A:CYS:HB3	1:48:A:ALA:H	2	1.12	0.09	1.12
(7,132)	1:36:A:SER:HB2	1:36:A:SER:H	2	1.12	0.38	1.12
(7,430)	1:124:A:TYR:HA	1:124:A:TYR:H	2	1.12	0.02	1.12
(4,208)	1:72:A:GLN:HA	1:75:A:ARG:H	2	1.12	0.14	1.12
(7,1)	1:3:A:THR:HA	1:3:A:THR:H	2	1.12	0.03	1.12
(4,207)	1:72:A:GLN:HA	1:74:A:HIS:H	2	1.12	0.04	1.12
(4,210)	1:72:A:GLN:H	1:74:A:HIS:H	2	1.12	0.22	1.12
(6,340)	1:82:A:PHE:HB3	1:83:A:LEU:H	2	1.12	0.5	1.12
(6,466)	1:111:A:ASN:HB3	1:110:A:GLU:H	2	1.12	0.01	1.12
(7,133)	1:37:A:LYS:HA	1:37:A:LYS:H	2	1.11	0.0	1.11
(4,145)	1:48:A:ALA:HA	1:52:A:LEU:H	2	1.1	0.02	1.1
(6,270)	1:65:A:CYS:HA	1:66:A:LEU:H	2	1.1	0.18	1.1
(7,85)	1:22:A:THR:H	1:22:A:THR:HA	2	1.1	0.06	1.1
(7,93)	1:25:A:THR:H	1:25:A:THR:HA	2	1.1	0.04	1.1
(7,432)	1:124:A:TYR:HB3	1:124:A:TYR:H	2	1.1	0.7	1.1
(4,92)	1:32:A:ILE:H	1:34:A:ALA:H	2	1.1	0.13	1.1
(7,135)	1:38:A:ASN:HA	1:38:A:ASN:H	2	1.1	0.0	1.1
(7,306)	1:89:A:ASN:HD22	1:89:A:ASN:H	2	1.1	0.07	1.1
(4,246)	1:82:A:PHE:HA	1:86:A:LEU:H	2	1.1	0.03	1.1
(7,326)	1:92:A:GLY:HA3	1:92:A:GLY:H	2	1.1	0.01	1.1
(4,127)	1:44:A:THR:HB	1:46:A:CYS:H	2	1.1	0.08	1.1
(4,252)	1:84:A:LYS:HA	1:88:A:ARG:H	2	1.1	0.24	1.1
(6,146)	1:34:A:ALA:HA	1:33:A:PHE:H	2	1.09	0.16	1.09
(4,24)	1:8:A:GLN:HA	1:12:A:LYS:H	2	1.08	0.4	1.08
(4,58)	1:17:A:LEU:HA	1:19:A:GLU:H	2	1.08	0.39	1.08
(6,389)	1:92:A:GLY:HA2	1:93:A:LEU:H	2	1.08	0.09	1.08
(7,212)	1:62:A:ASP:HA	1:62:A:ASP:H	2	1.08	0.04	1.08
(7,357)	1:103:A:GLU:HA	1:103:A:GLU:H	2	1.08	0.05	1.08
(4,9)	1:5:A:ILE:H	1:7:A:LEU:H	2	1.07	0.41	1.07
(4,323)	1:114:A:GLU:HA	1:118:A:THR:H	2	1.07	0.01	1.07
(6,323)	1:79:A:LEU:HB2	1:80:A:ILE:H	2	1.07	0.93	1.07
(4,330)	1:118:A:THR:HA	1:121:A:ARG:H	2	1.07	0.11	1.07
(4,345)	1:123:A:LYS:H	1:125:A:SER:H	2	1.07	0.33	1.07
(6,293)	1:73:A:PHE:HA	1:72:A:GLN:H	2	1.06	0.22	1.06
(2,49)	1:10:A:ILE:HD11	1:89:A:ASN:H	2	1.06	0.36	1.06

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,49)	1:10:A:ILE:HD12	1:89:A:ASN:H	2	1.06	0.36	1.06
(2,49)	1:10:A:ILE:HD13	1:89:A:ASN:H	2	1.06	0.36	1.06
(6,504)	1:119:A:ILE:HG12	1:120:A:MET:H	2	1.06	0.07	1.06
(7,373)	1:107:A:SER:HA	1:107:A:SER:H	2	1.06	0.04	1.06
(7,231)	1:69:A:THR:HA	1:69:A:THR:H	2	1.06	0.04	1.06
(4,286)	1:103:A:GLU:HG2	1:105:A:ASN:H	2	1.05	0.04	1.05
(4,286)	1:103:A:GLU:HG3	1:105:A:ASN:H	2	1.05	0.04	1.05
(4,346)	1:123:A:LYS:H	1:126:A:LYS:H	2	1.05	0.05	1.05
(6,477)	1:112:A:PHE:HB2	1:113:A:LEU:H	2	1.05	0.03	1.05
(7,72)	1:19:A:GLU:H	1:19:A:GLU:HB2	2	1.05	0.05	1.05
(7,72)	1:19:A:GLU:H	1:19:A:GLU:HB3	2	1.05	0.05	1.05
(6,104)	1:24:A:CYS:H	1:23:A:LEU:HB3	2	1.05	0.1	1.05
(4,215)	1:73:A:PHE:H	1:75:A:ARG:H	2	1.04	0.09	1.04
(7,324)	1:91:A:TRP:HE3	1:91:A:TRP:H	2	1.04	0.06	1.04
(7,112)	1:31:A:ASP:HA	1:31:A:ASP:H	2	1.04	0.01	1.04
(4,107)	1:40:A:THR:HA	1:42:A:LYS:H	2	1.04	0.02	1.04
(6,329)	1:80:A:ILE:HB	1:81:A:ARG:H	2	1.03	0.64	1.03
(6,139)	1:32:A:ILE:HB	1:33:A:PHE:H	2	1.03	0.06	1.03
(7,105)	1:29:A:VAL:HA	1:29:A:VAL:H	2	1.02	0.01	1.02
(7,144)	1:40:A:THR:HA	1:40:A:THR:H	2	1.02	0.01	1.02
(4,194)	1:72:A:GLN:HG3	1:69:A:THR:H	2	1.02	0.38	1.02
(4,216)	1:74:A:HIS:HA	1:76:A:HIS:H	2	1.02	0.59	1.02
(6,471)	1:111:A:ASN:HB2	1:112:A:PHE:H	2	1.02	0.07	1.02
(4,192)	1:69:A:THR:H	1:72:A:GLN:H	2	1.01	0.21	1.01
(7,281)	1:83:A:LEU:HB3	1:83:A:LEU:H	2	1.01	0.54	1.01
(6,202)	1:46:A:CYS:H	1:45:A:PHE:HB3	2	1.01	0.09	1.01
(6,203)	1:46:A:CYS:H	1:45:A:PHE:HB2	2	1.0	0.06	1.0
(7,123)	1:33:A:PHE:HB2	1:33:A:PHE:H	2	1.0	0.6	1.0
(4,136)	1:49:A:ALA:H	1:45:A:PHE:HE1	2	0.99	0.06	0.99
(4,136)	1:49:A:ALA:H	1:45:A:PHE:HE2	2	0.99	0.06	0.99
(4,53)	1:15:A:ASN:H	1:17:A:LEU:H	2	0.98	0.02	0.98
(4,89)	1:32:A:ILE:HB	1:34:A:ALA:H	2	0.98	0.04	0.98
(7,122)	1:33:A:PHE:HB3	1:33:A:PHE:H	2	0.97	0.55	0.97
(7,238)	1:71:A:GLN:HG2	1:71:A:GLN:H	2	0.97	0.01	0.97
(7,238)	1:71:A:GLN:HG3	1:71:A:GLN:H	2	0.97	0.01	0.97
(4,37)	1:11:A:ILE:HA	1:15:A:ASN:H	2	0.96	0.24	0.96
(6,174)	1:39:A:THR:HG21	1:40:A:THR:H	2	0.96	0.08	0.96
(6,174)	1:39:A:THR:HG22	1:40:A:THR:H	2	0.96	0.08	0.96
(6,174)	1:39:A:THR:HG23	1:40:A:THR:H	2	0.96	0.08	0.96
(6,264)	1:63:A:THR:H	1:64:A:ARG:H	2	0.96	0.36	0.96
(2,35)	1:69:A:THR:HG21	1:76:A:HIS:H	2	0.96	0.13	0.96
(2,35)	1:69:A:THR:HG22	1:76:A:HIS:H	2	0.96	0.13	0.96

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,35)	1:69:A:THR:HG23	1:76:A:HIS:H	2	0.96	0.13	0.96
(4,113)	1:43:A:GLU:HB3	1:40:A:THR:H	2	0.96	0.03	0.96
(6,255)	1:61:A:LYS:HA	1:62:A:ASP:H	2	0.96	0.2	0.96
(6,294)	1:73:A:PHE:HB3	1:72:A:GLN:H	2	0.95	0.03	0.95
(7,358)	1:103:A:GLU:HB2	1:103:A:GLU:H	2	0.95	0.09	0.95
(7,358)	1:103:A:GLU:HB3	1:103:A:GLU:H	2	0.95	0.09	0.95
(4,228)	1:77:A:LYS:HA	1:81:A:ARG:H	2	0.94	0.1	0.94
(6,77)	1:18:A:THR:H	1:17:A:LEU:HG	2	0.94	0.0	0.94
(7,363)	1:105:A:ASN:HB3	1:105:A:ASN:H	2	0.94	0.03	0.94
(6,165)	1:37:A:LYS:H	1:38:A:ASN:H	2	0.93	0.49	0.93
(6,367)	1:87:A:ASP:HB2	1:88:A:ARG:H	2	0.93	0.7	0.93
(4,78)	1:27:A:LEU:HB2	1:29:A:VAL:H	2	0.92	0.12	0.92
(4,78)	1:27:A:LEU:HB3	1:29:A:VAL:H	2	0.92	0.12	0.92
(7,162)	1:45:A:PHE:H	1:45:A:PHE:HB2	2	0.92	0.01	0.92
(6,80)	1:18:A:THR:H	1:19:A:GLU:H	2	0.92	0.48	0.92
(6,459)	1:109:A:LEU:HG	1:110:A:GLU:H	2	0.92	0.16	0.92
(4,143)	1:48:A:ALA:H	1:50:A:THR:H	2	0.92	0.1	0.92
(6,435)	1:104:A:ALA:HB1	1:105:A:ASN:H	2	0.92	0.16	0.92
(6,435)	1:104:A:ALA:HB2	1:105:A:ASN:H	2	0.92	0.16	0.92
(6,435)	1:104:A:ALA:HB3	1:105:A:ASN:H	2	0.92	0.16	0.92
(6,467)	1:111:A:ASN:HB2	1:110:A:GLU:H	2	0.92	0.01	0.92
(4,43)	1:13:A:THR:H	1:15:A:ASN:H	2	0.91	0.02	0.91
(4,139)	1:46:A:CYS:H	1:48:A:ALA:H	2	0.9	0.03	0.9
(7,208)	1:60:A:GLU:HB2	1:60:A:GLU:H	2	0.9	0.18	0.9
(7,208)	1:60:A:GLU:HB3	1:60:A:GLU:H	2	0.9	0.18	0.9
(4,179)	1:62:A:ASP:HA	1:64:A:ARG:H	2	0.89	0.02	0.89
(6,521)	1:124:A:TYR:HB2	1:123:A:LYS:H	2	0.89	0.32	0.89
(6,119)	1:28:A:THR:HA	1:29:A:VAL:H	2	0.87	0.01	0.87
(4,248)	1:83:A:LEU:H	1:85:A:ARG:H	2	0.86	0.1	0.86
(7,76)	1:20:A:GLN:H	1:20:A:GLN:HB3	2	0.86	0.65	0.86
(6,70)	1:17:A:LEU:HB3	1:16:A:SER:H	2	0.86	0.03	0.86
(6,274)	1:67:A:GLY:HA3	1:68:A:ALA:H	2	0.84	0.01	0.84
(4,212)	1:72:A:GLN:H	1:75:A:ARG:H	2	0.84	0.29	0.84
(4,223)	1:75:A:ARG:H	1:78:A:GLN:H	2	0.84	0.01	0.84
(6,412)	1:98:A:SER:HA	1:99:A:CYS:H	2	0.84	0.03	0.84
(7,364)	1:105:A:ASN:HB2	1:105:A:ASN:H	2	0.84	0.02	0.84
(6,22)	1:7:A:LEU:HB2	1:8:A:GLN:H	2	0.83	0.43	0.83
(6,22)	1:7:A:LEU:HB3	1:8:A:GLN:H	2	0.83	0.43	0.83
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB1	2	0.82	0.26	0.82
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB2	2	0.82	0.26	0.82
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB3	2	0.82	0.26	0.82
(7,201)	1:59:A:HIS:HD2	1:59:A:HIS:H	2	0.82	0.09	0.82

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,69)	1:17:A:LEU:HA	1:16:A:SER:H	2	0.82	0.02	0.82
(6,519)	1:124:A:TYR:HA	1:123:A:LYS:H	2	0.82	0.08	0.82
(4,242)	1:81:A:ARG:H	1:83:A:LEU:H	2	0.81	0.14	0.81
(6,259)	1:62:A:ASP:HA	1:63:A:THR:H	2	0.81	0.02	0.81
(2,4)	1:31:A:ASP:H	1:106:A:GLN:HB2	2	0.8	0.2	0.8
(2,4)	1:31:A:ASP:H	1:106:A:GLN:HB3	2	0.8	0.2	0.8
(4,48)	1:14:A:LEU:HA	1:17:A:LEU:H	2	0.8	0.2	0.8
(4,253)	1:84:A:LYS:H	1:86:A:LEU:H	2	0.79	0.01	0.79
(4,124)	1:43:A:GLU:HA	1:46:A:CYS:H	2	0.78	0.02	0.78
(7,239)	1:71:A:GLN:HE21	1:71:A:GLN:H	2	0.78	0.26	0.78
(7,239)	1:71:A:GLN:HE22	1:71:A:GLN:H	2	0.78	0.26	0.78
(4,256)	1:85:A:ARG:H	1:87:A:ASP:H	2	0.78	0.02	0.78
(6,169)	1:38:A:ASN:HB3	1:39:A:THR:H	2	0.78	0.04	0.78
(2,5)	1:31:A:ASP:H	1:106:A:GLN:HE21	2	0.76	0.43	0.76
(2,5)	1:31:A:ASP:H	1:106:A:GLN:HE22	2	0.76	0.43	0.76
(6,492)	1:117:A:LYS:HA	1:116:A:LEU:H	2	0.76	0.01	0.76
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG21	2	0.76	0.01	0.76
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG22	2	0.76	0.01	0.76
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG23	2	0.76	0.01	0.76
(7,37)	1:11:A:ILE:H	1:11:A:ILE:HG13	2	0.76	0.42	0.76
(6,12)	1:5:A:ILE:HB	1:6:A:THR:H	2	0.75	0.17	0.75
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG21	2	0.74	0.02	0.74
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG22	2	0.74	0.02	0.74
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG23	2	0.74	0.02	0.74
(7,88)	1:23:A:LEU:H	1:23:A:LEU:HG	2	0.74	0.24	0.74
(6,159)	1:36:A:SER:HB3	1:37:A:LYS:H	2	0.74	0.22	0.74
(7,15)	1:6:A:THR:H	1:6:A:THR:HG21	2	0.74	0.01	0.74
(7,15)	1:6:A:THR:H	1:6:A:THR:HG22	2	0.74	0.01	0.74
(7,15)	1:6:A:THR:H	1:6:A:THR:HG23	2	0.74	0.01	0.74
(7,394)	1:112:A:PHE:HB3	1:112:A:PHE:H	2	0.74	0.06	0.74
(4,46)	1:15:A:ASN:H	1:13:A:THR:HB	2	0.74	0.1	0.74
(6,75)	1:18:A:THR:H	1:17:A:LEU:HB3	2	0.74	0.03	0.74
(6,204)	1:45:A:PHE:H	1:46:A:CYS:HA	2	0.74	0.03	0.74
(7,217)	1:63:A:THR:HG21	1:63:A:THR:H	2	0.74	0.03	0.74
(7,217)	1:63:A:THR:HG22	1:63:A:THR:H	2	0.74	0.03	0.74
(7,217)	1:63:A:THR:HG23	1:63:A:THR:H	2	0.74	0.03	0.74
(7,257)	1:76:A:HIS:HD2	1:76:A:HIS:H	2	0.74	0.15	0.74
(6,341)	1:82:A:PHE:HB2	1:83:A:LEU:H	2	0.73	0.49	0.73
(6,424)	1:101:A:VAL:H	1:102:A:LYS:H	2	0.72	0.09	0.72
(6,150)	1:33:A:PHE:HA	1:34:A:ALA:H	2	0.72	0.07	0.72
(4,25)	1:8:A:GLN:H	1:10:A:ILE:H	2	0.71	0.13	0.71
(6,437)	1:104:A:ALA:HA	1:105:A:ASN:H	2	0.71	0.07	0.71

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,474)	1:112:A:PHE:HB2	1:111:A:ASN:H	2	0.71	0.02	0.71
(7,65)	1:17:A:LEU:H	1:17:A:LEU:HG	2	0.71	0.0	0.71
(7,321)	1:91:A:TRP:HD1	1:91:A:TRP:HA	2	0.71	0.24	0.71
(7,250)	1:74:A:HIS:HB2	1:74:A:HIS:H	2	0.7	0.03	0.7
(7,250)	1:74:A:HIS:HB3	1:74:A:HIS:H	2	0.7	0.03	0.7
(4,45)	1:15:A:ASN:H	1:13:A:THR:HA	2	0.7	0.24	0.7
(6,269)	1:65:A:CYS:HB2	1:66:A:LEU:H	2	0.7	0.36	0.7
(6,430)	1:102:A:LYS:H	1:103:A:GLU:H	2	0.7	0.01	0.7
(6,538)	1:128:A:SER:HA	1:129:A:SER:H	2	0.7	0.03	0.7
(4,311)	1:111:A:ASN:H	1:113:A:LEU:H	2	0.69	0.1	0.69
(4,334)	1:119:A:ILE:HA	1:123:A:LYS:H	2	0.69	0.12	0.69
(6,138)	1:32:A:ILE:H	1:33:A:PHE:H	2	0.69	0.18	0.69
(4,247)	1:82:A:PHE:H	1:84:A:LYS:H	2	0.68	0.12	0.68
(7,261)	1:79:A:LEU:HB2	1:79:A:LEU:H	2	0.68	0.11	0.68
(7,261)	1:79:A:LEU:HB3	1:79:A:LEU:H	2	0.68	0.11	0.68
(7,337)	1:95:A:GLY:HA2	1:95:A:GLY:H	2	0.68	0.01	0.68
(6,258)	1:62:A:ASP:HB2	1:63:A:THR:H	2	0.67	0.13	0.67
(6,11)	1:5:A:ILE:HG21	1:6:A:THR:H	2	0.66	0.12	0.66
(6,11)	1:5:A:ILE:HG22	1:6:A:THR:H	2	0.66	0.12	0.66
(6,11)	1:5:A:ILE:HG23	1:6:A:THR:H	2	0.66	0.12	0.66
(6,268)	1:65:A:CYS:HB3	1:66:A:LEU:H	2	0.66	0.01	0.66
(4,54)	1:16:A:SER:HA	1:18:A:THR:H	2	0.66	0.03	0.66
(4,105)	1:39:A:THR:HG21	1:43:A:GLU:H	2	0.65	0.42	0.65
(4,105)	1:39:A:THR:HG22	1:43:A:GLU:H	2	0.65	0.42	0.65
(4,105)	1:39:A:THR:HG23	1:43:A:GLU:H	2	0.65	0.42	0.65
(6,78)	1:18:A:THR:HA	1:19:A:GLU:H	2	0.65	0.21	0.65
(7,197)	1:57:A:SER:HB2	1:57:A:SER:H	2	0.65	0.04	0.65
(4,125)	1:43:A:GLU:H	1:45:A:PHE:H	2	0.64	0.04	0.64
(4,190)	1:72:A:GLN:HG2	1:68:A:ALA:H	2	0.64	0.29	0.64
(6,122)	1:28:A:THR:H	1:29:A:VAL:H	2	0.64	0.03	0.64
(6,455)	1:108:A:THR:HB	1:109:A:LEU:H	2	0.64	0.04	0.64
(7,187)	1:55:A:PHE:HB3	1:55:A:PHE:H	2	0.64	0.12	0.64
(6,160)	1:36:A:SER:HB2	1:37:A:LYS:H	2	0.62	0.25	0.62
(7,256)	1:76:A:HIS:HB2	1:76:A:HIS:H	2	0.62	0.09	0.62
(4,21)	1:7:A:LEU:H	1:9:A:GLU:H	2	0.62	0.16	0.62
(6,85)	1:19:A:GLU:HA	1:20:A:GLN:H	2	0.61	0.08	0.61
(6,156)	1:35:A:ALA:HA	1:36:A:SER:H	2	0.61	0.02	0.61
(6,84)	1:20:A:GLN:H	1:19:A:GLU:HB2	2	0.6	0.09	0.6
(6,84)	1:20:A:GLN:H	1:19:A:GLU:HB3	2	0.6	0.09	0.6
(6,170)	1:38:A:ASN:HB2	1:39:A:THR:H	2	0.6	0.12	0.6
(6,191)	1:44:A:THR:HB	1:45:A:PHE:H	2	0.6	0.05	0.6
(6,436)	1:104:A:ALA:HB1	1:105:A:ASN:HD21	2	0.6	0.04	0.6

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,436)	1:104:A:ALA:HB2	1:105:A:ASN:HD21	2	0.6	0.04	0.6
(6,436)	1:104:A:ALA:HB3	1:105:A:ASN:HD21	2	0.6	0.04	0.6
(4,47)	1:14:A:LEU:HA	1:16:A:SER:H	2	0.6	0.11	0.6
(6,180)	1:41:A:GLU:HA	1:42:A:LYS:H	2	0.6	0.01	0.6
(6,90)	1:20:A:GLN:H	1:21:A:LYS:H	2	0.6	0.16	0.6
(4,56)	1:16:A:SER:H	1:18:A:THR:H	2	0.59	0.05	0.59
(4,121)	1:43:A:GLU:HA	1:45:A:PHE:H	2	0.59	0.09	0.59
(4,19)	1:7:A:LEU:HA	1:10:A:ILE:H	2	0.58	0.12	0.58
(6,216)	1:50:A:THR:HB	1:51:A:VAL:H	2	0.58	0.1	0.58
(4,31)	1:12:A:LYS:H	1:9:A:GLU:HG2	2	0.58	0.08	0.58
(4,31)	1:12:A:LYS:H	1:9:A:GLU:HG3	2	0.58	0.08	0.58
(7,61)	1:16:A:SER:H	1:16:A:SER:HB2	2	0.57	0.11	0.57
(7,61)	1:16:A:SER:H	1:16:A:SER:HB3	2	0.57	0.11	0.57
(4,28)	1:9:A:GLU:HA	1:11:A:ILE:H	2	0.57	0.28	0.57
(6,196)	1:44:A:THR:H	1:45:A:PHE:HA	2	0.56	0.02	0.56
(7,299)	1:87:A:ASP:HB2	1:87:A:ASP:H	2	0.56	0.06	0.56
(7,117)	1:32:A:ILE:HG13	1:32:A:ILE:H	2	0.56	0.16	0.56
(4,116)	1:42:A:LYS:HA	1:46:A:CYS:H	2	0.56	0.14	0.56
(6,393)	1:93:A:LEU:HA	1:94:A:ALA:H	2	0.55	0.06	0.55
(7,279)	1:82:A:PHE:HB2	1:82:A:PHE:H	2	0.55	0.08	0.55
(6,9)	1:5:A:ILE:HG13	1:6:A:THR:H	2	0.55	0.04	0.55
(6,19)	1:7:A:LEU:H	1:6:A:THR:HG1	2	0.55	0.17	0.55
(7,90)	1:23:A:LEU:H	1:23:A:LEU:HB2	2	0.55	0.11	0.55
(6,76)	1:18:A:THR:H	1:17:A:LEU:HB2	2	0.55	0.01	0.55
(6,39)	1:11:A:ILE:H	1:10:A:ILE:HB	2	0.54	0.14	0.54
(6,177)	1:40:A:THR:HA	1:41:A:GLU:H	2	0.54	0.08	0.54
(4,13)	1:10:A:ILE:H	1:6:A:THR:HA	2	0.54	0.14	0.54
(4,120)	1:42:A:LYS:H	1:45:A:PHE:H	2	0.53	0.06	0.53
(6,137)	1:32:A:ILE:HA	1:33:A:PHE:H	2	0.52	0.01	0.52
(7,131)	1:36:A:SER:HB3	1:36:A:SER:H	2	0.52	0.1	0.52
(7,350)	1:101:A:VAL:HB	1:101:A:VAL:H	2	0.51	0.15	0.51
(6,53)	1:14:A:LEU:HA	1:15:A:ASN:H	2	0.5	0.03	0.5
(6,135)	1:31:A:ASP:H	1:32:A:ILE:H	2	0.5	0.04	0.5
(6,245)	1:57:A:SER:H	1:58:A:HIS:H	2	0.5	0.08	0.5
(6,307)	1:74:A:HIS:HA	1:75:A:ARG:H	2	0.5	0.07	0.5
(4,8)	1:5:A:ILE:HA	1:8:A:GLN:H	2	0.5	0.22	0.5
(6,20)	1:7:A:LEU:HA	1:8:A:GLN:H	2	0.5	0.0	0.5
(7,10)	1:5:A:ILE:H	1:5:A:ILE:HG12	2	0.5	0.05	0.5
(6,66)	1:16:A:SER:H	1:17:A:LEU:H	2	0.5	0.04	0.5
(6,377)	1:89:A:ASN:H	1:90:A:LEU:H	2	0.5	0.15	0.5
(6,318)	1:78:A:GLN:HA	1:79:A:LEU:H	2	0.49	0.01	0.49
(6,311)	1:76:A:HIS:HB3	1:77:A:LYS:H	2	0.48	0.34	0.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,388)	1:92:A:GLY:HA3	1:93:A:LEU:H	2	0.48	0.02	0.48
(7,247)	1:73:A:PHE:HB2	1:73:A:PHE:H	2	0.48	0.07	0.48
(6,65)	1:16:A:SER:HA	1:17:A:LEU:H	2	0.48	0.0	0.48
(7,200)	1:58:A:HIS:HB2	1:58:A:HIS:H	2	0.48	0.08	0.48
(6,248)	1:58:A:HIS:H	1:59:A:HIS:H	2	0.47	0.06	0.47
(6,350)	1:84:A:LYS:HA	1:85:A:ARG:H	2	0.47	0.0	0.47
(4,240)	1:81:A:ARG:HA	1:83:A:LEU:H	2	0.46	0.3	0.46
(7,262)	1:79:A:LEU:HB2	1:79:A:LEU:H	2	0.46	0.06	0.46
(4,50)	1:14:A:LEU:H	1:16:A:SER:H	2	0.46	0.12	0.46
(4,295)	1:111:A:ASN:HB2	1:108:A:THR:H	2	0.46	0.36	0.46
(6,309)	1:75:A:ARG:HA	1:76:A:HIS:H	2	0.46	0.01	0.46
(7,391)	1:111:A:ASN:HB3	1:111:A:ASN:H	2	0.46	0.0	0.46
(7,64)	1:17:A:LEU:H	1:17:A:LEU:HB2	2	0.46	0.0	0.46
(7,420)	1:120:A:MET:HB3	1:120:A:MET:H	2	0.46	0.0	0.46
(6,337)	1:81:A:ARG:HA	1:82:A:PHE:H	2	0.46	0.01	0.46
(7,114)	1:31:A:ASP:HB2	1:31:A:ASP:H	2	0.46	0.05	0.46
(7,193)	1:56:A:TYR:HB3	1:56:A:TYR:H	2	0.46	0.01	0.46
(6,151)	1:33:A:PHE:H	1:34:A:ALA:H	2	0.45	0.01	0.45
(6,49)	1:13:A:THR:HA	1:14:A:LEU:H	2	0.45	0.01	0.45
(6,220)	1:51:A:VAL:HA	1:52:A:LEU:H	2	0.45	0.01	0.45
(6,303)	1:73:A:PHE:HA	1:74:A:HIS:H	2	0.45	0.01	0.45
(6,364)	1:86:A:LEU:HA	1:87:A:ASP:H	2	0.45	0.01	0.45
(6,370)	1:88:A:ARG:HA	1:89:A:ASN:H	2	0.45	0.01	0.45
(4,251)	1:84:A:LYS:HA	1:87:A:ASP:H	2	0.45	0.02	0.45
(6,26)	1:8:A:GLN:HA	1:9:A:GLU:H	2	0.44	0.02	0.44
(6,40)	1:11:A:ILE:HA	1:12:A:LYS:H	2	0.44	0.01	0.44
(7,392)	1:111:A:ASN:HB2	1:111:A:ASN:H	2	0.44	0.02	0.44
(7,94)	1:25:A:THR:H	1:25:A:THR:HB	2	0.44	0.02	0.44
(4,249)	1:83:A:LEU:HA	1:85:A:ARG:H	2	0.44	0.06	0.44
(6,29)	1:9:A:GLU:HA	1:10:A:ILE:H	2	0.44	0.02	0.44
(6,188)	1:43:A:GLU:HA	1:44:A:THR:H	2	0.44	0.02	0.44
(7,172)	1:50:A:THR:HB	1:50:A:THR:H	2	0.44	0.08	0.44
(7,207)	1:60:A:GLU:HA	1:60:A:GLU:H	2	0.44	0.26	0.44
(6,21)	1:7:A:LEU:H	1:8:A:GLN:H	2	0.44	0.11	0.44
(6,237)	1:56:A:TYR:HE1	1:57:A:SER:H	2	0.44	0.01	0.44
(6,237)	1:56:A:TYR:HE2	1:57:A:SER:H	2	0.44	0.01	0.44
(4,324)	1:115:A:ARG:HA	1:117:A:LYS:H	2	0.43	0.04	0.43
(6,192)	1:44:A:THR:HA	1:45:A:PHE:H	2	0.43	0.01	0.43
(6,225)	1:53:A:ARG:HA	1:54:A:GLN:H	2	0.43	0.01	0.43
(6,226)	1:54:A:GLN:HA	1:55:A:PHE:H	2	0.43	0.0	0.43
(4,305)	1:110:A:GLU:HA	1:113:A:LEU:H	2	0.43	0.12	0.43
(7,29)	1:9:A:GLU:H	1:9:A:GLU:HB3	2	0.42	0.02	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,307)	1:111:A:ASN:HB3	1:114:A:GLU:H	2	0.42	0.09	0.42
(6,209)	1:47:A:ARG:HA	1:48:A:ALA:H	2	0.42	0.03	0.42
(6,475)	1:111:A:ASN:H	1:112:A:PHE:H	2	0.42	0.04	0.42
(6,47)	1:12:A:LYS:HA	1:13:A:THR:H	2	0.42	0.01	0.42
(7,81)	1:21:A:LYS:HA	1:21:A:LYS:H	2	0.42	0.27	0.42
(4,231)	1:78:A:GLN:H	1:80:A:ILE:H	2	0.42	0.26	0.42
(7,2)	1:3:A:THR:H	1:3:A:THR:HB	2	0.42	0.02	0.42
(7,14)	1:6:A:THR:H	1:6:A:THR:HB	2	0.42	0.04	0.42
(6,267)	1:65:A:CYS:H	1:66:A:LEU:H	2	0.42	0.2	0.42
(6,266)	1:64:A:ARG:H	1:65:A:CYS:H	2	0.41	0.21	0.41
(7,307)	1:89:A:ASN:HB3	1:89:A:ASN:H	2	0.41	0.04	0.41
(7,4)	1:4:A:ASP:HA	1:4:A:ASP:H	2	0.41	0.29	0.41
(6,182)	1:42:A:LYS:H	1:43:A:GLU:H	2	0.4	0.07	0.4
(7,142)	1:39:A:THR:HB	1:39:A:THR:H	2	0.4	0.15	0.4
(7,246)	1:73:A:PHE:HB3	1:73:A:PHE:H	2	0.4	0.12	0.4
(4,4)	1:6:A:THR:H	1:4:A:ASP:HB3	2	0.4	0.1	0.4
(4,153)	1:52:A:LEU:HA	1:55:A:PHE:H	2	0.39	0.06	0.39
(6,131)	1:30:A:THR:H	1:31:A:ASP:H	2	0.39	0.03	0.39
(4,338)	1:120:A:MET:H	1:123:A:LYS:H	2	0.38	0.04	0.38
(6,315)	1:76:A:HIS:H	1:77:A:LYS:H	2	0.38	0.21	0.38
(7,116)	1:32:A:ILE:HB	1:32:A:ILE:H	2	0.38	0.02	0.38
(4,146)	1:49:A:ALA:HA	1:51:A:VAL:H	2	0.38	0.08	0.38
(6,67)	1:17:A:LEU:H	1:16:A:SER:HB2	2	0.37	0.03	0.37
(6,67)	1:17:A:LEU:H	1:16:A:SER:HB3	2	0.37	0.03	0.37
(6,454)	1:108:A:THR:HA	1:109:A:LEU:H	2	0.37	0.02	0.37
(4,132)	1:45:A:PHE:H	1:48:A:ALA:H	2	0.36	0.02	0.36
(6,130)	1:30:A:THR:HG21	1:31:A:ASP:H	2	0.36	0.02	0.36
(6,130)	1:30:A:THR:HG22	1:31:A:ASP:H	2	0.36	0.02	0.36
(6,130)	1:30:A:THR:HG23	1:31:A:ASP:H	2	0.36	0.02	0.36
(6,189)	1:43:A:GLU:H	1:44:A:THR:H	2	0.36	0.07	0.36
(6,212)	1:48:A:ALA:H	1:49:A:ALA:H	2	0.36	0.05	0.36
(6,299)	1:72:A:GLN:H	1:73:A:PHE:H	2	0.36	0.0	0.36
(3,87)	1:107:A:SER:H	1:29:A:VAL:O	2	0.36	0.12	0.36
(4,155)	1:54:A:GLN:HA	1:56:A:TYR:H	2	0.36	0.04	0.36
(6,224)	1:51:A:VAL:H	1:52:A:LEU:H	2	0.35	0.03	0.35
(6,8)	1:5:A:ILE:H	1:6:A:THR:H	2	0.34	0.07	0.34
(6,199)	1:45:A:PHE:H	1:46:A:CYS:H	2	0.34	0.01	0.34
(6,494)	1:116:A:LEU:H	1:117:A:LYS:H	2	0.34	0.0	0.34
(6,320)	1:78:A:GLN:H	1:79:A:LEU:H	2	0.34	0.12	0.34
(6,490)	1:115:A:ARG:H	1:116:A:LEU:H	2	0.34	0.04	0.34
(4,29)	1:9:A:GLU:HA	1:12:A:LYS:H	2	0.33	0.05	0.33
(4,255)	1:85:A:ARG:HA	1:87:A:ASP:H	2	0.33	0.08	0.33

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,351)	1:84:A:LYS:H	1:85:A:ARG:H	2	0.32	0.08	0.32
(4,51)	1:15:A:ASN:HA	1:18:A:THR:H	2	0.32	0.15	0.32
(6,30)	1:9:A:GLU:H	1:10:A:ILE:H	2	0.32	0.01	0.32
(4,225)	1:76:A:HIS:H	1:78:A:GLN:H	2	0.31	0.06	0.31
(6,68)	1:17:A:LEU:H	1:16:A:SER:HB2	2	0.31	0.05	0.31
(6,517)	1:121:A:ARG:H	1:122:A:GLU:H	2	0.31	0.02	0.31
(4,114)	1:43:A:GLU:HG2	1:40:A:THR:H	2	0.3	0.1	0.3
(4,114)	1:43:A:GLU:HG3	1:40:A:THR:H	2	0.3	0.1	0.3
(6,317)	1:77:A:LYS:H	1:78:A:GLN:H	2	0.3	0.01	0.3
(6,241)	1:56:A:TYR:H	1:57:A:SER:H	2	0.3	0.04	0.3
(4,39)	1:12:A:LYS:HA	1:15:A:ASN:H	2	0.3	0.08	0.3
(6,235)	1:55:A:PHE:H	1:56:A:TYR:H	2	0.3	0.01	0.3
(6,210)	1:47:A:ARG:H	1:48:A:ALA:H	2	0.3	0.15	0.3
(6,112)	1:27:A:LEU:HA	1:28:A:THR:H	2	0.29	0.01	0.29
(6,349)	1:83:A:LEU:H	1:84:A:LYS:H	2	0.29	0.04	0.29
(7,109)	1:30:A:THR:HA	1:30:A:THR:H	2	0.29	0.04	0.29
(6,134)	1:31:A:ASP:HA	1:32:A:ILE:H	2	0.29	0.06	0.29
(4,83)	1:31:A:ASP:HA	1:34:A:ALA:H	2	0.29	0.14	0.29
(6,128)	1:30:A:THR:HA	1:31:A:ASP:H	2	0.29	0.04	0.29
(6,488)	1:114:A:GLU:H	1:115:A:ARG:H	2	0.29	0.02	0.29
(6,124)	1:29:A:VAL:HA	1:30:A:THR:H	2	0.28	0.06	0.28
(4,35)	1:11:A:ILE:HA	1:13:A:THR:H	2	0.28	0.03	0.28
(6,94)	1:21:A:LYS:HA	1:22:A:THR:H	2	0.28	0.01	0.28
(6,198)	1:44:A:THR:H	1:45:A:PHE:HB2	2	0.28	0.06	0.28
(7,188)	1:55:A:PHE:HB2	1:55:A:PHE:H	2	0.28	0.14	0.28
(6,218)	1:50:A:THR:H	1:51:A:VAL:H	2	0.27	0.04	0.27
(3,35)	1:57:A:SER:H	1:53:A:ARG:O	2	0.26	0.03	0.26
(3,55)	1:91:A:TRP:H	1:87:A:ASP:O	2	0.26	0.09	0.26
(6,310)	1:75:A:ARG:H	1:76:A:HIS:H	2	0.26	0.14	0.26
(6,359)	1:85:A:ARG:H	1:86:A:LEU:H	2	0.26	0.0	0.26
(6,429)	1:102:A:LYS:HA	1:103:A:GLU:H	2	0.26	0.07	0.26
(7,322)	1:91:A:TRP:HD1	1:91:A:TRP:HB3	2	0.26	0.06	0.26
(6,326)	1:79:A:LEU:H	1:80:A:ILE:H	2	0.25	0.09	0.25
(6,54)	1:14:A:LEU:H	1:15:A:ASN:H	2	0.24	0.04	0.24
(7,245)	1:73:A:PHE:HA	1:73:A:PHE:H	2	0.24	0.04	0.24
(7,300)	1:88:A:ARG:HA	1:88:A:ARG:H	2	0.24	0.04	0.24
(4,308)	1:111:A:ASN:HB2	1:114:A:GLU:H	2	0.24	0.08	0.24
(4,321)	1:114:A:GLU:HA	1:117:A:LYS:H	2	0.24	0.13	0.24
(7,32)	1:10:A:ILE:H	1:10:A:ILE:HA	2	0.24	0.05	0.24
(7,156)	1:44:A:THR:HA	1:44:A:THR:H	2	0.24	0.0	0.24
(7,205)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	2	0.23	0.0	0.23
(4,138)	1:46:A:CYS:HB2	1:48:A:ALA:H	2	0.23	0.07	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,328)	1:93:A:LEU:HA	1:93:A:LEU:H	2	0.23	0.06	0.23
(7,275)	1:82:A:PHE:HA	1:82:A:PHE:H	2	0.22	0.06	0.22
(7,45)	1:14:A:LEU:H	1:14:A:LEU:HA	2	0.22	0.01	0.22
(7,126)	1:34:A:ALA:HA	1:34:A:ALA:H	2	0.22	0.04	0.22
(6,501)	1:118:A:THR:H	1:119:A:ILE:H	2	0.22	0.07	0.22
(7,334)	1:94:A:ALA:HA	1:94:A:ALA:H	2	0.22	0.07	0.22
(7,41)	1:12:A:LYS:H	1:12:A:LYS:HA	2	0.22	0.02	0.22
(7,163)	1:46:A:CYS:HA	1:46:A:CYS:H	2	0.22	0.01	0.22
(4,123)	1:43:A:GLU:HG2	1:45:A:PHE:H	2	0.21	0.02	0.21
(4,123)	1:43:A:GLU:HG3	1:45:A:PHE:H	2	0.21	0.02	0.21
(7,297)	1:87:A:ASP:HA	1:87:A:ASP:H	2	0.21	0.05	0.21
(7,59)	1:15:A:ASN:H	1:15:A:ASN:HA	2	0.21	0.03	0.21
(7,406)	1:117:A:LYS:HA	1:117:A:LYS:H	2	0.2	0.0	0.2
(7,287)	1:85:A:ARG:HA	1:85:A:ARG:H	2	0.2	0.01	0.2
(4,226)	1:77:A:LYS:HA	1:80:A:ILE:H	2	0.2	0.05	0.2
(7,22)	1:8:A:GLN:HA	1:8:A:GLN:H	2	0.2	0.02	0.2
(7,43)	1:13:A:THR:H	1:13:A:THR:HA	2	0.2	0.04	0.2
(7,178)	1:52:A:LEU:HA	1:52:A:LEU:H	2	0.2	0.02	0.2
(7,272)	1:81:A:ARG:HA	1:81:A:ARG:H	2	0.2	0.01	0.2
(4,232)	1:79:A:LEU:HA	1:82:A:PHE:H	2	0.19	0.04	0.19
(7,7)	1:5:A:ILE:H	1:5:A:ILE:HA	2	0.19	0.02	0.19
(7,183)	1:54:A:GLN:HA	1:54:A:GLN:H	2	0.19	0.0	0.19
(7,259)	1:78:A:GLN:HA	1:78:A:GLN:H	2	0.19	0.05	0.19
(7,409)	1:118:A:THR:HA	1:118:A:THR:H	2	0.19	0.02	0.19
(6,227)	1:54:A:GLN:H	1:55:A:PHE:H	2	0.18	0.02	0.18
(7,186)	1:55:A:PHE:HA	1:55:A:PHE:H	2	0.18	0.01	0.18
(7,286)	1:84:A:LYS:HA	1:84:A:LYS:H	2	0.18	0.04	0.18
(1,1)	1:24:A:CYS:SG	1:65:A:CYS:SG	2	0.18	0.0	0.18
(1,2)	1:46:A:CYS:SG	1:99:A:CYS:SG	2	0.18	0.0	0.18
(1,3)	1:24:A:CYS:SG	1:65:A:CYS:SG	2	0.18	0.0	0.18
(1,4)	1:46:A:CYS:SG	1:99:A:CYS:SG	2	0.18	0.0	0.18
(1,5)	1:24:A:CYS:SG	1:65:A:CYS:SG	2	0.18	0.0	0.18
(1,6)	1:46:A:CYS:SG	1:99:A:CYS:SG	2	0.18	0.0	0.18
(7,128)	1:35:A:ALA:HA	1:35:A:ALA:H	2	0.18	0.02	0.18
(7,292)	1:86:A:LEU:HA	1:86:A:LEU:H	2	0.18	0.04	0.18
(7,171)	1:50:A:THR:HA	1:50:A:THR:H	2	0.17	0.01	0.17
(3,79)	1:123:A:LYS:H	1:119:A:ILE:O	2	0.16	0.02	0.16
(7,160)	1:45:A:PHE:H	1:45:A:PHE:HA	2	0.16	0.01	0.16
(7,174)	1:51:A:VAL:HA	1:51:A:VAL:H	2	0.16	0.01	0.16
(7,260)	1:79:A:LEU:HA	1:79:A:LEU:H	2	0.16	0.02	0.16
(6,48)	1:12:A:LYS:H	1:13:A:THR:H	2	0.16	0.04	0.16
(7,388)	1:111:A:ASN:HA	1:111:A:ASN:H	2	0.16	0.02	0.16

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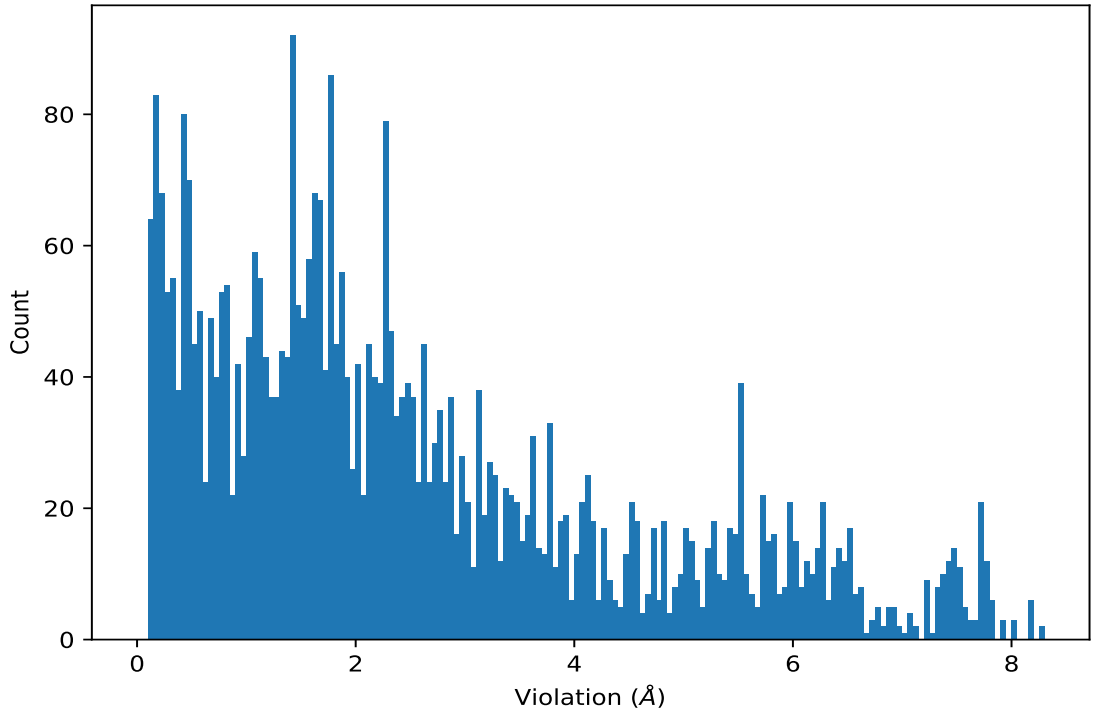
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(7,153)	1:43:A:GLU:HA	1:43:A:GLU:H	2	0.16	0.01	0.16
(7,169)	1:49:A:ALA:HA	1:49:A:ALA:H	2	0.16	0.03	0.16
(7,393)	1:112:A:PHE:HA	1:112:A:PHE:H	2	0.16	0.0	0.16
(7,403)	1:115:A:ARG:HA	1:115:A:ARG:H	2	0.16	0.02	0.16
(7,258)	1:77:A:LYS:HA	1:77:A:LYS:H	2	0.16	0.02	0.16
(6,208)	1:46:A:CYS:H	1:47:A:ARG:H	2	0.15	0.03	0.15
(7,60)	1:16:A:SER:H	1:16:A:SER:HA	2	0.15	0.0	0.15
(7,28)	1:9:A:GLU:H	1:9:A:GLU:HA	2	0.15	0.02	0.15
(7,235)	1:71:A:GLN:HA	1:71:A:GLN:H	2	0.14	0.02	0.14
(3,5)	1:13:A:THR:H	1:9:A:GLU:O	2	0.14	0.04	0.14
(7,13)	1:6:A:THR:H	1:6:A:THR:HA	2	0.14	0.02	0.14
(7,35)	1:11:A:ILE:HA	1:11:A:ILE:H	2	0.14	0.02	0.14
(7,87)	1:23:A:LEU:H	1:23:A:LEU:HA	2	0.12	0.01	0.12
(7,198)	1:58:A:HIS:HA	1:58:A:HIS:H	2	0.12	0.0	0.12

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations (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)
(7,331)	1:93:A:LEU:HG	1:93:A:LEU:H	2	8.27
(7,314)	1:90:A:LEU:HG	1:90:A:LEU:H	2	8.26
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD11	1	8.19
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD12	1	8.19
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD13	1	8.19
(7,21)	1:7:A:LEU:HD21	1:7:A:LEU:H	2	8.15
(7,21)	1:7:A:LEU:HD22	1:7:A:LEU:H	2	8.15
(7,21)	1:7:A:LEU:HD23	1:7:A:LEU:H	2	8.15
(6,420)	1:100:A:PRO:HB2	1:101:A:VAL:H	2	8.03
(7,291)	1:85:A:ARG:HG2	1:85:A:ARG:H	2	8.01
(7,74)	1:19:A:GLU:H	1:19:A:GLU:HG2	1	8.01
(7,19)	1:7:A:LEU:HG	1:7:A:LEU:H	1	7.9
(6,427)	1:102:A:LYS:HG2	1:103:A:GLU:H	2	7.9
(6,427)	1:102:A:LYS:HG3	1:103:A:GLU:H	2	7.9
(7,333)	1:93:A:LEU:HD21	1:93:A:LEU:H	2	7.82
(7,333)	1:93:A:LEU:HD22	1:93:A:LEU:H	2	7.82
(7,333)	1:93:A:LEU:HD23	1:93:A:LEU:H	2	7.82
(7,331)	1:93:A:LEU:HG	1:93:A:LEU:H	1	7.82
(7,302)	1:88:A:ARG:HG3	1:88:A:ARG:H	2	7.82
(7,265)	1:79:A:LEU:HG	1:79:A:LEU:H	2	7.82
(7,313)	1:90:A:LEU:HB2	1:90:A:LEU:H	1	7.8
(7,170)	1:49:A:ALA:HB1	1:49:A:ALA:H	1	7.8
(7,170)	1:49:A:ALA:HB2	1:49:A:ALA:H	1	7.8
(7,170)	1:49:A:ALA:HB3	1:49:A:ALA:H	1	7.8
(7,18)	1:7:A:LEU:HB2	1:7:A:LEU:H	2	7.76
(7,398)	1:113:A:LEU:HB2	1:113:A:LEU:H	2	7.75
(7,398)	1:113:A:LEU:HB3	1:113:A:LEU:H	2	7.75
(7,289)	1:85:A:ARG:HB2	1:85:A:ARG:H	1	7.75
(7,289)	1:85:A:ARG:HB3	1:85:A:ARG:H	1	7.75
(7,150)	1:42:A:LYS:HB2	1:42:A:LYS:H	2	7.75
(7,42)	1:12:A:LYS:H	1:12:A:LYS:HB2	1	7.75
(7,42)	1:12:A:LYS:H	1:12:A:LYS:HB3	1	7.75
(7,398)	1:113:A:LEU:HB2	1:113:A:LEU:H	1	7.74
(7,398)	1:113:A:LEU:HB3	1:113:A:LEU:H	1	7.74
(7,316)	1:90:A:LEU:HD21	1:90:A:LEU:H	2	7.74
(7,316)	1:90:A:LEU:HD22	1:90:A:LEU:H	2	7.74
(7,316)	1:90:A:LEU:HD23	1:90:A:LEU:H	2	7.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,301)	1:88:A:ARG:HB2	1:88:A:ARG:H	1	7.74
(7,301)	1:88:A:ARG:HB3	1:88:A:ARG:H	1	7.74
(7,170)	1:49:A:ALA:HB1	1:49:A:ALA:H	2	7.74
(7,170)	1:49:A:ALA:HB2	1:49:A:ALA:H	2	7.74
(7,170)	1:49:A:ALA:HB3	1:49:A:ALA:H	2	7.74
(7,47)	1:14:A:LEU:H	1:14:A:LEU:HB2	2	7.74
(7,42)	1:12:A:LYS:H	1:12:A:LYS:HB2	2	7.74
(7,42)	1:12:A:LYS:H	1:12:A:LYS:HB3	2	7.74
(7,282)	1:83:A:LEU:HB2	1:83:A:LEU:H	2	7.72
(7,180)	1:52:A:LEU:HB2	1:52:A:LEU:H	2	7.72
(7,26)	1:8:A:GLN:HB2	1:8:A:GLN:H	1	7.72
(6,184)	1:42:A:LYS:HB2	1:43:A:GLU:H	2	7.72
(6,527)	1:124:A:TYR:HB2	1:125:A:SER:H	2	7.71
(7,150)	1:42:A:LYS:HB2	1:42:A:LYS:H	1	7.7
(7,30)	1:9:A:GLU:H	1:9:A:GLU:HB2	1	7.7
(6,184)	1:42:A:LYS:HB2	1:43:A:GLU:H	1	7.7
(7,47)	1:14:A:LEU:H	1:14:A:LEU:HB2	1	7.69
(7,438)	1:126:A:LYS:HB2	1:126:A:LYS:H	1	7.67
(7,438)	1:126:A:LYS:HB2	1:126:A:LYS:H	2	7.67
(7,30)	1:9:A:GLU:H	1:9:A:GLU:HB2	2	7.64
(7,433)	1:124:A:TYR:HB2	1:124:A:TYR:H	2	7.61
(7,180)	1:52:A:LEU:HB2	1:52:A:LEU:H	1	7.61
(6,354)	1:85:A:ARG:HB2	1:86:A:LEU:H	2	7.59
(6,354)	1:85:A:ARG:HB3	1:86:A:LEU:H	2	7.59
(6,354)	1:85:A:ARG:HB2	1:86:A:LEU:H	1	7.58
(6,354)	1:85:A:ARG:HB3	1:86:A:LEU:H	1	7.58
(6,540)	1:129:A:SER:H	1:128:A:SER:H	1	7.56
(7,26)	1:8:A:GLN:HB2	1:8:A:GLN:H	2	7.55
(7,237)	1:71:A:GLN:HB2	1:71:A:GLN:H	1	7.54
(7,301)	1:88:A:ARG:HB2	1:88:A:ARG:H	2	7.52
(7,301)	1:88:A:ARG:HB3	1:88:A:ARG:H	2	7.52
(7,17)	1:7:A:LEU:HB3	1:7:A:LEU:H	1	7.52
(7,386)	1:110:A:GLU:HB2	1:110:A:GLU:H	1	7.51
(7,330)	1:93:A:LEU:HB2	1:93:A:LEU:H	1	7.51
(7,289)	1:85:A:ARG:HB2	1:85:A:ARG:H	2	7.51
(7,289)	1:85:A:ARG:HB3	1:85:A:ARG:H	2	7.51
(7,408)	1:117:A:LYS:HB2	1:117:A:LYS:H	2	7.5
(7,237)	1:71:A:GLN:HB2	1:71:A:GLN:H	2	7.5
(7,386)	1:110:A:GLU:HB2	1:110:A:GLU:H	2	7.49
(6,215)	1:49:A:ALA:HB1	1:50:A:THR:H	1	7.49
(6,215)	1:49:A:ALA:HB2	1:50:A:THR:H	1	7.49
(6,215)	1:49:A:ALA:HB3	1:50:A:THR:H	1	7.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,439)	1:126:A:LYS:HG3	1:126:A:LYS:H	1	7.48
(7,408)	1:117:A:LYS:HB2	1:117:A:LYS:H	1	7.48
(6,496)	1:117:A:LYS:HB3	1:118:A:THR:H	2	7.48
(6,213)	1:48:A:ALA:HB1	1:49:A:ALA:H	1	7.48
(6,213)	1:48:A:ALA:HB2	1:49:A:ALA:H	1	7.48
(6,213)	1:48:A:ALA:HB3	1:49:A:ALA:H	1	7.48
(7,429)	1:123:A:LYS:HB2	1:123:A:LYS:H	2	7.47
(6,496)	1:117:A:LYS:HB3	1:118:A:THR:H	1	7.46
(7,428)	1:123:A:LYS:HB3	1:123:A:LYS:H	2	7.45
(7,74)	1:19:A:GLU:H	1:19:A:GLU:HG2	2	7.45
(7,428)	1:123:A:LYS:HB3	1:123:A:LYS:H	1	7.44
(7,407)	1:117:A:LYS:HB3	1:117:A:LYS:H	2	7.44
(7,282)	1:83:A:LEU:HB2	1:83:A:LEU:H	1	7.44
(6,345)	1:83:A:LEU:HB2	1:84:A:LYS:H	2	7.44
(6,213)	1:48:A:ALA:HB1	1:49:A:ALA:H	2	7.44
(6,213)	1:48:A:ALA:HB2	1:49:A:ALA:H	2	7.44
(6,213)	1:48:A:ALA:HB3	1:49:A:ALA:H	2	7.44
(7,407)	1:117:A:LYS:HB3	1:117:A:LYS:H	1	7.42
(7,84)	1:21:A:LYS:HG2	1:21:A:LYS:H	1	7.41
(7,84)	1:21:A:LYS:HG3	1:21:A:LYS:H	1	7.41
(6,371)	1:88:A:ARG:HB2	1:89:A:ASN:H	2	7.41
(6,371)	1:88:A:ARG:HB3	1:89:A:ASN:H	2	7.41
(4,99)	1:35:A:ALA:HB1	1:37:A:LYS:H	2	7.39
(4,99)	1:35:A:ALA:HB2	1:37:A:LYS:H	2	7.39
(4,99)	1:35:A:ALA:HB3	1:37:A:LYS:H	2	7.39
(7,21)	1:7:A:LEU:HD21	1:7:A:LEU:H	1	7.38
(7,21)	1:7:A:LEU:HD22	1:7:A:LEU:H	1	7.38
(7,21)	1:7:A:LEU:HD23	1:7:A:LEU:H	1	7.38
(6,215)	1:49:A:ALA:HB1	1:50:A:THR:H	2	7.38
(6,215)	1:49:A:ALA:HB2	1:50:A:THR:H	2	7.38
(6,215)	1:49:A:ALA:HB3	1:50:A:THR:H	2	7.38
(7,48)	1:14:A:LEU:H	1:14:A:LEU:HG	2	7.37
(6,486)	1:113:A:LEU:H	1:114:A:GLU:H	1	7.35
(6,486)	1:113:A:LEU:H	1:114:A:GLU:H	2	7.34
(6,513)	1:120:A:MET:HB2	1:121:A:ARG:H	2	7.33
(4,100)	1:35:A:ALA:HB1	1:38:A:ASN:H	2	7.33
(4,100)	1:35:A:ALA:HB2	1:38:A:ASN:H	2	7.33
(4,100)	1:35:A:ALA:HB3	1:38:A:ASN:H	2	7.33
(7,429)	1:123:A:LYS:HB2	1:123:A:LYS:H	1	7.31
(6,513)	1:120:A:MET:HB2	1:121:A:ARG:H	1	7.31
(6,392)	1:93:A:LEU:HG	1:92:A:GLY:H	2	7.29
(6,540)	1:129:A:SER:H	1:128:A:SER:H	2	7.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,371)	1:88:A:ARG:HB2	1:89:A:ASN:H	1	7.24
(6,371)	1:88:A:ARG:HB3	1:89:A:ASN:H	1	7.24
(7,355)	1:102:A:LYS:HB2	1:102:A:LYS:H	1	7.23
(7,437)	1:126:A:LYS:HB3	1:126:A:LYS:H	2	7.22
(6,183)	1:42:A:LYS:HB3	1:43:A:GLU:H	2	7.22
(4,84)	1:31:A:ASP:HB3	1:33:A:PHE:H	2	7.22
(6,381)	1:90:A:LEU:HB2	1:91:A:TRP:H	1	7.21
(7,313)	1:90:A:LEU:HB2	1:90:A:LEU:H	2	7.2
(7,330)	1:93:A:LEU:HB2	1:93:A:LEU:H	2	7.12
(4,274)	1:92:A:GLY:HA2	1:94:A:ALA:H	2	7.12
(7,151)	1:42:A:LYS:HG3	1:42:A:LYS:H	1	7.08
(7,151)	1:42:A:LYS:HG3	1:42:A:LYS:H	2	7.07
(7,433)	1:124:A:TYR:HB2	1:124:A:TYR:H	1	7.06
(6,183)	1:42:A:LYS:HB3	1:43:A:GLU:H	1	7.06
(7,314)	1:90:A:LEU:HG	1:90:A:LEU:H	1	7.04
(7,78)	1:20:A:GLN:H	1:20:A:GLN:HG2	2	6.99
(7,78)	1:20:A:GLN:H	1:20:A:GLN:HG3	2	6.99
(7,82)	1:21:A:LYS:HB3	1:21:A:LYS:H	2	6.93
(7,332)	1:93:A:LEU:HD11	1:93:A:LEU:H	1	6.9
(7,332)	1:93:A:LEU:HD12	1:93:A:LEU:H	1	6.9
(7,332)	1:93:A:LEU:HD13	1:93:A:LEU:H	1	6.9
(4,30)	1:9:A:GLU:HA	1:13:A:THR:H	2	6.9
(4,275)	1:93:A:LEU:HA	1:95:A:GLY:H	2	6.89
(6,298)	1:72:A:GLN:HA	1:73:A:PHE:H	2	6.87
(7,356)	1:102:A:LYS:HG2	1:102:A:LYS:H	1	6.86
(7,356)	1:102:A:LYS:HG3	1:102:A:LYS:H	1	6.86
(6,420)	1:100:A:PRO:HB2	1:101:A:VAL:H	1	6.86
(4,354)	1:127:A:CYS:H	1:129:A:SER:H	2	6.84
(6,444)	1:106:A:GLN:H	1:105:A:ASN:H	2	6.83
(4,348)	1:124:A:TYR:HA	1:126:A:LYS:H	1	6.78
(6,380)	1:90:A:LEU:HB3	1:91:A:TRP:H	1	6.77
(4,272)	1:92:A:GLY:HA2	1:95:A:GLY:H	1	6.76
(4,180)	1:62:A:ASP:HB3	1:64:A:ARG:H	2	6.76
(4,30)	1:9:A:GLU:HA	1:13:A:THR:H	1	6.76
(7,290)	1:85:A:ARG:HG3	1:85:A:ARG:H	2	6.73
(4,164)	1:55:A:PHE:HA	1:58:A:HIS:H	1	6.71
(4,142)	1:47:A:ARG:HA	1:50:A:THR:H	2	6.7
(7,303)	1:88:A:ARG:HG2	1:88:A:ARG:H	2	6.65
(7,181)	1:52:A:LEU:HD11	1:52:A:LEU:H	1	6.64
(7,181)	1:52:A:LEU:HD12	1:52:A:LEU:H	1	6.64
(7,181)	1:52:A:LEU:HD13	1:52:A:LEU:H	1	6.64
(7,83)	1:21:A:LYS:HB2	1:21:A:LYS:H	1	6.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,512)	1:120:A:MET:HB3	1:121:A:ARG:H	2	6.64
(4,164)	1:55:A:PHE:HA	1:58:A:HIS:H	2	6.64
(6,512)	1:120:A:MET:HB3	1:121:A:ARG:H	1	6.62
(4,142)	1:47:A:ARG:HA	1:50:A:THR:H	1	6.61
(7,244)	1:72:A:GLN:HE21	1:72:A:GLN:H	1	6.6
(7,244)	1:72:A:GLN:HE22	1:72:A:GLN:H	1	6.6
(7,355)	1:102:A:LYS:HB2	1:102:A:LYS:H	2	6.59
(6,419)	1:100:A:PRO:HB3	1:101:A:VAL:H	2	6.59
(6,289)	1:71:A:GLN:HB2	1:72:A:GLN:H	1	6.58
(6,322)	1:79:A:LEU:HG	1:80:A:ILE:H	1	6.57
(6,298)	1:72:A:GLN:HA	1:73:A:PHE:H	1	6.57
(7,253)	1:75:A:ARG:HD2	1:75:A:ARG:H	2	6.54
(4,348)	1:124:A:TYR:HA	1:126:A:LYS:H	2	6.54
(4,59)	1:17:A:LEU:HA	1:20:A:GLN:H	1	6.54
(7,83)	1:21:A:LYS:HB2	1:21:A:LYS:H	2	6.53
(7,315)	1:90:A:LEU:HD11	1:90:A:LEU:H	2	6.52
(7,315)	1:90:A:LEU:HD12	1:90:A:LEU:H	2	6.52
(7,315)	1:90:A:LEU:HD13	1:90:A:LEU:H	2	6.52
(7,210)	1:60:A:GLU:HG2	1:60:A:GLU:H	2	6.52
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD11	2	6.52
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD12	2	6.52
(7,49)	1:14:A:LEU:H	1:14:A:LEU:HD13	2	6.52
(7,332)	1:93:A:LEU:HD11	1:93:A:LEU:H	2	6.51
(7,332)	1:93:A:LEU:HD12	1:93:A:LEU:H	2	6.51
(7,332)	1:93:A:LEU:HD13	1:93:A:LEU:H	2	6.51
(7,181)	1:52:A:LEU:HD11	1:52:A:LEU:H	2	6.5
(7,181)	1:52:A:LEU:HD12	1:52:A:LEU:H	2	6.5
(7,181)	1:52:A:LEU:HD13	1:52:A:LEU:H	2	6.5
(7,312)	1:90:A:LEU:HB3	1:90:A:LEU:H	1	6.49
(6,506)	1:119:A:ILE:HG22	1:120:A:MET:H	2	6.49
(7,18)	1:7:A:LEU:HB2	1:7:A:LEU:H	1	6.48
(7,17)	1:7:A:LEU:HB3	1:7:A:LEU:H	2	6.48
(6,534)	1:126:A:LYS:HB2	1:127:A:CYS:H	1	6.48
(6,282)	1:69:A:THR:HB	1:70:A:ALA:H	2	6.48
(7,312)	1:90:A:LEU:HB3	1:90:A:LEU:H	2	6.47
(7,149)	1:42:A:LYS:HB3	1:42:A:LYS:H	2	6.47
(6,289)	1:71:A:GLN:HB2	1:72:A:GLN:H	2	6.47
(7,329)	1:93:A:LEU:HB3	1:93:A:LEU:H	2	6.45
(7,179)	1:52:A:LEU:HB3	1:52:A:LEU:H	2	6.45
(7,46)	1:14:A:LEU:H	1:14:A:LEU:HB3	2	6.45
(7,437)	1:126:A:LYS:HB3	1:126:A:LYS:H	1	6.44
(6,15)	1:7:A:LEU:H	1:6:A:THR:HA	2	6.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,179)	1:52:A:LEU:HB3	1:52:A:LEU:H	1	6.43
(7,149)	1:42:A:LYS:HB3	1:42:A:LYS:H	1	6.43
(7,46)	1:14:A:LEU:H	1:14:A:LEU:HB3	1	6.43
(6,500)	1:118:A:THR:HA	1:119:A:ILE:H	2	6.43
(6,217)	1:50:A:THR:HA	1:51:A:VAL:H	1	6.43
(6,217)	1:50:A:THR:HA	1:51:A:VAL:H	2	6.43
(6,500)	1:118:A:THR:HA	1:119:A:ILE:H	1	6.42
(6,332)	1:80:A:ILE:HD11	1:81:A:ARG:H	1	6.42
(6,332)	1:80:A:ILE:HD12	1:81:A:ARG:H	1	6.42
(6,332)	1:80:A:ILE:HD13	1:81:A:ARG:H	1	6.42
(7,329)	1:93:A:LEU:HB3	1:93:A:LEU:H	1	6.4
(6,15)	1:7:A:LEU:H	1:6:A:THR:HA	1	6.4
(7,182)	1:52:A:LEU:HD21	1:52:A:LEU:H	1	6.38
(7,182)	1:52:A:LEU:HD22	1:52:A:LEU:H	1	6.38
(7,182)	1:52:A:LEU:HD23	1:52:A:LEU:H	1	6.38
(6,381)	1:90:A:LEU:HB2	1:91:A:TRP:H	2	6.38
(4,102)	1:36:A:SER:H	1:38:A:ASN:H	2	6.38
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD21	1	6.37
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD22	1	6.37
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD23	1	6.37
(4,177)	1:58:A:HIS:HA	1:60:A:GLU:H	1	6.37
(7,288)	1:85:A:ARG:HD2	1:85:A:ARG:H	2	6.36
(7,288)	1:85:A:ARG:HD3	1:85:A:ARG:H	2	6.36
(6,282)	1:69:A:THR:HB	1:70:A:ALA:H	1	6.34
(7,440)	1:126:A:LYS:HG2	1:126:A:LYS:H	1	6.32
(7,20)	1:7:A:LEU:HD11	1:7:A:LEU:H	1	6.31
(7,20)	1:7:A:LEU:HD12	1:7:A:LEU:H	1	6.31
(7,20)	1:7:A:LEU:HD13	1:7:A:LEU:H	1	6.31
(6,419)	1:100:A:PRO:HB3	1:101:A:VAL:H	1	6.31
(7,333)	1:93:A:LEU:HD21	1:93:A:LEU:H	1	6.3
(7,333)	1:93:A:LEU:HD22	1:93:A:LEU:H	1	6.3
(7,333)	1:93:A:LEU:HD23	1:93:A:LEU:H	1	6.3
(6,405)	1:96:A:LEU:HD11	1:97:A:ASN:H	1	6.3
(6,405)	1:96:A:LEU:HD12	1:97:A:ASN:H	1	6.3
(6,405)	1:96:A:LEU:HD13	1:97:A:ASN:H	1	6.3
(6,405)	1:96:A:LEU:HD21	1:97:A:ASN:H	1	6.3
(6,405)	1:96:A:LEU:HD22	1:97:A:ASN:H	1	6.3
(6,405)	1:96:A:LEU:HD23	1:97:A:ASN:H	1	6.3
(4,161)	1:55:A:PHE:HE1	1:59:A:HIS:H	1	6.29
(4,161)	1:55:A:PHE:HE2	1:59:A:HIS:H	1	6.29
(4,349)	1:124:A:TYR:H	1:126:A:LYS:H	2	6.28
(4,180)	1:62:A:ASP:HB3	1:64:A:ARG:H	1	6.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,157)	1:55:A:PHE:HD1	1:58:A:HIS:H	2	6.28
(4,157)	1:55:A:PHE:HD2	1:58:A:HIS:H	2	6.28
(7,315)	1:90:A:LEU:HD11	1:90:A:LEU:H	1	6.27
(7,315)	1:90:A:LEU:HD12	1:90:A:LEU:H	1	6.27
(7,315)	1:90:A:LEU:HD13	1:90:A:LEU:H	1	6.27
(4,97)	1:34:A:ALA:H	1:36:A:SER:H	2	6.26
(7,24)	1:8:A:GLN:HG2	1:8:A:GLN:H	1	6.25
(6,392)	1:93:A:LEU:HG	1:92:A:GLY:H	1	6.25
(7,182)	1:52:A:LEU:HD21	1:52:A:LEU:H	2	6.24
(7,182)	1:52:A:LEU:HD22	1:52:A:LEU:H	2	6.24
(7,182)	1:52:A:LEU:HD23	1:52:A:LEU:H	2	6.24
(7,19)	1:7:A:LEU:HG	1:7:A:LEU:H	2	6.24
(6,533)	1:126:A:LYS:HB3	1:127:A:CYS:H	2	6.24
(7,244)	1:72:A:GLN:HE21	1:72:A:GLN:H	2	6.22
(7,244)	1:72:A:GLN:HE22	1:72:A:GLN:H	2	6.22
(7,20)	1:7:A:LEU:HD11	1:7:A:LEU:H	2	6.21
(7,20)	1:7:A:LEU:HD12	1:7:A:LEU:H	2	6.21
(7,20)	1:7:A:LEU:HD13	1:7:A:LEU:H	2	6.21
(6,378)	1:90:A:LEU:HG	1:89:A:ASN:H	2	6.21
(4,65)	1:21:A:LYS:HA	1:23:A:LEU:H	2	6.21
(7,48)	1:14:A:LEU:H	1:14:A:LEU:HG	1	6.2
(6,345)	1:83:A:LEU:HB2	1:84:A:LYS:H	1	6.2
(6,391)	1:93:A:LEU:HD11	1:92:A:GLY:H	2	6.19
(6,391)	1:93:A:LEU:HD12	1:92:A:GLY:H	2	6.19
(6,391)	1:93:A:LEU:HD13	1:92:A:GLY:H	2	6.19
(6,391)	1:93:A:LEU:HD21	1:92:A:GLY:H	2	6.19
(6,391)	1:93:A:LEU:HD22	1:92:A:GLY:H	2	6.19
(6,391)	1:93:A:LEU:HD23	1:92:A:GLY:H	2	6.19
(6,273)	1:66:A:LEU:HB2	1:67:A:GLY:H	2	6.19
(6,273)	1:66:A:LEU:HB3	1:67:A:GLY:H	2	6.19
(6,497)	1:117:A:LYS:HB2	1:118:A:THR:H	2	6.18
(6,497)	1:117:A:LYS:HB2	1:118:A:THR:H	1	6.15
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD21	2	6.14
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD22	2	6.14
(7,50)	1:14:A:LEU:H	1:14:A:LEU:HD23	2	6.14
(6,395)	1:93:A:LEU:HD11	1:94:A:ALA:H	1	6.14
(6,395)	1:93:A:LEU:HD12	1:94:A:ALA:H	1	6.14
(6,395)	1:93:A:LEU:HD13	1:94:A:ALA:H	1	6.14
(6,395)	1:93:A:LEU:HD21	1:94:A:ALA:H	1	6.14
(6,395)	1:93:A:LEU:HD22	1:94:A:ALA:H	1	6.14
(6,395)	1:93:A:LEU:HD23	1:94:A:ALA:H	1	6.14
(4,274)	1:92:A:GLY:HA2	1:94:A:ALA:H	1	6.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,427)	1:102:A:LYS:HG2	1:103:A:GLU:H	1	6.11
(6,427)	1:102:A:LYS:HG3	1:103:A:GLU:H	1	6.11
(4,84)	1:31:A:ASP:HB3	1:33:A:PHE:H	1	6.1
(7,273)	1:81:A:ARG:HD3	1:81:A:ARG:H	1	6.09
(4,152)	1:51:A:VAL:HA	1:55:A:PHE:H	2	6.08
(4,99)	1:35:A:ALA:HB1	1:37:A:LYS:H	1	6.08
(4,99)	1:35:A:ALA:HB2	1:37:A:LYS:H	1	6.08
(4,99)	1:35:A:ALA:HB3	1:37:A:LYS:H	1	6.08
(6,95)	1:21:A:LYS:HB3	1:22:A:THR:H	1	6.06
(4,275)	1:93:A:LEU:HA	1:95:A:GLY:H	1	6.06
(4,181)	1:62:A:ASP:HB2	1:64:A:ARG:H	2	6.04
(7,78)	1:20:A:GLN:H	1:20:A:GLN:HG2	1	6.03
(7,78)	1:20:A:GLN:H	1:20:A:GLN:HG3	1	6.03
(6,95)	1:21:A:LYS:HB3	1:22:A:THR:H	2	6.03
(6,355)	1:85:A:ARG:HG3	1:86:A:LEU:H	1	6.02
(6,296)	1:72:A:GLN:HB3	1:73:A:PHE:H	1	6.02
(6,3)	1:3:A:THR:HG21	1:4:A:ASP:H	2	6.02
(6,3)	1:3:A:THR:HG22	1:4:A:ASP:H	2	6.02
(6,3)	1:3:A:THR:HG23	1:4:A:ASP:H	2	6.02
(4,134)	1:45:A:PHE:HA	1:49:A:ALA:H	1	6.02
(6,3)	1:3:A:THR:HG21	1:4:A:ASP:H	1	6.01
(6,3)	1:3:A:THR:HG22	1:4:A:ASP:H	1	6.01
(6,3)	1:3:A:THR:HG23	1:4:A:ASP:H	1	6.01
(4,134)	1:45:A:PHE:HA	1:49:A:ALA:H	2	6.01
(6,426)	1:102:A:LYS:HB2	1:103:A:GLU:H	2	6.0
(7,400)	1:113:A:LEU:HD11	1:113:A:LEU:H	2	5.99
(7,400)	1:113:A:LEU:HD12	1:113:A:LEU:H	2	5.99
(7,400)	1:113:A:LEU:HD13	1:113:A:LEU:H	2	5.99
(7,316)	1:90:A:LEU:HD21	1:90:A:LEU:H	1	5.99
(7,316)	1:90:A:LEU:HD22	1:90:A:LEU:H	1	5.99
(7,316)	1:90:A:LEU:HD23	1:90:A:LEU:H	1	5.99
(7,152)	1:42:A:LYS:HG2	1:42:A:LYS:H	1	5.98
(7,82)	1:21:A:LYS:HB3	1:21:A:LYS:H	1	5.97
(6,527)	1:124:A:TYR:HB2	1:125:A:SER:H	1	5.97
(4,349)	1:124:A:TYR:H	1:126:A:LYS:H	1	5.97
(4,344)	1:122:A:GLU:HA	1:125:A:SER:H	1	5.97
(4,344)	1:122:A:GLU:HA	1:125:A:SER:H	2	5.97
(6,395)	1:93:A:LEU:HD11	1:94:A:ALA:H	2	5.96
(6,395)	1:93:A:LEU:HD12	1:94:A:ALA:H	2	5.96
(6,395)	1:93:A:LEU:HD13	1:94:A:ALA:H	2	5.96
(6,395)	1:93:A:LEU:HD21	1:94:A:ALA:H	2	5.96
(6,395)	1:93:A:LEU:HD22	1:94:A:ALA:H	2	5.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,395)	1:93:A:LEU:HD23	1:94:A:ALA:H	2	5.96
(7,400)	1:113:A:LEU:HD11	1:113:A:LEU:H	1	5.95
(7,400)	1:113:A:LEU:HD12	1:113:A:LEU:H	1	5.95
(7,400)	1:113:A:LEU:HD13	1:113:A:LEU:H	1	5.95
(7,152)	1:42:A:LYS:HG2	1:42:A:LYS:H	2	5.93
(6,426)	1:102:A:LYS:HB2	1:103:A:GLU:H	1	5.93
(6,96)	1:21:A:LYS:HB2	1:22:A:THR:H	2	5.93
(6,322)	1:79:A:LEU:HG	1:80:A:ILE:H	2	5.92
(6,297)	1:72:A:GLN:HB2	1:73:A:PHE:H	1	5.92
(6,168)	1:39:A:THR:HG1	1:38:A:ASN:H	1	5.92
(4,219)	1:74:A:HIS:H	1:76:A:HIS:H	2	5.92
(6,394)	1:93:A:LEU:HG	1:94:A:ALA:H	2	5.91
(6,413)	1:98:A:SER:H	1:99:A:CYS:H	1	5.88
(4,85)	1:31:A:ASP:HB2	1:33:A:PHE:H	2	5.87
(7,84)	1:21:A:LYS:HG2	1:21:A:LYS:H	2	5.86
(7,84)	1:21:A:LYS:HG3	1:21:A:LYS:H	2	5.86
(6,506)	1:119:A:ILE:HG22	1:120:A:MET:H	1	5.86
(6,249)	1:59:A:HIS:HD1	1:60:A:GLU:H	2	5.86
(4,152)	1:51:A:VAL:HA	1:55:A:PHE:H	1	5.86
(7,356)	1:102:A:LYS:HG2	1:102:A:LYS:H	2	5.85
(7,356)	1:102:A:LYS:HG3	1:102:A:LYS:H	2	5.85
(6,533)	1:126:A:LYS:HB3	1:127:A:CYS:H	1	5.83
(6,356)	1:85:A:ARG:HG2	1:86:A:LEU:H	2	5.83
(4,331)	1:118:A:THR:H	1:120:A:MET:H	2	5.83
(7,274)	1:81:A:ARG:HD2	1:81:A:ARG:H	2	5.82
(4,258)	1:86:A:LEU:HA	1:90:A:LEU:H	1	5.82
(6,332)	1:80:A:ILE:HD11	1:81:A:ARG:H	2	5.81
(6,332)	1:80:A:ILE:HD12	1:81:A:ARG:H	2	5.81
(6,332)	1:80:A:ILE:HD13	1:81:A:ARG:H	2	5.81
(4,206)	1:72:A:GLN:HB2	1:75:A:ARG:H	1	5.81
(4,111)	1:40:A:THR:HG21	1:44:A:THR:H	1	5.81
(4,111)	1:40:A:THR:HG22	1:44:A:THR:H	1	5.81
(4,111)	1:40:A:THR:HG23	1:44:A:THR:H	1	5.81
(4,98)	1:35:A:ALA:H	1:37:A:LYS:H	2	5.81
(4,14)	1:8:A:GLN:H	1:6:A:THR:HA	1	5.81
(6,485)	1:113:A:LEU:HD21	1:114:A:GLU:H	2	5.8
(6,485)	1:113:A:LEU:HD22	1:114:A:GLU:H	2	5.8
(6,485)	1:113:A:LEU:HD23	1:114:A:GLU:H	2	5.8
(4,191)	1:69:A:THR:H	1:71:A:GLN:H	2	5.79
(4,161)	1:55:A:PHE:HE1	1:59:A:HIS:H	2	5.79
(4,161)	1:55:A:PHE:HE2	1:59:A:HIS:H	2	5.79
(6,414)	1:100:A:PRO:HG3	1:99:A:CYS:H	2	5.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,163)	1:37:A:LYS:HB2	1:36:A:SER:H	1	5.77
(6,163)	1:37:A:LYS:HB3	1:36:A:SER:H	1	5.77
(6,297)	1:72:A:GLN:HB2	1:73:A:PHE:H	2	5.76
(6,485)	1:113:A:LEU:HD21	1:114:A:GLU:H	1	5.75
(6,485)	1:113:A:LEU:HD22	1:114:A:GLU:H	1	5.75
(6,485)	1:113:A:LEU:HD23	1:114:A:GLU:H	1	5.75
(6,394)	1:93:A:LEU:HG	1:94:A:ALA:H	1	5.75
(4,32)	1:13:A:THR:H	1:9:A:GLU:HB3	1	5.75
(4,268)	1:91:A:TRP:H	1:93:A:LEU:H	2	5.74
(7,439)	1:126:A:LYS:HG3	1:126:A:LYS:H	2	5.73
(6,413)	1:98:A:SER:H	1:99:A:CYS:H	2	5.73
(7,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	1	5.72
(7,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	1	5.72
(7,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	1	5.72
(7,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	2	5.72
(7,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	2	5.72
(7,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	2	5.72
(7,288)	1:85:A:ARG:HD2	1:85:A:ARG:H	1	5.72
(7,288)	1:85:A:ARG:HD3	1:85:A:ARG:H	1	5.72
(7,252)	1:75:A:ARG:HD3	1:75:A:ARG:H	2	5.72
(4,258)	1:86:A:LEU:HA	1:90:A:LEU:H	2	5.72
(7,341)	1:96:A:LEU:HD11	1:96:A:LEU:H	2	5.71
(7,341)	1:96:A:LEU:HD12	1:96:A:LEU:H	2	5.71
(7,341)	1:96:A:LEU:HD13	1:96:A:LEU:H	2	5.71
(7,341)	1:96:A:LEU:HD21	1:96:A:LEU:H	2	5.71
(7,341)	1:96:A:LEU:HD22	1:96:A:LEU:H	2	5.71
(7,341)	1:96:A:LEU:HD23	1:96:A:LEU:H	2	5.71
(4,129)	1:44:A:THR:HA	1:48:A:ALA:H	1	5.71
(6,534)	1:126:A:LYS:HB2	1:127:A:CYS:H	2	5.7
(4,257)	1:86:A:LEU:H	1:88:A:ARG:H	2	5.7
(4,18)	1:7:A:LEU:HA	1:9:A:GLU:H	1	5.69
(4,157)	1:55:A:PHE:HD1	1:58:A:HIS:H	1	5.68
(4,157)	1:55:A:PHE:HD2	1:58:A:HIS:H	1	5.68
(4,18)	1:7:A:LEU:HA	1:9:A:GLU:H	2	5.67
(7,265)	1:79:A:LEU:HG	1:79:A:LEU:H	1	5.66
(6,87)	1:20:A:GLN:HB2	1:19:A:GLU:H	2	5.64
(4,206)	1:72:A:GLN:HB2	1:75:A:ARG:H	2	5.64
(6,525)	1:124:A:TYR:HD1	1:125:A:SER:H	1	5.63
(6,525)	1:124:A:TYR:HD2	1:125:A:SER:H	1	5.63
(7,417)	1:119:A:ILE:HG22	1:119:A:ILE:H	2	5.61
(4,257)	1:86:A:LEU:H	1:88:A:ARG:H	1	5.61
(4,191)	1:69:A:THR:H	1:71:A:GLN:H	1	5.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,444)	1:106:A:GLN:H	1:105:A:ASN:H	1	5.6
(4,14)	1:8:A:GLN:H	1:6:A:THR:HA	2	5.6
(7,302)	1:88:A:ARG:HG3	1:88:A:ARG:H	1	5.58
(7,27)	1:8:A:GLN:HE21	1:8:A:GLN:H	2	5.58
(7,27)	1:8:A:GLN:HE22	1:8:A:GLN:H	2	5.58
(6,356)	1:85:A:ARG:HG2	1:86:A:LEU:H	1	5.58
(6,284)	1:69:A:THR:H	1:70:A:ALA:H	2	5.58
(4,32)	1:13:A:THR:H	1:9:A:GLU:HB3	2	5.57
(7,399)	1:113:A:LEU:HG	1:113:A:LEU:H	2	5.56
(7,24)	1:8:A:GLN:HG2	1:8:A:GLN:H	2	5.56
(7,399)	1:113:A:LEU:HG	1:113:A:LEU:H	1	5.55
(7,290)	1:85:A:ARG:HG3	1:85:A:ARG:H	1	5.55
(6,380)	1:90:A:LEU:HB3	1:91:A:TRP:H	2	5.55
(4,199)	1:69:A:THR:HG21	1:72:A:GLN:HE21	1	5.55
(4,199)	1:69:A:THR:HG21	1:72:A:GLN:HE22	1	5.55
(4,199)	1:69:A:THR:HG22	1:72:A:GLN:HE21	1	5.55
(4,199)	1:69:A:THR:HG22	1:72:A:GLN:HE22	1	5.55
(4,199)	1:69:A:THR:HG23	1:72:A:GLN:HE21	1	5.55
(4,199)	1:69:A:THR:HG23	1:72:A:GLN:HE22	1	5.55
(4,198)	1:69:A:THR:HG21	1:72:A:GLN:HE21	1	5.55
(4,198)	1:69:A:THR:HG21	1:72:A:GLN:HE22	1	5.55
(4,198)	1:69:A:THR:HG22	1:72:A:GLN:HE21	1	5.55
(4,198)	1:69:A:THR:HG22	1:72:A:GLN:HE22	1	5.55
(4,198)	1:69:A:THR:HG23	1:72:A:GLN:HE21	1	5.55
(4,198)	1:69:A:THR:HG23	1:72:A:GLN:HE22	1	5.55
(4,331)	1:118:A:THR:H	1:120:A:MET:H	1	5.54
(4,129)	1:44:A:THR:HA	1:48:A:ALA:H	2	5.54
(7,273)	1:81:A:ARG:HD3	1:81:A:ARG:H	2	5.53
(4,268)	1:91:A:TRP:H	1:93:A:LEU:H	1	5.53
(7,418)	1:119:A:ILE:HD11	1:119:A:ILE:H	1	5.52
(7,418)	1:119:A:ILE:HD12	1:119:A:ILE:H	1	5.52
(7,418)	1:119:A:ILE:HD13	1:119:A:ILE:H	1	5.52
(7,303)	1:88:A:ARG:HG2	1:88:A:ARG:H	1	5.52
(6,272)	1:66:A:LEU:HD11	1:67:A:GLY:H	1	5.52
(6,272)	1:66:A:LEU:HD12	1:67:A:GLY:H	1	5.52
(6,272)	1:66:A:LEU:HD13	1:67:A:GLY:H	1	5.52
(6,272)	1:66:A:LEU:HD21	1:67:A:GLY:H	1	5.52
(6,272)	1:66:A:LEU:HD22	1:67:A:GLY:H	1	5.52
(6,272)	1:66:A:LEU:HD23	1:67:A:GLY:H	1	5.52
(4,309)	1:111:A:ASN:HA	1:113:A:LEU:H	1	5.52
(4,111)	1:40:A:THR:HG21	1:44:A:THR:H	2	5.51
(4,111)	1:40:A:THR:HG22	1:44:A:THR:H	2	5.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,111)	1:40:A:THR:HG23	1:44:A:THR:H	2	5.51
(6,403)	1:96:A:LEU:HD11	1:95:A:GLY:H	2	5.5
(6,403)	1:96:A:LEU:HD12	1:95:A:GLY:H	2	5.5
(6,403)	1:96:A:LEU:HD13	1:95:A:GLY:H	2	5.5
(6,403)	1:96:A:LEU:HD21	1:95:A:GLY:H	2	5.5
(6,403)	1:96:A:LEU:HD22	1:95:A:GLY:H	2	5.5
(6,403)	1:96:A:LEU:HD23	1:95:A:GLY:H	2	5.5
(7,253)	1:75:A:ARG:HD2	1:75:A:ARG:H	1	5.48
(6,96)	1:21:A:LYS:HB2	1:22:A:THR:H	1	5.47
(4,343)	1:122:A:GLU:HA	1:124:A:TYR:H	2	5.46
(2,31)	1:23:A:LEU:HD11	1:68:A:ALA:H	2	5.46
(2,31)	1:23:A:LEU:HD12	1:68:A:ALA:H	2	5.46
(2,31)	1:23:A:LEU:HD13	1:68:A:ALA:H	2	5.46
(2,31)	1:23:A:LEU:HD21	1:68:A:ALA:H	2	5.46
(2,31)	1:23:A:LEU:HD22	1:68:A:ALA:H	2	5.46
(2,31)	1:23:A:LEU:HD23	1:68:A:ALA:H	2	5.46
(7,440)	1:126:A:LYS:HG2	1:126:A:LYS:H	2	5.45
(6,484)	1:113:A:LEU:HD11	1:114:A:GLU:H	1	5.45
(6,484)	1:113:A:LEU:HD12	1:114:A:GLU:H	1	5.45
(6,484)	1:113:A:LEU:HD13	1:114:A:GLU:H	1	5.45
(6,484)	1:113:A:LEU:HD11	1:114:A:GLU:H	2	5.45
(6,484)	1:113:A:LEU:HD12	1:114:A:GLU:H	2	5.45
(6,484)	1:113:A:LEU:HD13	1:114:A:GLU:H	2	5.45
(6,284)	1:69:A:THR:H	1:70:A:ALA:H	1	5.44
(6,62)	1:16:A:SER:H	1:15:A:ASN:HD21	2	5.42
(6,62)	1:16:A:SER:H	1:15:A:ASN:HD22	2	5.42
(6,61)	1:16:A:SER:H	1:15:A:ASN:HD21	2	5.42
(6,61)	1:16:A:SER:H	1:15:A:ASN:HD22	2	5.42
(4,150)	1:50:A:THR:HA	1:52:A:LEU:H	1	5.42
(6,144)	1:32:A:ILE:HD11	1:33:A:PHE:HE1	1	5.41
(6,144)	1:32:A:ILE:HD11	1:33:A:PHE:HE2	1	5.41
(6,144)	1:32:A:ILE:HD12	1:33:A:PHE:HE1	1	5.41
(6,144)	1:32:A:ILE:HD12	1:33:A:PHE:HE2	1	5.41
(6,144)	1:32:A:ILE:HD13	1:33:A:PHE:HE1	1	5.41
(6,144)	1:32:A:ILE:HD13	1:33:A:PHE:HE2	1	5.41
(4,264)	1:88:A:ARG:HB2	1:90:A:LEU:H	1	5.41
(4,264)	1:88:A:ARG:HB3	1:90:A:LEU:H	1	5.41
(7,252)	1:75:A:ARG:HD3	1:75:A:ARG:H	1	5.4
(4,150)	1:50:A:THR:HA	1:52:A:LEU:H	2	5.4
(4,141)	1:47:A:ARG:H	1:50:A:THR:H	2	5.4
(7,417)	1:119:A:ILE:HG22	1:119:A:ILE:H	1	5.39
(6,296)	1:72:A:GLN:HB3	1:73:A:PHE:H	2	5.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,456)	1:109:A:LEU:HA	1:108:A:THR:H	2	5.38
(6,355)	1:85:A:ARG:HG3	1:86:A:LEU:H	2	5.37
(7,210)	1:60:A:GLU:HG2	1:60:A:GLU:H	1	5.36
(4,220)	1:74:A:HIS:H	1:77:A:LYS:H	2	5.36
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG21	1	5.36
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG22	1	5.36
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG23	1	5.36
(4,156)	1:55:A:PHE:HD1	1:57:A:SER:H	1	5.35
(4,156)	1:55:A:PHE:HD2	1:57:A:SER:H	1	5.35
(4,147)	1:49:A:ALA:HB1	1:52:A:LEU:H	1	5.35
(4,147)	1:49:A:ALA:HB2	1:52:A:LEU:H	1	5.35
(4,147)	1:49:A:ALA:HB3	1:52:A:LEU:H	1	5.35
(7,274)	1:81:A:ARG:HD2	1:81:A:ARG:H	1	5.34
(6,295)	1:73:A:PHE:HB2	1:72:A:GLN:H	2	5.34
(4,165)	1:55:A:PHE:HA	1:59:A:HIS:H	1	5.34
(7,291)	1:85:A:ARG:HG2	1:85:A:ARG:H	1	5.33
(6,378)	1:90:A:LEU:HG	1:89:A:ASN:H	1	5.31
(6,522)	1:124:A:TYR:HD1	1:123:A:LYS:H	2	5.3
(6,522)	1:124:A:TYR:HD2	1:123:A:LYS:H	2	5.3
(4,312)	1:111:A:ASN:H	1:114:A:GLU:H	2	5.3
(4,147)	1:49:A:ALA:HB1	1:52:A:LEU:H	2	5.3
(4,147)	1:49:A:ALA:HB2	1:52:A:LEU:H	2	5.3
(4,147)	1:49:A:ALA:HB3	1:52:A:LEU:H	2	5.3
(4,98)	1:35:A:ALA:H	1:37:A:LYS:H	1	5.3
(7,27)	1:8:A:GLN:HE21	1:8:A:GLN:H	1	5.29
(7,27)	1:8:A:GLN:HE22	1:8:A:GLN:H	1	5.29
(4,254)	1:85:A:ARG:HB2	1:87:A:ASP:H	2	5.29
(4,254)	1:85:A:ARG:HB3	1:87:A:ASP:H	2	5.29
(4,95)	1:34:A:ALA:HB1	1:38:A:ASN:H	1	5.28
(4,95)	1:34:A:ALA:HB2	1:38:A:ASN:H	1	5.28
(4,95)	1:34:A:ALA:HB3	1:38:A:ASN:H	1	5.28
(4,312)	1:111:A:ASN:H	1:114:A:GLU:H	1	5.27
(4,85)	1:31:A:ASP:HB2	1:33:A:PHE:H	1	5.27
(4,254)	1:85:A:ARG:HB2	1:87:A:ASP:H	1	5.25
(4,254)	1:85:A:ARG:HB3	1:87:A:ASP:H	1	5.25
(6,415)	1:100:A:PRO:HG2	1:99:A:CYS:H	2	5.24
(4,309)	1:111:A:ASN:HA	1:113:A:LEU:H	2	5.24
(4,167)	1:55:A:PHE:HB3	1:57:A:SER:H	2	5.22
(4,181)	1:62:A:ASP:HB2	1:64:A:ARG:H	1	5.21
(4,167)	1:55:A:PHE:HB3	1:57:A:SER:H	1	5.21
(4,95)	1:34:A:ALA:HB1	1:38:A:ASN:H	2	5.21
(4,95)	1:34:A:ALA:HB2	1:38:A:ASN:H	2	5.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,95)	1:34:A:ALA:HB3	1:38:A:ASN:H	2	5.21
(7,277)	1:82:A:PHE:HD1	1:82:A:PHE:H	2	5.2
(7,277)	1:82:A:PHE:HD2	1:82:A:PHE:H	2	5.2
(6,163)	1:37:A:LYS:HB2	1:36:A:SER:H	2	5.2
(6,163)	1:37:A:LYS:HB3	1:36:A:SER:H	2	5.2
(4,156)	1:55:A:PHE:HD1	1:57:A:SER:H	2	5.2
(4,156)	1:55:A:PHE:HD2	1:57:A:SER:H	2	5.2
(4,34)	1:13:A:THR:H	1:9:A:GLU:HG2	1	5.16
(4,34)	1:13:A:THR:H	1:9:A:GLU:HG3	1	5.16
(4,141)	1:47:A:ARG:H	1:50:A:THR:H	1	5.15
(4,112)	1:43:A:GLU:HA	1:40:A:THR:H	2	5.15
(4,108)	1:40:A:THR:HA	1:43:A:GLU:H	1	5.15
(4,34)	1:13:A:THR:H	1:9:A:GLU:HG2	2	5.14
(4,34)	1:13:A:THR:H	1:9:A:GLU:HG3	2	5.14
(6,353)	1:85:A:ARG:HD2	1:86:A:LEU:H	2	5.13
(6,353)	1:85:A:ARG:HD3	1:86:A:LEU:H	2	5.13
(6,295)	1:73:A:PHE:HB2	1:72:A:GLN:H	1	5.13
(6,86)	1:20:A:GLN:HB3	1:19:A:GLU:H	1	5.13
(4,272)	1:92:A:GLY:HA2	1:95:A:GLY:H	2	5.12
(4,219)	1:74:A:HIS:H	1:76:A:HIS:H	1	5.12
(4,59)	1:17:A:LEU:HA	1:20:A:GLN:H	2	5.11
(4,220)	1:74:A:HIS:H	1:77:A:LYS:H	1	5.1
(7,226)	1:66:A:LEU:HD11	1:66:A:LEU:H	2	5.09
(7,226)	1:66:A:LEU:HD12	1:66:A:LEU:H	2	5.09
(7,226)	1:66:A:LEU:HD13	1:66:A:LEU:H	2	5.09
(7,226)	1:66:A:LEU:HD21	1:66:A:LEU:H	2	5.09
(7,226)	1:66:A:LEU:HD22	1:66:A:LEU:H	2	5.09
(7,226)	1:66:A:LEU:HD23	1:66:A:LEU:H	2	5.09
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG21	1	5.08
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG22	1	5.08
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG23	1	5.08
(4,100)	1:35:A:ALA:HB1	1:38:A:ASN:H	1	5.07
(4,100)	1:35:A:ALA:HB2	1:38:A:ASN:H	1	5.07
(4,100)	1:35:A:ALA:HB3	1:38:A:ASN:H	1	5.07
(2,6)	1:31:A:ASP:H	1:105:A:ASN:HB2	1	5.06
(2,6)	1:31:A:ASP:H	1:105:A:ASN:HB3	1	5.06
(4,269)	1:91:A:TRP:HA	1:93:A:LEU:H	1	5.05
(4,205)	1:72:A:GLN:HB3	1:75:A:ARG:H	2	5.04
(4,264)	1:88:A:ARG:HB2	1:90:A:LEU:H	2	5.03
(4,264)	1:88:A:ARG:HB3	1:90:A:LEU:H	2	5.03
(4,160)	1:55:A:PHE:HE1	1:58:A:HIS:H	2	5.03
(4,160)	1:55:A:PHE:HE2	1:58:A:HIS:H	2	5.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG21	2	5.03
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG22	2	5.03
(4,17)	1:9:A:GLU:H	1:6:A:THR:HG23	2	5.03
(6,515)	1:120:A:MET:HG2	1:121:A:ARG:H	2	5.01
(4,108)	1:40:A:THR:HA	1:43:A:GLU:H	2	5.01
(2,32)	1:23:A:LEU:HD11	1:72:A:GLN:HE21	2	5.01
(2,32)	1:23:A:LEU:HD12	1:72:A:GLN:HE21	2	5.01
(2,32)	1:23:A:LEU:HD13	1:72:A:GLN:HE21	2	5.01
(2,32)	1:23:A:LEU:HD21	1:72:A:GLN:HE21	2	5.01
(2,32)	1:23:A:LEU:HD22	1:72:A:GLN:HE21	2	5.01
(2,32)	1:23:A:LEU:HD23	1:72:A:GLN:HE21	2	5.01
(4,343)	1:122:A:GLU:HA	1:124:A:TYR:H	1	4.99
(6,514)	1:120:A:MET:HG3	1:121:A:ARG:H	1	4.98
(4,205)	1:72:A:GLN:HB3	1:75:A:ARG:H	1	4.98
(4,112)	1:43:A:GLU:HA	1:40:A:THR:H	1	4.98
(4,354)	1:127:A:CYS:H	1:129:A:SER:H	1	4.97
(6,87)	1:20:A:GLN:HB2	1:19:A:GLU:H	1	4.96
(6,353)	1:85:A:ARG:HD2	1:86:A:LEU:H	1	4.95
(6,353)	1:85:A:ARG:HD3	1:86:A:LEU:H	1	4.95
(4,175)	1:57:A:SER:HB2	1:59:A:HIS:H	2	4.95
(4,175)	1:57:A:SER:HB3	1:59:A:HIS:H	2	4.95
(6,515)	1:120:A:MET:HG2	1:121:A:ARG:H	1	4.94
(4,260)	1:87:A:ASP:HB3	1:90:A:LEU:H	1	4.94
(4,73)	1:25:A:THR:H	1:27:A:LEU:H	1	4.94
(6,514)	1:120:A:MET:HG3	1:121:A:ARG:H	2	4.93
(4,73)	1:25:A:THR:H	1:27:A:LEU:H	2	4.93
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG21	2	4.93
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG22	2	4.93
(4,16)	1:8:A:GLN:H	1:6:A:THR:HG23	2	4.93
(4,165)	1:55:A:PHE:HA	1:59:A:HIS:H	2	4.89
(4,102)	1:36:A:SER:H	1:38:A:ASN:H	1	4.89
(4,266)	1:89:A:ASN:HA	1:93:A:LEU:H	2	4.87
(4,63)	1:18:A:THR:HG1	1:20:A:GLN:H	2	4.87
(4,266)	1:89:A:ASN:HA	1:93:A:LEU:H	1	4.85
(4,276)	1:93:A:LEU:HA	1:96:A:LEU:H	2	4.83
(7,310)	1:89:A:ASN:HB2	1:89:A:ASN:HD21	2	4.82
(7,310)	1:89:A:ASN:HB2	1:89:A:ASN:HD22	2	4.82
(7,310)	1:89:A:ASN:HB3	1:89:A:ASN:HD21	2	4.82
(7,310)	1:89:A:ASN:HB3	1:89:A:ASN:HD22	2	4.82
(6,391)	1:93:A:LEU:HD11	1:92:A:GLY:H	1	4.82
(6,391)	1:93:A:LEU:HD12	1:92:A:GLY:H	1	4.82
(6,391)	1:93:A:LEU:HD13	1:92:A:GLY:H	1	4.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,391)	1:93:A:LEU:HD21	1:92:A:GLY:H	1	4.82
(6,391)	1:93:A:LEU:HD22	1:92:A:GLY:H	1	4.82
(6,391)	1:93:A:LEU:HD23	1:92:A:GLY:H	1	4.82
(7,80)	1:20:A:GLN:HE21	1:20:A:GLN:HG2	2	4.81
(7,80)	1:20:A:GLN:HE21	1:20:A:GLN:HG3	2	4.81
(7,80)	1:20:A:GLN:HE22	1:20:A:GLN:HG2	2	4.81
(7,80)	1:20:A:GLN:HE22	1:20:A:GLN:HG3	2	4.81
(6,167)	1:39:A:THR:HB	1:38:A:ASN:H	2	4.81
(4,168)	1:55:A:PHE:HB3	1:58:A:HIS:H	1	4.81
(4,175)	1:57:A:SER:HB2	1:59:A:HIS:H	1	4.8
(4,175)	1:57:A:SER:HB3	1:59:A:HIS:H	1	4.8
(4,269)	1:91:A:TRP:HA	1:93:A:LEU:H	2	4.79
(4,97)	1:34:A:ALA:H	1:36:A:SER:H	1	4.77
(6,17)	1:6:A:THR:H	1:7:A:LEU:HA	2	4.75
(4,261)	1:87:A:ASP:HB2	1:90:A:LEU:H	1	4.75
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD11	2	4.74
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD12	2	4.74
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD13	2	4.74
(7,80)	1:20:A:GLN:HE21	1:20:A:GLN:HG2	1	4.73
(7,80)	1:20:A:GLN:HE21	1:20:A:GLN:HG3	1	4.73
(7,80)	1:20:A:GLN:HE22	1:20:A:GLN:HG2	1	4.73
(7,80)	1:20:A:GLN:HE22	1:20:A:GLN:HG3	1	4.73
(6,357)	1:86:A:LEU:HD11	1:85:A:ARG:H	2	4.73
(6,357)	1:86:A:LEU:HD12	1:85:A:ARG:H	2	4.73
(6,357)	1:86:A:LEU:HD13	1:85:A:ARG:H	2	4.73
(6,116)	1:27:A:LEU:HD11	1:28:A:THR:H	1	4.73
(6,116)	1:27:A:LEU:HD12	1:28:A:THR:H	1	4.73
(6,116)	1:27:A:LEU:HD13	1:28:A:THR:H	1	4.73
(4,160)	1:55:A:PHE:HE1	1:58:A:HIS:H	1	4.72
(4,160)	1:55:A:PHE:HE2	1:58:A:HIS:H	1	4.72
(4,33)	1:13:A:THR:H	1:9:A:GLU:HB2	1	4.71
(4,33)	1:13:A:THR:H	1:9:A:GLU:HB2	2	4.7
(6,17)	1:6:A:THR:H	1:7:A:LEU:HA	1	4.68
(4,196)	1:69:A:THR:HG21	1:71:A:GLN:H	2	4.66
(4,196)	1:69:A:THR:HG22	1:71:A:GLN:H	2	4.66
(4,196)	1:69:A:THR:HG23	1:71:A:GLN:H	2	4.66
(4,197)	1:69:A:THR:HG21	1:72:A:GLN:H	2	4.65
(4,197)	1:69:A:THR:HG22	1:72:A:GLN:H	2	4.65
(4,197)	1:69:A:THR:HG23	1:72:A:GLN:H	2	4.65
(6,116)	1:27:A:LEU:HD11	1:28:A:THR:H	2	4.62
(6,116)	1:27:A:LEU:HD12	1:28:A:THR:H	2	4.62
(6,116)	1:27:A:LEU:HD13	1:28:A:THR:H	2	4.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,168)	1:55:A:PHE:HB3	1:58:A:HIS:H	2	4.62
(6,339)	1:82:A:PHE:HD1	1:83:A:LEU:H	1	4.6
(6,339)	1:82:A:PHE:HD2	1:83:A:LEU:H	1	4.6
(4,199)	1:69:A:THR:HG21	1:72:A:GLN:HE21	2	4.6
(4,199)	1:69:A:THR:HG21	1:72:A:GLN:HE22	2	4.6
(4,199)	1:69:A:THR:HG22	1:72:A:GLN:HE21	2	4.6
(4,199)	1:69:A:THR:HG22	1:72:A:GLN:HE22	2	4.6
(4,199)	1:69:A:THR:HG23	1:72:A:GLN:HE21	2	4.6
(4,199)	1:69:A:THR:HG23	1:72:A:GLN:HE22	2	4.6
(4,198)	1:69:A:THR:HG21	1:72:A:GLN:HE21	2	4.6
(4,198)	1:69:A:THR:HG21	1:72:A:GLN:HE22	2	4.6
(4,198)	1:69:A:THR:HG22	1:72:A:GLN:HE21	2	4.6
(4,198)	1:69:A:THR:HG22	1:72:A:GLN:HE22	2	4.6
(4,198)	1:69:A:THR:HG23	1:72:A:GLN:HE21	2	4.6
(4,198)	1:69:A:THR:HG23	1:72:A:GLN:HE22	2	4.6
(6,522)	1:124:A:TYR:HD1	1:123:A:LYS:H	1	4.58
(6,522)	1:124:A:TYR:HD2	1:123:A:LYS:H	1	4.58
(4,63)	1:18:A:THR:HG1	1:20:A:GLN:H	1	4.58
(6,256)	1:61:A:LYS:H	1:62:A:ASP:H	1	4.56
(6,272)	1:66:A:LEU:HD11	1:67:A:GLY:H	2	4.54
(6,272)	1:66:A:LEU:HD12	1:67:A:GLY:H	2	4.54
(6,272)	1:66:A:LEU:HD13	1:67:A:GLY:H	2	4.54
(6,272)	1:66:A:LEU:HD21	1:67:A:GLY:H	2	4.54
(6,272)	1:66:A:LEU:HD22	1:67:A:GLY:H	2	4.54
(6,272)	1:66:A:LEU:HD23	1:67:A:GLY:H	2	4.54
(2,26)	1:96:A:LEU:HD11	1:46:A:CYS:H	2	4.54
(2,26)	1:96:A:LEU:HD12	1:46:A:CYS:H	2	4.54
(2,26)	1:96:A:LEU:HD13	1:46:A:CYS:H	2	4.54
(2,26)	1:96:A:LEU:HD21	1:46:A:CYS:H	2	4.54
(2,26)	1:96:A:LEU:HD22	1:46:A:CYS:H	2	4.54
(2,26)	1:96:A:LEU:HD23	1:46:A:CYS:H	2	4.54
(6,27)	1:8:A:GLN:HB3	1:9:A:GLU:H	2	4.53
(6,93)	1:20:A:GLN:HG2	1:21:A:LYS:H	1	4.52
(6,93)	1:20:A:GLN:HG3	1:21:A:LYS:H	1	4.52
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD11	2	4.51
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD12	2	4.51
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD13	2	4.51
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD21	2	4.51
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD22	2	4.51
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD23	2	4.51
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD11	1	4.49
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD12	1	4.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD13	1	4.49
(6,358)	1:86:A:LEU:HD21	1:85:A:ARG:H	2	4.47
(6,358)	1:86:A:LEU:HD22	1:85:A:ARG:H	2	4.47
(6,358)	1:86:A:LEU:HD23	1:85:A:ARG:H	2	4.47
(4,49)	1:14:A:LEU:HA	1:18:A:THR:H	2	4.45
(2,22)	1:96:A:LEU:HD11	1:43:A:GLU:H	2	4.45
(2,22)	1:96:A:LEU:HD12	1:43:A:GLU:H	2	4.45
(2,22)	1:96:A:LEU:HD13	1:43:A:GLU:H	2	4.45
(2,22)	1:96:A:LEU:HD21	1:43:A:GLU:H	2	4.45
(2,22)	1:96:A:LEU:HD22	1:43:A:GLU:H	2	4.45
(2,22)	1:96:A:LEU:HD23	1:43:A:GLU:H	2	4.45
(7,108)	1:29:A:VAL:HG21	1:29:A:VAL:H	2	4.44
(7,108)	1:29:A:VAL:HG22	1:29:A:VAL:H	2	4.44
(7,108)	1:29:A:VAL:HG23	1:29:A:VAL:H	2	4.44
(3,85)	1:30:A:THR:H	1:106:A:GLN:O	2	4.42
(4,211)	1:72:A:GLN:H	1:76:A:HIS:H	1	4.4
(6,28)	1:8:A:GLN:HB2	1:9:A:GLU:H	1	4.39
(4,315)	1:112:A:PHE:HD1	1:116:A:LEU:H	2	4.38
(4,315)	1:112:A:PHE:HD2	1:116:A:LEU:H	2	4.38
(4,197)	1:69:A:THR:HG21	1:72:A:GLN:H	1	4.37
(4,197)	1:69:A:THR:HG22	1:72:A:GLN:H	1	4.37
(4,197)	1:69:A:THR:HG23	1:72:A:GLN:H	1	4.37
(7,79)	1:20:A:GLN:H	1:20:A:GLN:HE21	2	4.33
(7,79)	1:20:A:GLN:H	1:20:A:GLN:HE22	2	4.33
(6,167)	1:39:A:THR:HB	1:38:A:ASN:H	1	4.31
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD11	2	4.31
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD12	2	4.31
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD13	2	4.31
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD21	2	4.31
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD22	2	4.31
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD23	2	4.31
(4,281)	1:96:A:LEU:HD11	1:99:A:CYS:H	1	4.29
(4,281)	1:96:A:LEU:HD12	1:99:A:CYS:H	1	4.29
(4,281)	1:96:A:LEU:HD13	1:99:A:CYS:H	1	4.29
(4,281)	1:96:A:LEU:HD21	1:99:A:CYS:H	1	4.29
(4,281)	1:96:A:LEU:HD22	1:99:A:CYS:H	1	4.29
(4,281)	1:96:A:LEU:HD23	1:99:A:CYS:H	1	4.29
(3,85)	1:30:A:THR:H	1:106:A:GLN:O	1	4.27
(4,261)	1:87:A:ASP:HB2	1:90:A:LEU:H	2	4.26
(4,196)	1:69:A:THR:HG21	1:71:A:GLN:H	1	4.26
(4,196)	1:69:A:THR:HG22	1:71:A:GLN:H	1	4.26
(4,196)	1:69:A:THR:HG23	1:71:A:GLN:H	1	4.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:96:A:LEU:HD11	1:45:A:PHE:H	2	4.26
(2,24)	1:96:A:LEU:HD12	1:45:A:PHE:H	2	4.26
(2,24)	1:96:A:LEU:HD13	1:45:A:PHE:H	2	4.26
(2,24)	1:96:A:LEU:HD21	1:45:A:PHE:H	2	4.26
(2,24)	1:96:A:LEU:HD22	1:45:A:PHE:H	2	4.26
(2,24)	1:96:A:LEU:HD23	1:45:A:PHE:H	2	4.26
(6,456)	1:109:A:LEU:HA	1:108:A:THR:H	1	4.24
(6,86)	1:20:A:GLN:HB3	1:19:A:GLU:H	2	4.24
(4,260)	1:87:A:ASP:HB3	1:90:A:LEU:H	2	4.23
(7,359)	1:103:A:GLU:HG2	1:103:A:GLU:H	1	4.22
(7,359)	1:103:A:GLU:HG3	1:103:A:GLU:H	1	4.22
(4,49)	1:14:A:LEU:HA	1:18:A:THR:H	1	4.21
(6,324)	1:79:A:LEU:HD11	1:80:A:ILE:H	2	4.19
(6,324)	1:79:A:LEU:HD12	1:80:A:ILE:H	2	4.19
(6,324)	1:79:A:LEU:HD13	1:80:A:ILE:H	2	4.19
(6,324)	1:79:A:LEU:HD21	1:80:A:ILE:H	2	4.19
(6,324)	1:79:A:LEU:HD22	1:80:A:ILE:H	2	4.19
(6,324)	1:79:A:LEU:HD23	1:80:A:ILE:H	2	4.19
(7,309)	1:89:A:ASN:HA	1:89:A:ASN:HD21	1	4.18
(7,309)	1:89:A:ASN:HA	1:89:A:ASN:HD22	1	4.18
(6,250)	1:59:A:HIS:HB2	1:60:A:GLU:H	2	4.18
(6,250)	1:59:A:HIS:HB3	1:60:A:GLU:H	2	4.18
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD11	2	4.18
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD12	2	4.18
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD13	2	4.18
(7,310)	1:89:A:ASN:HB2	1:89:A:ASN:HD21	1	4.17
(7,310)	1:89:A:ASN:HB2	1:89:A:ASN:HD22	1	4.17
(7,310)	1:89:A:ASN:HB3	1:89:A:ASN:HD21	1	4.17
(7,310)	1:89:A:ASN:HB3	1:89:A:ASN:HD22	1	4.17
(4,211)	1:72:A:GLN:H	1:76:A:HIS:H	2	4.17
(4,79)	1:28:A:THR:HA	1:30:A:THR:H	1	4.14
(2,6)	1:31:A:ASP:H	1:105:A:ASN:HB2	2	4.14
(2,6)	1:31:A:ASP:H	1:105:A:ASN:HB3	2	4.14
(6,324)	1:79:A:LEU:HD11	1:80:A:ILE:H	1	4.13
(6,324)	1:79:A:LEU:HD12	1:80:A:ILE:H	1	4.13
(6,324)	1:79:A:LEU:HD13	1:80:A:ILE:H	1	4.13
(6,324)	1:79:A:LEU:HD21	1:80:A:ILE:H	1	4.13
(6,324)	1:79:A:LEU:HD22	1:80:A:ILE:H	1	4.13
(6,324)	1:79:A:LEU:HD23	1:80:A:ILE:H	1	4.13
(4,55)	1:16:A:SER:HB2	1:19:A:GLU:H	2	4.13
(4,55)	1:16:A:SER:HB3	1:19:A:GLU:H	2	4.13
(6,44)	1:12:A:LYS:H	1:11:A:ILE:HG13	2	4.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:23:A:LEU:HD11	1:72:A:GLN:HE22	2	4.12
(2,33)	1:23:A:LEU:HD12	1:72:A:GLN:HE22	2	4.12
(2,33)	1:23:A:LEU:HD13	1:72:A:GLN:HE22	2	4.12
(2,33)	1:23:A:LEU:HD21	1:72:A:GLN:HE22	2	4.12
(2,33)	1:23:A:LEU:HD22	1:72:A:GLN:HE22	2	4.12
(2,33)	1:23:A:LEU:HD23	1:72:A:GLN:HE22	2	4.12
(7,341)	1:96:A:LEU:HD11	1:96:A:LEU:H	1	4.11
(7,341)	1:96:A:LEU:HD12	1:96:A:LEU:H	1	4.11
(7,341)	1:96:A:LEU:HD13	1:96:A:LEU:H	1	4.11
(7,341)	1:96:A:LEU:HD21	1:96:A:LEU:H	1	4.11
(7,341)	1:96:A:LEU:HD22	1:96:A:LEU:H	1	4.11
(7,341)	1:96:A:LEU:HD23	1:96:A:LEU:H	1	4.11
(4,65)	1:21:A:LYS:HA	1:23:A:LEU:H	1	4.11
(2,23)	1:96:A:LEU:HD11	1:44:A:THR:H	2	4.1
(2,23)	1:96:A:LEU:HD12	1:44:A:THR:H	2	4.1
(2,23)	1:96:A:LEU:HD13	1:44:A:THR:H	2	4.1
(2,23)	1:96:A:LEU:HD21	1:44:A:THR:H	2	4.1
(2,23)	1:96:A:LEU:HD22	1:44:A:THR:H	2	4.1
(2,23)	1:96:A:LEU:HD23	1:44:A:THR:H	2	4.1
(2,31)	1:23:A:LEU:HD11	1:68:A:ALA:H	1	4.09
(2,31)	1:23:A:LEU:HD12	1:68:A:ALA:H	1	4.09
(2,31)	1:23:A:LEU:HD13	1:68:A:ALA:H	1	4.09
(2,31)	1:23:A:LEU:HD21	1:68:A:ALA:H	1	4.09
(2,31)	1:23:A:LEU:HD22	1:68:A:ALA:H	1	4.09
(2,31)	1:23:A:LEU:HD23	1:68:A:ALA:H	1	4.09
(7,418)	1:119:A:ILE:HD11	1:119:A:ILE:H	2	4.08
(7,418)	1:119:A:ILE:HD12	1:119:A:ILE:H	2	4.08
(7,418)	1:119:A:ILE:HD13	1:119:A:ILE:H	2	4.08
(4,280)	1:96:A:LEU:HD11	1:98:A:SER:H	1	4.05
(4,280)	1:96:A:LEU:HD12	1:98:A:SER:H	1	4.05
(4,280)	1:96:A:LEU:HD13	1:98:A:SER:H	1	4.05
(4,280)	1:96:A:LEU:HD21	1:98:A:SER:H	1	4.05
(4,280)	1:96:A:LEU:HD22	1:98:A:SER:H	1	4.05
(4,280)	1:96:A:LEU:HD23	1:98:A:SER:H	1	4.05
(6,273)	1:66:A:LEU:HB2	1:67:A:GLY:H	1	4.04
(6,273)	1:66:A:LEU:HB3	1:67:A:GLY:H	1	4.04
(4,22)	1:7:A:LEU:H	1:11:A:ILE:H	1	4.04
(7,404)	1:115:A:ARG:H	1:115:A:ARG:HE	1	4.03
(6,404)	1:96:A:LEU:HB2	1:97:A:ASN:H	1	4.03
(6,404)	1:96:A:LEU:HB3	1:97:A:ASN:H	1	4.03
(6,145)	1:32:A:ILE:HD11	1:33:A:PHE:HZ	1	4.03
(6,145)	1:32:A:ILE:HD12	1:33:A:PHE:HZ	1	4.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,145)	1:32:A:ILE:HD13	1:33:A:PHE:HZ	1	4.03
(7,79)	1:20:A:GLN:H	1:20:A:GLN:HE21	1	4.02
(7,79)	1:20:A:GLN:H	1:20:A:GLN:HE22	1	4.02
(7,431)	1:124:A:TYR:HD1	1:124:A:TYR:H	2	4.0
(7,431)	1:124:A:TYR:HD2	1:124:A:TYR:H	2	4.0
(6,510)	1:120:A:MET:HB3	1:119:A:ILE:H	1	3.99
(4,151)	1:51:A:VAL:H	1:55:A:PHE:H	2	3.99
(4,315)	1:112:A:PHE:HD1	1:116:A:LEU:H	1	3.97
(4,315)	1:112:A:PHE:HD2	1:116:A:LEU:H	1	3.97
(6,441)	1:105:A:ASN:HB3	1:106:A:GLN:H	1	3.95
(4,296)	1:108:A:THR:HB	1:111:A:ASN:H	2	3.95
(4,267)	1:90:A:LEU:H	1:93:A:LEU:H	2	3.93
(6,432)	1:103:A:GLU:HG2	1:104:A:ALA:H	2	3.92
(6,432)	1:103:A:GLU:HG3	1:104:A:ALA:H	2	3.92
(2,22)	1:96:A:LEU:HD11	1:43:A:GLU:H	1	3.92
(2,22)	1:96:A:LEU:HD12	1:43:A:GLU:H	1	3.92
(2,22)	1:96:A:LEU:HD13	1:43:A:GLU:H	1	3.92
(2,22)	1:96:A:LEU:HD21	1:43:A:GLU:H	1	3.92
(2,22)	1:96:A:LEU:HD22	1:43:A:GLU:H	1	3.92
(2,22)	1:96:A:LEU:HD23	1:43:A:GLU:H	1	3.92
(6,423)	1:101:A:VAL:HG21	1:102:A:LYS:H	2	3.91
(6,423)	1:101:A:VAL:HG22	1:102:A:LYS:H	2	3.91
(6,423)	1:101:A:VAL:HG23	1:102:A:LYS:H	2	3.91
(6,405)	1:96:A:LEU:HD11	1:97:A:ASN:H	2	3.91
(6,405)	1:96:A:LEU:HD12	1:97:A:ASN:H	2	3.91
(6,405)	1:96:A:LEU:HD13	1:97:A:ASN:H	2	3.91
(6,405)	1:96:A:LEU:HD21	1:97:A:ASN:H	2	3.91
(6,405)	1:96:A:LEU:HD22	1:97:A:ASN:H	2	3.91
(6,405)	1:96:A:LEU:HD23	1:97:A:ASN:H	2	3.91
(4,22)	1:7:A:LEU:H	1:11:A:ILE:H	2	3.91
(7,190)	1:56:A:TYR:HD1	1:56:A:TYR:H	2	3.9
(7,190)	1:56:A:TYR:HD2	1:56:A:TYR:H	2	3.9
(6,510)	1:120:A:MET:HB3	1:119:A:ILE:H	2	3.9
(6,525)	1:124:A:TYR:HD1	1:125:A:SER:H	2	3.89
(6,525)	1:124:A:TYR:HD2	1:125:A:SER:H	2	3.89
(4,293)	1:108:A:THR:HG21	1:111:A:ASN:HD21	2	3.88
(4,293)	1:108:A:THR:HG21	1:111:A:ASN:HD22	2	3.88
(4,293)	1:108:A:THR:HG22	1:111:A:ASN:HD21	2	3.88
(4,293)	1:108:A:THR:HG22	1:111:A:ASN:HD22	2	3.88
(4,293)	1:108:A:THR:HG23	1:111:A:ASN:HD21	2	3.88
(4,293)	1:108:A:THR:HG23	1:111:A:ASN:HD22	2	3.88
(6,249)	1:59:A:HIS:HD2	1:60:A:GLU:H	1	3.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:96:A:LEU:HD11	1:46:A:CYS:H	1	3.86
(2,26)	1:96:A:LEU:HD12	1:46:A:CYS:H	1	3.86
(2,26)	1:96:A:LEU:HD13	1:46:A:CYS:H	1	3.86
(2,26)	1:96:A:LEU:HD21	1:46:A:CYS:H	1	3.86
(2,26)	1:96:A:LEU:HD22	1:46:A:CYS:H	1	3.86
(2,26)	1:96:A:LEU:HD23	1:46:A:CYS:H	1	3.86
(7,276)	1:82:A:PHE:HE1	1:82:A:PHE:H	2	3.82
(7,276)	1:82:A:PHE:HE2	1:82:A:PHE:H	2	3.82
(4,280)	1:96:A:LEU:HD11	1:98:A:SER:H	2	3.82
(4,280)	1:96:A:LEU:HD12	1:98:A:SER:H	2	3.82
(4,280)	1:96:A:LEU:HD13	1:98:A:SER:H	2	3.82
(4,280)	1:96:A:LEU:HD21	1:98:A:SER:H	2	3.82
(4,280)	1:96:A:LEU:HD22	1:98:A:SER:H	2	3.82
(4,280)	1:96:A:LEU:HD23	1:98:A:SER:H	2	3.82
(4,159)	1:55:A:PHE:HE1	1:57:A:SER:H	2	3.81
(4,159)	1:55:A:PHE:HE2	1:57:A:SER:H	2	3.81
(4,151)	1:51:A:VAL:H	1:55:A:PHE:H	1	3.81
(7,372)	1:106:A:GLN:HG2	1:106:A:GLN:HE21	2	3.8
(7,372)	1:106:A:GLN:HG2	1:106:A:GLN:HE22	2	3.8
(7,372)	1:106:A:GLN:HG3	1:106:A:GLN:HE21	2	3.8
(7,372)	1:106:A:GLN:HG3	1:106:A:GLN:HE22	2	3.8
(4,79)	1:28:A:THR:HA	1:30:A:THR:H	2	3.8
(6,232)	1:56:A:TYR:HD1	1:55:A:PHE:H	2	3.79
(6,232)	1:56:A:TYR:HD2	1:55:A:PHE:H	2	3.79
(4,292)	1:108:A:THR:HG21	1:111:A:ASN:H	2	3.79
(4,292)	1:108:A:THR:HG22	1:111:A:ASN:H	2	3.79
(4,292)	1:108:A:THR:HG23	1:111:A:ASN:H	2	3.79
(2,34)	1:69:A:THR:HG21	1:75:A:ARG:H	1	3.79
(2,34)	1:69:A:THR:HG22	1:75:A:ARG:H	1	3.79
(2,34)	1:69:A:THR:HG23	1:75:A:ARG:H	1	3.79
(2,18)	1:8:A:GLN:H	1:124:A:TYR:HE1	2	3.79
(2,18)	1:8:A:GLN:H	1:124:A:TYR:HE2	2	3.79
(7,372)	1:106:A:GLN:HG2	1:106:A:GLN:HE21	1	3.78
(7,372)	1:106:A:GLN:HG2	1:106:A:GLN:HE22	1	3.78
(7,372)	1:106:A:GLN:HG3	1:106:A:GLN:HE21	1	3.78
(7,372)	1:106:A:GLN:HG3	1:106:A:GLN:HE22	1	3.78
(4,267)	1:90:A:LEU:H	1:93:A:LEU:H	1	3.77
(2,43)	1:30:A:THR:HG21	1:106:A:GLN:HE21	1	3.77
(2,43)	1:30:A:THR:HG21	1:106:A:GLN:HE22	1	3.77
(2,43)	1:30:A:THR:HG22	1:106:A:GLN:HE21	1	3.77
(2,43)	1:30:A:THR:HG22	1:106:A:GLN:HE22	1	3.77
(2,43)	1:30:A:THR:HG23	1:106:A:GLN:HE21	1	3.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,43)	1:30:A:THR:HG23	1:106:A:GLN:HE22	1	3.77
(7,139)	1:38:A:ASN:HB2	1:38:A:ASN:HD21	2	3.76
(7,139)	1:38:A:ASN:HB2	1:38:A:ASN:HD22	2	3.76
(7,111)	1:30:A:THR:HG21	1:30:A:THR:H	2	3.76
(7,111)	1:30:A:THR:HG22	1:30:A:THR:H	2	3.76
(7,111)	1:30:A:THR:HG23	1:30:A:THR:H	2	3.76
(4,135)	1:48:A:ALA:H	1:45:A:PHE:HE1	2	3.75
(4,135)	1:48:A:ALA:H	1:45:A:PHE:HE2	2	3.75
(7,447)	1:129:A:SER:HB2	1:129:A:SER:H	2	3.74
(7,447)	1:129:A:SER:HB3	1:129:A:SER:H	2	3.74
(6,31)	1:10:A:ILE:H	1:9:A:GLU:HB2	1	3.74
(6,31)	1:10:A:ILE:H	1:9:A:GLU:HB3	1	3.74
(7,190)	1:56:A:TYR:HD1	1:56:A:TYR:H	1	3.73
(7,190)	1:56:A:TYR:HD2	1:56:A:TYR:H	1	3.73
(7,365)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	2	3.72
(7,365)	1:105:A:ASN:HB3	1:105:A:ASN:HD22	2	3.72
(6,302)	1:73:A:PHE:HD1	1:74:A:HIS:H	2	3.72
(6,302)	1:73:A:PHE:HD2	1:74:A:HIS:H	2	3.72
(6,357)	1:86:A:LEU:HD11	1:85:A:ARG:H	1	3.7
(6,357)	1:86:A:LEU:HD12	1:85:A:ARG:H	1	3.7
(6,357)	1:86:A:LEU:HD13	1:85:A:ARG:H	1	3.7
(2,46)	1:33:A:PHE:HE1	1:116:A:LEU:H	1	3.69
(2,46)	1:33:A:PHE:HE2	1:116:A:LEU:H	1	3.69
(7,111)	1:30:A:THR:HG21	1:30:A:THR:H	1	3.68
(7,111)	1:30:A:THR:HG22	1:30:A:THR:H	1	3.68
(7,111)	1:30:A:THR:HG23	1:30:A:THR:H	1	3.68
(7,352)	1:101:A:VAL:HG21	1:101:A:VAL:H	1	3.66
(7,352)	1:101:A:VAL:HG22	1:101:A:VAL:H	1	3.66
(7,352)	1:101:A:VAL:HG23	1:101:A:VAL:H	1	3.66
(6,445)	1:106:A:GLN:HB2	1:107:A:SER:H	2	3.66
(6,445)	1:106:A:GLN:HB3	1:107:A:SER:H	2	3.66
(6,415)	1:100:A:PRO:HG2	1:99:A:CYS:H	1	3.66
(6,358)	1:86:A:LEU:HD21	1:85:A:ARG:H	1	3.66
(6,358)	1:86:A:LEU:HD22	1:85:A:ARG:H	1	3.66
(6,358)	1:86:A:LEU:HD23	1:85:A:ARG:H	1	3.66
(6,339)	1:82:A:PHE:HD1	1:83:A:LEU:H	2	3.65
(6,339)	1:82:A:PHE:HD2	1:83:A:LEU:H	2	3.65
(2,40)	1:45:A:PHE:HD1	1:94:A:ALA:H	1	3.65
(2,40)	1:45:A:PHE:HD2	1:94:A:ALA:H	1	3.65
(4,293)	1:108:A:THR:HG21	1:111:A:ASN:HD21	1	3.64
(4,293)	1:108:A:THR:HG21	1:111:A:ASN:HD22	1	3.64
(4,293)	1:108:A:THR:HG22	1:111:A:ASN:HD21	1	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,293)	1:108:A:THR:HG22	1:111:A:ASN:HD22	1	3.64
(4,293)	1:108:A:THR:HG23	1:111:A:ASN:HD21	1	3.64
(4,293)	1:108:A:THR:HG23	1:111:A:ASN:HD22	1	3.64
(4,159)	1:55:A:PHE:HE1	1:57:A:SER:H	1	3.64
(4,159)	1:55:A:PHE:HE2	1:57:A:SER:H	1	3.64
(6,27)	1:8:A:GLN:HB3	1:9:A:GLU:H	1	3.63
(2,24)	1:96:A:LEU:HD11	1:45:A:PHE:H	1	3.63
(2,24)	1:96:A:LEU:HD12	1:45:A:PHE:H	1	3.63
(2,24)	1:96:A:LEU:HD13	1:45:A:PHE:H	1	3.63
(2,24)	1:96:A:LEU:HD21	1:45:A:PHE:H	1	3.63
(2,24)	1:96:A:LEU:HD22	1:45:A:PHE:H	1	3.63
(2,24)	1:96:A:LEU:HD23	1:45:A:PHE:H	1	3.63
(7,365)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	1	3.62
(7,365)	1:105:A:ASN:HB3	1:105:A:ASN:HD22	1	3.62
(6,335)	1:82:A:PHE:HD1	1:81:A:ARG:H	2	3.62
(6,335)	1:82:A:PHE:HD2	1:81:A:ARG:H	2	3.62
(7,369)	1:106:A:GLN:HA	1:106:A:GLN:HE21	1	3.61
(7,369)	1:106:A:GLN:HA	1:106:A:GLN:HE22	1	3.61
(7,108)	1:29:A:VAL:HG21	1:29:A:VAL:H	1	3.61
(7,108)	1:29:A:VAL:HG22	1:29:A:VAL:H	1	3.61
(7,108)	1:29:A:VAL:HG23	1:29:A:VAL:H	1	3.61
(7,232)	1:69:A:THR:HG21	1:69:A:THR:H	1	3.6
(7,232)	1:69:A:THR:HG22	1:69:A:THR:H	1	3.6
(7,232)	1:69:A:THR:HG23	1:69:A:THR:H	1	3.6
(6,461)	1:109:A:LEU:HD21	1:110:A:GLU:H	2	3.59
(6,461)	1:109:A:LEU:HD22	1:110:A:GLU:H	2	3.59
(6,461)	1:109:A:LEU:HD23	1:110:A:GLU:H	2	3.59
(7,371)	1:106:A:GLN:HG2	1:106:A:GLN:H	2	3.58
(7,371)	1:106:A:GLN:HG3	1:106:A:GLN:H	2	3.58
(6,478)	1:112:A:PHE:HD1	1:113:A:LEU:H	1	3.58
(6,478)	1:112:A:PHE:HD2	1:113:A:LEU:H	1	3.58
(6,431)	1:103:A:GLU:HB2	1:104:A:ALA:H	2	3.58
(6,431)	1:103:A:GLU:HB3	1:104:A:ALA:H	2	3.58
(7,107)	1:29:A:VAL:HG11	1:29:A:VAL:H	2	3.56
(7,107)	1:29:A:VAL:HG12	1:29:A:VAL:H	2	3.56
(7,107)	1:29:A:VAL:HG13	1:29:A:VAL:H	2	3.56
(6,478)	1:112:A:PHE:HD1	1:113:A:LEU:H	2	3.56
(6,478)	1:112:A:PHE:HD2	1:113:A:LEU:H	2	3.56
(6,302)	1:73:A:PHE:HD1	1:74:A:HIS:H	1	3.56
(6,302)	1:73:A:PHE:HD2	1:74:A:HIS:H	1	3.56
(6,287)	1:70:A:ALA:H	1:71:A:GLN:H	2	3.56
(6,232)	1:56:A:TYR:HD1	1:55:A:PHE:H	1	3.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,232)	1:56:A:TYR:HD2	1:55:A:PHE:H	1	3.56
(7,191)	1:56:A:TYR:HE1	1:56:A:TYR:H	2	3.54
(7,191)	1:56:A:TYR:HE2	1:56:A:TYR:H	2	3.54
(6,499)	1:118:A:THR:HG21	1:119:A:ILE:H	2	3.54
(6,499)	1:118:A:THR:HG22	1:119:A:ILE:H	2	3.54
(6,499)	1:118:A:THR:HG23	1:119:A:ILE:H	2	3.54
(7,359)	1:103:A:GLU:HG2	1:103:A:GLU:H	2	3.53
(7,359)	1:103:A:GLU:HG3	1:103:A:GLU:H	2	3.53
(2,34)	1:69:A:THR:HG21	1:75:A:ARG:H	2	3.53
(2,34)	1:69:A:THR:HG22	1:75:A:ARG:H	2	3.53
(2,34)	1:69:A:THR:HG23	1:75:A:ARG:H	2	3.53
(4,135)	1:48:A:ALA:H	1:45:A:PHE:HE1	1	3.52
(4,135)	1:48:A:ALA:H	1:45:A:PHE:HE2	1	3.52
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD11	2	3.5
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD12	2	3.5
(2,17)	1:124:A:TYR:H	1:11:A:ILE:HD13	2	3.5
(2,40)	1:45:A:PHE:HD1	1:94:A:ALA:H	2	3.49
(2,40)	1:45:A:PHE:HD2	1:94:A:ALA:H	2	3.49
(6,440)	1:106:A:GLN:HE21	1:105:A:ASN:H	1	3.48
(6,440)	1:106:A:GLN:HE22	1:105:A:ASN:H	1	3.48
(4,177)	1:58:A:HIS:HA	1:60:A:GLU:H	2	3.48
(4,149)	1:50:A:THR:H	1:52:A:LEU:H	2	3.48
(6,201)	1:46:A:CYS:H	1:45:A:PHE:HD1	2	3.47
(6,201)	1:46:A:CYS:H	1:45:A:PHE:HD2	2	3.47
(6,115)	1:27:A:LEU:HG	1:28:A:THR:H	2	3.47
(4,184)	1:66:A:LEU:HD11	1:63:A:THR:H	2	3.46
(4,184)	1:66:A:LEU:HD12	1:63:A:THR:H	2	3.46
(4,184)	1:66:A:LEU:HD13	1:63:A:THR:H	2	3.46
(4,184)	1:66:A:LEU:HD21	1:63:A:THR:H	2	3.46
(4,184)	1:66:A:LEU:HD22	1:63:A:THR:H	2	3.46
(4,184)	1:66:A:LEU:HD23	1:63:A:THR:H	2	3.46
(7,232)	1:69:A:THR:HG21	1:69:A:THR:H	2	3.45
(7,232)	1:69:A:THR:HG22	1:69:A:THR:H	2	3.45
(7,232)	1:69:A:THR:HG23	1:69:A:THR:H	2	3.45
(6,31)	1:10:A:ILE:H	1:9:A:GLU:HB2	2	3.45
(6,31)	1:10:A:ILE:H	1:9:A:GLU:HB3	2	3.45
(4,276)	1:93:A:LEU:HA	1:96:A:LEU:H	1	3.45
(6,384)	1:91:A:TRP:HE3	1:92:A:GLY:H	2	3.44
(6,115)	1:27:A:LEU:HG	1:28:A:THR:H	1	3.44
(7,191)	1:56:A:TYR:HE1	1:56:A:TYR:H	1	3.43
(7,191)	1:56:A:TYR:HE2	1:56:A:TYR:H	1	3.43
(7,351)	1:101:A:VAL:HG11	1:101:A:VAL:H	2	3.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,351)	1:101:A:VAL:HG12	1:101:A:VAL:H	2	3.42
(7,351)	1:101:A:VAL:HG13	1:101:A:VAL:H	2	3.42
(7,139)	1:38:A:ASN:HB2	1:38:A:ASN:HD21	1	3.42
(7,139)	1:38:A:ASN:HB2	1:38:A:ASN:HD22	1	3.42
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD11	1	3.42
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD12	1	3.42
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD13	1	3.42
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD21	1	3.42
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD22	1	3.42
(4,186)	1:64:A:ARG:H	1:66:A:LEU:HD23	1	3.42
(2,38)	1:56:A:TYR:HE1	1:87:A:ASP:H	2	3.42
(2,38)	1:56:A:TYR:HE2	1:87:A:ASP:H	2	3.42
(6,143)	1:32:A:ILE:HD11	1:33:A:PHE:H	1	3.41
(6,143)	1:32:A:ILE:HD12	1:33:A:PHE:H	1	3.41
(6,143)	1:32:A:ILE:HD13	1:33:A:PHE:H	1	3.41
(2,37)	1:56:A:TYR:HD1	1:84:A:LYS:H	1	3.41
(2,37)	1:56:A:TYR:HD2	1:84:A:LYS:H	1	3.41
(6,201)	1:46:A:CYS:H	1:45:A:PHE:HD1	1	3.4
(6,201)	1:46:A:CYS:H	1:45:A:PHE:HD2	1	3.4
(6,452)	1:107:A:SER:H	1:108:A:THR:H	2	3.39
(6,287)	1:70:A:ALA:H	1:71:A:GLN:H	1	3.39
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG21	2	3.39
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG22	2	3.39
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG23	2	3.39
(4,149)	1:50:A:THR:H	1:52:A:LEU:H	1	3.39
(7,138)	1:38:A:ASN:HB3	1:38:A:ASN:HD21	1	3.38
(7,138)	1:38:A:ASN:HB3	1:38:A:ASN:HD22	1	3.38
(4,283)	1:101:A:VAL:HG11	1:103:A:GLU:H	2	3.36
(4,283)	1:101:A:VAL:HG12	1:103:A:GLU:H	2	3.36
(4,283)	1:101:A:VAL:HG13	1:103:A:GLU:H	2	3.36
(4,283)	1:101:A:VAL:HG21	1:103:A:GLU:H	2	3.36
(4,283)	1:101:A:VAL:HG22	1:103:A:GLU:H	2	3.36
(4,283)	1:101:A:VAL:HG23	1:103:A:GLU:H	2	3.36
(6,445)	1:106:A:GLN:HB2	1:107:A:SER:H	1	3.35
(6,445)	1:106:A:GLN:HB3	1:107:A:SER:H	1	3.35
(6,152)	1:33:A:PHE:HD1	1:34:A:ALA:H	2	3.35
(6,152)	1:33:A:PHE:HD2	1:34:A:ALA:H	2	3.35
(2,44)	1:28:A:THR:HG21	1:108:A:THR:H	1	3.35
(2,44)	1:28:A:THR:HG22	1:108:A:THR:H	1	3.35
(2,44)	1:28:A:THR:HG23	1:108:A:THR:H	1	3.35
(6,283)	1:69:A:THR:HG21	1:70:A:ALA:H	2	3.34
(6,283)	1:69:A:THR:HG22	1:70:A:ALA:H	2	3.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,283)	1:69:A:THR:HG23	1:70:A:ALA:H	2	3.34
(2,23)	1:96:A:LEU:HD11	1:44:A:THR:H	1	3.34
(2,23)	1:96:A:LEU:HD12	1:44:A:THR:H	1	3.34
(2,23)	1:96:A:LEU:HD13	1:44:A:THR:H	1	3.34
(2,23)	1:96:A:LEU:HD21	1:44:A:THR:H	1	3.34
(2,23)	1:96:A:LEU:HD22	1:44:A:THR:H	1	3.34
(2,23)	1:96:A:LEU:HD23	1:44:A:THR:H	1	3.34
(6,453)	1:108:A:THR:HG21	1:109:A:LEU:H	2	3.33
(6,453)	1:108:A:THR:HG22	1:109:A:LEU:H	2	3.33
(6,453)	1:108:A:THR:HG23	1:109:A:LEU:H	2	3.33
(7,270)	1:80:A:ILE:HG21	1:80:A:ILE:H	1	3.3
(7,270)	1:80:A:ILE:HG22	1:80:A:ILE:H	1	3.3
(7,270)	1:80:A:ILE:HG23	1:80:A:ILE:H	1	3.3
(6,327)	1:80:A:ILE:HG21	1:79:A:LEU:H	1	3.29
(6,327)	1:80:A:ILE:HG22	1:79:A:LEU:H	1	3.29
(6,327)	1:80:A:ILE:HG23	1:79:A:LEU:H	1	3.29
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG21	2	3.29
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG22	2	3.29
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG23	2	3.29
(6,526)	1:124:A:TYR:HB3	1:125:A:SER:H	1	3.28
(6,98)	1:22:A:THR:H	1:23:A:LEU:H	2	3.27
(4,184)	1:66:A:LEU:HD11	1:63:A:THR:H	1	3.27
(4,184)	1:66:A:LEU:HD12	1:63:A:THR:H	1	3.27
(4,184)	1:66:A:LEU:HD13	1:63:A:THR:H	1	3.27
(4,184)	1:66:A:LEU:HD21	1:63:A:THR:H	1	3.27
(4,184)	1:66:A:LEU:HD22	1:63:A:THR:H	1	3.27
(4,184)	1:66:A:LEU:HD23	1:63:A:THR:H	1	3.27
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG21	1	3.26
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG22	1	3.26
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG23	1	3.26
(4,292)	1:108:A:THR:HG21	1:111:A:ASN:H	1	3.26
(4,292)	1:108:A:THR:HG22	1:111:A:ASN:H	1	3.26
(4,292)	1:108:A:THR:HG23	1:111:A:ASN:H	1	3.26
(7,370)	1:106:A:GLN:HB2	1:106:A:GLN:H	1	3.25
(7,370)	1:106:A:GLN:HB3	1:106:A:GLN:H	1	3.25
(7,389)	1:111:A:ASN:HA	1:111:A:ASN:HD21	1	3.24
(7,389)	1:111:A:ASN:HA	1:111:A:ASN:HD22	1	3.24
(6,28)	1:8:A:GLN:HB2	1:9:A:GLU:H	2	3.24
(4,270)	1:91:A:TRP:HE3	1:93:A:LEU:H	1	3.24
(6,132)	1:31:A:ASP:HB3	1:32:A:ILE:H	2	3.23
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD11	1	3.23
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD12	1	3.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD13	1	3.23
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD21	1	3.23
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD22	1	3.23
(4,3)	1:4:A:ASP:H	1:7:A:LEU:HD23	1	3.23
(6,483)	1:113:A:LEU:HG	1:114:A:GLU:H	2	3.22
(6,461)	1:109:A:LEU:HD21	1:110:A:GLU:H	1	3.22
(6,461)	1:109:A:LEU:HD22	1:110:A:GLU:H	1	3.22
(6,461)	1:109:A:LEU:HD23	1:110:A:GLU:H	1	3.22
(6,403)	1:96:A:LEU:HD11	1:95:A:GLY:H	1	3.22
(6,403)	1:96:A:LEU:HD12	1:95:A:GLY:H	1	3.22
(6,403)	1:96:A:LEU:HD13	1:95:A:GLY:H	1	3.22
(6,403)	1:96:A:LEU:HD21	1:95:A:GLY:H	1	3.22
(6,403)	1:96:A:LEU:HD22	1:95:A:GLY:H	1	3.22
(6,403)	1:96:A:LEU:HD23	1:95:A:GLY:H	1	3.22
(7,370)	1:106:A:GLN:HB2	1:106:A:GLN:H	2	3.21
(7,370)	1:106:A:GLN:HB3	1:106:A:GLN:H	2	3.21
(6,483)	1:113:A:LEU:HG	1:114:A:GLU:H	1	3.21
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD21	1	3.2
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD22	1	3.2
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD23	1	3.2
(7,411)	1:118:A:THR:HG21	1:118:A:THR:H	2	3.19
(7,411)	1:118:A:THR:HG22	1:118:A:THR:H	2	3.19
(7,411)	1:118:A:THR:HG23	1:118:A:THR:H	2	3.19
(6,330)	1:80:A:ILE:HG12	1:81:A:ARG:H	1	3.19
(6,330)	1:80:A:ILE:HG13	1:81:A:ARG:H	1	3.19
(2,28)	1:29:A:VAL:HG11	1:55:A:PHE:H	2	3.19
(2,28)	1:29:A:VAL:HG12	1:55:A:PHE:H	2	3.19
(2,28)	1:29:A:VAL:HG13	1:55:A:PHE:H	2	3.19
(6,288)	1:71:A:GLN:HB3	1:72:A:GLN:H	1	3.18
(4,80)	1:28:A:THR:HB	1:30:A:THR:H	1	3.18
(2,13)	1:30:A:THR:HG21	1:103:A:GLU:H	2	3.18
(2,13)	1:30:A:THR:HG22	1:103:A:GLU:H	2	3.18
(2,13)	1:30:A:THR:HG23	1:103:A:GLU:H	2	3.18
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD21	1	3.16
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD22	1	3.16
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD23	1	3.16
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD11	1	3.16
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD12	1	3.16
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD13	1	3.16
(7,351)	1:101:A:VAL:HG11	1:101:A:VAL:H	1	3.15
(7,351)	1:101:A:VAL:HG12	1:101:A:VAL:H	1	3.15
(7,351)	1:101:A:VAL:HG13	1:101:A:VAL:H	1	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,168)	1:39:A:THR:HG1	1:38:A:ASN:H	2	3.15
(6,25)	1:7:A:LEU:HD11	1:8:A:GLN:H	1	3.15
(6,25)	1:7:A:LEU:HD12	1:8:A:GLN:H	1	3.15
(6,25)	1:7:A:LEU:HD13	1:8:A:GLN:H	1	3.15
(6,25)	1:7:A:LEU:HD21	1:8:A:GLN:H	1	3.15
(6,25)	1:7:A:LEU:HD22	1:8:A:GLN:H	1	3.15
(6,25)	1:7:A:LEU:HD23	1:8:A:GLN:H	1	3.15
(6,24)	1:7:A:LEU:HD11	1:8:A:GLN:H	1	3.15
(6,24)	1:7:A:LEU:HD12	1:8:A:GLN:H	1	3.15
(6,24)	1:7:A:LEU:HD13	1:8:A:GLN:H	1	3.15
(6,24)	1:7:A:LEU:HD21	1:8:A:GLN:H	1	3.15
(6,24)	1:7:A:LEU:HD22	1:8:A:GLN:H	1	3.15
(6,24)	1:7:A:LEU:HD23	1:8:A:GLN:H	1	3.15
(4,314)	1:112:A:PHE:HD1	1:115:A:ARG:H	2	3.15
(4,314)	1:112:A:PHE:HD2	1:115:A:ARG:H	2	3.15
(7,431)	1:124:A:TYR:HD1	1:124:A:TYR:H	1	3.14
(7,431)	1:124:A:TYR:HD2	1:124:A:TYR:H	1	3.14
(7,366)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	1	3.14
(7,366)	1:105:A:ASN:HB2	1:105:A:ASN:HD22	1	3.14
(6,292)	1:72:A:GLN:HG2	1:71:A:GLN:H	2	3.13
(6,292)	1:72:A:GLN:HG3	1:71:A:GLN:H	2	3.13
(6,88)	1:20:A:GLN:HE21	1:19:A:GLU:HB2	2	3.12
(6,88)	1:20:A:GLN:HE21	1:19:A:GLU:HB3	2	3.12
(6,88)	1:20:A:GLN:HE22	1:19:A:GLU:HB2	2	3.12
(6,88)	1:20:A:GLN:HE22	1:19:A:GLU:HB3	2	3.12
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD21	2	3.11
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD22	2	3.11
(7,67)	1:17:A:LEU:H	1:17:A:LEU:HD23	2	3.11
(6,414)	1:100:A:PRO:HG3	1:99:A:CYS:H	1	3.11
(2,13)	1:30:A:THR:HG21	1:103:A:GLU:H	1	3.11
(2,13)	1:30:A:THR:HG22	1:103:A:GLU:H	1	3.11
(2,13)	1:30:A:THR:HG23	1:103:A:GLU:H	1	3.11
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD11	2	3.1
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD12	2	3.1
(7,12)	1:5:A:ILE:H	1:5:A:ILE:HD13	2	3.1
(7,368)	1:106:A:GLN:HA	1:106:A:GLN:H	2	3.09
(7,124)	1:33:A:PHE:HD1	1:33:A:PHE:H	2	3.09
(7,124)	1:33:A:PHE:HD2	1:33:A:PHE:H	2	3.09
(4,271)	1:92:A:GLY:HA3	1:95:A:GLY:H	1	3.09
(7,51)	1:15:A:ASN:H	1:15:A:ASN:HD21	1	3.08
(4,299)	1:108:A:THR:H	1:111:A:ASN:HD21	2	3.08
(4,299)	1:108:A:THR:H	1:111:A:ASN:HD22	2	3.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,55)	1:16:A:SER:HB2	1:19:A:GLU:H	1	3.08
(4,55)	1:16:A:SER:HB3	1:19:A:GLU:H	1	3.08
(7,368)	1:106:A:GLN:HA	1:106:A:GLN:H	1	3.06
(6,417)	1:100:A:PRO:HD3	1:99:A:CYS:H	2	3.06
(7,296)	1:86:A:LEU:HD21	1:86:A:LEU:H	2	3.05
(7,296)	1:86:A:LEU:HD22	1:86:A:LEU:H	2	3.05
(7,296)	1:86:A:LEU:HD23	1:86:A:LEU:H	2	3.05
(6,185)	1:43:A:GLU:HG2	1:42:A:LYS:H	1	3.04
(6,185)	1:43:A:GLU:HG3	1:42:A:LYS:H	1	3.04
(4,270)	1:91:A:TRP:HE3	1:93:A:LEU:H	2	3.03
(7,366)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	2	3.02
(7,366)	1:105:A:ASN:HB2	1:105:A:ASN:HD22	2	3.02
(7,295)	1:86:A:LEU:HD11	1:86:A:LEU:H	2	3.02
(7,295)	1:86:A:LEU:HD12	1:86:A:LEU:H	2	3.02
(7,295)	1:86:A:LEU:HD13	1:86:A:LEU:H	2	3.02
(7,226)	1:66:A:LEU:HD11	1:66:A:LEU:H	1	3.01
(7,226)	1:66:A:LEU:HD12	1:66:A:LEU:H	1	3.01
(7,226)	1:66:A:LEU:HD13	1:66:A:LEU:H	1	3.01
(7,226)	1:66:A:LEU:HD21	1:66:A:LEU:H	1	3.01
(7,226)	1:66:A:LEU:HD22	1:66:A:LEU:H	1	3.01
(7,226)	1:66:A:LEU:HD23	1:66:A:LEU:H	1	3.01
(6,233)	1:55:A:PHE:HD1	1:56:A:TYR:H	1	3.01
(6,233)	1:55:A:PHE:HD2	1:56:A:TYR:H	1	3.01
(4,314)	1:112:A:PHE:HD1	1:115:A:ARG:H	1	3.01
(4,314)	1:112:A:PHE:HD2	1:115:A:ARG:H	1	3.01
(6,440)	1:106:A:GLN:HE21	1:105:A:ASN:H	2	2.99
(6,440)	1:106:A:GLN:HE22	1:105:A:ASN:H	2	2.99
(6,425)	1:102:A:LYS:HB3	1:103:A:GLU:H	1	2.99
(6,140)	1:32:A:ILE:HG13	1:33:A:PHE:H	1	2.99
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD21	2	2.99
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD22	2	2.99
(6,107)	1:24:A:CYS:H	1:23:A:LEU:HD23	2	2.99
(2,41)	1:30:A:THR:HA	1:105:A:ASN:H	2	2.99
(6,283)	1:69:A:THR:HG21	1:70:A:ALA:H	1	2.98
(6,283)	1:69:A:THR:HG22	1:70:A:ALA:H	1	2.98
(6,283)	1:69:A:THR:HG23	1:70:A:ALA:H	1	2.98
(7,125)	1:33:A:PHE:HE1	1:33:A:PHE:H	2	2.97
(7,125)	1:33:A:PHE:HE2	1:33:A:PHE:H	2	2.97
(6,449)	1:107:A:SER:HB2	1:108:A:THR:H	2	2.97
(6,449)	1:107:A:SER:HB3	1:108:A:THR:H	2	2.97
(2,12)	1:30:A:THR:HG21	1:104:A:ALA:H	2	2.97
(2,12)	1:30:A:THR:HG22	1:104:A:ALA:H	2	2.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:30:A:THR:HG23	1:104:A:ALA:H	2	2.97
(7,354)	1:102:A:LYS:HB3	1:102:A:LYS:H	2	2.96
(7,140)	1:38:A:ASN:HD21	1:38:A:ASN:H	2	2.96
(7,140)	1:38:A:ASN:HD22	1:38:A:ASN:H	2	2.96
(4,285)	1:103:A:GLU:HB2	1:105:A:ASN:H	1	2.96
(4,285)	1:103:A:GLU:HB3	1:105:A:ASN:H	1	2.96
(4,96)	1:34:A:ALA:HA	1:36:A:SER:H	1	2.96
(7,389)	1:111:A:ASN:HA	1:111:A:ASN:HD21	2	2.95
(7,389)	1:111:A:ASN:HA	1:111:A:ASN:HD22	2	2.95
(6,93)	1:20:A:GLN:HG2	1:21:A:LYS:H	2	2.95
(6,93)	1:20:A:GLN:HG3	1:21:A:LYS:H	2	2.95
(6,446)	1:106:A:GLN:HG2	1:107:A:SER:H	2	2.94
(6,446)	1:106:A:GLN:HG3	1:107:A:SER:H	2	2.94
(4,281)	1:96:A:LEU:HD11	1:99:A:CYS:H	2	2.94
(4,281)	1:96:A:LEU:HD12	1:99:A:CYS:H	2	2.94
(4,281)	1:96:A:LEU:HD13	1:99:A:CYS:H	2	2.94
(4,281)	1:96:A:LEU:HD21	1:99:A:CYS:H	2	2.94
(4,281)	1:96:A:LEU:HD22	1:99:A:CYS:H	2	2.94
(4,281)	1:96:A:LEU:HD23	1:99:A:CYS:H	2	2.94
(4,158)	1:55:A:PHE:HE1	1:59:A:HIS:HD2	1	2.94
(4,158)	1:55:A:PHE:HE2	1:59:A:HIS:HD2	1	2.94
(7,124)	1:33:A:PHE:HD1	1:33:A:PHE:H	1	2.93
(7,124)	1:33:A:PHE:HD2	1:33:A:PHE:H	1	2.93
(3,86)	1:30:A:THR:N	1:106:A:GLN:O	2	2.92
(7,396)	1:112:A:PHE:HD1	1:112:A:PHE:H	2	2.91
(7,396)	1:112:A:PHE:HD2	1:112:A:PHE:H	2	2.91
(6,450)	1:107:A:SER:HB2	1:108:A:THR:H	2	2.91
(7,371)	1:106:A:GLN:HG2	1:106:A:GLN:H	1	2.9
(7,371)	1:106:A:GLN:HG3	1:106:A:GLN:H	1	2.9
(6,256)	1:61:A:LYS:H	1:62:A:ASP:H	2	2.89
(6,72)	1:17:A:LEU:HG	1:16:A:SER:H	2	2.89
(4,351)	1:125:A:SER:HA	1:127:A:CYS:H	2	2.89
(6,126)	1:29:A:VAL:HG11	1:30:A:THR:H	1	2.88
(6,126)	1:29:A:VAL:HG12	1:30:A:THR:H	1	2.88
(6,126)	1:29:A:VAL:HG13	1:30:A:THR:H	1	2.88
(4,351)	1:125:A:SER:HA	1:127:A:CYS:H	1	2.88
(7,125)	1:33:A:PHE:HE1	1:33:A:PHE:H	1	2.87
(7,125)	1:33:A:PHE:HE2	1:33:A:PHE:H	1	2.87
(6,416)	1:99:A:CYS:HA	1:100:A:PRO:HD2	1	2.87
(6,416)	1:99:A:CYS:HA	1:100:A:PRO:HD3	1	2.87
(6,288)	1:71:A:GLN:HB3	1:72:A:GLN:H	2	2.87
(6,279)	1:69:A:THR:HG21	1:68:A:ALA:H	1	2.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,279)	1:69:A:THR:HG22	1:68:A:ALA:H	1	2.87
(6,279)	1:69:A:THR:HG23	1:68:A:ALA:H	1	2.87
(6,262)	1:63:A:THR:HG21	1:64:A:ARG:H	1	2.87
(6,262)	1:63:A:THR:HG22	1:64:A:ARG:H	1	2.87
(6,262)	1:63:A:THR:HG23	1:64:A:ARG:H	1	2.87
(6,62)	1:16:A:SER:H	1:15:A:ASN:HD21	1	2.86
(6,62)	1:16:A:SER:H	1:15:A:ASN:HD22	1	2.86
(6,61)	1:16:A:SER:H	1:15:A:ASN:HD21	1	2.86
(6,61)	1:16:A:SER:H	1:15:A:ASN:HD22	1	2.86
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD11	2	2.85
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD12	2	2.85
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD13	2	2.85
(6,432)	1:103:A:GLU:HG2	1:104:A:ALA:H	1	2.85
(6,432)	1:103:A:GLU:HG3	1:104:A:ALA:H	1	2.85
(2,39)	1:56:A:TYR:HE1	1:88:A:ARG:H	1	2.85
(2,39)	1:56:A:TYR:HE2	1:88:A:ARG:H	1	2.85
(2,33)	1:23:A:LEU:HD11	1:72:A:GLN:HE22	1	2.85
(2,33)	1:23:A:LEU:HD12	1:72:A:GLN:HE22	1	2.85
(2,33)	1:23:A:LEU:HD13	1:72:A:GLN:HE22	1	2.85
(2,33)	1:23:A:LEU:HD21	1:72:A:GLN:HE22	1	2.85
(2,33)	1:23:A:LEU:HD22	1:72:A:GLN:HE22	1	2.85
(2,33)	1:23:A:LEU:HD23	1:72:A:GLN:HE22	1	2.85
(7,404)	1:115:A:ARG:H	1:115:A:ARG:HE	2	2.84
(7,396)	1:112:A:PHE:HD1	1:112:A:PHE:H	1	2.84
(7,396)	1:112:A:PHE:HD2	1:112:A:PHE:H	1	2.84
(6,375)	1:89:A:ASN:HB2	1:90:A:LEU:H	2	2.84
(6,72)	1:17:A:LEU:HG	1:16:A:SER:H	1	2.84
(7,248)	1:73:A:PHE:HD1	1:73:A:PHE:H	1	2.83
(7,248)	1:73:A:PHE:HD2	1:73:A:PHE:H	1	2.83
(7,248)	1:73:A:PHE:HD1	1:73:A:PHE:H	2	2.83
(7,248)	1:73:A:PHE:HD2	1:73:A:PHE:H	2	2.83
(6,443)	1:105:A:ASN:H	1:106:A:GLN:H	2	2.83
(7,277)	1:82:A:PHE:HD1	1:82:A:PHE:H	1	2.82
(7,277)	1:82:A:PHE:HD2	1:82:A:PHE:H	1	2.82
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD11	1	2.82
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD12	1	2.82
(7,66)	1:17:A:LEU:H	1:17:A:LEU:HD13	1	2.82
(6,154)	1:34:A:ALA:HB1	1:35:A:ALA:H	2	2.82
(6,154)	1:34:A:ALA:HB2	1:35:A:ALA:H	2	2.82
(6,154)	1:34:A:ALA:HB3	1:35:A:ALA:H	2	2.82
(4,283)	1:101:A:VAL:HG11	1:103:A:GLU:H	1	2.82
(4,283)	1:101:A:VAL:HG12	1:103:A:GLU:H	1	2.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,283)	1:101:A:VAL:HG13	1:103:A:GLU:H	1	2.82
(4,283)	1:101:A:VAL:HG21	1:103:A:GLU:H	1	2.82
(4,283)	1:101:A:VAL:HG22	1:103:A:GLU:H	1	2.82
(4,283)	1:101:A:VAL:HG23	1:103:A:GLU:H	1	2.82
(2,32)	1:23:A:LEU:HD11	1:72:A:GLN:HE21	1	2.8
(2,32)	1:23:A:LEU:HD12	1:72:A:GLN:HE21	1	2.8
(2,32)	1:23:A:LEU:HD13	1:72:A:GLN:HE21	1	2.8
(2,32)	1:23:A:LEU:HD21	1:72:A:GLN:HE21	1	2.8
(2,32)	1:23:A:LEU:HD22	1:72:A:GLN:HE21	1	2.8
(2,32)	1:23:A:LEU:HD23	1:72:A:GLN:HE21	1	2.8
(6,460)	1:109:A:LEU:HD11	1:110:A:GLU:H	2	2.79
(6,460)	1:109:A:LEU:HD12	1:110:A:GLU:H	2	2.79
(6,460)	1:109:A:LEU:HD13	1:110:A:GLU:H	2	2.79
(2,44)	1:28:A:THR:HG1	1:108:A:THR:H	2	2.79
(7,347)	1:99:A:CYS:HB3	1:99:A:CYS:H	2	2.78
(6,505)	1:119:A:ILE:HG21	1:120:A:MET:H	1	2.78
(6,292)	1:72:A:GLN:HG2	1:71:A:GLN:H	1	2.78
(6,292)	1:72:A:GLN:HG3	1:71:A:GLN:H	1	2.78
(7,104)	1:28:A:THR:HG21	1:28:A:THR:H	1	2.77
(7,104)	1:28:A:THR:HG22	1:28:A:THR:H	1	2.77
(7,104)	1:28:A:THR:HG23	1:28:A:THR:H	1	2.77
(2,29)	1:29:A:VAL:HG21	1:55:A:PHE:H	1	2.77
(2,29)	1:29:A:VAL:HG22	1:55:A:PHE:H	1	2.77
(2,29)	1:29:A:VAL:HG23	1:55:A:PHE:H	1	2.77
(7,138)	1:38:A:ASN:HB3	1:38:A:ASN:HD21	2	2.76
(7,138)	1:38:A:ASN:HB3	1:38:A:ASN:HD22	2	2.76
(6,404)	1:96:A:LEU:HB2	1:97:A:ASN:H	2	2.76
(6,404)	1:96:A:LEU:HB3	1:97:A:ASN:H	2	2.76
(6,279)	1:69:A:THR:HG21	1:68:A:ALA:H	2	2.76
(6,279)	1:69:A:THR:HG22	1:68:A:ALA:H	2	2.76
(6,279)	1:69:A:THR:HG23	1:68:A:ALA:H	2	2.76
(6,439)	1:106:A:GLN:HG2	1:105:A:ASN:H	1	2.75
(6,439)	1:106:A:GLN:HG3	1:105:A:ASN:H	1	2.75
(6,379)	1:90:A:LEU:HA	1:91:A:TRP:H	2	2.75
(6,246)	1:58:A:HIS:HB2	1:59:A:HIS:H	1	2.75
(6,246)	1:58:A:HIS:HB3	1:59:A:HIS:H	1	2.75
(4,296)	1:108:A:THR:HB	1:111:A:ASN:H	1	2.75
(2,39)	1:56:A:TYR:HE1	1:88:A:ARG:H	2	2.75
(2,39)	1:56:A:TYR:HE2	1:88:A:ARG:H	2	2.75
(7,325)	1:91:A:TRP:HB2	1:91:A:TRP:H	2	2.74
(7,325)	1:91:A:TRP:HB3	1:91:A:TRP:H	2	2.74
(7,104)	1:28:A:THR:HG21	1:28:A:THR:H	2	2.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,104)	1:28:A:THR:HG22	1:28:A:THR:H	2	2.74
(7,104)	1:28:A:THR:HG23	1:28:A:THR:H	2	2.74
(6,402)	1:96:A:LEU:HB2	1:95:A:GLY:H	2	2.74
(6,402)	1:96:A:LEU:HB3	1:95:A:GLY:H	2	2.74
(4,234)	1:82:A:PHE:HD1	1:79:A:LEU:H	2	2.74
(4,234)	1:82:A:PHE:HD2	1:79:A:LEU:H	2	2.74
(6,526)	1:124:A:TYR:HB3	1:125:A:SER:H	2	2.73
(7,447)	1:129:A:SER:HB2	1:129:A:SER:H	1	2.72
(7,447)	1:129:A:SER:HB3	1:129:A:SER:H	1	2.72
(6,385)	1:91:A:TRP:HB2	1:92:A:GLY:H	2	2.72
(6,385)	1:91:A:TRP:HB3	1:92:A:GLY:H	2	2.72
(4,352)	1:125:A:SER:HA	1:128:A:SER:H	2	2.72
(2,28)	1:29:A:VAL:HG11	1:55:A:PHE:H	1	2.72
(2,28)	1:29:A:VAL:HG12	1:55:A:PHE:H	1	2.72
(2,28)	1:29:A:VAL:HG13	1:55:A:PHE:H	1	2.72
(7,414)	1:119:A:ILE:HG13	1:119:A:ILE:H	2	2.71
(7,325)	1:91:A:TRP:HB2	1:91:A:TRP:H	1	2.71
(7,325)	1:91:A:TRP:HB3	1:91:A:TRP:H	1	2.71
(7,107)	1:29:A:VAL:HG11	1:29:A:VAL:H	1	2.71
(7,107)	1:29:A:VAL:HG12	1:29:A:VAL:H	1	2.71
(7,107)	1:29:A:VAL:HG13	1:29:A:VAL:H	1	2.71
(6,6)	1:5:A:ILE:H	1:4:A:ASP:HB3	2	2.71
(7,443)	1:128:A:SER:HA	1:128:A:SER:H	2	2.7
(7,221)	1:65:A:CYS:HB2	1:65:A:CYS:H	2	2.7
(6,277)	1:68:A:ALA:HA	1:69:A:THR:H	2	2.7
(4,285)	1:103:A:GLU:HB2	1:105:A:ASN:H	2	2.7
(4,285)	1:103:A:GLU:HB3	1:105:A:ASN:H	2	2.7
(6,499)	1:118:A:THR:HG1	1:119:A:ILE:H	1	2.69
(6,416)	1:99:A:CYS:HA	1:100:A:PRO:HD2	2	2.69
(6,416)	1:99:A:CYS:HA	1:100:A:PRO:HD3	2	2.69
(4,328)	1:117:A:LYS:HA	1:121:A:ARG:H	1	2.69
(4,259)	1:87:A:ASP:HA	1:90:A:LEU:H	1	2.69
(6,411)	1:98:A:SER:HB2	1:99:A:CYS:H	2	2.68
(6,411)	1:98:A:SER:HB3	1:99:A:CYS:H	2	2.68
(6,152)	1:33:A:PHE:HD1	1:34:A:ALA:H	1	2.68
(6,152)	1:33:A:PHE:HD2	1:34:A:ALA:H	1	2.68
(6,142)	1:32:A:ILE:HG21	1:33:A:PHE:H	1	2.68
(6,142)	1:32:A:ILE:HG22	1:33:A:PHE:H	1	2.68
(6,142)	1:32:A:ILE:HG23	1:33:A:PHE:H	1	2.68
(6,91)	1:20:A:GLN:HB3	1:21:A:LYS:H	2	2.67
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG21	1	2.67
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG22	1	2.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,83)	1:19:A:GLU:H	1:18:A:THR:HG23	1	2.67
(4,288)	1:104:A:ALA:HB1	1:106:A:GLN:HE21	2	2.67
(4,288)	1:104:A:ALA:HB1	1:106:A:GLN:HE22	2	2.67
(4,288)	1:104:A:ALA:HB2	1:106:A:GLN:HE21	2	2.67
(4,288)	1:104:A:ALA:HB2	1:106:A:GLN:HE22	2	2.67
(4,288)	1:104:A:ALA:HB3	1:106:A:GLN:HE21	2	2.67
(4,288)	1:104:A:ALA:HB3	1:106:A:GLN:HE22	2	2.67
(4,350)	1:125:A:SER:HB2	1:127:A:CYS:H	2	2.66
(4,350)	1:125:A:SER:HB3	1:127:A:CYS:H	2	2.66
(7,382)	1:109:A:LEU:HD11	1:109:A:LEU:H	1	2.65
(7,382)	1:109:A:LEU:HD12	1:109:A:LEU:H	1	2.65
(7,382)	1:109:A:LEU:HD13	1:109:A:LEU:H	1	2.65
(6,140)	1:32:A:ILE:HG13	1:33:A:PHE:H	2	2.65
(4,110)	1:40:A:THR:HG21	1:43:A:GLU:H	1	2.65
(4,110)	1:40:A:THR:HG22	1:43:A:GLU:H	1	2.65
(4,110)	1:40:A:THR:HG23	1:43:A:GLU:H	1	2.65
(4,62)	1:18:A:THR:H	1:20:A:GLN:H	1	2.65
(7,348)	1:99:A:CYS:HB2	1:99:A:CYS:H	2	2.64
(6,410)	1:97:A:ASN:H	1:98:A:SER:H	2	2.64
(6,331)	1:80:A:ILE:HG21	1:81:A:ARG:H	2	2.64
(6,331)	1:80:A:ILE:HG22	1:81:A:ARG:H	2	2.64
(6,331)	1:80:A:ILE:HG23	1:81:A:ARG:H	2	2.64
(6,179)	1:40:A:THR:HG21	1:41:A:GLU:H	1	2.64
(6,179)	1:40:A:THR:HG22	1:41:A:GLU:H	1	2.64
(6,179)	1:40:A:THR:HG23	1:41:A:GLU:H	1	2.64
(4,238)	1:80:A:ILE:HA	1:84:A:LYS:H	1	2.64
(6,460)	1:109:A:LEU:HD11	1:110:A:GLU:H	1	2.63
(6,460)	1:109:A:LEU:HD12	1:110:A:GLU:H	1	2.63
(6,460)	1:109:A:LEU:HD13	1:110:A:GLU:H	1	2.63
(6,360)	1:86:A:LEU:HB2	1:87:A:ASP:H	2	2.63
(6,360)	1:86:A:LEU:HB3	1:87:A:ASP:H	2	2.63
(6,179)	1:40:A:THR:HG21	1:41:A:GLU:H	2	2.63
(6,179)	1:40:A:THR:HG22	1:41:A:GLU:H	2	2.63
(6,179)	1:40:A:THR:HG23	1:41:A:GLU:H	2	2.63
(4,104)	1:37:A:LYS:H	1:39:A:THR:H	2	2.63
(4,110)	1:40:A:THR:HG21	1:43:A:GLU:H	2	2.62
(4,110)	1:40:A:THR:HG22	1:43:A:GLU:H	2	2.62
(4,110)	1:40:A:THR:HG23	1:43:A:GLU:H	2	2.62
(3,86)	1:30:A:THR:N	1:106:A:GLN:O	1	2.62
(7,177)	1:51:A:VAL:HG21	1:51:A:VAL:H	2	2.61
(7,177)	1:51:A:VAL:HG22	1:51:A:VAL:H	2	2.61
(7,177)	1:51:A:VAL:HG23	1:51:A:VAL:H	2	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,397)	1:94:A:ALA:HB1	1:95:A:GLY:H	1	2.61
(6,397)	1:94:A:ALA:HB2	1:95:A:GLY:H	1	2.61
(6,397)	1:94:A:ALA:HB3	1:95:A:GLY:H	1	2.61
(6,385)	1:91:A:TRP:HB2	1:92:A:GLY:H	1	2.61
(6,385)	1:91:A:TRP:HB3	1:92:A:GLY:H	1	2.61
(7,243)	1:72:A:GLN:HE21	1:72:A:GLN:H	1	2.6
(7,243)	1:72:A:GLN:HE22	1:72:A:GLN:H	1	2.6
(6,441)	1:105:A:ASN:HB3	1:106:A:GLN:H	2	2.6
(6,387)	1:91:A:TRP:H	1:92:A:GLY:H	1	2.6
(6,344)	1:83:A:LEU:HB3	1:84:A:LYS:H	1	2.6
(2,46)	1:33:A:PHE:HE1	1:116:A:LEU:H	2	2.6
(2,46)	1:33:A:PHE:HE2	1:116:A:LEU:H	2	2.6
(6,409)	1:97:A:ASN:HA	1:98:A:SER:H	1	2.59
(4,328)	1:117:A:LYS:HA	1:121:A:ARG:H	2	2.59
(4,259)	1:87:A:ASP:HA	1:90:A:LEU:H	2	2.59
(4,213)	1:73:A:PHE:HB2	1:75:A:ARG:H	1	2.59
(4,213)	1:73:A:PHE:HB3	1:75:A:ARG:H	1	2.59
(6,423)	1:101:A:VAL:HG21	1:102:A:LYS:H	1	2.58
(6,423)	1:101:A:VAL:HG22	1:102:A:LYS:H	1	2.58
(6,423)	1:101:A:VAL:HG23	1:102:A:LYS:H	1	2.58
(2,14)	1:30:A:THR:HG21	1:105:A:ASN:H	1	2.58
(2,14)	1:30:A:THR:HG22	1:105:A:ASN:H	1	2.58
(2,14)	1:30:A:THR:HG23	1:105:A:ASN:H	1	2.58
(6,491)	1:116:A:LEU:H	1:115:A:ARG:HE	2	2.57
(7,119)	1:32:A:ILE:HG21	1:32:A:ILE:H	1	2.56
(7,119)	1:32:A:ILE:HG22	1:32:A:ILE:H	1	2.56
(7,119)	1:32:A:ILE:HG23	1:32:A:ILE:H	1	2.56
(6,539)	1:128:A:SER:H	1:129:A:SER:H	1	2.56
(6,457)	1:109:A:LEU:HB3	1:110:A:GLU:H	2	2.56
(6,397)	1:94:A:ALA:HB1	1:95:A:GLY:H	2	2.56
(6,397)	1:94:A:ALA:HB2	1:95:A:GLY:H	2	2.56
(6,397)	1:94:A:ALA:HB3	1:95:A:GLY:H	2	2.56
(6,360)	1:86:A:LEU:HB2	1:87:A:ASP:H	1	2.56
(6,360)	1:86:A:LEU:HB3	1:87:A:ASP:H	1	2.56
(4,350)	1:125:A:SER:HB2	1:127:A:CYS:H	1	2.56
(4,350)	1:125:A:SER:HB3	1:127:A:CYS:H	1	2.56
(6,463)	1:110:A:GLU:HB3	1:111:A:ASN:H	1	2.55
(6,453)	1:108:A:THR:HG21	1:109:A:LEU:H	1	2.55
(6,453)	1:108:A:THR:HG22	1:109:A:LEU:H	1	2.55
(6,453)	1:108:A:THR:HG23	1:109:A:LEU:H	1	2.55
(6,300)	1:73:A:PHE:HB3	1:74:A:HIS:H	2	2.55
(4,93)	1:32:A:ILE:HG21	1:34:A:ALA:H	1	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,93)	1:32:A:ILE:HG22	1:34:A:ALA:H	1	2.55
(4,93)	1:32:A:ILE:HG23	1:34:A:ALA:H	1	2.55
(6,498)	1:118:A:THR:HB	1:119:A:ILE:H	1	2.54
(6,185)	1:43:A:GLU:HG2	1:42:A:LYS:H	2	2.54
(6,185)	1:43:A:GLU:HG3	1:42:A:LYS:H	2	2.54
(6,158)	1:35:A:ALA:H	1:36:A:SER:H	1	2.54
(4,282)	1:96:A:LEU:HA	1:98:A:SER:H	2	2.54
(4,103)	1:37:A:LYS:HA	1:39:A:THR:H	2	2.54
(7,203)	1:59:A:HIS:HB3	1:59:A:HIS:H	2	2.53
(6,328)	1:80:A:ILE:HD11	1:79:A:LEU:H	2	2.53
(6,328)	1:80:A:ILE:HD12	1:79:A:LEU:H	2	2.53
(6,328)	1:80:A:ILE:HD13	1:79:A:LEU:H	2	2.53
(6,157)	1:35:A:ALA:HB1	1:36:A:SER:H	2	2.53
(6,157)	1:35:A:ALA:HB2	1:36:A:SER:H	2	2.53
(6,157)	1:35:A:ALA:HB3	1:36:A:SER:H	2	2.53
(6,507)	1:119:A:ILE:HD11	1:120:A:MET:H	1	2.52
(6,507)	1:119:A:ILE:HD12	1:120:A:MET:H	1	2.52
(6,507)	1:119:A:ILE:HD13	1:120:A:MET:H	1	2.52
(6,434)	1:103:A:GLU:H	1:104:A:ALA:H	1	2.52
(4,93)	1:32:A:ILE:HG21	1:34:A:ALA:H	2	2.52
(4,93)	1:32:A:ILE:HG22	1:34:A:ALA:H	2	2.52
(4,93)	1:32:A:ILE:HG23	1:34:A:ALA:H	2	2.52
(7,382)	1:109:A:LEU:HD11	1:109:A:LEU:H	2	2.51
(7,382)	1:109:A:LEU:HD12	1:109:A:LEU:H	2	2.51
(7,382)	1:109:A:LEU:HD13	1:109:A:LEU:H	2	2.51
(4,109)	1:40:A:THR:HG21	1:42:A:LYS:H	2	2.51
(4,109)	1:40:A:THR:HG22	1:42:A:LYS:H	2	2.51
(4,109)	1:40:A:THR:HG23	1:42:A:LYS:H	2	2.51
(6,262)	1:63:A:THR:HG21	1:64:A:ARG:H	2	2.5
(6,262)	1:63:A:THR:HG22	1:64:A:ARG:H	2	2.5
(6,262)	1:63:A:THR:HG23	1:64:A:ARG:H	2	2.5
(7,203)	1:59:A:HIS:HB3	1:59:A:HIS:H	1	2.49
(6,45)	1:12:A:LYS:H	1:11:A:ILE:HG12	2	2.49
(7,295)	1:86:A:LEU:HD11	1:86:A:LEU:H	1	2.48
(7,295)	1:86:A:LEU:HD12	1:86:A:LEU:H	1	2.48
(7,295)	1:86:A:LEU:HD13	1:86:A:LEU:H	1	2.48
(6,438)	1:104:A:ALA:H	1:105:A:ASN:H	2	2.48
(4,279)	1:96:A:LEU:HB2	1:98:A:SER:H	2	2.48
(4,279)	1:96:A:LEU:HB3	1:98:A:SER:H	2	2.48
(4,62)	1:18:A:THR:H	1:20:A:GLN:H	2	2.48
(7,136)	1:38:A:ASN:HB3	1:38:A:ASN:H	2	2.47
(6,379)	1:90:A:LEU:HA	1:91:A:TRP:H	1	2.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,385)	1:110:A:GLU:HB3	1:110:A:GLU:H	2	2.46
(7,106)	1:29:A:VAL:HB	1:29:A:VAL:H	1	2.46
(7,56)	1:15:A:ASN:HB3	1:15:A:ASN:HD21	2	2.46
(7,56)	1:15:A:ASN:HB3	1:15:A:ASN:HD22	2	2.46
(7,55)	1:15:A:ASN:HB3	1:15:A:ASN:HD21	2	2.46
(7,55)	1:15:A:ASN:HB3	1:15:A:ASN:HD22	2	2.46
(6,465)	1:110:A:GLU:HG2	1:111:A:ASN:H	1	2.46
(6,465)	1:110:A:GLU:HG3	1:111:A:ASN:H	1	2.46
(6,463)	1:110:A:GLU:HB3	1:111:A:ASN:H	2	2.46
(6,422)	1:101:A:VAL:HG11	1:102:A:LYS:H	1	2.46
(6,422)	1:101:A:VAL:HG12	1:102:A:LYS:H	1	2.46
(6,422)	1:101:A:VAL:HG13	1:102:A:LYS:H	1	2.46
(6,261)	1:63:A:THR:HB	1:64:A:ARG:H	1	2.46
(6,143)	1:32:A:ILE:HD11	1:33:A:PHE:H	2	2.46
(6,143)	1:32:A:ILE:HD12	1:33:A:PHE:H	2	2.46
(6,143)	1:32:A:ILE:HD13	1:33:A:PHE:H	2	2.46
(6,117)	1:27:A:LEU:HD21	1:28:A:THR:H	1	2.46
(6,117)	1:27:A:LEU:HD22	1:28:A:THR:H	1	2.46
(6,117)	1:27:A:LEU:HD23	1:28:A:THR:H	1	2.46
(7,385)	1:110:A:GLU:HB3	1:110:A:GLU:H	1	2.45
(7,159)	1:45:A:PHE:H	1:45:A:PHE:HD1	1	2.45
(7,159)	1:45:A:PHE:H	1:45:A:PHE:HD2	1	2.45
(6,537)	1:127:A:CYS:HB2	1:128:A:SER:H	2	2.45
(6,537)	1:127:A:CYS:HB3	1:128:A:SER:H	2	2.45
(6,476)	1:112:A:PHE:HB3	1:113:A:LEU:H	2	2.45
(6,422)	1:101:A:VAL:HG11	1:102:A:LYS:H	2	2.45
(6,422)	1:101:A:VAL:HG12	1:102:A:LYS:H	2	2.45
(6,422)	1:101:A:VAL:HG13	1:102:A:LYS:H	2	2.45
(7,159)	1:45:A:PHE:H	1:45:A:PHE:HD1	2	2.44
(7,159)	1:45:A:PHE:H	1:45:A:PHE:HD2	2	2.44
(6,142)	1:32:A:ILE:HG21	1:33:A:PHE:H	2	2.44
(6,142)	1:32:A:ILE:HG22	1:33:A:PHE:H	2	2.44
(6,142)	1:32:A:ILE:HG23	1:33:A:PHE:H	2	2.44
(6,117)	1:27:A:LEU:HD21	1:28:A:THR:H	2	2.44
(6,117)	1:27:A:LEU:HD22	1:28:A:THR:H	2	2.44
(6,117)	1:27:A:LEU:HD23	1:28:A:THR:H	2	2.44
(4,148)	1:50:A:THR:HG21	1:52:A:LEU:H	1	2.44
(4,148)	1:50:A:THR:HG22	1:52:A:LEU:H	1	2.44
(4,148)	1:50:A:THR:HG23	1:52:A:LEU:H	1	2.44
(6,384)	1:91:A:TRP:HE3	1:92:A:GLY:H	1	2.43
(6,158)	1:35:A:ALA:H	1:36:A:SER:H	2	2.43
(6,81)	1:18:A:THR:H	1:19:A:GLU:HB2	2	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,81)	1:18:A:THR:H	1:19:A:GLU:HB3	2	2.43
(6,491)	1:116:A:LEU:H	1:115:A:ARG:HE	1	2.42
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD11	1	2.42
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD12	1	2.42
(6,42)	1:12:A:LYS:H	1:11:A:ILE:HD13	1	2.42
(4,80)	1:28:A:THR:HB	1:30:A:THR:H	2	2.42
(7,376)	1:108:A:THR:HB	1:108:A:THR:H	1	2.41
(7,86)	1:22:A:THR:H	1:22:A:THR:HG21	2	2.41
(7,86)	1:22:A:THR:H	1:22:A:THR:HG22	2	2.41
(7,86)	1:22:A:THR:H	1:22:A:THR:HG23	2	2.41
(7,51)	1:15:A:ASN:H	1:15:A:ASN:HD21	2	2.41
(6,465)	1:110:A:GLU:HG2	1:111:A:ASN:H	2	2.41
(6,465)	1:110:A:GLU:HG3	1:111:A:ASN:H	2	2.41
(6,402)	1:96:A:LEU:HB2	1:95:A:GLY:H	1	2.41
(6,402)	1:96:A:LEU:HB3	1:95:A:GLY:H	1	2.41
(6,305)	1:74:A:HIS:HB2	1:75:A:ARG:H	2	2.41
(6,305)	1:74:A:HIS:HB3	1:75:A:ARG:H	2	2.41
(6,253)	1:60:A:GLU:H	1:61:A:LYS:H	1	2.41
(6,246)	1:58:A:HIS:HB2	1:59:A:HIS:H	2	2.41
(6,246)	1:58:A:HIS:HB3	1:59:A:HIS:H	2	2.41
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG21	2	2.41
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG22	2	2.41
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG23	2	2.41
(7,416)	1:119:A:ILE:HG21	1:119:A:ILE:H	1	2.4
(7,345)	1:98:A:SER:HB2	1:98:A:SER:H	2	2.4
(7,345)	1:98:A:SER:HB3	1:98:A:SER:H	2	2.4
(6,300)	1:73:A:PHE:HB3	1:74:A:HIS:H	1	2.4
(6,233)	1:55:A:PHE:HD1	1:56:A:TYR:H	2	2.4
(6,233)	1:55:A:PHE:HD2	1:56:A:TYR:H	2	2.4
(6,157)	1:35:A:ALA:HB1	1:36:A:SER:H	1	2.4
(6,157)	1:35:A:ALA:HB2	1:36:A:SER:H	1	2.4
(6,157)	1:35:A:ALA:HB3	1:36:A:SER:H	1	2.4
(2,12)	1:30:A:THR:HG21	1:104:A:ALA:H	1	2.39
(2,12)	1:30:A:THR:HG22	1:104:A:ALA:H	1	2.39
(2,12)	1:30:A:THR:HG23	1:104:A:ALA:H	1	2.39
(2,29)	1:29:A:VAL:HG21	1:55:A:PHE:H	2	2.38
(2,29)	1:29:A:VAL:HG22	1:55:A:PHE:H	2	2.38
(2,29)	1:29:A:VAL:HG23	1:55:A:PHE:H	2	2.38
(6,476)	1:112:A:PHE:HB3	1:113:A:LEU:H	1	2.37
(6,347)	1:83:A:LEU:HD21	1:84:A:LYS:H	1	2.37
(6,347)	1:83:A:LEU:HD22	1:84:A:LYS:H	1	2.37
(6,347)	1:83:A:LEU:HD23	1:84:A:LYS:H	1	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD11	2	2.37
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD12	2	2.37
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD13	2	2.37
(4,303)	1:112:A:PHE:HB2	1:110:A:GLU:H	2	2.37
(4,303)	1:112:A:PHE:HB3	1:110:A:GLU:H	2	2.37
(4,148)	1:50:A:THR:HG21	1:52:A:LEU:H	2	2.37
(4,148)	1:50:A:THR:HG22	1:52:A:LEU:H	2	2.37
(4,148)	1:50:A:THR:HG23	1:52:A:LEU:H	2	2.37
(6,390)	1:92:A:GLY:H	1:93:A:LEU:H	2	2.36
(6,263)	1:63:A:THR:HA	1:64:A:ARG:H	2	2.36
(4,213)	1:73:A:PHE:HB2	1:75:A:ARG:H	2	2.36
(4,213)	1:73:A:PHE:HB3	1:75:A:ARG:H	2	2.36
(7,204)	1:59:A:HIS:HB2	1:59:A:HIS:H	1	2.35
(6,446)	1:106:A:GLN:HG2	1:107:A:SER:H	1	2.35
(6,446)	1:106:A:GLN:HG3	1:107:A:SER:H	1	2.35
(7,444)	1:128:A:SER:HB3	1:128:A:SER:H	1	2.34
(7,347)	1:99:A:CYS:HB3	1:99:A:CYS:H	1	2.34
(7,77)	1:20:A:GLN:H	1:20:A:GLN:HB2	1	2.34
(4,299)	1:108:A:THR:H	1:111:A:ASN:HD21	1	2.34
(4,299)	1:108:A:THR:H	1:111:A:ASN:HD22	1	2.34
(4,1)	1:4:A:ASP:HA	1:7:A:LEU:H	2	2.34
(2,14)	1:30:A:THR:HG21	1:105:A:ASN:H	2	2.34
(2,14)	1:30:A:THR:HG22	1:105:A:ASN:H	2	2.34
(2,14)	1:30:A:THR:HG23	1:105:A:ASN:H	2	2.34
(6,411)	1:98:A:SER:HB2	1:99:A:CYS:H	1	2.33
(6,411)	1:98:A:SER:HB3	1:99:A:CYS:H	1	2.33
(6,181)	1:41:A:GLU:H	1:42:A:LYS:H	1	2.33
(6,2)	1:4:A:ASP:H	1:3:A:THR:HB	1	2.33
(4,109)	1:40:A:THR:HG21	1:42:A:LYS:H	1	2.33
(4,109)	1:40:A:THR:HG22	1:42:A:LYS:H	1	2.33
(4,109)	1:40:A:THR:HG23	1:42:A:LYS:H	1	2.33
(2,19)	1:112:A:PHE:HD1	1:32:A:ILE:H	1	2.33
(2,19)	1:112:A:PHE:HD2	1:32:A:ILE:H	1	2.33
(7,376)	1:108:A:THR:HB	1:108:A:THR:H	2	2.32
(6,470)	1:111:A:ASN:HB3	1:112:A:PHE:H	1	2.32
(6,25)	1:7:A:LEU:HD11	1:8:A:GLN:H	2	2.32
(6,25)	1:7:A:LEU:HD12	1:8:A:GLN:H	2	2.32
(6,25)	1:7:A:LEU:HD13	1:8:A:GLN:H	2	2.32
(6,25)	1:7:A:LEU:HD21	1:8:A:GLN:H	2	2.32
(6,25)	1:7:A:LEU:HD22	1:8:A:GLN:H	2	2.32
(6,25)	1:7:A:LEU:HD23	1:8:A:GLN:H	2	2.32
(6,24)	1:7:A:LEU:HD11	1:8:A:GLN:H	2	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,24)	1:7:A:LEU:HD12	1:8:A:GLN:H	2	2.32
(6,24)	1:7:A:LEU:HD13	1:8:A:GLN:H	2	2.32
(6,24)	1:7:A:LEU:HD21	1:8:A:GLN:H	2	2.32
(6,24)	1:7:A:LEU:HD22	1:8:A:GLN:H	2	2.32
(6,24)	1:7:A:LEU:HD23	1:8:A:GLN:H	2	2.32
(7,442)	1:127:A:CYS:HB2	1:127:A:CYS:H	2	2.31
(7,442)	1:127:A:CYS:HB3	1:127:A:CYS:H	2	2.31
(7,374)	1:107:A:SER:HB2	1:107:A:SER:H	2	2.31
(7,374)	1:107:A:SER:HB3	1:107:A:SER:H	2	2.31
(7,317)	1:91:A:TRP:HA	1:91:A:TRP:H	2	2.31
(7,204)	1:59:A:HIS:HB2	1:59:A:HIS:H	2	2.31
(7,77)	1:20:A:GLN:H	1:20:A:GLN:HB2	2	2.31
(6,530)	1:125:A:SER:HB2	1:126:A:LYS:H	2	2.31
(6,530)	1:125:A:SER:HB3	1:126:A:LYS:H	2	2.31
(6,147)	1:34:A:ALA:HB1	1:33:A:PHE:H	2	2.31
(6,147)	1:34:A:ALA:HB2	1:33:A:PHE:H	2	2.31
(6,147)	1:34:A:ALA:HB3	1:33:A:PHE:H	2	2.31
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD11	2	2.31
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD12	2	2.31
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD13	2	2.31
(7,369)	1:106:A:GLN:HA	1:106:A:GLN:HE21	2	2.3
(7,369)	1:106:A:GLN:HA	1:106:A:GLN:HE22	2	2.3
(7,129)	1:35:A:ALA:HB1	1:35:A:ALA:H	1	2.3
(7,129)	1:35:A:ALA:HB2	1:35:A:ALA:H	1	2.3
(7,129)	1:35:A:ALA:HB3	1:35:A:ALA:H	1	2.3
(7,95)	1:25:A:THR:H	1:25:A:THR:HG21	1	2.3
(7,95)	1:25:A:THR:H	1:25:A:THR:HG22	1	2.3
(7,95)	1:25:A:THR:H	1:25:A:THR:HG23	1	2.3
(6,363)	1:86:A:LEU:HD21	1:87:A:ASP:H	1	2.3
(6,363)	1:86:A:LEU:HD22	1:87:A:ASP:H	1	2.3
(6,363)	1:86:A:LEU:HD23	1:87:A:ASP:H	1	2.3
(4,170)	1:56:A:TYR:HA	1:58:A:HIS:H	2	2.3
(3,83)	1:29:A:VAL:H	1:107:A:SER:O	2	2.3
(2,1)	1:29:A:VAL:H	1:107:A:SER:H	2	2.3
(7,343)	1:97:A:ASN:HB2	1:97:A:ASN:H	2	2.29
(7,343)	1:97:A:ASN:HB3	1:97:A:ASN:H	2	2.29
(7,335)	1:94:A:ALA:HB1	1:94:A:ALA:H	1	2.29
(7,335)	1:94:A:ALA:HB2	1:94:A:ALA:H	1	2.29
(7,335)	1:94:A:ALA:HB3	1:94:A:ALA:H	1	2.29
(7,143)	1:39:A:THR:HG21	1:39:A:THR:H	2	2.29
(7,143)	1:39:A:THR:HG22	1:39:A:THR:H	2	2.29
(7,143)	1:39:A:THR:HG23	1:39:A:THR:H	2	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,328)	1:80:A:ILE:HD11	1:79:A:LEU:H	1	2.29
(6,328)	1:80:A:ILE:HD12	1:79:A:LEU:H	1	2.29
(6,328)	1:80:A:ILE:HD13	1:79:A:LEU:H	1	2.29
(6,277)	1:68:A:ALA:HA	1:69:A:THR:H	1	2.29
(7,176)	1:51:A:VAL:HG11	1:51:A:VAL:H	2	2.28
(7,176)	1:51:A:VAL:HG12	1:51:A:VAL:H	2	2.28
(7,176)	1:51:A:VAL:HG13	1:51:A:VAL:H	2	2.28
(4,303)	1:112:A:PHE:HB2	1:110:A:GLU:H	1	2.28
(4,303)	1:112:A:PHE:HB3	1:110:A:GLU:H	1	2.28
(4,271)	1:92:A:GLY:HA3	1:95:A:GLY:H	2	2.28
(4,202)	1:70:A:ALA:HB1	1:74:A:HIS:H	1	2.28
(4,202)	1:70:A:ALA:HB2	1:74:A:HIS:H	1	2.28
(4,202)	1:70:A:ALA:HB3	1:74:A:HIS:H	1	2.28
(2,1)	1:29:A:VAL:H	1:107:A:SER:H	1	2.28
(7,361)	1:104:A:ALA:HB1	1:104:A:ALA:H	1	2.27
(7,361)	1:104:A:ALA:HB2	1:104:A:ALA:H	1	2.27
(7,361)	1:104:A:ALA:HB3	1:104:A:ALA:H	1	2.27
(7,348)	1:99:A:CYS:HB2	1:99:A:CYS:H	1	2.27
(7,234)	1:70:A:ALA:HB1	1:70:A:ALA:H	1	2.27
(7,234)	1:70:A:ALA:HB2	1:70:A:ALA:H	1	2.27
(7,234)	1:70:A:ALA:HB3	1:70:A:ALA:H	1	2.27
(7,129)	1:35:A:ALA:HB1	1:35:A:ALA:H	2	2.27
(7,129)	1:35:A:ALA:HB2	1:35:A:ALA:H	2	2.27
(7,129)	1:35:A:ALA:HB3	1:35:A:ALA:H	2	2.27
(6,181)	1:41:A:GLU:H	1:42:A:LYS:H	2	2.27
(6,147)	1:34:A:ALA:HB1	1:33:A:PHE:H	1	2.27
(6,147)	1:34:A:ALA:HB2	1:33:A:PHE:H	1	2.27
(6,147)	1:34:A:ALA:HB3	1:33:A:PHE:H	1	2.27
(4,332)	1:119:A:ILE:HD11	1:121:A:ARG:H	1	2.27
(4,332)	1:119:A:ILE:HD12	1:121:A:ARG:H	1	2.27
(4,332)	1:119:A:ILE:HD13	1:121:A:ARG:H	1	2.27
(4,297)	1:108:A:THR:HA	1:110:A:GLU:H	1	2.27
(4,273)	1:92:A:GLY:HA3	1:94:A:ALA:H	2	2.27
(7,284)	1:83:A:LEU:HD11	1:83:A:LEU:H	2	2.26
(7,284)	1:83:A:LEU:HD12	1:83:A:LEU:H	2	2.26
(7,284)	1:83:A:LEU:HD13	1:83:A:LEU:H	2	2.26
(6,194)	1:44:A:THR:H	1:45:A:PHE:HD1	2	2.26
(6,194)	1:44:A:THR:H	1:45:A:PHE:HD2	2	2.26
(6,35)	1:10:A:ILE:H	1:11:A:ILE:HG12	2	2.26
(6,35)	1:10:A:ILE:H	1:11:A:ILE:HG13	2	2.26
(4,341)	1:121:A:ARG:H	1:123:A:LYS:H	1	2.26
(2,48)	1:12:A:LYS:HB2	1:125:A:SER:H	2	2.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,48)	1:12:A:LYS:HB3	1:125:A:SER:H	2	2.26
(2,36)	1:56:A:TYR:HD1	1:83:A:LEU:H	1	2.26
(2,36)	1:56:A:TYR:HD2	1:83:A:LEU:H	1	2.26
(2,19)	1:112:A:PHE:HD1	1:32:A:ILE:H	2	2.26
(2,19)	1:112:A:PHE:HD2	1:32:A:ILE:H	2	2.26
(7,335)	1:94:A:ALA:HB1	1:94:A:ALA:H	2	2.25
(7,335)	1:94:A:ALA:HB2	1:94:A:ALA:H	2	2.25
(7,335)	1:94:A:ALA:HB3	1:94:A:ALA:H	2	2.25
(7,177)	1:51:A:VAL:HG21	1:51:A:VAL:H	1	2.25
(7,177)	1:51:A:VAL:HG22	1:51:A:VAL:H	1	2.25
(7,177)	1:51:A:VAL:HG23	1:51:A:VAL:H	1	2.25
(6,346)	1:83:A:LEU:HD11	1:84:A:LYS:H	1	2.25
(6,346)	1:83:A:LEU:HD12	1:84:A:LYS:H	1	2.25
(6,346)	1:83:A:LEU:HD13	1:84:A:LYS:H	1	2.25
(2,41)	1:30:A:THR:HA	1:105:A:ASN:H	1	2.25
(7,234)	1:70:A:ALA:HB1	1:70:A:ALA:H	2	2.24
(7,234)	1:70:A:ALA:HB2	1:70:A:ALA:H	2	2.24
(7,234)	1:70:A:ALA:HB3	1:70:A:ALA:H	2	2.24
(6,539)	1:128:A:SER:H	1:129:A:SER:H	2	2.24
(2,50)	1:93:A:LEU:HD11	1:6:A:THR:H	1	2.24
(2,50)	1:93:A:LEU:HD12	1:6:A:THR:H	1	2.24
(2,50)	1:93:A:LEU:HD13	1:6:A:THR:H	1	2.24
(2,50)	1:93:A:LEU:HD21	1:6:A:THR:H	1	2.24
(2,50)	1:93:A:LEU:HD22	1:6:A:THR:H	1	2.24
(2,50)	1:93:A:LEU:HD23	1:6:A:THR:H	1	2.24
(7,374)	1:107:A:SER:HB2	1:107:A:SER:H	1	2.23
(7,374)	1:107:A:SER:HB3	1:107:A:SER:H	1	2.23
(7,296)	1:86:A:LEU:HD21	1:86:A:LEU:H	1	2.23
(7,296)	1:86:A:LEU:HD22	1:86:A:LEU:H	1	2.23
(7,296)	1:86:A:LEU:HD23	1:86:A:LEU:H	1	2.23
(4,1)	1:4:A:ASP:HA	1:7:A:LEU:H	1	2.23
(7,343)	1:97:A:ASN:HB2	1:97:A:ASN:H	1	2.22
(7,343)	1:97:A:ASN:HB3	1:97:A:ASN:H	1	2.22
(7,243)	1:72:A:GLN:HE21	1:72:A:GLN:H	2	2.22
(7,243)	1:72:A:GLN:HE22	1:72:A:GLN:H	2	2.22
(6,457)	1:109:A:LEU:HB3	1:110:A:GLU:H	1	2.22
(6,5)	1:4:A:ASP:H	1:5:A:ILE:H	1	2.22
(7,360)	1:104:A:ALA:HA	1:104:A:ALA:H	1	2.21
(6,362)	1:86:A:LEU:HD11	1:87:A:ASP:H	1	2.21
(6,362)	1:86:A:LEU:HD12	1:87:A:ASP:H	1	2.21
(6,362)	1:86:A:LEU:HD13	1:87:A:ASP:H	1	2.21
(6,121)	1:28:A:THR:HG21	1:29:A:VAL:H	2	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,121)	1:28:A:THR:HG22	1:29:A:VAL:H	2	2.21
(6,121)	1:28:A:THR:HG23	1:29:A:VAL:H	2	2.21
(6,7)	1:5:A:ILE:H	1:4:A:ASP:HB2	1	2.21
(4,277)	1:94:A:ALA:HA	1:96:A:LEU:H	1	2.21
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD11	1	2.21
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD12	1	2.21
(2,16)	1:121:A:ARG:H	1:11:A:ILE:HD13	1	2.21
(7,383)	1:109:A:LEU:HD21	1:109:A:LEU:H	2	2.2
(7,383)	1:109:A:LEU:HD22	1:109:A:LEU:H	2	2.2
(7,383)	1:109:A:LEU:HD23	1:109:A:LEU:H	2	2.2
(6,425)	1:102:A:LYS:HB3	1:103:A:GLU:H	2	2.2
(4,339)	1:121:A:ARG:HA	1:123:A:LYS:H	1	2.2
(4,229)	1:77:A:LYS:H	1:79:A:LEU:H	2	2.19
(2,47)	1:33:A:PHE:HZ	1:116:A:LEU:H	1	2.19
(2,45)	1:33:A:PHE:HD1	1:115:A:ARG:H	2	2.19
(2,45)	1:33:A:PHE:HD2	1:115:A:ARG:H	2	2.19
(7,384)	1:110:A:GLU:HA	1:110:A:GLU:H	1	2.18
(7,384)	1:110:A:GLU:HA	1:110:A:GLU:H	2	2.18
(6,408)	1:97:A:ASN:HB2	1:98:A:SER:H	2	2.18
(6,408)	1:97:A:ASN:HB3	1:98:A:SER:H	2	2.18
(6,219)	1:50:A:THR:HG21	1:51:A:VAL:H	1	2.18
(6,219)	1:50:A:THR:HG22	1:51:A:VAL:H	1	2.18
(6,219)	1:50:A:THR:HG23	1:51:A:VAL:H	1	2.18
(6,71)	1:17:A:LEU:HB2	1:16:A:SER:H	2	2.18
(7,412)	1:119:A:ILE:HA	1:119:A:ILE:H	2	2.17
(7,211)	1:61:A:LYS:HA	1:61:A:LYS:H	1	2.17
(7,233)	1:70:A:ALA:HA	1:70:A:ALA:H	1	2.16
(7,219)	1:65:A:CYS:HA	1:65:A:CYS:H	1	2.16
(6,362)	1:86:A:LEU:HD11	1:87:A:ASP:H	2	2.16
(6,362)	1:86:A:LEU:HD12	1:87:A:ASP:H	2	2.16
(6,362)	1:86:A:LEU:HD13	1:87:A:ASP:H	2	2.16
(6,250)	1:59:A:HIS:HB2	1:60:A:GLU:H	1	2.16
(6,250)	1:59:A:HIS:HB3	1:60:A:GLU:H	1	2.16
(6,194)	1:44:A:THR:H	1:45:A:PHE:HD1	1	2.16
(6,194)	1:44:A:THR:H	1:45:A:PHE:HD2	1	2.16
(6,144)	1:32:A:ILE:HD11	1:33:A:PHE:HE1	2	2.16
(6,144)	1:32:A:ILE:HD11	1:33:A:PHE:HE2	2	2.16
(6,144)	1:32:A:ILE:HD12	1:33:A:PHE:HE1	2	2.16
(6,144)	1:32:A:ILE:HD12	1:33:A:PHE:HE2	2	2.16
(6,144)	1:32:A:ILE:HD13	1:33:A:PHE:HE1	2	2.16
(6,144)	1:32:A:ILE:HD13	1:33:A:PHE:HE2	2	2.16
(4,170)	1:56:A:TYR:HA	1:58:A:HIS:H	1	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,354)	1:102:A:LYS:HB3	1:102:A:LYS:H	1	2.15
(7,346)	1:99:A:CYS:HA	1:99:A:CYS:H	2	2.15
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG21	2	2.15
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG22	2	2.15
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG23	2	2.15
(6,121)	1:28:A:THR:HG21	1:29:A:VAL:H	1	2.15
(6,121)	1:28:A:THR:HG22	1:29:A:VAL:H	1	2.15
(6,121)	1:28:A:THR:HG23	1:29:A:VAL:H	1	2.15
(2,45)	1:33:A:PHE:HD1	1:115:A:ARG:H	1	2.15
(2,45)	1:33:A:PHE:HD2	1:115:A:ARG:H	1	2.15
(7,271)	1:80:A:ILE:HD11	1:80:A:ILE:H	2	2.14
(7,271)	1:80:A:ILE:HD12	1:80:A:ILE:H	2	2.14
(7,271)	1:80:A:ILE:HD13	1:80:A:ILE:H	2	2.14
(6,530)	1:125:A:SER:HB2	1:126:A:LYS:H	1	2.14
(6,530)	1:125:A:SER:HB3	1:126:A:LYS:H	1	2.14
(6,346)	1:83:A:LEU:HD11	1:84:A:LYS:H	2	2.14
(6,346)	1:83:A:LEU:HD12	1:84:A:LYS:H	2	2.14
(6,346)	1:83:A:LEU:HD13	1:84:A:LYS:H	2	2.14
(2,27)	1:96:A:LEU:HB2	1:46:A:CYS:H	2	2.14
(2,27)	1:96:A:LEU:HB3	1:46:A:CYS:H	2	2.14
(7,442)	1:127:A:CYS:HB2	1:127:A:CYS:H	1	2.13
(7,442)	1:127:A:CYS:HB3	1:127:A:CYS:H	1	2.13
(7,360)	1:104:A:ALA:HA	1:104:A:ALA:H	2	2.13
(7,305)	1:89:A:ASN:HD21	1:89:A:ASN:H	1	2.13
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG21	1	2.13
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG22	1	2.13
(6,37)	1:11:A:ILE:H	1:10:A:ILE:HG23	1	2.13
(4,229)	1:77:A:LYS:H	1:79:A:LEU:H	1	2.13
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG21	1	2.13
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG22	1	2.13
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG23	1	2.13
(7,416)	1:119:A:ILE:HG21	1:119:A:ILE:H	2	2.12
(7,412)	1:119:A:ILE:HA	1:119:A:ILE:H	1	2.12
(7,383)	1:109:A:LEU:HD21	1:109:A:LEU:H	1	2.12
(7,383)	1:109:A:LEU:HD22	1:109:A:LEU:H	1	2.12
(7,383)	1:109:A:LEU:HD23	1:109:A:LEU:H	1	2.12
(7,353)	1:102:A:LYS:HA	1:102:A:LYS:H	2	2.12
(6,408)	1:97:A:ASN:HB2	1:98:A:SER:H	1	2.12
(6,408)	1:97:A:ASN:HB3	1:98:A:SER:H	1	2.12
(6,71)	1:17:A:LEU:HB2	1:16:A:SER:H	1	2.12
(4,353)	1:126:A:LYS:HA	1:128:A:SER:H	2	2.12
(7,202)	1:59:A:HIS:HA	1:59:A:HIS:H	1	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,202)	1:59:A:HIS:HA	1:59:A:HIS:H	2	2.11
(6,470)	1:111:A:ASN:HB3	1:112:A:PHE:H	2	2.11
(4,306)	1:110:A:GLU:H	1:112:A:PHE:H	2	2.11
(7,443)	1:128:A:SER:HA	1:128:A:SER:H	1	2.1
(7,233)	1:70:A:ALA:HA	1:70:A:ALA:H	2	2.1
(7,219)	1:65:A:CYS:HA	1:65:A:CYS:H	2	2.1
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD11	1	2.1
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD12	1	2.1
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD13	1	2.1
(6,166)	1:37:A:LYS:HB2	1:38:A:ASN:H	1	2.1
(6,166)	1:37:A:LYS:HB3	1:38:A:ASN:H	1	2.1
(2,48)	1:12:A:LYS:HB2	1:125:A:SER:H	1	2.1
(2,48)	1:12:A:LYS:HB3	1:125:A:SER:H	1	2.1
(7,346)	1:99:A:CYS:HA	1:99:A:CYS:H	1	2.09
(7,211)	1:61:A:LYS:HA	1:61:A:LYS:H	2	2.09
(6,507)	1:119:A:ILE:HD11	1:120:A:MET:H	2	2.09
(6,507)	1:119:A:ILE:HD12	1:120:A:MET:H	2	2.09
(6,507)	1:119:A:ILE:HD13	1:120:A:MET:H	2	2.09
(7,342)	1:97:A:ASN:HA	1:97:A:ASN:H	1	2.08
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD11	2	2.08
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD12	2	2.08
(7,34)	1:10:A:ILE:H	1:10:A:ILE:HD13	2	2.08
(4,262)	1:87:A:ASP:H	1:89:A:ASN:H	1	2.08
(7,353)	1:102:A:LYS:HA	1:102:A:LYS:H	1	2.07
(7,342)	1:97:A:ASN:HA	1:97:A:ASN:H	2	2.07
(7,317)	1:91:A:TRP:HA	1:91:A:TRP:H	1	2.07
(6,219)	1:50:A:THR:HG21	1:51:A:VAL:H	2	2.07
(6,219)	1:50:A:THR:HG22	1:51:A:VAL:H	2	2.07
(6,219)	1:50:A:THR:HG23	1:51:A:VAL:H	2	2.07
(6,133)	1:31:A:ASP:HB2	1:32:A:ILE:H	2	2.07
(4,341)	1:121:A:ARG:H	1:123:A:LYS:H	2	2.07
(4,317)	1:112:A:PHE:H	1:114:A:GLU:H	2	2.07
(7,377)	1:108:A:THR:HG21	1:108:A:THR:H	1	2.06
(7,377)	1:108:A:THR:HG22	1:108:A:THR:H	1	2.06
(7,377)	1:108:A:THR:HG23	1:108:A:THR:H	1	2.06
(7,387)	1:110:A:GLU:HG2	1:110:A:GLU:H	1	2.05
(7,387)	1:110:A:GLU:HG3	1:110:A:GLU:H	1	2.05
(7,387)	1:110:A:GLU:HG2	1:110:A:GLU:H	2	2.05
(7,387)	1:110:A:GLU:HG3	1:110:A:GLU:H	2	2.05
(7,338)	1:96:A:LEU:HA	1:96:A:LEU:H	1	2.05
(6,431)	1:103:A:GLU:HB2	1:104:A:ALA:H	1	2.05
(6,431)	1:103:A:GLU:HB3	1:104:A:ALA:H	1	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,260)	1:62:A:ASP:H	1:63:A:THR:H	2	2.05
(6,251)	1:59:A:HIS:HA	1:60:A:GLU:H	1	2.05
(6,16)	1:7:A:LEU:H	1:6:A:THR:HB	1	2.05
(4,287)	1:103:A:GLU:HA	1:105:A:ASN:H	1	2.05
(4,106)	1:40:A:THR:H	1:43:A:GLU:H	2	2.05
(7,345)	1:98:A:SER:HB2	1:98:A:SER:H	1	2.04
(7,345)	1:98:A:SER:HB3	1:98:A:SER:H	1	2.04
(7,338)	1:96:A:LEU:HA	1:96:A:LEU:H	2	2.04
(7,103)	1:28:A:THR:HB	1:28:A:THR:H	2	2.04
(7,58)	1:15:A:ASN:HB2	1:15:A:ASN:HD21	1	2.04
(7,58)	1:15:A:ASN:HB2	1:15:A:ASN:HD22	1	2.04
(7,57)	1:15:A:ASN:HB2	1:15:A:ASN:HD21	1	2.04
(7,57)	1:15:A:ASN:HB2	1:15:A:ASN:HD22	1	2.04
(4,263)	1:88:A:ARG:H	1:90:A:LEU:H	1	2.04
(6,239)	1:56:A:TYR:HB2	1:57:A:SER:H	1	2.03
(6,82)	1:19:A:GLU:H	1:18:A:THR:HB	1	2.03
(2,20)	1:105:A:ASN:HB2	1:34:A:ALA:H	1	2.03
(2,20)	1:105:A:ASN:HB3	1:34:A:ALA:H	1	2.03
(7,103)	1:28:A:THR:HB	1:28:A:THR:H	1	2.02
(6,321)	1:79:A:LEU:HB2	1:80:A:ILE:H	2	2.02
(6,321)	1:79:A:LEU:HB3	1:80:A:ILE:H	2	2.02
(6,190)	1:44:A:THR:HG21	1:45:A:PHE:H	1	2.02
(6,190)	1:44:A:THR:HG22	1:45:A:PHE:H	1	2.02
(6,190)	1:44:A:THR:HG23	1:45:A:PHE:H	1	2.02
(6,38)	1:11:A:ILE:H	1:10:A:ILE:HG12	2	2.02
(6,38)	1:11:A:ILE:H	1:10:A:ILE:HG13	2	2.02
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD11	1	2.02
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD12	1	2.02
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD13	1	2.02
(7,3)	1:3:A:THR:H	1:3:A:THR:HG21	1	2.01
(7,3)	1:3:A:THR:H	1:3:A:THR:HG22	1	2.01
(7,3)	1:3:A:THR:H	1:3:A:THR:HG23	1	2.01
(4,335)	1:119:A:ILE:H	1:121:A:ARG:H	1	2.01
(4,306)	1:110:A:GLU:H	1:112:A:PHE:H	1	2.01
(6,323)	1:79:A:LEU:HB2	1:80:A:ILE:H	2	2.0
(7,95)	1:25:A:THR:H	1:25:A:THR:HG21	2	1.98
(7,95)	1:25:A:THR:H	1:25:A:THR:HG22	2	1.98
(7,95)	1:25:A:THR:H	1:25:A:THR:HG23	2	1.98
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD11	2	1.98
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD12	2	1.98
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD13	2	1.98
(6,418)	1:100:A:PRO:HD2	1:99:A:CYS:H	2	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,133)	1:45:A:PHE:HA	1:48:A:ALA:H	2	1.98
(6,190)	1:44:A:THR:HG21	1:45:A:PHE:H	2	1.97
(6,190)	1:44:A:THR:HG22	1:45:A:PHE:H	2	1.97
(6,190)	1:44:A:THR:HG23	1:45:A:PHE:H	2	1.97
(4,317)	1:112:A:PHE:H	1:114:A:GLU:H	1	1.97
(4,288)	1:104:A:ALA:HB1	1:106:A:GLN:HE21	1	1.97
(4,288)	1:104:A:ALA:HB1	1:106:A:GLN:HE22	1	1.97
(4,288)	1:104:A:ALA:HB2	1:106:A:GLN:HE21	1	1.97
(4,288)	1:104:A:ALA:HB2	1:106:A:GLN:HE22	1	1.97
(4,288)	1:104:A:ALA:HB3	1:106:A:GLN:HE21	1	1.97
(4,288)	1:104:A:ALA:HB3	1:106:A:GLN:HE22	1	1.97
(7,309)	1:89:A:ASN:HA	1:89:A:ASN:HD21	2	1.96
(7,309)	1:89:A:ASN:HA	1:89:A:ASN:HD22	2	1.96
(7,86)	1:22:A:THR:H	1:22:A:THR:HG21	1	1.96
(7,86)	1:22:A:THR:H	1:22:A:THR:HG22	1	1.96
(7,86)	1:22:A:THR:H	1:22:A:THR:HG23	1	1.96
(6,452)	1:107:A:SER:H	1:108:A:THR:H	1	1.96
(4,173)	1:56:A:TYR:H	1:58:A:HIS:H	2	1.96
(4,140)	1:47:A:ARG:H	1:49:A:ALA:H	2	1.96
(7,136)	1:38:A:ASN:HB3	1:38:A:ASN:H	1	1.95
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD11	1	1.95
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD12	1	1.95
(7,40)	1:11:A:ILE:H	1:11:A:ILE:HD13	1	1.95
(6,537)	1:127:A:CYS:HB2	1:128:A:SER:H	1	1.95
(6,537)	1:127:A:CYS:HB3	1:128:A:SER:H	1	1.95
(4,325)	1:115:A:ARG:H	1:117:A:LYS:H	2	1.95
(4,313)	1:112:A:PHE:HB2	1:115:A:ARG:H	2	1.95
(4,313)	1:112:A:PHE:HB3	1:115:A:ARG:H	2	1.95
(4,224)	1:76:A:HIS:HB2	1:78:A:GLN:H	1	1.95
(4,224)	1:76:A:HIS:HB3	1:78:A:GLN:H	1	1.95
(2,8)	1:28:A:THR:HG21	1:108:A:THR:H	1	1.95
(2,8)	1:28:A:THR:HG22	1:108:A:THR:H	1	1.95
(2,8)	1:28:A:THR:HG23	1:108:A:THR:H	1	1.95
(7,444)	1:128:A:SER:HB3	1:128:A:SER:H	2	1.94
(7,9)	1:5:A:ILE:H	1:5:A:ILE:HG13	1	1.94
(6,38)	1:11:A:ILE:H	1:10:A:ILE:HG12	1	1.94
(6,38)	1:11:A:ILE:H	1:10:A:ILE:HG13	1	1.94
(4,325)	1:115:A:ARG:H	1:117:A:LYS:H	1	1.94
(4,289)	1:106:A:GLN:HB2	1:108:A:THR:H	2	1.94
(4,289)	1:106:A:GLN:HB3	1:108:A:THR:H	2	1.94
(4,313)	1:112:A:PHE:HB2	1:115:A:ARG:H	1	1.93
(4,313)	1:112:A:PHE:HB3	1:115:A:ARG:H	1	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,289)	1:106:A:GLN:HB2	1:108:A:THR:H	1	1.93
(4,289)	1:106:A:GLN:HB3	1:108:A:THR:H	1	1.93
(2,18)	1:8:A:GLN:H	1:124:A:TYR:HE1	1	1.93
(2,18)	1:8:A:GLN:H	1:124:A:TYR:HE2	1	1.93
(6,387)	1:91:A:TRP:H	1:92:A:GLY:H	2	1.92
(6,375)	1:89:A:ASN:HB2	1:90:A:LEU:H	1	1.92
(6,91)	1:20:A:GLN:HB3	1:21:A:LYS:H	1	1.92
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD11	1	1.92
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD12	1	1.92
(6,34)	1:10:A:ILE:H	1:11:A:ILE:HD13	1	1.92
(6,141)	1:32:A:ILE:HG12	1:33:A:PHE:H	2	1.91
(2,42)	1:30:A:THR:HA	1:106:A:GLN:HE21	1	1.91
(2,42)	1:30:A:THR:HA	1:106:A:GLN:HE22	1	1.91
(2,38)	1:56:A:TYR:HE1	1:87:A:ASP:H	1	1.91
(2,38)	1:56:A:TYR:HE2	1:87:A:ASP:H	1	1.91
(2,27)	1:96:A:LEU:HB2	1:46:A:CYS:H	1	1.91
(2,27)	1:96:A:LEU:HB3	1:46:A:CYS:H	1	1.91
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD21	2	1.9
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD22	2	1.9
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD23	2	1.9
(6,472)	1:112:A:PHE:HD1	1:111:A:ASN:H	2	1.9
(6,472)	1:112:A:PHE:HD2	1:111:A:ASN:H	2	1.9
(6,305)	1:74:A:HIS:HB2	1:75:A:ARG:H	1	1.9
(6,305)	1:74:A:HIS:HB3	1:75:A:ARG:H	1	1.9
(6,127)	1:29:A:VAL:HG21	1:30:A:THR:H	2	1.9
(6,127)	1:29:A:VAL:HG22	1:30:A:THR:H	2	1.9
(6,127)	1:29:A:VAL:HG23	1:30:A:THR:H	2	1.9
(6,109)	1:25:A:THR:H	1:24:A:CYS:HB2	2	1.9
(4,131)	1:45:A:PHE:H	1:47:A:ARG:H	2	1.9
(2,9)	1:29:A:VAL:H	1:109:A:LEU:H	1	1.9
(7,271)	1:80:A:ILE:HD11	1:80:A:ILE:H	1	1.89
(7,271)	1:80:A:ILE:HD12	1:80:A:ILE:H	1	1.89
(7,271)	1:80:A:ILE:HD13	1:80:A:ILE:H	1	1.89
(6,439)	1:106:A:GLN:HG2	1:105:A:ASN:H	2	1.89
(6,439)	1:106:A:GLN:HG3	1:105:A:ASN:H	2	1.89
(6,401)	1:95:A:GLY:HA2	1:96:A:LEU:H	2	1.89
(6,363)	1:86:A:LEU:HD21	1:87:A:ASP:H	2	1.89
(6,363)	1:86:A:LEU:HD22	1:87:A:ASP:H	2	1.89
(6,363)	1:86:A:LEU:HD23	1:87:A:ASP:H	2	1.89
(4,335)	1:119:A:ILE:H	1:121:A:ARG:H	2	1.89
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG21	2	1.89
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG22	2	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,15)	1:10:A:ILE:H	1:6:A:THR:HG23	2	1.89
(7,189)	1:55:A:PHE:HD1	1:55:A:PHE:H	2	1.88
(7,189)	1:55:A:PHE:HD2	1:55:A:PHE:H	2	1.88
(7,184)	1:54:A:GLN:HG2	1:54:A:GLN:H	1	1.88
(7,184)	1:54:A:GLN:HG3	1:54:A:GLN:H	1	1.88
(7,69)	1:18:A:THR:H	1:18:A:THR:HG21	2	1.88
(7,69)	1:18:A:THR:H	1:18:A:THR:HG22	2	1.88
(7,69)	1:18:A:THR:H	1:18:A:THR:HG23	2	1.88
(6,239)	1:56:A:TYR:HB2	1:57:A:SER:H	2	1.88
(6,92)	1:20:A:GLN:HB2	1:21:A:LYS:H	1	1.88
(4,173)	1:56:A:TYR:H	1:58:A:HIS:H	1	1.88
(7,120)	1:32:A:ILE:HD11	1:32:A:ILE:H	2	1.87
(7,120)	1:32:A:ILE:HD12	1:32:A:ILE:H	2	1.87
(7,120)	1:32:A:ILE:HD13	1:32:A:ILE:H	2	1.87
(7,119)	1:32:A:ILE:HG21	1:32:A:ILE:H	2	1.87
(7,119)	1:32:A:ILE:HG22	1:32:A:ILE:H	2	1.87
(7,119)	1:32:A:ILE:HG23	1:32:A:ILE:H	2	1.87
(6,401)	1:95:A:GLY:HA2	1:96:A:LEU:H	1	1.87
(6,280)	1:68:A:ALA:HB1	1:69:A:THR:H	2	1.87
(6,280)	1:68:A:ALA:HB2	1:69:A:THR:H	2	1.87
(6,280)	1:68:A:ALA:HB3	1:69:A:THR:H	2	1.87
(6,89)	1:20:A:GLN:HA	1:21:A:LYS:H	2	1.87
(4,300)	1:109:A:LEU:HD11	1:113:A:LEU:H	2	1.87
(4,300)	1:109:A:LEU:HD12	1:113:A:LEU:H	2	1.87
(4,300)	1:109:A:LEU:HD13	1:113:A:LEU:H	2	1.87
(6,406)	1:96:A:LEU:HA	1:97:A:ASN:H	2	1.86
(6,132)	1:31:A:ASP:HB3	1:32:A:ILE:H	1	1.86
(4,297)	1:108:A:THR:HA	1:110:A:GLU:H	2	1.86
(4,86)	1:31:A:ASP:HB3	1:34:A:ALA:H	1	1.86
(6,447)	1:106:A:GLN:HA	1:107:A:SER:H	1	1.85
(6,89)	1:20:A:GLN:HA	1:21:A:LYS:H	1	1.85
(6,535)	1:126:A:LYS:HA	1:127:A:CYS:H	2	1.84
(4,326)	1:116:A:LEU:H	1:118:A:THR:H	1	1.84
(7,189)	1:55:A:PHE:HD1	1:55:A:PHE:H	1	1.83
(7,189)	1:55:A:PHE:HD2	1:55:A:PHE:H	1	1.83
(7,168)	1:48:A:ALA:HB1	1:48:A:ALA:H	1	1.83
(7,168)	1:48:A:ALA:HB2	1:48:A:ALA:H	1	1.83
(7,168)	1:48:A:ALA:HB3	1:48:A:ALA:H	1	1.83
(4,214)	1:73:A:PHE:HA	1:75:A:ARG:H	1	1.83
(4,140)	1:47:A:ARG:H	1:49:A:ALA:H	1	1.83
(2,30)	1:29:A:VAL:HG11	1:56:A:TYR:H	2	1.83
(2,30)	1:29:A:VAL:HG12	1:56:A:TYR:H	2	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:29:A:VAL:HG13	1:56:A:TYR:H	2	1.83
(2,30)	1:29:A:VAL:HG21	1:56:A:TYR:H	2	1.83
(2,30)	1:29:A:VAL:HG22	1:56:A:TYR:H	2	1.83
(2,30)	1:29:A:VAL:HG23	1:56:A:TYR:H	2	1.83
(2,10)	1:28:A:THR:HA	1:109:A:LEU:H	1	1.83
(7,9)	1:5:A:ILE:H	1:5:A:ILE:HG13	2	1.82
(6,347)	1:83:A:LEU:HD21	1:84:A:LYS:H	2	1.82
(6,347)	1:83:A:LEU:HD22	1:84:A:LYS:H	2	1.82
(6,347)	1:83:A:LEU:HD23	1:84:A:LYS:H	2	1.82
(6,205)	1:46:A:CYS:HB3	1:47:A:ARG:H	1	1.82
(6,195)	1:44:A:THR:HG21	1:45:A:PHE:HD1	1	1.82
(6,195)	1:44:A:THR:HG21	1:45:A:PHE:HD2	1	1.82
(6,195)	1:44:A:THR:HG22	1:45:A:PHE:HD1	1	1.82
(6,195)	1:44:A:THR:HG22	1:45:A:PHE:HD2	1	1.82
(6,195)	1:44:A:THR:HG23	1:45:A:PHE:HD1	1	1.82
(6,195)	1:44:A:THR:HG23	1:45:A:PHE:HD2	1	1.82
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG21	1	1.82
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG22	1	1.82
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG23	1	1.82
(4,201)	1:70:A:ALA:HB1	1:73:A:PHE:H	2	1.82
(4,201)	1:70:A:ALA:HB2	1:73:A:PHE:H	2	1.82
(4,201)	1:70:A:ALA:HB3	1:73:A:PHE:H	2	1.82
(6,447)	1:106:A:GLN:HA	1:107:A:SER:H	2	1.81
(6,101)	1:23:A:LEU:HA	1:24:A:CYS:H	1	1.81
(4,304)	1:110:A:GLU:HA	1:112:A:PHE:H	2	1.81
(4,278)	1:94:A:ALA:H	1:96:A:LEU:H	2	1.81
(7,432)	1:124:A:TYR:HB3	1:124:A:TYR:H	1	1.8
(7,413)	1:119:A:ILE:HB	1:119:A:ILE:H	1	1.8
(7,220)	1:65:A:CYS:HB3	1:65:A:CYS:H	1	1.8
(7,140)	1:38:A:ASN:HD21	1:38:A:ASN:H	1	1.8
(7,140)	1:38:A:ASN:HD22	1:38:A:ASN:H	1	1.8
(4,320)	1:113:A:LEU:H	1:115:A:ARG:H	2	1.8
(4,204)	1:71:A:GLN:HG2	1:75:A:ARG:H	1	1.8
(4,204)	1:71:A:GLN:HG3	1:75:A:ARG:H	1	1.8
(7,361)	1:104:A:ALA:HB1	1:104:A:ALA:H	2	1.79
(7,361)	1:104:A:ALA:HB2	1:104:A:ALA:H	2	1.79
(7,361)	1:104:A:ALA:HB3	1:104:A:ALA:H	2	1.79
(7,158)	1:44:A:THR:HG21	1:44:A:THR:H	1	1.79
(7,158)	1:44:A:THR:HG22	1:44:A:THR:H	1	1.79
(7,158)	1:44:A:THR:HG23	1:44:A:THR:H	1	1.79
(7,147)	1:41:A:GLU:HB2	1:41:A:GLU:H	2	1.79
(7,147)	1:41:A:GLU:HB3	1:41:A:GLU:H	2	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,472)	1:112:A:PHE:HD1	1:111:A:ASN:H	1	1.79
(6,472)	1:112:A:PHE:HD2	1:111:A:ASN:H	1	1.79
(6,410)	1:97:A:ASN:H	1:98:A:SER:H	1	1.79
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD11	2	1.79
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD12	2	1.79
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD13	2	1.79
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD21	2	1.79
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD22	2	1.79
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD23	2	1.79
(4,339)	1:121:A:ARG:HA	1:123:A:LYS:H	2	1.79
(4,326)	1:116:A:LEU:H	1:118:A:THR:H	2	1.79
(4,133)	1:45:A:PHE:HA	1:48:A:ALA:H	1	1.79
(2,15)	1:120:A:MET:H	1:11:A:ILE:HG12	1	1.79
(2,15)	1:120:A:MET:H	1:11:A:ILE:HG13	1	1.79
(7,276)	1:82:A:PHE:HE1	1:82:A:PHE:H	1	1.78
(7,276)	1:82:A:PHE:HE2	1:82:A:PHE:H	1	1.78
(7,127)	1:34:A:ALA:HB1	1:34:A:ALA:H	1	1.78
(7,127)	1:34:A:ALA:HB2	1:34:A:ALA:H	1	1.78
(7,127)	1:34:A:ALA:HB3	1:34:A:ALA:H	1	1.78
(4,227)	1:77:A:LYS:HA	1:79:A:LEU:H	2	1.78
(4,185)	1:64:A:ARG:H	1:66:A:LEU:H	1	1.78
(7,293)	1:86:A:LEU:HB2	1:86:A:LEU:H	1	1.77
(7,293)	1:86:A:LEU:HB3	1:86:A:LEU:H	1	1.77
(7,168)	1:48:A:ALA:HB1	1:48:A:ALA:H	2	1.77
(7,168)	1:48:A:ALA:HB2	1:48:A:ALA:H	2	1.77
(7,168)	1:48:A:ALA:HB3	1:48:A:ALA:H	2	1.77
(7,158)	1:44:A:THR:HG21	1:44:A:THR:H	2	1.77
(7,158)	1:44:A:THR:HG22	1:44:A:THR:H	2	1.77
(7,158)	1:44:A:THR:HG23	1:44:A:THR:H	2	1.77
(6,448)	1:106:A:GLN:H	1:107:A:SER:H	1	1.77
(6,306)	1:74:A:HIS:HB2	1:75:A:ARG:H	1	1.77
(6,280)	1:68:A:ALA:HB1	1:69:A:THR:H	1	1.77
(6,280)	1:68:A:ALA:HB2	1:69:A:THR:H	1	1.77
(6,280)	1:68:A:ALA:HB3	1:69:A:THR:H	1	1.77
(6,260)	1:62:A:ASP:H	1:63:A:THR:H	1	1.77
(6,110)	1:24:A:CYS:HA	1:25:A:THR:H	1	1.77
(6,110)	1:24:A:CYS:HA	1:25:A:THR:H	2	1.77
(4,209)	1:72:A:GLN:HA	1:76:A:HIS:H	1	1.77
(4,94)	1:34:A:ALA:HB1	1:37:A:LYS:H	2	1.77
(4,94)	1:34:A:ALA:HB2	1:37:A:LYS:H	2	1.77
(4,94)	1:34:A:ALA:HB3	1:37:A:LYS:H	2	1.77
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD11	2	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD12	2	1.77
(4,26)	1:8:A:GLN:H	1:11:A:ILE:HD13	2	1.77
(7,426)	1:122:A:GLU:HB2	1:122:A:GLU:H	2	1.76
(7,426)	1:122:A:GLU:HB3	1:122:A:GLU:H	2	1.76
(7,411)	1:118:A:THR:HG21	1:118:A:THR:H	1	1.76
(7,411)	1:118:A:THR:HG22	1:118:A:THR:H	1	1.76
(7,411)	1:118:A:THR:HG23	1:118:A:THR:H	1	1.76
(7,339)	1:96:A:LEU:HB2	1:96:A:LEU:H	1	1.76
(7,339)	1:96:A:LEU:HB3	1:96:A:LEU:H	1	1.76
(7,194)	1:56:A:TYR:HB2	1:56:A:TYR:H	1	1.76
(7,194)	1:56:A:TYR:HB2	1:56:A:TYR:H	2	1.76
(7,173)	1:50:A:THR:HG21	1:50:A:THR:H	2	1.76
(7,173)	1:50:A:THR:HG22	1:50:A:THR:H	2	1.76
(7,173)	1:50:A:THR:HG23	1:50:A:THR:H	2	1.76
(7,127)	1:34:A:ALA:HB1	1:34:A:ALA:H	2	1.76
(7,127)	1:34:A:ALA:HB2	1:34:A:ALA:H	2	1.76
(7,127)	1:34:A:ALA:HB3	1:34:A:ALA:H	2	1.76
(6,101)	1:23:A:LEU:HA	1:24:A:CYS:H	2	1.76
(6,92)	1:20:A:GLN:HB2	1:21:A:LYS:H	2	1.76
(4,329)	1:117:A:LYS:H	1:119:A:ILE:H	2	1.76
(4,278)	1:94:A:ALA:H	1:96:A:LEU:H	1	1.76
(4,201)	1:70:A:ALA:HB1	1:73:A:PHE:H	1	1.76
(4,201)	1:70:A:ALA:HB2	1:73:A:PHE:H	1	1.76
(4,201)	1:70:A:ALA:HB3	1:73:A:PHE:H	1	1.76
(3,84)	1:29:A:VAL:N	1:107:A:SER:O	2	1.76
(2,15)	1:120:A:MET:H	1:11:A:ILE:HG12	2	1.76
(2,15)	1:120:A:MET:H	1:11:A:ILE:HG13	2	1.76
(7,305)	1:89:A:ASN:HD21	1:89:A:ASN:H	2	1.75
(7,173)	1:50:A:THR:HG21	1:50:A:THR:H	1	1.75
(7,173)	1:50:A:THR:HG22	1:50:A:THR:H	1	1.75
(7,173)	1:50:A:THR:HG23	1:50:A:THR:H	1	1.75
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD11	2	1.75
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD12	2	1.75
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD13	2	1.75
(4,42)	1:12:A:LYS:H	1:15:A:ASN:HB2	1	1.75
(4,42)	1:12:A:LYS:H	1:15:A:ASN:HB3	1	1.75
(7,185)	1:54:A:GLN:HB2	1:54:A:GLN:H	2	1.74
(7,185)	1:54:A:GLN:HB3	1:54:A:GLN:H	2	1.74
(7,137)	1:38:A:ASN:HB2	1:38:A:ASN:H	1	1.74
(7,69)	1:18:A:THR:H	1:18:A:THR:HG21	1	1.74
(7,69)	1:18:A:THR:H	1:18:A:THR:HG22	1	1.74
(7,69)	1:18:A:THR:H	1:18:A:THR:HG23	1	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,320)	1:113:A:LEU:H	1:115:A:ARG:H	1	1.74
(2,43)	1:30:A:THR:HG21	1:106:A:GLN:HE21	2	1.74
(2,43)	1:30:A:THR:HG21	1:106:A:GLN:HE22	2	1.74
(2,43)	1:30:A:THR:HG22	1:106:A:GLN:HE21	2	1.74
(2,43)	1:30:A:THR:HG22	1:106:A:GLN:HE22	2	1.74
(2,43)	1:30:A:THR:HG23	1:106:A:GLN:HE21	2	1.74
(2,43)	1:30:A:THR:HG23	1:106:A:GLN:HE22	2	1.74
(7,421)	1:120:A:MET:HB2	1:120:A:MET:H	2	1.73
(6,327)	1:80:A:ILE:HG21	1:79:A:LEU:H	2	1.73
(6,327)	1:80:A:ILE:HG22	1:79:A:LEU:H	2	1.73
(6,327)	1:80:A:ILE:HG23	1:79:A:LEU:H	2	1.73
(4,86)	1:31:A:ASP:HB3	1:34:A:ALA:H	2	1.73
(7,339)	1:96:A:LEU:HB2	1:96:A:LEU:H	2	1.72
(7,339)	1:96:A:LEU:HB3	1:96:A:LEU:H	2	1.72
(7,229)	1:68:A:ALA:HA	1:68:A:ALA:H	1	1.72
(7,73)	1:19:A:GLU:H	1:19:A:GLU:HG3	1	1.72
(6,531)	1:125:A:SER:HA	1:126:A:LYS:H	1	1.72
(6,428)	1:103:A:GLU:HG2	1:102:A:LYS:H	2	1.72
(6,428)	1:103:A:GLU:HG3	1:102:A:LYS:H	2	1.72
(6,319)	1:79:A:LEU:HB2	1:78:A:GLN:H	1	1.72
(6,319)	1:79:A:LEU:HB3	1:78:A:GLN:H	1	1.72
(6,126)	1:29:A:VAL:HG11	1:30:A:THR:H	2	1.72
(6,126)	1:29:A:VAL:HG12	1:30:A:THR:H	2	1.72
(6,126)	1:29:A:VAL:HG13	1:30:A:THR:H	2	1.72
(7,308)	1:89:A:ASN:HB2	1:89:A:ASN:H	1	1.71
(7,229)	1:68:A:ALA:HA	1:68:A:ALA:H	2	1.71
(6,308)	1:74:A:HIS:H	1:75:A:ARG:H	1	1.71
(4,342)	1:122:A:GLU:H	1:124:A:TYR:H	2	1.71
(4,336)	1:120:A:MET:HA	1:123:A:LYS:H	1	1.71
(4,304)	1:110:A:GLU:HA	1:112:A:PHE:H	1	1.71
(4,227)	1:77:A:LYS:HA	1:79:A:LEU:H	1	1.71
(4,94)	1:34:A:ALA:HB1	1:37:A:LYS:H	1	1.71
(4,94)	1:34:A:ALA:HB2	1:37:A:LYS:H	1	1.71
(4,94)	1:34:A:ALA:HB3	1:37:A:LYS:H	1	1.71
(4,2)	1:4:A:ASP:HA	1:6:A:THR:H	1	1.71
(7,344)	1:98:A:SER:HA	1:98:A:SER:H	1	1.7
(7,130)	1:36:A:SER:HA	1:36:A:SER:H	2	1.7
(6,535)	1:126:A:LYS:HA	1:127:A:CYS:H	1	1.7
(6,344)	1:83:A:LEU:HB3	1:84:A:LYS:H	2	1.7
(6,195)	1:44:A:THR:HG21	1:45:A:PHE:HD1	2	1.7
(6,195)	1:44:A:THR:HG21	1:45:A:PHE:HD2	2	1.7
(6,195)	1:44:A:THR:HG22	1:45:A:PHE:HD1	2	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,195)	1:44:A:THR:HG22	1:45:A:PHE:HD2	2	1.7
(6,195)	1:44:A:THR:HG23	1:45:A:PHE:HD1	2	1.7
(6,195)	1:44:A:THR:HG23	1:45:A:PHE:HD2	2	1.7
(6,13)	1:5:A:ILE:HD11	1:6:A:THR:H	2	1.7
(6,13)	1:5:A:ILE:HD12	1:6:A:THR:H	2	1.7
(6,13)	1:5:A:ILE:HD13	1:6:A:THR:H	2	1.7
(4,195)	1:72:A:GLN:HG2	1:69:A:THR:H	1	1.7
(7,441)	1:127:A:CYS:HA	1:127:A:CYS:H	1	1.69
(7,421)	1:120:A:MET:HB2	1:120:A:MET:H	1	1.69
(7,270)	1:80:A:ILE:HG21	1:80:A:ILE:H	2	1.69
(7,270)	1:80:A:ILE:HG22	1:80:A:ILE:H	2	1.69
(7,270)	1:80:A:ILE:HG23	1:80:A:ILE:H	2	1.69
(4,319)	1:113:A:LEU:HA	1:117:A:LYS:H	1	1.69
(4,144)	1:48:A:ALA:HA	1:51:A:VAL:H	1	1.69
(4,96)	1:34:A:ALA:HA	1:36:A:SER:H	2	1.69
(2,20)	1:105:A:ASN:HB2	1:34:A:ALA:H	2	1.69
(2,20)	1:105:A:ASN:HB3	1:34:A:ALA:H	2	1.69
(7,222)	1:66:A:LEU:HA	1:66:A:LEU:H	2	1.68
(7,120)	1:32:A:ILE:HD11	1:32:A:ILE:H	1	1.68
(7,120)	1:32:A:ILE:HD12	1:32:A:ILE:H	1	1.68
(7,120)	1:32:A:ILE:HD13	1:32:A:ILE:H	1	1.68
(7,70)	1:18:A:THR:H	1:18:A:THR:HB	2	1.68
(7,56)	1:15:A:ASN:HB3	1:15:A:ASN:HD21	1	1.68
(7,56)	1:15:A:ASN:HB3	1:15:A:ASN:HD22	1	1.68
(7,55)	1:15:A:ASN:HB3	1:15:A:ASN:HD21	1	1.68
(7,55)	1:15:A:ASN:HB3	1:15:A:ASN:HD22	1	1.68
(6,421)	1:101:A:VAL:HB	1:102:A:LYS:H	1	1.68
(6,409)	1:97:A:ASN:HA	1:98:A:SER:H	2	1.68
(7,327)	1:92:A:GLY:HA2	1:92:A:GLY:H	1	1.67
(7,228)	1:67:A:GLY:HA2	1:67:A:GLY:H	2	1.67
(6,331)	1:80:A:ILE:HG21	1:81:A:ARG:H	1	1.67
(6,331)	1:80:A:ILE:HG22	1:81:A:ARG:H	1	1.67
(6,331)	1:80:A:ILE:HG23	1:81:A:ARG:H	1	1.67
(6,329)	1:80:A:ILE:HB	1:81:A:ARG:H	2	1.67
(6,229)	1:54:A:GLN:HB2	1:55:A:PHE:H	2	1.67
(6,229)	1:54:A:GLN:HB3	1:55:A:PHE:H	2	1.67
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG21	2	1.67
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG22	2	1.67
(6,52)	1:14:A:LEU:H	1:13:A:THR:HG23	2	1.67
(4,202)	1:70:A:ALA:HB1	1:74:A:HIS:H	2	1.67
(4,202)	1:70:A:ALA:HB2	1:74:A:HIS:H	2	1.67
(4,202)	1:70:A:ALA:HB3	1:74:A:HIS:H	2	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:28:A:THR:HA	1:109:A:LEU:H	2	1.67
(7,380)	1:109:A:LEU:HB2	1:109:A:LEU:H	1	1.66
(7,352)	1:101:A:VAL:HG21	1:101:A:VAL:H	2	1.66
(7,352)	1:101:A:VAL:HG22	1:101:A:VAL:H	2	1.66
(7,352)	1:101:A:VAL:HG23	1:101:A:VAL:H	2	1.66
(6,503)	1:119:A:ILE:HG13	1:120:A:MET:H	2	1.66
(6,434)	1:103:A:GLU:H	1:104:A:ALA:H	2	1.66
(6,407)	1:96:A:LEU:H	1:97:A:ASN:H	1	1.66
(6,286)	1:70:A:ALA:HA	1:71:A:GLN:H	2	1.66
(6,251)	1:59:A:HIS:HA	1:60:A:GLU:H	2	1.66
(6,229)	1:54:A:GLN:HB2	1:55:A:PHE:H	1	1.66
(6,229)	1:54:A:GLN:HB3	1:55:A:PHE:H	1	1.66
(4,337)	1:120:A:MET:HA	1:122:A:GLU:H	1	1.66
(4,224)	1:76:A:HIS:HB2	1:78:A:GLN:H	2	1.66
(4,224)	1:76:A:HIS:HB3	1:78:A:GLN:H	2	1.66
(2,8)	1:28:A:THR:HG21	1:108:A:THR:H	2	1.66
(2,8)	1:28:A:THR:HG22	1:108:A:THR:H	2	1.66
(2,8)	1:28:A:THR:HG23	1:108:A:THR:H	2	1.66
(7,3)	1:3:A:THR:H	1:3:A:THR:HG21	2	1.65
(7,3)	1:3:A:THR:H	1:3:A:THR:HG22	2	1.65
(7,3)	1:3:A:THR:H	1:3:A:THR:HG23	2	1.65
(6,374)	1:89:A:ASN:HB3	1:90:A:LEU:H	2	1.65
(6,136)	1:32:A:ILE:HG12	1:31:A:ASP:H	2	1.65
(6,136)	1:32:A:ILE:HG13	1:31:A:ASP:H	2	1.65
(6,58)	1:15:A:ASN:HD21	1:14:A:LEU:HA	1	1.65
(6,58)	1:15:A:ASN:HD22	1:14:A:LEU:HA	1	1.65
(6,57)	1:15:A:ASN:HD21	1:14:A:LEU:HA	1	1.65
(6,57)	1:15:A:ASN:HD22	1:14:A:LEU:HA	1	1.65
(4,347)	1:124:A:TYR:HA	1:127:A:CYS:H	2	1.65
(4,302)	1:109:A:LEU:HA	1:112:A:PHE:H	1	1.65
(4,302)	1:109:A:LEU:HA	1:112:A:PHE:H	2	1.65
(4,61)	1:18:A:THR:HA	1:20:A:GLN:H	2	1.65
(7,426)	1:122:A:GLU:HB2	1:122:A:GLU:H	1	1.64
(7,426)	1:122:A:GLU:HB3	1:122:A:GLU:H	1	1.64
(6,428)	1:103:A:GLU:HG2	1:102:A:LYS:H	1	1.64
(6,428)	1:103:A:GLU:HG3	1:102:A:LYS:H	1	1.64
(6,244)	1:57:A:SER:HA	1:58:A:HIS:H	2	1.64
(6,125)	1:29:A:VAL:H	1:30:A:THR:H	1	1.64
(7,435)	1:125:A:SER:HB2	1:125:A:SER:H	2	1.63
(7,435)	1:125:A:SER:HB3	1:125:A:SER:H	2	1.63
(7,413)	1:119:A:ILE:HB	1:119:A:ILE:H	2	1.63
(7,155)	1:43:A:GLU:HG2	1:43:A:GLU:H	1	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,155)	1:43:A:GLU:HG3	1:43:A:GLU:H	1	1.63
(6,520)	1:124:A:TYR:HB3	1:123:A:LYS:H	1	1.63
(6,400)	1:95:A:GLY:HA3	1:96:A:LEU:H	1	1.63
(6,367)	1:87:A:ASP:HB2	1:88:A:ARG:H	1	1.63
(4,300)	1:109:A:LEU:HD11	1:113:A:LEU:H	1	1.63
(4,300)	1:109:A:LEU:HD12	1:113:A:LEU:H	1	1.63
(4,300)	1:109:A:LEU:HD13	1:113:A:LEU:H	1	1.63
(4,238)	1:80:A:ILE:HA	1:84:A:LYS:H	2	1.63
(4,11)	1:6:A:THR:H	1:8:A:GLN:H	1	1.63
(2,30)	1:29:A:VAL:HG11	1:56:A:TYR:H	1	1.63
(2,30)	1:29:A:VAL:HG12	1:56:A:TYR:H	1	1.63
(2,30)	1:29:A:VAL:HG13	1:56:A:TYR:H	1	1.63
(2,30)	1:29:A:VAL:HG21	1:56:A:TYR:H	1	1.63
(2,30)	1:29:A:VAL:HG22	1:56:A:TYR:H	1	1.63
(2,30)	1:29:A:VAL:HG23	1:56:A:TYR:H	1	1.63
(7,52)	1:15:A:ASN:H	1:15:A:ASN:HD22	1	1.62
(7,31)	1:9:A:GLU:H	1:9:A:GLU:HG2	2	1.62
(7,31)	1:9:A:GLU:H	1:9:A:GLU:HG3	2	1.62
(6,449)	1:107:A:SER:HB2	1:108:A:THR:H	1	1.62
(6,449)	1:107:A:SER:HB3	1:108:A:THR:H	1	1.62
(4,347)	1:124:A:TYR:HA	1:127:A:CYS:H	1	1.62
(4,329)	1:117:A:LYS:H	1:119:A:ILE:H	1	1.62
(4,294)	1:111:A:ASN:HB3	1:108:A:THR:H	2	1.62
(4,262)	1:87:A:ASP:H	1:89:A:ASN:H	2	1.62
(7,230)	1:68:A:ALA:HB1	1:68:A:ALA:H	2	1.61
(7,230)	1:68:A:ALA:HB2	1:68:A:ALA:H	2	1.61
(7,230)	1:68:A:ALA:HB3	1:68:A:ALA:H	2	1.61
(6,366)	1:87:A:ASP:HB3	1:88:A:ARG:H	2	1.61
(6,340)	1:82:A:PHE:HB3	1:83:A:LEU:H	1	1.61
(6,314)	1:76:A:HIS:HA	1:77:A:LYS:H	2	1.61
(6,286)	1:70:A:ALA:HA	1:71:A:GLN:H	1	1.61
(6,236)	1:56:A:TYR:HD1	1:57:A:SER:H	2	1.61
(6,236)	1:56:A:TYR:HD2	1:57:A:SER:H	2	1.61
(6,73)	1:17:A:LEU:HA	1:18:A:THR:H	2	1.61
(4,216)	1:74:A:HIS:HA	1:76:A:HIS:H	2	1.61
(7,147)	1:41:A:GLU:HB2	1:41:A:GLU:H	1	1.6
(7,147)	1:41:A:GLU:HB3	1:41:A:GLU:H	1	1.6
(7,58)	1:15:A:ASN:HB2	1:15:A:ASN:HD21	2	1.6
(7,58)	1:15:A:ASN:HB2	1:15:A:ASN:HD22	2	1.6
(7,57)	1:15:A:ASN:HB2	1:15:A:ASN:HD21	2	1.6
(7,57)	1:15:A:ASN:HB2	1:15:A:ASN:HD22	2	1.6
(6,443)	1:105:A:ASN:H	1:106:A:GLN:H	1	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,314)	1:76:A:HIS:HA	1:77:A:LYS:H	1	1.6
(4,310)	1:111:A:ASN:HA	1:114:A:GLU:H	1	1.6
(7,285)	1:83:A:LEU:HD21	1:83:A:LEU:H	2	1.59
(7,285)	1:83:A:LEU:HD22	1:83:A:LEU:H	2	1.59
(7,285)	1:83:A:LEU:HD23	1:83:A:LEU:H	2	1.59
(7,230)	1:68:A:ALA:HB1	1:68:A:ALA:H	1	1.59
(7,230)	1:68:A:ALA:HB2	1:68:A:ALA:H	1	1.59
(7,230)	1:68:A:ALA:HB3	1:68:A:ALA:H	1	1.59
(7,221)	1:65:A:CYS:HB2	1:65:A:CYS:H	1	1.59
(7,123)	1:33:A:PHE:HB2	1:33:A:PHE:H	1	1.59
(6,531)	1:125:A:SER:HA	1:126:A:LYS:H	2	1.59
(6,133)	1:31:A:ASP:HB2	1:32:A:ILE:H	1	1.59
(4,279)	1:96:A:LEU:HB2	1:98:A:SER:H	1	1.59
(4,279)	1:96:A:LEU:HB3	1:98:A:SER:H	1	1.59
(4,243)	1:82:A:PHE:HD1	1:85:A:ARG:H	2	1.59
(4,243)	1:82:A:PHE:HD2	1:85:A:ARG:H	2	1.59
(7,380)	1:109:A:LEU:HB2	1:109:A:LEU:H	2	1.58
(7,164)	1:46:A:CYS:HB3	1:46:A:CYS:H	2	1.58
(7,154)	1:43:A:GLU:HB2	1:43:A:GLU:H	2	1.58
(7,154)	1:43:A:GLU:HB3	1:43:A:GLU:H	2	1.58
(6,442)	1:105:A:ASN:HA	1:106:A:GLN:H	2	1.58
(6,400)	1:95:A:GLY:HA3	1:96:A:LEU:H	2	1.58
(6,236)	1:56:A:TYR:HD1	1:57:A:SER:H	1	1.58
(6,236)	1:56:A:TYR:HD2	1:57:A:SER:H	1	1.58
(6,127)	1:29:A:VAL:HG21	1:30:A:THR:H	1	1.58
(6,127)	1:29:A:VAL:HG22	1:30:A:THR:H	1	1.58
(6,127)	1:29:A:VAL:HG23	1:30:A:THR:H	1	1.58
(6,125)	1:29:A:VAL:H	1:30:A:THR:H	2	1.58
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD11	1	1.58
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD12	1	1.58
(6,106)	1:24:A:CYS:H	1:23:A:LEU:HD13	1	1.58
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG21	2	1.58
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG22	2	1.58
(6,43)	1:12:A:LYS:H	1:11:A:ILE:HG23	2	1.58
(4,336)	1:120:A:MET:HA	1:123:A:LYS:H	2	1.58
(4,333)	1:119:A:ILE:HA	1:122:A:GLU:H	1	1.58
(7,293)	1:86:A:LEU:HB2	1:86:A:LEU:H	2	1.57
(7,293)	1:86:A:LEU:HB3	1:86:A:LEU:H	2	1.57
(7,185)	1:54:A:GLN:HB2	1:54:A:GLN:H	1	1.57
(7,185)	1:54:A:GLN:HB3	1:54:A:GLN:H	1	1.57
(6,390)	1:92:A:GLY:H	1:93:A:LEU:H	1	1.57
(6,376)	1:89:A:ASN:HA	1:90:A:LEU:H	1	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,245)	1:82:A:PHE:HA	1:85:A:ARG:H	2	1.57
(7,145)	1:40:A:THR:HG21	1:40:A:THR:H	2	1.56
(7,145)	1:40:A:THR:HG22	1:40:A:THR:H	2	1.56
(7,145)	1:40:A:THR:HG23	1:40:A:THR:H	2	1.56
(6,335)	1:82:A:PHE:HD1	1:81:A:ARG:H	1	1.56
(6,335)	1:82:A:PHE:HD2	1:81:A:ARG:H	1	1.56
(6,281)	1:69:A:THR:HA	1:70:A:ALA:H	1	1.56
(6,73)	1:17:A:LEU:HA	1:18:A:THR:H	1	1.56
(4,265)	1:89:A:ASN:HA	1:92:A:GLY:H	1	1.56
(7,381)	1:109:A:LEU:HG	1:109:A:LEU:H	2	1.55
(7,281)	1:83:A:LEU:HB3	1:83:A:LEU:H	1	1.55
(6,244)	1:57:A:SER:HA	1:58:A:HIS:H	1	1.55
(6,240)	1:56:A:TYR:HA	1:57:A:SER:H	2	1.55
(6,44)	1:12:A:LYS:H	1:11:A:ILE:HG13	1	1.55
(5,3)	1:10:A:ILE:HA	1:14:A:LEU:H	1	1.55
(4,230)	1:78:A:GLN:HA	1:80:A:ILE:H	1	1.55
(4,10)	1:5:A:ILE:H	1:8:A:GLN:HB2	1	1.55
(4,10)	1:5:A:ILE:H	1:8:A:GLN:HB3	1	1.55
(7,435)	1:125:A:SER:HB2	1:125:A:SER:H	1	1.54
(7,435)	1:125:A:SER:HB3	1:125:A:SER:H	1	1.54
(6,398)	1:94:A:ALA:HA	1:95:A:GLY:H	1	1.54
(6,398)	1:94:A:ALA:HA	1:95:A:GLY:H	2	1.54
(6,238)	1:56:A:TYR:HB3	1:57:A:SER:H	1	1.54
(6,186)	1:43:A:GLU:HB2	1:44:A:THR:H	1	1.54
(6,186)	1:43:A:GLU:HB3	1:44:A:THR:H	1	1.54
(7,381)	1:109:A:LEU:HG	1:109:A:LEU:H	1	1.53
(7,97)	1:27:A:LEU:HB3	1:27:A:LEU:H	2	1.53
(6,498)	1:118:A:THR:HB	1:119:A:ILE:H	2	1.53
(6,407)	1:96:A:LEU:H	1:97:A:ASN:H	2	1.53
(6,240)	1:56:A:TYR:HA	1:57:A:SER:H	1	1.53
(4,250)	1:84:A:LYS:HA	1:86:A:LEU:H	2	1.53
(4,131)	1:45:A:PHE:H	1:47:A:ARG:H	1	1.53
(4,90)	1:32:A:ILE:HA	1:34:A:ALA:H	2	1.53
(7,165)	1:46:A:CYS:HB2	1:46:A:CYS:H	1	1.52
(7,122)	1:33:A:PHE:HB3	1:33:A:PHE:H	2	1.52
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD11	1	1.52
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD12	1	1.52
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD13	1	1.52
(7,31)	1:9:A:GLU:H	1:9:A:GLU:HG2	1	1.52
(7,31)	1:9:A:GLU:H	1:9:A:GLU:HG3	1	1.52
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD11	1	1.52
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD12	1	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD13	1	1.52
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD21	1	1.52
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD22	1	1.52
(6,383)	1:91:A:TRP:HE3	1:90:A:LEU:HD23	1	1.52
(6,321)	1:79:A:LEU:HB2	1:80:A:ILE:H	1	1.52
(6,321)	1:79:A:LEU:HB3	1:80:A:ILE:H	1	1.52
(6,18)	1:6:A:THR:H	1:7:A:LEU:HB2	2	1.52
(6,18)	1:6:A:THR:H	1:7:A:LEU:HB3	2	1.52
(4,316)	1:112:A:PHE:HA	1:115:A:ARG:H	1	1.52
(4,171)	1:56:A:TYR:HA	1:59:A:HIS:H	1	1.52
(7,132)	1:36:A:SER:HB2	1:36:A:SER:H	1	1.51
(7,97)	1:27:A:LEU:HB3	1:27:A:LEU:H	1	1.51
(7,76)	1:20:A:GLN:H	1:20:A:GLN:HB3	1	1.51
(7,23)	1:8:A:GLN:HG3	1:8:A:GLN:H	1	1.51
(6,473)	1:112:A:PHE:HB3	1:111:A:ASN:H	2	1.51
(6,372)	1:88:A:ARG:HA	1:89:A:ASN:HD21	1	1.51
(6,372)	1:88:A:ARG:HA	1:89:A:ASN:HD22	1	1.51
(6,230)	1:55:A:PHE:HB3	1:56:A:TYR:H	1	1.51
(6,118)	1:27:A:LEU:H	1:28:A:THR:H	1	1.51
(4,298)	1:108:A:THR:H	1:111:A:ASN:H	1	1.51
(4,119)	1:42:A:LYS:H	1:44:A:THR:H	2	1.51
(2,37)	1:56:A:TYR:HD1	1:84:A:LYS:H	2	1.51
(2,37)	1:56:A:TYR:HD2	1:84:A:LYS:H	2	1.51
(6,16)	1:7:A:LEU:H	1:6:A:THR:HB	2	1.5
(4,90)	1:32:A:ILE:HA	1:34:A:ALA:H	1	1.5
(6,348)	1:83:A:LEU:HA	1:84:A:LYS:H	2	1.49
(6,333)	1:80:A:ILE:HA	1:81:A:ARG:H	1	1.49
(4,214)	1:73:A:PHE:HA	1:75:A:ARG:H	2	1.49
(7,284)	1:83:A:LEU:HD11	1:83:A:LEU:H	1	1.48
(7,284)	1:83:A:LEU:HD12	1:83:A:LEU:H	1	1.48
(7,284)	1:83:A:LEU:HD13	1:83:A:LEU:H	1	1.48
(6,524)	1:123:A:LYS:H	1:124:A:TYR:H	1	1.48
(6,502)	1:119:A:ILE:HB	1:120:A:MET:H	1	1.48
(6,482)	1:113:A:LEU:HB2	1:114:A:GLU:H	2	1.48
(6,482)	1:113:A:LEU:HB3	1:114:A:GLU:H	2	1.48
(6,468)	1:110:A:GLU:HA	1:111:A:ASN:H	2	1.48
(6,336)	1:82:A:PHE:HB2	1:81:A:ARG:H	1	1.48
(6,336)	1:82:A:PHE:HB3	1:81:A:ARG:H	1	1.48
(6,214)	1:49:A:ALA:HA	1:50:A:THR:H	2	1.48
(6,211)	1:48:A:ALA:HA	1:49:A:ALA:H	2	1.48
(6,13)	1:5:A:ILE:HD11	1:6:A:THR:H	1	1.48
(6,13)	1:5:A:ILE:HD12	1:6:A:THR:H	1	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,13)	1:5:A:ILE:HD13	1:6:A:THR:H	1	1.48
(6,7)	1:5:A:ILE:H	1:4:A:ASP:HB2	2	1.48
(4,340)	1:121:A:ARG:HA	1:124:A:TYR:H	2	1.48
(4,244)	1:82:A:PHE:HA	1:84:A:LYS:H	2	1.48
(4,24)	1:8:A:GLN:HA	1:12:A:LYS:H	2	1.48
(4,10)	1:5:A:ILE:H	1:8:A:GLN:HB2	2	1.48
(4,10)	1:5:A:ILE:H	1:8:A:GLN:HB3	2	1.48
(4,9)	1:5:A:ILE:H	1:7:A:LEU:H	2	1.48
(7,323)	1:91:A:TRP:HD1	1:91:A:TRP:HB2	1	1.47
(7,308)	1:89:A:ASN:HB2	1:89:A:ASN:H	2	1.47
(6,511)	1:120:A:MET:HA	1:121:A:ARG:H	1	1.47
(6,495)	1:117:A:LYS:HA	1:118:A:THR:H	2	1.47
(6,493)	1:116:A:LEU:HA	1:117:A:LYS:H	1	1.47
(6,481)	1:113:A:LEU:HA	1:114:A:GLU:H	1	1.47
(6,468)	1:110:A:GLU:HA	1:111:A:ASN:H	1	1.47
(6,352)	1:85:A:ARG:HA	1:86:A:LEU:H	2	1.47
(6,325)	1:79:A:LEU:HA	1:80:A:ILE:H	1	1.47
(6,325)	1:79:A:LEU:HA	1:80:A:ILE:H	2	1.47
(6,234)	1:55:A:PHE:HA	1:56:A:TYR:H	1	1.47
(6,32)	1:10:A:ILE:HA	1:11:A:ILE:H	1	1.47
(4,58)	1:17:A:LEU:HA	1:19:A:GLU:H	2	1.47
(6,508)	1:119:A:ILE:HA	1:120:A:MET:H	2	1.46
(6,493)	1:116:A:LEU:HA	1:117:A:LYS:H	2	1.46
(6,479)	1:112:A:PHE:HA	1:113:A:LEU:H	1	1.46
(6,368)	1:87:A:ASP:HA	1:88:A:ARG:H	1	1.46
(6,342)	1:82:A:PHE:HA	1:83:A:LEU:H	2	1.46
(6,265)	1:64:A:ARG:HA	1:65:A:CYS:H	2	1.46
(6,263)	1:63:A:THR:HA	1:64:A:ARG:H	1	1.46
(6,247)	1:58:A:HIS:HA	1:59:A:HIS:H	2	1.46
(6,214)	1:49:A:ALA:HA	1:50:A:THR:H	1	1.46
(6,211)	1:48:A:ALA:HA	1:49:A:ALA:H	1	1.46
(6,207)	1:46:A:CYS:HA	1:47:A:ARG:H	1	1.46
(6,207)	1:46:A:CYS:HA	1:47:A:ARG:H	2	1.46
(6,32)	1:10:A:ILE:HA	1:11:A:ILE:H	2	1.46
(7,228)	1:67:A:GLY:HA2	1:67:A:GLY:H	1	1.45
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD11	2	1.45
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD12	2	1.45
(7,91)	1:23:A:LEU:H	1:23:A:LEU:HD13	2	1.45
(6,529)	1:124:A:TYR:H	1:125:A:SER:H	2	1.45
(6,528)	1:124:A:TYR:HA	1:125:A:SER:H	1	1.45
(6,523)	1:123:A:LYS:HA	1:124:A:TYR:H	2	1.45
(6,516)	1:121:A:ARG:HA	1:122:A:GLU:H	1	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,511)	1:120:A:MET:HA	1:121:A:ARG:H	2	1.45
(6,502)	1:119:A:ILE:HB	1:120:A:MET:H	2	1.45
(6,495)	1:117:A:LYS:HA	1:118:A:THR:H	1	1.45
(6,481)	1:113:A:LEU:HA	1:114:A:GLU:H	2	1.45
(6,442)	1:105:A:ASN:HA	1:106:A:GLN:H	1	1.45
(6,348)	1:83:A:LEU:HA	1:84:A:LYS:H	1	1.45
(6,234)	1:55:A:PHE:HA	1:56:A:TYR:H	2	1.45
(6,200)	1:45:A:PHE:HA	1:46:A:CYS:H	1	1.45
(6,59)	1:15:A:ASN:HA	1:16:A:SER:H	1	1.45
(4,322)	1:114:A:GLU:H	1:117:A:LYS:H	1	1.45
(4,318)	1:113:A:LEU:HA	1:116:A:LEU:H	1	1.45
(4,52)	1:15:A:ASN:HA	1:17:A:LEU:H	1	1.45
(4,40)	1:12:A:LYS:HA	1:16:A:SER:H	1	1.45
(7,145)	1:40:A:THR:HG21	1:40:A:THR:H	1	1.44
(7,145)	1:40:A:THR:HG22	1:40:A:THR:H	1	1.44
(7,145)	1:40:A:THR:HG23	1:40:A:THR:H	1	1.44
(7,100)	1:27:A:LEU:HD11	1:27:A:LEU:H	2	1.44
(7,100)	1:27:A:LEU:HD12	1:27:A:LEU:H	2	1.44
(7,100)	1:27:A:LEU:HD13	1:27:A:LEU:H	2	1.44
(6,536)	1:126:A:LYS:H	1:127:A:CYS:H	1	1.44
(6,528)	1:124:A:TYR:HA	1:125:A:SER:H	2	1.44
(6,516)	1:121:A:ARG:HA	1:122:A:GLU:H	2	1.44
(6,508)	1:119:A:ILE:HA	1:120:A:MET:H	1	1.44
(6,489)	1:115:A:ARG:HA	1:116:A:LEU:H	1	1.44
(6,489)	1:115:A:ARG:HA	1:116:A:LEU:H	2	1.44
(6,386)	1:91:A:TRP:HA	1:92:A:GLY:H	1	1.44
(6,368)	1:87:A:ASP:HA	1:88:A:ARG:H	2	1.44
(6,316)	1:77:A:LYS:HA	1:78:A:GLN:H	1	1.44
(6,316)	1:77:A:LYS:HA	1:78:A:GLN:H	2	1.44
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG21	1	1.44
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG22	1	1.44
(6,99)	1:23:A:LEU:H	1:22:A:THR:HG23	1	1.44
(6,59)	1:15:A:ASN:HA	1:16:A:SER:H	2	1.44
(6,2)	1:4:A:ASP:H	1:3:A:THR:HB	2	1.44
(4,322)	1:114:A:GLU:H	1:117:A:LYS:H	2	1.44
(7,220)	1:65:A:CYS:HB3	1:65:A:CYS:H	2	1.43
(7,164)	1:46:A:CYS:HB3	1:46:A:CYS:H	1	1.43
(7,154)	1:43:A:GLU:HB2	1:43:A:GLU:H	1	1.43
(7,154)	1:43:A:GLU:HB3	1:43:A:GLU:H	1	1.43
(6,523)	1:123:A:LYS:HA	1:124:A:TYR:H	1	1.43
(6,487)	1:114:A:GLU:HA	1:115:A:ARG:H	1	1.43
(6,487)	1:114:A:GLU:HA	1:115:A:ARG:H	2	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,448)	1:106:A:GLN:H	1:107:A:SER:H	2	1.43
(6,399)	1:94:A:ALA:H	1:95:A:GLY:H	1	1.43
(6,386)	1:91:A:TRP:HA	1:92:A:GLY:H	2	1.43
(6,336)	1:82:A:PHE:HB2	1:81:A:ARG:H	2	1.43
(6,336)	1:82:A:PHE:HB3	1:81:A:ARG:H	2	1.43
(6,333)	1:80:A:ILE:HA	1:81:A:ARG:H	2	1.43
(6,265)	1:64:A:ARG:HA	1:65:A:CYS:H	1	1.43
(6,247)	1:58:A:HIS:HA	1:59:A:HIS:H	1	1.43
(6,200)	1:45:A:PHE:HA	1:46:A:CYS:H	2	1.43
(7,70)	1:18:A:THR:H	1:18:A:THR:HB	1	1.42
(6,482)	1:113:A:LEU:HB2	1:114:A:GLU:H	1	1.42
(6,482)	1:113:A:LEU:HB3	1:114:A:GLU:H	1	1.42
(6,479)	1:112:A:PHE:HA	1:113:A:LEU:H	2	1.42
(6,352)	1:85:A:ARG:HA	1:86:A:LEU:H	1	1.42
(6,290)	1:71:A:GLN:HA	1:72:A:GLN:H	2	1.42
(6,285)	1:70:A:ALA:HB1	1:71:A:GLN:H	1	1.42
(6,285)	1:70:A:ALA:HB2	1:71:A:GLN:H	1	1.42
(6,285)	1:70:A:ALA:HB3	1:71:A:GLN:H	1	1.42
(6,281)	1:69:A:THR:HA	1:70:A:ALA:H	2	1.42
(6,165)	1:37:A:LYS:H	1:38:A:ASN:H	2	1.42
(6,102)	1:23:A:LEU:H	1:24:A:CYS:H	1	1.42
(4,337)	1:120:A:MET:HA	1:122:A:GLU:H	2	1.42
(4,301)	1:109:A:LEU:HD21	1:113:A:LEU:H	1	1.42
(4,301)	1:109:A:LEU:HD22	1:113:A:LEU:H	1	1.42
(4,301)	1:109:A:LEU:HD23	1:113:A:LEU:H	1	1.42
(4,193)	1:69:A:THR:H	1:73:A:PHE:H	2	1.42
(2,49)	1:10:A:ILE:HD11	1:89:A:ASN:H	2	1.42
(2,49)	1:10:A:ILE:HD12	1:89:A:ASN:H	2	1.42
(2,49)	1:10:A:ILE:HD13	1:89:A:ASN:H	2	1.42
(6,342)	1:82:A:PHE:HA	1:83:A:LEU:H	1	1.41
(6,290)	1:71:A:GLN:HA	1:72:A:GLN:H	1	1.41
(6,118)	1:27:A:LEU:H	1:28:A:THR:H	2	1.41
(6,80)	1:18:A:THR:H	1:19:A:GLU:H	2	1.41
(4,310)	1:111:A:ASN:HA	1:114:A:GLU:H	2	1.41
(4,250)	1:84:A:LYS:HA	1:86:A:LEU:H	1	1.41
(4,235)	1:82:A:PHE:HB2	1:79:A:LEU:H	2	1.41
(4,235)	1:82:A:PHE:HB3	1:79:A:LEU:H	2	1.41
(4,193)	1:69:A:THR:H	1:73:A:PHE:H	1	1.41
(4,126)	1:44:A:THR:HA	1:46:A:CYS:H	1	1.41
(4,52)	1:15:A:ASN:HA	1:17:A:LEU:H	2	1.41
(4,44)	1:13:A:THR:H	1:15:A:ASN:HB2	1	1.41
(4,44)	1:13:A:THR:H	1:15:A:ASN:HB3	1	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,236)	1:71:A:GLN:HB3	1:71:A:GLN:H	1	1.4
(7,137)	1:38:A:ASN:HB2	1:38:A:ASN:H	2	1.4
(6,382)	1:90:A:LEU:H	1:91:A:TRP:H	1	1.4
(6,376)	1:89:A:ASN:HA	1:90:A:LEU:H	2	1.4
(4,345)	1:123:A:LYS:H	1:125:A:SER:H	1	1.4
(4,194)	1:72:A:GLN:HG3	1:69:A:THR:H	2	1.4
(7,319)	1:91:A:TRP:HE3	1:91:A:TRP:HB3	2	1.39
(7,98)	1:27:A:LEU:HB2	1:27:A:LEU:H	2	1.39
(6,102)	1:23:A:LEU:H	1:24:A:CYS:H	2	1.39
(4,277)	1:94:A:ALA:HA	1:96:A:LEU:H	2	1.39
(7,445)	1:128:A:SER:HB2	1:128:A:SER:H	1	1.38
(7,390)	1:111:A:ASN:HD21	1:111:A:ASN:H	1	1.38
(7,390)	1:111:A:ASN:HD22	1:111:A:ASN:H	1	1.38
(7,390)	1:111:A:ASN:HD21	1:111:A:ASN:H	2	1.38
(7,390)	1:111:A:ASN:HD22	1:111:A:ASN:H	2	1.38
(7,379)	1:109:A:LEU:HB3	1:109:A:LEU:H	2	1.38
(6,524)	1:123:A:LYS:H	1:124:A:TYR:H	2	1.38
(6,509)	1:119:A:ILE:H	1:120:A:MET:H	2	1.38
(6,129)	1:30:A:THR:HB	1:31:A:ASP:H	2	1.38
(4,316)	1:112:A:PHE:HA	1:115:A:ARG:H	2	1.38
(4,106)	1:40:A:THR:H	1:43:A:GLU:H	1	1.38
(7,415)	1:119:A:ILE:HG12	1:119:A:ILE:H	2	1.37
(7,236)	1:71:A:GLN:HB3	1:71:A:GLN:H	2	1.37
(6,529)	1:124:A:TYR:H	1:125:A:SER:H	1	1.37
(6,308)	1:74:A:HIS:H	1:75:A:ARG:H	2	1.37
(6,230)	1:55:A:PHE:HB3	1:56:A:TYR:H	2	1.37
(6,186)	1:43:A:GLU:HB2	1:44:A:THR:H	2	1.37
(6,186)	1:43:A:GLU:HB3	1:44:A:THR:H	2	1.37
(4,233)	1:79:A:LEU:HA	1:83:A:LEU:H	2	1.37
(4,154)	1:52:A:LEU:HA	1:56:A:TYR:H	1	1.37
(4,119)	1:42:A:LYS:H	1:44:A:THR:H	1	1.37
(6,505)	1:119:A:ILE:HG21	1:120:A:MET:H	2	1.36
(6,365)	1:86:A:LEU:H	1:87:A:ASP:H	2	1.36
(7,323)	1:91:A:TRP:HD1	1:91:A:TRP:HB2	2	1.35
(7,155)	1:43:A:GLU:HG2	1:43:A:GLU:H	2	1.35
(7,155)	1:43:A:GLU:HG3	1:43:A:GLU:H	2	1.35
(6,509)	1:119:A:ILE:H	1:120:A:MET:H	1	1.35
(6,205)	1:46:A:CYS:HB3	1:47:A:ARG:H	2	1.35
(6,58)	1:15:A:ASN:HD21	1:14:A:LEU:HA	2	1.35
(6,58)	1:15:A:ASN:HD22	1:14:A:LEU:HA	2	1.35
(6,57)	1:15:A:ASN:HD21	1:14:A:LEU:HA	2	1.35
(6,57)	1:15:A:ASN:HD22	1:14:A:LEU:HA	2	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,104)	1:37:A:LYS:H	1:39:A:THR:H	1	1.35
(7,216)	1:63:A:THR:HB	1:63:A:THR:H	1	1.34
(7,165)	1:46:A:CYS:HB2	1:46:A:CYS:H	2	1.34
(6,480)	1:112:A:PHE:H	1:113:A:LEU:H	1	1.34
(6,473)	1:112:A:PHE:HB3	1:111:A:ASN:H	1	1.34
(6,469)	1:110:A:GLU:H	1:111:A:ASN:H	2	1.34
(6,285)	1:70:A:ALA:HB1	1:71:A:GLN:H	2	1.34
(6,285)	1:70:A:ALA:HB2	1:71:A:GLN:H	2	1.34
(6,285)	1:70:A:ALA:HB3	1:71:A:GLN:H	2	1.34
(4,318)	1:113:A:LEU:HA	1:116:A:LEU:H	2	1.34
(4,298)	1:108:A:THR:H	1:111:A:ASN:H	2	1.34
(4,221)	1:75:A:ARG:HA	1:77:A:LYS:H	1	1.34
(4,128)	1:44:A:THR:HA	1:47:A:ARG:H	2	1.34
(6,480)	1:112:A:PHE:H	1:113:A:LEU:H	2	1.33
(6,108)	1:25:A:THR:H	1:24:A:CYS:HB3	2	1.33
(4,327)	1:117:A:LYS:HA	1:120:A:MET:H	2	1.33
(4,252)	1:84:A:LYS:HA	1:88:A:ARG:H	1	1.33
(4,210)	1:72:A:GLN:H	1:74:A:HIS:H	1	1.33
(4,126)	1:44:A:THR:HA	1:46:A:CYS:H	2	1.33
(4,12)	1:6:A:THR:H	1:9:A:GLU:H	1	1.33
(7,327)	1:92:A:GLY:HA2	1:92:A:GLY:H	2	1.32
(7,209)	1:60:A:GLU:HG3	1:60:A:GLU:H	2	1.32
(7,134)	1:37:A:LYS:HB2	1:37:A:LYS:H	2	1.32
(7,134)	1:37:A:LYS:HB3	1:37:A:LYS:H	2	1.32
(6,469)	1:110:A:GLU:H	1:111:A:ASN:H	1	1.32
(6,264)	1:63:A:THR:H	1:64:A:ARG:H	1	1.32
(6,136)	1:32:A:ILE:HG12	1:31:A:ASP:H	1	1.32
(6,136)	1:32:A:ILE:HG13	1:31:A:ASP:H	1	1.32
(4,195)	1:72:A:GLN:HG2	1:69:A:THR:H	2	1.32
(4,117)	1:42:A:LYS:HA	1:44:A:THR:H	2	1.32
(7,266)	1:80:A:ILE:HA	1:80:A:ILE:H	2	1.31
(7,216)	1:63:A:THR:HB	1:63:A:THR:H	2	1.31
(7,134)	1:37:A:LYS:HB2	1:37:A:LYS:H	1	1.31
(7,134)	1:37:A:LYS:HB3	1:37:A:LYS:H	1	1.31
(6,238)	1:56:A:TYR:HB3	1:57:A:SER:H	2	1.31
(6,129)	1:30:A:THR:HB	1:31:A:ASP:H	1	1.31
(4,342)	1:122:A:GLU:H	1:124:A:TYR:H	1	1.31
(4,319)	1:113:A:LEU:HA	1:117:A:LYS:H	2	1.31
(7,422)	1:120:A:MET:HG3	1:120:A:MET:H	1	1.3
(4,294)	1:111:A:ASN:HB3	1:108:A:THR:H	1	1.3
(4,243)	1:82:A:PHE:HD1	1:85:A:ARG:H	1	1.3
(4,243)	1:82:A:PHE:HD2	1:85:A:ARG:H	1	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	1:28:A:THR:HG21	1:109:A:LEU:H	2	1.3
(2,11)	1:28:A:THR:HG22	1:109:A:LEU:H	2	1.3
(2,11)	1:28:A:THR:HG23	1:109:A:LEU:H	2	1.3
(7,375)	1:108:A:THR:HA	1:108:A:THR:H	1	1.29
(7,227)	1:67:A:GLY:HA3	1:67:A:GLY:H	2	1.29
(6,270)	1:65:A:CYS:HA	1:66:A:LEU:H	1	1.29
(6,45)	1:12:A:LYS:H	1:11:A:ILE:HG12	1	1.29
(6,6)	1:5:A:ILE:H	1:4:A:ASP:HB3	1	1.29
(7,434)	1:125:A:SER:HA	1:125:A:SER:H	2	1.28
(7,254)	1:76:A:HIS:HA	1:76:A:HIS:H	1	1.28
(7,100)	1:27:A:LEU:HD11	1:27:A:LEU:H	1	1.28
(7,100)	1:27:A:LEU:HD12	1:27:A:LEU:H	1	1.28
(7,100)	1:27:A:LEU:HD13	1:27:A:LEU:H	1	1.28
(6,293)	1:73:A:PHE:HA	1:72:A:GLN:H	2	1.28
(2,11)	1:28:A:THR:HG21	1:109:A:LEU:H	1	1.28
(2,11)	1:28:A:THR:HG22	1:109:A:LEU:H	1	1.28
(2,11)	1:28:A:THR:HG23	1:109:A:LEU:H	1	1.28
(7,378)	1:109:A:LEU:HA	1:109:A:LEU:H	1	1.27
(6,462)	1:109:A:LEU:H	1:110:A:GLU:H	2	1.27
(4,200)	1:70:A:ALA:HB1	1:72:A:GLN:H	2	1.27
(4,200)	1:70:A:ALA:HB2	1:72:A:GLN:H	2	1.27
(4,200)	1:70:A:ALA:HB3	1:72:A:GLN:H	2	1.27
(4,75)	1:25:A:THR:HA	1:27:A:LEU:H	2	1.27
(4,20)	1:7:A:LEU:HA	1:11:A:ILE:H	1	1.27
(7,446)	1:129:A:SER:HA	1:129:A:SER:H	2	1.26
(6,458)	1:109:A:LEU:HB2	1:110:A:GLU:H	2	1.26
(6,141)	1:32:A:ILE:HG12	1:33:A:PHE:H	1	1.26
(6,22)	1:7:A:LEU:HB2	1:8:A:GLN:H	2	1.26
(6,22)	1:7:A:LEU:HB3	1:8:A:GLN:H	2	1.26
(4,263)	1:88:A:ARG:H	1:90:A:LEU:H	2	1.26
(4,208)	1:72:A:GLN:HA	1:75:A:ARG:H	1	1.26
(4,154)	1:52:A:LEU:HA	1:56:A:TYR:H	2	1.26
(6,536)	1:126:A:LYS:H	1:127:A:CYS:H	2	1.25
(6,396)	1:93:A:LEU:H	1:94:A:ALA:H	1	1.25
(6,369)	1:87:A:ASP:H	1:88:A:ARG:H	1	1.25
(6,146)	1:34:A:ALA:HA	1:33:A:PHE:H	2	1.25
(4,301)	1:109:A:LEU:HD21	1:113:A:LEU:H	2	1.25
(4,301)	1:109:A:LEU:HD22	1:113:A:LEU:H	2	1.25
(4,301)	1:109:A:LEU:HD23	1:113:A:LEU:H	2	1.25
(4,171)	1:56:A:TYR:HA	1:59:A:HIS:H	2	1.25
(7,434)	1:125:A:SER:HA	1:125:A:SER:H	1	1.24
(7,423)	1:120:A:MET:HG2	1:120:A:MET:H	2	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD21	1	1.24
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD22	1	1.24
(7,92)	1:23:A:LEU:H	1:23:A:LEU:HD23	1	1.24
(6,365)	1:86:A:LEU:H	1:87:A:ASP:H	1	1.24
(6,304)	1:73:A:PHE:H	1:74:A:HIS:H	2	1.24
(4,144)	1:48:A:ALA:HA	1:51:A:VAL:H	2	1.24
(7,419)	1:120:A:MET:HA	1:120:A:MET:H	1	1.23
(7,311)	1:90:A:LEU:HA	1:90:A:LEU:H	2	1.23
(7,285)	1:83:A:LEU:HD21	1:83:A:LEU:H	1	1.23
(7,285)	1:83:A:LEU:HD22	1:83:A:LEU:H	1	1.23
(7,285)	1:83:A:LEU:HD23	1:83:A:LEU:H	1	1.23
(7,192)	1:56:A:TYR:HA	1:56:A:TYR:H	1	1.23
(6,464)	1:110:A:GLU:HB2	1:111:A:ASN:H	1	1.23
(4,92)	1:32:A:ILE:H	1:34:A:ALA:H	2	1.23
(7,423)	1:120:A:MET:HG2	1:120:A:MET:H	1	1.22
(7,166)	1:47:A:ARG:HA	1:47:A:ARG:H	1	1.22
(7,16)	1:7:A:LEU:HA	1:7:A:LEU:H	1	1.22
(6,438)	1:104:A:ALA:H	1:105:A:ASN:H	1	1.22
(6,341)	1:82:A:PHE:HB2	1:83:A:LEU:H	2	1.22
(6,257)	1:62:A:ASP:HB3	1:63:A:THR:H	2	1.22
(6,81)	1:18:A:THR:H	1:19:A:GLU:HB2	1	1.22
(6,81)	1:18:A:THR:H	1:19:A:GLU:HB3	1	1.22
(4,192)	1:69:A:THR:H	1:72:A:GLN:H	2	1.22
(4,137)	1:46:A:CYS:HB3	1:48:A:ALA:H	1	1.22
(4,12)	1:6:A:THR:H	1:9:A:GLU:H	2	1.22
(7,379)	1:109:A:LEU:HB3	1:109:A:LEU:H	1	1.21
(7,241)	1:72:A:GLN:HG3	1:72:A:GLN:H	2	1.21
(7,167)	1:48:A:ALA:HA	1:48:A:ALA:H	1	1.21
(7,101)	1:27:A:LEU:HD21	1:27:A:LEU:H	2	1.21
(7,101)	1:27:A:LEU:HD22	1:27:A:LEU:H	2	1.21
(7,101)	1:27:A:LEU:HD23	1:27:A:LEU:H	2	1.21
(6,521)	1:124:A:TYR:HB2	1:123:A:LYS:H	2	1.21
(4,244)	1:82:A:PHE:HA	1:84:A:LYS:H	1	1.21
(4,117)	1:42:A:LYS:HA	1:44:A:THR:H	1	1.21
(4,37)	1:11:A:ILE:HA	1:15:A:ASN:H	1	1.21
(7,405)	1:116:A:LEU:HA	1:116:A:LEU:H	1	1.2
(7,280)	1:83:A:LEU:HA	1:83:A:LEU:H	1	1.2
(7,192)	1:56:A:TYR:HA	1:56:A:TYR:H	2	1.2
(4,234)	1:82:A:PHE:HD1	1:79:A:LEU:H	1	1.2
(4,234)	1:82:A:PHE:HD2	1:79:A:LEU:H	1	1.2
(4,122)	1:43:A:GLU:HB2	1:45:A:PHE:H	2	1.2
(4,122)	1:43:A:GLU:HB3	1:45:A:PHE:H	2	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,11)	1:6:A:THR:H	1:8:A:GLN:H	2	1.2
(7,405)	1:116:A:LEU:HA	1:116:A:LEU:H	2	1.19
(7,397)	1:113:A:LEU:HA	1:113:A:LEU:H	1	1.19
(7,378)	1:109:A:LEU:HA	1:109:A:LEU:H	2	1.19
(7,280)	1:83:A:LEU:HA	1:83:A:LEU:H	2	1.19
(4,287)	1:103:A:GLU:HA	1:105:A:ASN:H	2	1.19
(4,122)	1:43:A:GLU:HB2	1:45:A:PHE:H	1	1.19
(4,122)	1:43:A:GLU:HB3	1:45:A:PHE:H	1	1.19
(2,5)	1:31:A:ASP:H	1:106:A:GLN:HE21	1	1.19
(2,5)	1:31:A:ASP:H	1:106:A:GLN:HE22	1	1.19
(7,424)	1:121:A:ARG:HA	1:121:A:ARG:H	1	1.18
(7,424)	1:121:A:ARG:HA	1:121:A:ARG:H	2	1.18
(7,397)	1:113:A:LEU:HA	1:113:A:LEU:H	2	1.18
(7,215)	1:63:A:THR:HA	1:63:A:THR:H	1	1.18
(7,130)	1:36:A:SER:HA	1:36:A:SER:H	1	1.18
(7,73)	1:19:A:GLU:H	1:19:A:GLU:HG3	2	1.18
(6,319)	1:79:A:LEU:HB2	1:78:A:GLN:H	2	1.18
(6,319)	1:79:A:LEU:HB3	1:78:A:GLN:H	2	1.18
(4,330)	1:118:A:THR:HA	1:121:A:ARG:H	2	1.18
(4,327)	1:117:A:LYS:HA	1:120:A:MET:H	1	1.18
(4,130)	1:44:A:THR:H	1:47:A:ARG:H	2	1.18
(4,127)	1:44:A:THR:HB	1:46:A:CYS:H	1	1.18
(2,9)	1:29:A:VAL:H	1:109:A:LEU:H	2	1.18
(7,402)	1:114:A:GLU:HA	1:114:A:GLU:H	1	1.17
(7,306)	1:89:A:ASN:HD22	1:89:A:ASN:H	2	1.17
(7,85)	1:22:A:THR:H	1:22:A:THR:HA	1	1.17
(7,37)	1:11:A:ILE:H	1:11:A:ILE:HG13	2	1.17
(6,464)	1:110:A:GLU:HB2	1:111:A:ASN:H	2	1.17
(6,389)	1:92:A:GLY:HA2	1:93:A:LEU:H	1	1.17
(6,301)	1:73:A:PHE:HB2	1:74:A:HIS:H	2	1.17
(7,402)	1:114:A:GLU:HA	1:114:A:GLU:H	2	1.16
(7,167)	1:48:A:ALA:HA	1:48:A:ALA:H	2	1.16
(7,106)	1:29:A:VAL:HB	1:29:A:VAL:H	2	1.16
(6,406)	1:96:A:LEU:HA	1:97:A:ASN:H	1	1.16
(6,255)	1:61:A:LYS:HA	1:62:A:ASP:H	2	1.16
(4,207)	1:72:A:GLN:HA	1:74:A:HIS:H	1	1.16
(7,446)	1:129:A:SER:HA	1:129:A:SER:H	1	1.15
(7,436)	1:126:A:LYS:HA	1:126:A:LYS:H	2	1.15
(7,430)	1:124:A:TYR:HA	1:124:A:TYR:H	1	1.15
(7,311)	1:90:A:LEU:HA	1:90:A:LEU:H	1	1.15
(7,93)	1:25:A:THR:H	1:25:A:THR:HA	2	1.15
(7,16)	1:7:A:LEU:HA	1:7:A:LEU:H	2	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,1)	1:3:A:THR:HA	1:3:A:THR:H	2	1.15
(6,382)	1:90:A:LEU:H	1:91:A:TRP:H	2	1.15
(6,104)	1:24:A:CYS:H	1:23:A:LEU:HB3	2	1.15
(4,333)	1:119:A:ILE:HA	1:122:A:GLU:H	2	1.15
(4,245)	1:82:A:PHE:HA	1:85:A:ARG:H	1	1.15
(7,436)	1:126:A:LYS:HA	1:126:A:LYS:H	1	1.14
(7,419)	1:120:A:MET:HA	1:120:A:MET:H	2	1.14
(7,375)	1:108:A:THR:HA	1:108:A:THR:H	2	1.14
(7,166)	1:47:A:ARG:HA	1:47:A:ARG:H	2	1.14
(6,532)	1:125:A:SER:H	1:126:A:LYS:H	2	1.14
(6,462)	1:109:A:LEU:H	1:110:A:GLU:H	1	1.14
(6,399)	1:94:A:ALA:H	1:95:A:GLY:H	2	1.14
(6,301)	1:73:A:PHE:HB2	1:74:A:HIS:H	1	1.14
(4,235)	1:82:A:PHE:HB2	1:79:A:LEU:H	1	1.14
(4,235)	1:82:A:PHE:HB3	1:79:A:LEU:H	1	1.14
(4,215)	1:73:A:PHE:H	1:75:A:ARG:H	1	1.14
(7,266)	1:80:A:ILE:HA	1:80:A:ILE:H	1	1.13
(6,504)	1:119:A:ILE:HG12	1:120:A:MET:H	1	1.13
(6,466)	1:111:A:ASN:HB3	1:110:A:GLU:H	1	1.13
(6,396)	1:93:A:LEU:H	1:94:A:ALA:H	2	1.13
(6,374)	1:89:A:ASN:HB3	1:90:A:LEU:H	1	1.13
(4,212)	1:72:A:GLN:H	1:75:A:ARG:H	1	1.13
(4,145)	1:48:A:ALA:HA	1:52:A:LEU:H	1	1.13
(7,415)	1:119:A:ILE:HG12	1:119:A:ILE:H	1	1.12
(7,357)	1:103:A:GLU:HA	1:103:A:GLU:H	2	1.12
(7,212)	1:62:A:ASP:HA	1:62:A:ASP:H	1	1.12
(6,532)	1:125:A:SER:H	1:126:A:LYS:H	1	1.12
(6,458)	1:109:A:LEU:HB2	1:110:A:GLU:H	1	1.12
(4,246)	1:82:A:PHE:HA	1:86:A:LEU:H	1	1.12
(7,254)	1:76:A:HIS:HA	1:76:A:HIS:H	2	1.11
(7,133)	1:37:A:LYS:HA	1:37:A:LYS:H	1	1.11
(7,133)	1:37:A:LYS:HA	1:37:A:LYS:H	2	1.11
(7,101)	1:27:A:LEU:HD21	1:27:A:LEU:H	1	1.11
(7,101)	1:27:A:LEU:HD22	1:27:A:LEU:H	1	1.11
(7,101)	1:27:A:LEU:HD23	1:27:A:LEU:H	1	1.11
(6,306)	1:74:A:HIS:HB2	1:75:A:ARG:H	2	1.11
(6,257)	1:62:A:ASP:HB3	1:63:A:THR:H	1	1.11
(4,130)	1:44:A:THR:H	1:47:A:ARG:H	1	1.11
(7,430)	1:124:A:TYR:HA	1:124:A:TYR:H	2	1.1
(7,373)	1:107:A:SER:HA	1:107:A:SER:H	1	1.1
(7,326)	1:92:A:GLY:HA3	1:92:A:GLY:H	1	1.1
(7,324)	1:91:A:TRP:HE3	1:91:A:TRP:H	2	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,319)	1:91:A:TRP:HE3	1:91:A:TRP:HB3	1	1.1
(7,135)	1:38:A:ASN:HA	1:38:A:ASN:H	1	1.1
(7,135)	1:38:A:ASN:HA	1:38:A:ASN:H	2	1.1
(7,72)	1:19:A:GLU:H	1:19:A:GLU:HB2	2	1.1
(7,72)	1:19:A:GLU:H	1:19:A:GLU:HB3	2	1.1
(6,466)	1:111:A:ASN:HB3	1:110:A:GLU:H	2	1.1
(4,346)	1:123:A:LYS:H	1:126:A:LYS:H	2	1.1
(7,326)	1:92:A:GLY:HA3	1:92:A:GLY:H	2	1.09
(7,231)	1:69:A:THR:HA	1:69:A:THR:H	1	1.09
(7,118)	1:32:A:ILE:HG12	1:32:A:ILE:H	2	1.09
(7,1)	1:3:A:THR:HA	1:3:A:THR:H	1	1.09
(6,202)	1:46:A:CYS:H	1:45:A:PHE:HB3	2	1.09
(6,139)	1:32:A:ILE:HB	1:33:A:PHE:H	2	1.09
(4,286)	1:103:A:GLU:HG2	1:105:A:ASN:H	1	1.09
(4,286)	1:103:A:GLU:HG3	1:105:A:ASN:H	1	1.09
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB1	2	1.09
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB2	2	1.09
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB3	2	1.09
(7,445)	1:128:A:SER:HB2	1:128:A:SER:H	2	1.08
(7,222)	1:66:A:LEU:HA	1:66:A:LEU:H	1	1.08
(7,215)	1:63:A:THR:HA	1:63:A:THR:H	2	1.08
(7,208)	1:60:A:GLU:HB2	1:60:A:GLU:H	1	1.08
(7,208)	1:60:A:GLU:HB3	1:60:A:GLU:H	1	1.08
(7,143)	1:39:A:THR:HG21	1:39:A:THR:H	1	1.08
(7,143)	1:39:A:THR:HG22	1:39:A:THR:H	1	1.08
(7,143)	1:39:A:THR:HG23	1:39:A:THR:H	1	1.08
(6,477)	1:112:A:PHE:HB2	1:113:A:LEU:H	2	1.08
(6,471)	1:111:A:ASN:HB2	1:112:A:PHE:H	1	1.08
(6,459)	1:109:A:LEU:HG	1:110:A:GLU:H	2	1.08
(4,332)	1:119:A:ILE:HD11	1:121:A:ARG:H	2	1.08
(4,332)	1:119:A:ILE:HD12	1:121:A:ARG:H	2	1.08
(4,332)	1:119:A:ILE:HD13	1:121:A:ARG:H	2	1.08
(4,323)	1:114:A:GLU:HA	1:118:A:THR:H	1	1.08
(4,178)	1:59:A:HIS:HA	1:62:A:ASP:H	2	1.08
(4,145)	1:48:A:ALA:HA	1:52:A:LEU:H	2	1.08
(2,35)	1:69:A:THR:HG21	1:76:A:HIS:H	2	1.08
(2,35)	1:69:A:THR:HG22	1:76:A:HIS:H	2	1.08
(2,35)	1:69:A:THR:HG23	1:76:A:HIS:H	2	1.08
(7,98)	1:27:A:LEU:HB2	1:27:A:LEU:H	1	1.07
(6,503)	1:119:A:ILE:HG13	1:120:A:MET:H	1	1.07
(6,435)	1:104:A:ALA:HB1	1:105:A:ASN:H	2	1.07
(6,435)	1:104:A:ALA:HB2	1:105:A:ASN:H	2	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,435)	1:104:A:ALA:HB3	1:105:A:ASN:H	2	1.07
(6,304)	1:73:A:PHE:H	1:74:A:HIS:H	1	1.07
(6,223)	1:51:A:VAL:HG21	1:52:A:LEU:H	2	1.07
(6,223)	1:51:A:VAL:HG22	1:52:A:LEU:H	2	1.07
(6,223)	1:51:A:VAL:HG23	1:52:A:LEU:H	2	1.07
(4,246)	1:82:A:PHE:HA	1:86:A:LEU:H	2	1.07
(4,233)	1:79:A:LEU:HA	1:83:A:LEU:H	1	1.07
(4,207)	1:72:A:GLN:HA	1:74:A:HIS:H	2	1.07
(4,105)	1:39:A:THR:HG21	1:43:A:GLU:H	2	1.07
(4,105)	1:39:A:THR:HG22	1:43:A:GLU:H	2	1.07
(4,105)	1:39:A:THR:HG23	1:43:A:GLU:H	2	1.07
(7,93)	1:25:A:THR:H	1:25:A:THR:HA	1	1.06
(6,269)	1:65:A:CYS:HB2	1:66:A:LEU:H	2	1.06
(6,203)	1:46:A:CYS:H	1:45:A:PHE:HB2	2	1.06
(4,323)	1:114:A:GLU:HA	1:118:A:THR:H	2	1.06
(4,221)	1:75:A:ARG:HA	1:77:A:LYS:H	2	1.06
(4,44)	1:13:A:THR:H	1:15:A:ASN:HB2	2	1.06
(4,44)	1:13:A:THR:H	1:15:A:ASN:HB3	2	1.06
(7,269)	1:80:A:ILE:HG12	1:80:A:ILE:H	1	1.05
(7,112)	1:31:A:ASP:HA	1:31:A:ASP:H	1	1.05
(4,136)	1:49:A:ALA:H	1:45:A:PHE:HE1	2	1.05
(4,136)	1:49:A:ALA:H	1:45:A:PHE:HE2	2	1.05
(4,128)	1:44:A:THR:HA	1:47:A:ARG:H	1	1.05
(4,107)	1:40:A:THR:HA	1:42:A:LYS:H	1	1.05
(7,441)	1:127:A:CYS:HA	1:127:A:CYS:H	2	1.04
(7,358)	1:103:A:GLU:HB2	1:103:A:GLU:H	1	1.04
(7,358)	1:103:A:GLU:HB3	1:103:A:GLU:H	1	1.04
(7,239)	1:71:A:GLN:HE21	1:71:A:GLN:H	1	1.04
(7,239)	1:71:A:GLN:HE22	1:71:A:GLN:H	1	1.04
(7,212)	1:62:A:ASP:HA	1:62:A:ASP:H	2	1.04
(7,85)	1:22:A:THR:H	1:22:A:THR:HA	2	1.04
(6,174)	1:39:A:THR:HG21	1:40:A:THR:H	2	1.04
(6,174)	1:39:A:THR:HG22	1:40:A:THR:H	2	1.04
(6,174)	1:39:A:THR:HG23	1:40:A:THR:H	2	1.04
(5,3)	1:10:A:ILE:HA	1:14:A:LEU:H	2	1.04
(4,228)	1:77:A:LYS:HA	1:81:A:ARG:H	2	1.04
(4,200)	1:70:A:ALA:HB1	1:72:A:GLN:H	1	1.04
(4,200)	1:70:A:ALA:HB2	1:72:A:GLN:H	1	1.04
(4,200)	1:70:A:ALA:HB3	1:72:A:GLN:H	1	1.04
(4,78)	1:27:A:LEU:HB2	1:29:A:VAL:H	2	1.04
(4,78)	1:27:A:LEU:HB3	1:29:A:VAL:H	2	1.04
(4,2)	1:4:A:ASP:HA	1:6:A:THR:H	2	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:94:A:ALA:HA	1:46:A:CYS:H	1	1.04
(7,422)	1:120:A:MET:HG3	1:120:A:MET:H	2	1.03
(7,357)	1:103:A:GLU:HA	1:103:A:GLU:H	1	1.03
(7,306)	1:89:A:ASN:HD22	1:89:A:ASN:H	1	1.03
(7,227)	1:67:A:GLY:HA3	1:67:A:GLY:H	1	1.03
(7,144)	1:40:A:THR:HA	1:40:A:THR:H	2	1.03
(7,112)	1:31:A:ASP:HA	1:31:A:ASP:H	2	1.03
(7,105)	1:29:A:VAL:HA	1:29:A:VAL:H	2	1.03
(4,137)	1:46:A:CYS:HB3	1:48:A:ALA:H	2	1.03
(7,373)	1:107:A:SER:HA	1:107:A:SER:H	2	1.02
(7,344)	1:98:A:SER:HA	1:98:A:SER:H	2	1.02
(7,231)	1:69:A:THR:HA	1:69:A:THR:H	2	1.02
(7,144)	1:40:A:THR:HA	1:40:A:THR:H	1	1.02
(7,105)	1:29:A:VAL:HA	1:29:A:VAL:H	1	1.02
(6,477)	1:112:A:PHE:HB2	1:113:A:LEU:H	1	1.02
(6,369)	1:87:A:ASP:H	1:88:A:ARG:H	2	1.02
(4,143)	1:48:A:ALA:H	1:50:A:THR:H	2	1.02
(4,107)	1:40:A:THR:HA	1:42:A:LYS:H	2	1.02
(4,286)	1:103:A:GLU:HG2	1:105:A:ASN:H	2	1.01
(4,286)	1:103:A:GLU:HG3	1:105:A:ASN:H	2	1.01
(4,127)	1:44:A:THR:HB	1:46:A:CYS:H	2	1.01
(4,89)	1:32:A:ILE:HB	1:34:A:ALA:H	2	1.01
(4,20)	1:7:A:LEU:HA	1:11:A:ILE:H	2	1.01
(7,414)	1:119:A:ILE:HG13	1:119:A:ILE:H	1	1.0
(7,72)	1:19:A:GLU:H	1:19:A:GLU:HB2	1	1.0
(7,72)	1:19:A:GLU:H	1:19:A:GLU:HB3	1	1.0
(4,346)	1:123:A:LYS:H	1:126:A:LYS:H	1	1.0
(4,53)	1:15:A:ASN:H	1:17:A:LEU:H	1	1.0
(7,324)	1:91:A:TRP:HE3	1:91:A:TRP:H	1	0.99
(6,504)	1:119:A:ILE:HG12	1:120:A:MET:H	2	0.99
(6,389)	1:92:A:GLY:HA2	1:93:A:LEU:H	2	0.99
(6,108)	1:25:A:THR:H	1:24:A:CYS:HB3	1	0.99
(4,113)	1:43:A:GLU:HB3	1:40:A:THR:H	2	0.99
(4,48)	1:14:A:LEU:HA	1:17:A:LEU:H	2	0.99
(2,4)	1:31:A:ASP:H	1:106:A:GLN:HB2	2	0.99
(2,4)	1:31:A:ASP:H	1:106:A:GLN:HB3	2	0.99
(7,238)	1:71:A:GLN:HG2	1:71:A:GLN:H	2	0.98
(7,238)	1:71:A:GLN:HG3	1:71:A:GLN:H	2	0.98
(7,88)	1:23:A:LEU:H	1:23:A:LEU:HG	2	0.98
(6,294)	1:73:A:PHE:HB3	1:72:A:GLN:H	2	0.98
(4,208)	1:72:A:GLN:HA	1:75:A:ARG:H	2	0.98
(7,363)	1:105:A:ASN:HB3	1:105:A:ASN:H	1	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,139)	1:32:A:ILE:HB	1:33:A:PHE:H	1	0.97
(6,98)	1:22:A:THR:H	1:23:A:LEU:H	1	0.97
(6,35)	1:10:A:ILE:H	1:11:A:ILE:HG12	1	0.97
(6,35)	1:10:A:ILE:H	1:11:A:ILE:HG13	1	0.97
(4,273)	1:92:A:GLY:HA3	1:94:A:ALA:H	1	0.97
(4,248)	1:83:A:LEU:H	1:85:A:ARG:H	2	0.97
(4,92)	1:32:A:ILE:H	1:34:A:ALA:H	1	0.97
(7,238)	1:71:A:GLN:HG2	1:71:A:GLN:H	1	0.96
(7,238)	1:71:A:GLN:HG3	1:71:A:GLN:H	1	0.96
(6,159)	1:36:A:SER:HB3	1:37:A:LYS:H	2	0.96
(6,18)	1:6:A:THR:H	1:7:A:LEU:HB2	1	0.96
(6,18)	1:6:A:THR:H	1:7:A:LEU:HB3	1	0.96
(4,330)	1:118:A:THR:HA	1:121:A:ARG:H	1	0.96
(4,53)	1:15:A:ASN:H	1:17:A:LEU:H	2	0.96
(7,321)	1:91:A:TRP:HD1	1:91:A:TRP:HA	2	0.95
(6,471)	1:111:A:ASN:HB2	1:112:A:PHE:H	2	0.95
(6,104)	1:24:A:CYS:H	1:23:A:LEU:HB3	1	0.95
(4,242)	1:81:A:ARG:H	1:83:A:LEU:H	2	0.95
(4,215)	1:73:A:PHE:H	1:75:A:ARG:H	2	0.95
(4,209)	1:72:A:GLN:HA	1:76:A:HIS:H	2	0.95
(4,176)	1:58:A:HIS:H	1:60:A:GLU:H	1	0.95
(4,42)	1:12:A:LYS:H	1:15:A:ASN:HB2	2	0.95
(4,42)	1:12:A:LYS:H	1:15:A:ASN:HB3	2	0.95
(4,41)	1:12:A:LYS:H	1:14:A:LEU:H	2	0.95
(6,77)	1:18:A:THR:H	1:17:A:LEU:HG	2	0.94
(4,89)	1:32:A:ILE:HB	1:34:A:ALA:H	1	0.94
(4,45)	1:15:A:ASN:H	1:13:A:THR:HA	2	0.94
(2,36)	1:56:A:TYR:HD1	1:83:A:LEU:H	2	0.94
(2,36)	1:56:A:TYR:HD2	1:83:A:LEU:H	2	0.94
(7,162)	1:45:A:PHE:H	1:45:A:PHE:HB2	1	0.93
(6,242)	1:57:A:SER:HB3	1:58:A:HIS:H	1	0.93
(6,203)	1:46:A:CYS:H	1:45:A:PHE:HB2	1	0.93
(6,146)	1:34:A:ALA:HA	1:33:A:PHE:H	1	0.93
(6,77)	1:18:A:THR:H	1:17:A:LEU:HG	1	0.93
(4,190)	1:72:A:GLN:HG2	1:68:A:ALA:H	2	0.93
(4,139)	1:46:A:CYS:H	1:48:A:ALA:H	1	0.93
(4,43)	1:13:A:THR:H	1:15:A:ASN:H	1	0.93
(7,162)	1:45:A:PHE:H	1:45:A:PHE:HB2	2	0.92
(6,467)	1:111:A:ASN:HB2	1:110:A:GLU:H	2	0.92
(6,294)	1:73:A:PHE:HB3	1:72:A:GLN:H	1	0.92
(6,270)	1:65:A:CYS:HA	1:66:A:LEU:H	2	0.92
(6,202)	1:46:A:CYS:H	1:45:A:PHE:HB3	1	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,12)	1:5:A:ILE:HB	1:6:A:THR:H	2	0.92
(4,185)	1:64:A:ARG:H	1:66:A:LEU:H	2	0.92
(4,136)	1:49:A:ALA:H	1:45:A:PHE:HE1	1	0.92
(4,136)	1:49:A:ALA:H	1:45:A:PHE:HE2	1	0.92
(4,113)	1:43:A:GLU:HB3	1:40:A:THR:H	1	0.92
(7,201)	1:59:A:HIS:HD2	1:59:A:HIS:H	2	0.91
(6,467)	1:111:A:ASN:HB2	1:110:A:GLU:H	1	0.91
(4,239)	1:80:A:ILE:H	1:82:A:PHE:H	1	0.91
(4,179)	1:62:A:ASP:HA	1:64:A:ARG:H	2	0.91
(7,363)	1:105:A:ASN:HB3	1:105:A:ASN:H	2	0.9
(6,330)	1:80:A:ILE:HG12	1:81:A:ARG:H	2	0.9
(6,330)	1:80:A:ILE:HG13	1:81:A:ARG:H	2	0.9
(4,218)	1:74:A:HIS:HA	1:78:A:GLN:H	2	0.9
(4,210)	1:72:A:GLN:H	1:74:A:HIS:H	2	0.9
(7,25)	1:8:A:GLN:HB3	1:8:A:GLN:H	2	0.89
(6,519)	1:124:A:TYR:HA	1:123:A:LYS:H	1	0.89
(6,23)	1:7:A:LEU:HG	1:8:A:GLN:H	1	0.89
(4,43)	1:13:A:THR:H	1:15:A:ASN:H	2	0.89
(7,257)	1:76:A:HIS:HD2	1:76:A:HIS:H	1	0.88
(6,174)	1:39:A:THR:HG21	1:40:A:THR:H	1	0.88
(6,174)	1:39:A:THR:HG22	1:40:A:THR:H	1	0.88
(6,174)	1:39:A:THR:HG23	1:40:A:THR:H	1	0.88
(6,119)	1:28:A:THR:HA	1:29:A:VAL:H	1	0.88
(6,70)	1:17:A:LEU:HB3	1:16:A:SER:H	2	0.88
(4,340)	1:121:A:ARG:HA	1:124:A:TYR:H	1	0.88
(4,101)	1:36:A:SER:HA	1:38:A:ASN:H	2	0.88
(6,412)	1:98:A:SER:HA	1:99:A:CYS:H	2	0.87
(6,160)	1:36:A:SER:HB2	1:37:A:LYS:H	1	0.87
(6,138)	1:32:A:ILE:H	1:33:A:PHE:H	2	0.87
(4,179)	1:62:A:ASP:HA	1:64:A:ARG:H	1	0.87
(4,139)	1:46:A:CYS:H	1:48:A:ALA:H	2	0.87
(7,358)	1:103:A:GLU:HB2	1:103:A:GLU:H	2	0.86
(7,358)	1:103:A:GLU:HB3	1:103:A:GLU:H	2	0.86
(6,119)	1:28:A:THR:HA	1:29:A:VAL:H	2	0.86
(6,78)	1:18:A:THR:HA	1:19:A:GLU:H	2	0.86
(4,252)	1:84:A:LYS:HA	1:88:A:ARG:H	2	0.86
(7,364)	1:105:A:ASN:HB2	1:105:A:ASN:H	1	0.85
(7,53)	1:15:A:ASN:H	1:15:A:ASN:HB3	2	0.85
(6,421)	1:101:A:VAL:HB	1:102:A:LYS:H	2	0.85
(6,293)	1:73:A:PHE:HA	1:72:A:GLN:H	1	0.85
(6,274)	1:67:A:GLY:HA3	1:68:A:ALA:H	2	0.85
(6,171)	1:38:A:ASN:HA	1:39:A:THR:H	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,290)	1:106:A:GLN:HG2	1:108:A:THR:H	2	0.85
(4,290)	1:106:A:GLN:HG3	1:108:A:THR:H	2	0.85
(4,228)	1:77:A:LYS:HA	1:81:A:ARG:H	1	0.85
(4,28)	1:9:A:GLU:HA	1:11:A:ILE:H	1	0.85
(7,268)	1:80:A:ILE:HG13	1:80:A:ILE:H	2	0.84
(6,274)	1:67:A:GLY:HA3	1:68:A:ALA:H	1	0.84
(6,69)	1:17:A:LEU:HA	1:16:A:SER:H	2	0.84
(4,223)	1:75:A:ARG:H	1:78:A:GLN:H	1	0.84
(4,46)	1:15:A:ASN:H	1:13:A:THR:HB	1	0.84
(4,25)	1:8:A:GLN:H	1:10:A:ILE:H	2	0.84
(6,311)	1:76:A:HIS:HB3	1:77:A:LYS:H	2	0.83
(6,259)	1:62:A:ASP:HA	1:63:A:THR:H	2	0.83
(6,97)	1:22:A:THR:HA	1:23:A:LEU:H	1	0.83
(6,70)	1:17:A:LEU:HB3	1:16:A:SER:H	1	0.83
(4,223)	1:75:A:ARG:H	1:78:A:GLN:H	2	0.83
(2,35)	1:69:A:THR:HG21	1:76:A:HIS:H	1	0.83
(2,35)	1:69:A:THR:HG22	1:76:A:HIS:H	1	0.83
(2,35)	1:69:A:THR:HG23	1:76:A:HIS:H	1	0.83
(7,364)	1:105:A:ASN:HB2	1:105:A:ASN:H	2	0.82
(6,424)	1:101:A:VAL:H	1:102:A:LYS:H	2	0.82
(4,295)	1:111:A:ASN:HB2	1:108:A:THR:H	1	0.82
(4,187)	1:67:A:GLY:HA3	1:69:A:THR:H	1	0.82
(7,294)	1:86:A:LEU:HG	1:86:A:LEU:H	2	0.81
(6,169)	1:38:A:ASN:HB3	1:39:A:THR:H	2	0.81
(4,334)	1:119:A:ILE:HA	1:123:A:LYS:H	2	0.81
(4,174)	1:57:A:SER:HA	1:60:A:GLU:H	1	0.81
(4,143)	1:48:A:ALA:H	1:50:A:THR:H	1	0.81
(4,78)	1:27:A:LEU:HB2	1:29:A:VAL:H	1	0.81
(4,78)	1:27:A:LEU:HB3	1:29:A:VAL:H	1	0.81
(2,50)	1:93:A:LEU:HD11	1:6:A:THR:H	2	0.81
(2,50)	1:93:A:LEU:HD12	1:6:A:THR:H	2	0.81
(2,50)	1:93:A:LEU:HD13	1:6:A:THR:H	2	0.81
(2,50)	1:93:A:LEU:HD21	1:6:A:THR:H	2	0.81
(2,50)	1:93:A:LEU:HD22	1:6:A:THR:H	2	0.81
(2,50)	1:93:A:LEU:HD23	1:6:A:THR:H	2	0.81
(7,394)	1:112:A:PHE:HB3	1:112:A:PHE:H	2	0.8
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG21	1	0.8
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG22	1	0.8
(7,39)	1:11:A:ILE:H	1:11:A:ILE:HG23	1	0.8
(6,412)	1:98:A:SER:HA	1:99:A:CYS:H	1	0.8
(6,258)	1:62:A:ASP:HB2	1:63:A:THR:H	1	0.8
(6,166)	1:37:A:LYS:HB2	1:38:A:ASN:H	2	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,166)	1:37:A:LYS:HB3	1:38:A:ASN:H	2	0.8
(6,79)	1:18:A:THR:H	1:19:A:GLU:HA	2	0.8
(4,253)	1:84:A:LYS:H	1:86:A:LEU:H	1	0.8
(4,247)	1:82:A:PHE:H	1:84:A:LYS:H	1	0.8
(4,192)	1:69:A:THR:H	1:72:A:GLN:H	1	0.8
(4,124)	1:43:A:GLU:HA	1:46:A:CYS:H	2	0.8
(7,52)	1:15:A:ASN:H	1:15:A:ASN:HD22	2	0.79
(6,259)	1:62:A:ASP:HA	1:63:A:THR:H	1	0.79
(6,154)	1:34:A:ALA:HB1	1:35:A:ALA:H	1	0.79
(6,154)	1:34:A:ALA:HB2	1:35:A:ALA:H	1	0.79
(6,154)	1:34:A:ALA:HB3	1:35:A:ALA:H	1	0.79
(6,150)	1:33:A:PHE:HA	1:34:A:ALA:H	2	0.79
(6,69)	1:17:A:LEU:HA	1:16:A:SER:H	1	0.79
(4,311)	1:111:A:ASN:H	1:113:A:LEU:H	1	0.79
(4,256)	1:85:A:ARG:H	1:87:A:ASP:H	1	0.79
(7,261)	1:79:A:LEU:HB2	1:79:A:LEU:H	1	0.78
(7,261)	1:79:A:LEU:HB3	1:79:A:LEU:H	1	0.78
(7,176)	1:51:A:VAL:HG11	1:51:A:VAL:H	1	0.78
(7,176)	1:51:A:VAL:HG12	1:51:A:VAL:H	1	0.78
(7,176)	1:51:A:VAL:HG13	1:51:A:VAL:H	1	0.78
(6,437)	1:104:A:ALA:HA	1:105:A:ASN:H	1	0.78
(6,11)	1:5:A:ILE:HG21	1:6:A:THR:H	2	0.78
(6,11)	1:5:A:ILE:HG22	1:6:A:THR:H	2	0.78
(6,11)	1:5:A:ILE:HG23	1:6:A:THR:H	2	0.78
(4,253)	1:84:A:LYS:H	1:86:A:LEU:H	2	0.78
(4,21)	1:7:A:LEU:H	1:9:A:GLU:H	2	0.78
(2,47)	1:33:A:PHE:HZ	1:116:A:LEU:H	2	0.78
(6,46)	1:12:A:LYS:H	1:11:A:ILE:HB	1	0.77
(4,124)	1:43:A:GLU:HA	1:46:A:CYS:H	1	0.77
(7,217)	1:63:A:THR:HG21	1:63:A:THR:H	1	0.76
(7,217)	1:63:A:THR:HG22	1:63:A:THR:H	1	0.76
(7,217)	1:63:A:THR:HG23	1:63:A:THR:H	1	0.76
(7,187)	1:55:A:PHE:HB3	1:55:A:PHE:H	2	0.76
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG21	2	0.76
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG22	2	0.76
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG23	2	0.76
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG21	2	0.76
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG22	2	0.76
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG23	2	0.76
(6,492)	1:117:A:LYS:HA	1:116:A:LEU:H	1	0.76
(6,459)	1:109:A:LEU:HG	1:110:A:GLU:H	1	0.76
(6,435)	1:104:A:ALA:HB1	1:105:A:ASN:H	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,435)	1:104:A:ALA:HB2	1:105:A:ASN:H	1	0.76
(6,435)	1:104:A:ALA:HB3	1:105:A:ASN:H	1	0.76
(6,204)	1:45:A:PHE:H	1:46:A:CYS:HA	1	0.76
(6,75)	1:18:A:THR:H	1:17:A:LEU:HB3	2	0.76
(4,256)	1:85:A:ARG:H	1:87:A:ASP:H	2	0.76
(4,248)	1:83:A:LEU:H	1:85:A:ARG:H	1	0.76
(4,240)	1:81:A:ARG:HA	1:83:A:LEU:H	2	0.76
(4,188)	1:67:A:GLY:HA2	1:69:A:THR:H	1	0.76
(7,15)	1:6:A:THR:H	1:6:A:THR:HG21	2	0.75
(7,15)	1:6:A:THR:H	1:6:A:THR:HG22	2	0.75
(7,15)	1:6:A:THR:H	1:6:A:THR:HG23	2	0.75
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG21	1	0.75
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG22	1	0.75
(7,11)	1:5:A:ILE:H	1:5:A:ILE:HG23	1	0.75
(6,492)	1:117:A:LYS:HA	1:116:A:LEU:H	2	0.75
(6,255)	1:61:A:LYS:HA	1:62:A:ASP:H	1	0.75
(6,90)	1:20:A:GLN:H	1:21:A:LYS:H	2	0.75
(7,250)	1:74:A:HIS:HB2	1:74:A:HIS:H	2	0.74
(7,250)	1:74:A:HIS:HB3	1:74:A:HIS:H	2	0.74
(7,201)	1:59:A:HIS:HD2	1:59:A:HIS:H	1	0.74
(7,132)	1:36:A:SER:HB2	1:36:A:SER:H	2	0.74
(6,519)	1:124:A:TYR:HA	1:123:A:LYS:H	2	0.74
(6,169)	1:38:A:ASN:HB3	1:39:A:THR:H	1	0.74
(4,345)	1:123:A:LYS:H	1:125:A:SER:H	2	0.74
(4,230)	1:78:A:GLN:HA	1:80:A:ILE:H	2	0.74
(4,64)	1:21:A:LYS:H	1:19:A:GLU:HG2	1	0.74
(4,64)	1:21:A:LYS:H	1:19:A:GLU:HG3	1	0.74
(2,42)	1:30:A:THR:HA	1:106:A:GLN:HE21	2	0.74
(2,42)	1:30:A:THR:HA	1:106:A:GLN:HE22	2	0.74
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG21	1	0.73
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG22	1	0.73
(7,33)	1:10:A:ILE:H	1:10:A:ILE:HG23	1	0.73
(7,15)	1:6:A:THR:H	1:6:A:THR:HG21	1	0.73
(7,15)	1:6:A:THR:H	1:6:A:THR:HG22	1	0.73
(7,15)	1:6:A:THR:H	1:6:A:THR:HG23	1	0.73
(6,538)	1:128:A:SER:HA	1:129:A:SER:H	2	0.73
(6,474)	1:112:A:PHE:HB2	1:111:A:ASN:H	2	0.73
(6,366)	1:87:A:ASP:HB3	1:88:A:ARG:H	1	0.73
(7,208)	1:60:A:GLU:HB2	1:60:A:GLU:H	2	0.72
(7,208)	1:60:A:GLU:HB3	1:60:A:GLU:H	2	0.72
(7,117)	1:32:A:ILE:HG13	1:32:A:ILE:H	1	0.72
(6,170)	1:38:A:ASN:HB2	1:39:A:THR:H	2	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,149)	1:33:A:PHE:HB2	1:34:A:ALA:H	1	0.72
(6,19)	1:7:A:LEU:H	1:6:A:THR:HG1	1	0.72
(4,37)	1:11:A:ILE:HA	1:15:A:ASN:H	2	0.72
(4,8)	1:5:A:ILE:HA	1:8:A:GLN:H	2	0.72
(2,2)	1:31:A:ASP:H	1:107:A:SER:H	1	0.72
(7,256)	1:76:A:HIS:HB2	1:76:A:HIS:H	1	0.71
(7,217)	1:63:A:THR:HG21	1:63:A:THR:H	2	0.71
(7,217)	1:63:A:THR:HG22	1:63:A:THR:H	2	0.71
(7,217)	1:63:A:THR:HG23	1:63:A:THR:H	2	0.71
(7,65)	1:17:A:LEU:H	1:17:A:LEU:HG	1	0.71
(7,65)	1:17:A:LEU:H	1:17:A:LEU:HG	2	0.71
(6,430)	1:102:A:LYS:H	1:103:A:GLU:H	1	0.71
(6,204)	1:45:A:PHE:H	1:46:A:CYS:HA	2	0.71
(6,75)	1:18:A:THR:H	1:17:A:LEU:HB3	1	0.71
(4,47)	1:14:A:LEU:HA	1:16:A:SER:H	2	0.71
(7,207)	1:60:A:GLU:HA	1:60:A:GLU:H	2	0.7
(7,4)	1:4:A:ASP:HA	1:4:A:ASP:H	2	0.7
(6,84)	1:20:A:GLN:H	1:19:A:GLU:HB2	2	0.7
(6,84)	1:20:A:GLN:H	1:19:A:GLU:HB3	2	0.7
(4,116)	1:42:A:LYS:HA	1:46:A:CYS:H	1	0.7
(4,61)	1:18:A:THR:HA	1:20:A:GLN:H	1	0.7
(4,19)	1:7:A:LEU:HA	1:10:A:ILE:H	2	0.7
(2,49)	1:10:A:ILE:HD11	1:89:A:ASN:H	1	0.7
(2,49)	1:10:A:ILE:HD12	1:89:A:ASN:H	1	0.7
(2,49)	1:10:A:ILE:HD13	1:89:A:ASN:H	1	0.7
(7,337)	1:95:A:GLY:HA2	1:95:A:GLY:H	1	0.69
(7,197)	1:57:A:SER:HB2	1:57:A:SER:H	2	0.69
(7,81)	1:21:A:LYS:HA	1:21:A:LYS:H	1	0.69
(6,474)	1:112:A:PHE:HB2	1:111:A:ASN:H	1	0.69
(6,85)	1:19:A:GLU:HA	1:20:A:GLN:H	2	0.69
(6,39)	1:11:A:ILE:H	1:10:A:ILE:HB	2	0.69
(4,125)	1:43:A:GLU:H	1:45:A:PHE:H	2	0.69
(4,58)	1:17:A:LEU:HA	1:19:A:GLU:H	1	0.69
(4,54)	1:16:A:SER:HA	1:18:A:THR:H	1	0.69
(7,61)	1:16:A:SER:H	1:16:A:SER:HB2	2	0.68
(7,61)	1:16:A:SER:H	1:16:A:SER:HB3	2	0.68
(6,430)	1:102:A:LYS:H	1:103:A:GLU:H	2	0.68
(6,261)	1:63:A:THR:HB	1:64:A:ARG:H	2	0.68
(6,216)	1:50:A:THR:HB	1:51:A:VAL:H	2	0.68
(4,231)	1:78:A:GLN:H	1:80:A:ILE:H	1	0.68
(4,121)	1:43:A:GLU:HA	1:45:A:PHE:H	2	0.68
(4,24)	1:8:A:GLN:HA	1:12:A:LYS:H	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,394)	1:112:A:PHE:HB3	1:112:A:PHE:H	1	0.67
(7,250)	1:74:A:HIS:HB2	1:74:A:HIS:H	1	0.67
(7,250)	1:74:A:HIS:HB3	1:74:A:HIS:H	1	0.67
(6,455)	1:108:A:THR:HB	1:109:A:LEU:H	1	0.67
(6,312)	1:76:A:HIS:HB2	1:77:A:LYS:H	1	0.67
(6,268)	1:65:A:CYS:HB3	1:66:A:LEU:H	1	0.67
(4,242)	1:81:A:ARG:H	1:83:A:LEU:H	1	0.67
(4,13)	1:10:A:ILE:H	1:6:A:THR:HA	1	0.67
(7,350)	1:101:A:VAL:HB	1:101:A:VAL:H	2	0.66
(7,337)	1:95:A:GLY:HA2	1:95:A:GLY:H	2	0.66
(7,90)	1:23:A:LEU:H	1:23:A:LEU:HB2	1	0.66
(6,538)	1:128:A:SER:HA	1:129:A:SER:H	1	0.66
(6,268)	1:65:A:CYS:HB3	1:66:A:LEU:H	2	0.66
(6,122)	1:28:A:THR:H	1:29:A:VAL:H	2	0.66
(6,109)	1:25:A:THR:H	1:24:A:CYS:HB2	1	0.66
(6,82)	1:19:A:GLU:H	1:18:A:THR:HB	2	0.66
(6,1)	1:3:A:THR:HA	1:4:A:ASP:H	1	0.66
(4,31)	1:12:A:LYS:H	1:9:A:GLU:HG2	2	0.66
(4,31)	1:12:A:LYS:H	1:9:A:GLU:HG3	2	0.66
(4,9)	1:5:A:ILE:H	1:7:A:LEU:H	1	0.66
(6,191)	1:44:A:THR:HB	1:45:A:PHE:H	1	0.65
(6,150)	1:33:A:PHE:HA	1:34:A:ALA:H	1	0.65
(6,437)	1:104:A:ALA:HA	1:105:A:ASN:H	2	0.64
(6,436)	1:104:A:ALA:HB1	1:105:A:ASN:HD21	2	0.64
(6,436)	1:104:A:ALA:HB2	1:105:A:ASN:HD21	2	0.64
(6,436)	1:104:A:ALA:HB3	1:105:A:ASN:HD21	2	0.64
(6,377)	1:89:A:ASN:H	1:90:A:LEU:H	1	0.64
(4,194)	1:72:A:GLN:HG3	1:69:A:THR:H	1	0.64
(4,56)	1:16:A:SER:H	1:18:A:THR:H	1	0.64
(7,299)	1:87:A:ASP:HB2	1:87:A:ASP:H	1	0.63
(7,279)	1:82:A:PHE:HB2	1:82:A:PHE:H	2	0.63
(6,424)	1:101:A:VAL:H	1:102:A:LYS:H	1	0.63
(6,156)	1:35:A:ALA:HA	1:36:A:SER:H	1	0.63
(4,241)	1:81:A:ARG:HA	1:84:A:LYS:H	2	0.63
(4,46)	1:15:A:ASN:H	1:13:A:THR:HB	2	0.63
(7,131)	1:36:A:SER:HB3	1:36:A:SER:H	2	0.62
(6,393)	1:93:A:LEU:HA	1:94:A:ALA:H	2	0.62
(6,340)	1:82:A:PHE:HB3	1:83:A:LEU:H	2	0.62
(6,267)	1:65:A:CYS:H	1:66:A:LEU:H	1	0.62
(6,266)	1:64:A:ARG:H	1:65:A:CYS:H	1	0.62
(6,177)	1:40:A:THR:HA	1:41:A:GLU:H	1	0.62
(4,217)	1:74:A:HIS:HA	1:77:A:LYS:H	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,54)	1:16:A:SER:HA	1:18:A:THR:H	2	0.62
(7,197)	1:57:A:SER:HB2	1:57:A:SER:H	1	0.61
(6,180)	1:41:A:GLU:HA	1:42:A:LYS:H	2	0.61
(6,122)	1:28:A:THR:H	1:29:A:VAL:H	1	0.61
(7,175)	1:51:A:VAL:HB	1:51:A:VAL:H	1	0.6
(7,54)	1:15:A:ASN:H	1:15:A:ASN:HB2	1	0.6
(6,455)	1:108:A:THR:HB	1:109:A:LEU:H	2	0.6
(6,315)	1:76:A:HIS:H	1:77:A:LYS:H	2	0.6
(6,264)	1:63:A:THR:H	1:64:A:ARG:H	2	0.6
(4,125)	1:43:A:GLU:H	1:45:A:PHE:H	1	0.6
(4,48)	1:14:A:LEU:HA	1:17:A:LEU:H	1	0.6
(2,4)	1:31:A:ASP:H	1:106:A:GLN:HB2	1	0.6
(2,4)	1:31:A:ASP:H	1:106:A:GLN:HB3	1	0.6
(7,257)	1:76:A:HIS:HD2	1:76:A:HIS:H	2	0.59
(6,245)	1:57:A:SER:H	1:58:A:HIS:H	2	0.59
(6,228)	1:54:A:GLN:HG2	1:55:A:PHE:H	2	0.59
(6,228)	1:54:A:GLN:HG3	1:55:A:PHE:H	2	0.59
(6,196)	1:44:A:THR:H	1:45:A:PHE:HA	2	0.59
(6,180)	1:41:A:GLU:HA	1:42:A:LYS:H	1	0.59
(6,156)	1:35:A:ALA:HA	1:36:A:SER:H	2	0.59
(6,9)	1:5:A:ILE:HG13	1:6:A:THR:H	2	0.59
(4,311)	1:111:A:ASN:H	1:113:A:LEU:H	2	0.59
(4,120)	1:42:A:LYS:H	1:45:A:PHE:H	2	0.59
(4,50)	1:14:A:LEU:H	1:16:A:SER:H	1	0.59
(7,264)	1:79:A:LEU:HD21	1:79:A:LEU:H	2	0.58
(7,264)	1:79:A:LEU:HD22	1:79:A:LEU:H	2	0.58
(7,264)	1:79:A:LEU:HD23	1:79:A:LEU:H	2	0.58
(6,307)	1:74:A:HIS:HA	1:75:A:ARG:H	1	0.58
(6,243)	1:57:A:SER:HB2	1:58:A:HIS:H	2	0.58
(6,12)	1:5:A:ILE:HB	1:6:A:THR:H	1	0.58
(4,25)	1:8:A:GLN:H	1:10:A:ILE:H	1	0.58
(7,261)	1:79:A:LEU:HB2	1:79:A:LEU:H	2	0.57
(7,261)	1:79:A:LEU:HB3	1:79:A:LEU:H	2	0.57
(6,521)	1:124:A:TYR:HB2	1:123:A:LYS:H	1	0.57
(6,450)	1:107:A:SER:HB2	1:108:A:THR:H	1	0.57
(4,334)	1:119:A:ILE:HA	1:123:A:LYS:H	1	0.57
(4,236)	1:80:A:ILE:HA	1:82:A:PHE:H	1	0.57
(6,436)	1:104:A:ALA:HB1	1:105:A:ASN:HD21	1	0.56
(6,436)	1:104:A:ALA:HB2	1:105:A:ASN:HD21	1	0.56
(6,436)	1:104:A:ALA:HB3	1:105:A:ASN:HD21	1	0.56
(4,247)	1:82:A:PHE:H	1:84:A:LYS:H	2	0.56
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB1	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB2	1	0.56
(2,7)	1:31:A:ASP:H	1:104:A:ALA:HB3	1	0.56
(7,247)	1:73:A:PHE:HB2	1:73:A:PHE:H	1	0.55
(7,200)	1:58:A:HIS:HB2	1:58:A:HIS:H	1	0.55
(7,142)	1:39:A:THR:HB	1:39:A:THR:H	2	0.55
(7,10)	1:5:A:ILE:H	1:5:A:ILE:HG12	1	0.55
(6,191)	1:44:A:THR:HB	1:45:A:PHE:H	2	0.55
(6,76)	1:18:A:THR:H	1:17:A:LEU:HB2	1	0.55
(6,11)	1:5:A:ILE:HG21	1:6:A:THR:H	1	0.55
(6,11)	1:5:A:ILE:HG22	1:6:A:THR:H	1	0.55
(6,11)	1:5:A:ILE:HG23	1:6:A:THR:H	1	0.55
(4,212)	1:72:A:GLN:H	1:75:A:ARG:H	2	0.55
(7,242)	1:72:A:GLN:HG2	1:72:A:GLN:H	1	0.54
(6,258)	1:62:A:ASP:HB2	1:63:A:THR:H	2	0.54
(6,196)	1:44:A:THR:H	1:45:A:PHE:HA	1	0.54
(6,172)	1:38:A:ASN:H	1:39:A:THR:H	2	0.54
(6,135)	1:31:A:ASP:H	1:32:A:ILE:H	1	0.54
(6,76)	1:18:A:THR:H	1:17:A:LEU:HB2	2	0.54
(6,21)	1:7:A:LEU:H	1:8:A:GLN:H	2	0.54
(4,305)	1:110:A:GLU:HA	1:113:A:LEU:H	1	0.54
(4,56)	1:16:A:SER:H	1:18:A:THR:H	2	0.54
(7,262)	1:79:A:LEU:HB2	1:79:A:LEU:H	2	0.53
(7,256)	1:76:A:HIS:HB2	1:76:A:HIS:H	2	0.53
(7,239)	1:71:A:GLN:HE21	1:71:A:GLN:H	2	0.53
(7,239)	1:71:A:GLN:HE22	1:71:A:GLN:H	2	0.53
(6,361)	1:86:A:LEU:HG	1:87:A:ASP:H	1	0.53
(6,248)	1:58:A:HIS:H	1:59:A:HIS:H	2	0.53
(6,137)	1:32:A:ILE:HA	1:33:A:PHE:H	2	0.53
(6,85)	1:19:A:GLU:HA	1:20:A:GLN:H	1	0.53
(6,66)	1:16:A:SER:H	1:17:A:LEU:H	2	0.53
(6,53)	1:14:A:LEU:HA	1:15:A:ASN:H	2	0.53
(7,246)	1:73:A:PHE:HB3	1:73:A:PHE:H	2	0.52
(7,172)	1:50:A:THR:HB	1:50:A:THR:H	1	0.52
(6,159)	1:36:A:SER:HB3	1:37:A:LYS:H	1	0.52
(6,137)	1:32:A:ILE:HA	1:33:A:PHE:H	1	0.52
(7,263)	1:79:A:LEU:HD11	1:79:A:LEU:H	2	0.51
(7,263)	1:79:A:LEU:HD12	1:79:A:LEU:H	2	0.51
(7,263)	1:79:A:LEU:HD13	1:79:A:LEU:H	2	0.51
(7,187)	1:55:A:PHE:HB3	1:55:A:PHE:H	1	0.51
(7,114)	1:31:A:ASP:HB2	1:31:A:ASP:H	2	0.51
(7,88)	1:23:A:LEU:H	1:23:A:LEU:HG	1	0.51
(6,388)	1:92:A:GLY:HA3	1:93:A:LEU:H	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,138)	1:32:A:ILE:H	1:33:A:PHE:H	1	0.51
(6,84)	1:20:A:GLN:H	1:19:A:GLU:HB2	1	0.51
(6,84)	1:20:A:GLN:H	1:19:A:GLU:HB3	1	0.51
(6,9)	1:5:A:ILE:HG13	1:6:A:THR:H	1	0.51
(4,307)	1:111:A:ASN:HB3	1:114:A:GLU:H	1	0.51
(7,299)	1:87:A:ASP:HB2	1:87:A:ASP:H	2	0.5
(6,318)	1:78:A:GLN:HA	1:79:A:LEU:H	2	0.5
(6,20)	1:7:A:LEU:HA	1:8:A:GLN:H	1	0.5
(6,20)	1:7:A:LEU:HA	1:8:A:GLN:H	2	0.5
(4,282)	1:96:A:LEU:HA	1:98:A:SER:H	1	0.5
(4,249)	1:83:A:LEU:HA	1:85:A:ARG:H	2	0.5
(4,121)	1:43:A:GLU:HA	1:45:A:PHE:H	1	0.5
(4,31)	1:12:A:LYS:H	1:9:A:GLU:HG2	1	0.5
(4,31)	1:12:A:LYS:H	1:9:A:GLU:HG3	1	0.5
(4,27)	1:10:A:ILE:H	1:8:A:GLN:HA	2	0.5
(6,393)	1:93:A:LEU:HA	1:94:A:ALA:H	1	0.49
(6,221)	1:51:A:VAL:HB	1:52:A:LEU:H	1	0.49
(6,216)	1:50:A:THR:HB	1:51:A:VAL:H	1	0.49
(6,170)	1:38:A:ASN:HB2	1:39:A:THR:H	1	0.49
(4,203)	1:71:A:GLN:HA	1:75:A:ARG:H	1	0.49
(4,47)	1:14:A:LEU:HA	1:16:A:SER:H	1	0.49
(4,4)	1:6:A:THR:H	1:4:A:ASP:HB3	2	0.49
(7,279)	1:82:A:PHE:HB2	1:82:A:PHE:H	1	0.48
(7,199)	1:58:A:HIS:HB3	1:58:A:HIS:H	2	0.48
(6,318)	1:78:A:GLN:HA	1:79:A:LEU:H	1	0.48
(6,309)	1:75:A:ARG:HA	1:76:A:HIS:H	2	0.48
(6,182)	1:42:A:LYS:H	1:43:A:GLU:H	1	0.48
(6,65)	1:16:A:SER:HA	1:17:A:LEU:H	1	0.48
(6,65)	1:16:A:SER:HA	1:17:A:LEU:H	2	0.48
(6,64)	1:16:A:SER:H	1:15:A:ASN:HB2	1	0.48
(6,53)	1:14:A:LEU:HA	1:15:A:ASN:H	1	0.48
(4,237)	1:80:A:ILE:HA	1:83:A:LEU:H	1	0.48
(7,391)	1:111:A:ASN:HB3	1:111:A:ASN:H	2	0.47
(7,321)	1:91:A:TRP:HD1	1:91:A:TRP:HA	1	0.47
(7,281)	1:83:A:LEU:HB3	1:83:A:LEU:H	2	0.47
(7,94)	1:25:A:THR:H	1:25:A:THR:HB	1	0.47
(6,350)	1:84:A:LYS:HA	1:85:A:ARG:H	1	0.47
(6,350)	1:84:A:LYS:HA	1:85:A:ARG:H	2	0.47
(6,151)	1:33:A:PHE:H	1:34:A:ALA:H	2	0.47
(6,135)	1:31:A:ASP:H	1:32:A:ILE:H	2	0.47
(6,5)	1:4:A:ASP:H	1:5:A:ILE:H	2	0.47
(4,324)	1:115:A:ARG:HA	1:117:A:LYS:H	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,251)	1:84:A:LYS:HA	1:87:A:ASP:H	2	0.47
(4,120)	1:42:A:LYS:H	1:45:A:PHE:H	1	0.47
(4,45)	1:15:A:ASN:H	1:13:A:THR:HA	1	0.47
(4,19)	1:7:A:LEU:HA	1:10:A:ILE:H	1	0.47
(3,87)	1:107:A:SER:H	1:29:A:VAL:O	2	0.47
(7,420)	1:120:A:MET:HB3	1:120:A:MET:H	1	0.46
(7,420)	1:120:A:MET:HB3	1:120:A:MET:H	2	0.46
(7,392)	1:111:A:ASN:HB2	1:111:A:ASN:H	1	0.46
(7,391)	1:111:A:ASN:HB3	1:111:A:ASN:H	1	0.46
(7,193)	1:56:A:TYR:HB3	1:56:A:TYR:H	2	0.46
(7,64)	1:17:A:LEU:H	1:17:A:LEU:HB2	1	0.46
(7,64)	1:17:A:LEU:H	1:17:A:LEU:HB2	2	0.46
(7,61)	1:16:A:SER:H	1:16:A:SER:HB2	1	0.46
(7,61)	1:16:A:SER:H	1:16:A:SER:HB3	1	0.46
(6,475)	1:111:A:ASN:H	1:112:A:PHE:H	2	0.46
(6,388)	1:92:A:GLY:HA3	1:93:A:LEU:H	1	0.46
(6,370)	1:88:A:ARG:HA	1:89:A:ASN:H	2	0.46
(6,364)	1:86:A:LEU:HA	1:87:A:ASP:H	2	0.46
(6,337)	1:81:A:ARG:HA	1:82:A:PHE:H	1	0.46
(6,334)	1:80:A:ILE:H	1:81:A:ARG:H	1	0.46
(6,320)	1:78:A:GLN:H	1:79:A:LEU:H	1	0.46
(6,303)	1:73:A:PHE:HA	1:74:A:HIS:H	1	0.46
(6,220)	1:51:A:VAL:HA	1:52:A:LEU:H	2	0.46
(6,188)	1:43:A:GLU:HA	1:44:A:THR:H	2	0.46
(6,177)	1:40:A:THR:HA	1:41:A:GLU:H	2	0.46
(6,66)	1:16:A:SER:H	1:17:A:LEU:H	1	0.46
(6,49)	1:13:A:THR:HA	1:14:A:LEU:H	2	0.46
(6,29)	1:9:A:GLU:HA	1:10:A:ILE:H	2	0.46
(6,26)	1:8:A:GLN:HA	1:9:A:GLU:H	2	0.46
(4,87)	1:31:A:ASP:HB2	1:34:A:ALA:H	2	0.46
(4,51)	1:15:A:ASN:HA	1:18:A:THR:H	1	0.46
(7,307)	1:89:A:ASN:HB3	1:89:A:ASN:H	1	0.45
(7,278)	1:82:A:PHE:HB3	1:82:A:PHE:H	1	0.45
(7,193)	1:56:A:TYR:HB3	1:56:A:TYR:H	1	0.45
(7,14)	1:6:A:THR:H	1:6:A:THR:HB	1	0.45
(7,10)	1:5:A:ILE:H	1:5:A:ILE:HG12	2	0.45
(6,337)	1:81:A:ARG:HA	1:82:A:PHE:H	2	0.45
(6,309)	1:75:A:ARG:HA	1:76:A:HIS:H	1	0.45
(6,209)	1:47:A:ARG:HA	1:48:A:ALA:H	2	0.45
(6,40)	1:11:A:ILE:HA	1:12:A:LYS:H	2	0.45
(4,153)	1:52:A:LEU:HA	1:55:A:PHE:H	1	0.45
(4,146)	1:49:A:ALA:HA	1:51:A:VAL:H	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:7:A:LEU:H	1:9:A:GLU:H	1	0.45
(7,90)	1:23:A:LEU:H	1:23:A:LEU:HB2	2	0.44
(7,29)	1:9:A:GLU:H	1:9:A:GLU:HB3	1	0.44
(7,2)	1:3:A:THR:H	1:3:A:THR:HB	2	0.44
(6,370)	1:88:A:ARG:HA	1:89:A:ASN:H	1	0.44
(6,364)	1:86:A:LEU:HA	1:87:A:ASP:H	1	0.44
(6,303)	1:73:A:PHE:HA	1:74:A:HIS:H	2	0.44
(6,237)	1:56:A:TYR:HE1	1:57:A:SER:H	2	0.44
(6,237)	1:56:A:TYR:HE2	1:57:A:SER:H	2	0.44
(6,225)	1:53:A:ARG:HA	1:54:A:GLN:H	2	0.44
(6,220)	1:51:A:VAL:HA	1:52:A:LEU:H	1	0.44
(6,210)	1:47:A:ARG:H	1:48:A:ALA:H	2	0.44
(6,192)	1:44:A:THR:HA	1:45:A:PHE:H	2	0.44
(6,165)	1:37:A:LYS:H	1:38:A:ASN:H	1	0.44
(6,151)	1:33:A:PHE:H	1:34:A:ALA:H	1	0.44
(6,90)	1:20:A:GLN:H	1:21:A:LYS:H	1	0.44
(6,80)	1:18:A:THR:H	1:19:A:GLU:H	1	0.44
(6,78)	1:18:A:THR:HA	1:19:A:GLU:H	1	0.44
(6,49)	1:13:A:THR:HA	1:14:A:LEU:H	1	0.44
(6,40)	1:11:A:ILE:HA	1:12:A:LYS:H	1	0.44
(4,81)	1:30:A:THR:HG21	1:32:A:ILE:H	1	0.44
(4,81)	1:30:A:THR:HG22	1:32:A:ILE:H	1	0.44
(4,81)	1:30:A:THR:HG23	1:32:A:ILE:H	1	0.44
(7,392)	1:111:A:ASN:HB2	1:111:A:ASN:H	2	0.43
(6,307)	1:74:A:HIS:HA	1:75:A:ARG:H	2	0.43
(6,253)	1:60:A:GLU:H	1:61:A:LYS:H	2	0.43
(6,237)	1:56:A:TYR:HE1	1:57:A:SER:H	1	0.43
(6,237)	1:56:A:TYR:HE2	1:57:A:SER:H	1	0.43
(6,226)	1:54:A:GLN:HA	1:55:A:PHE:H	1	0.43
(6,226)	1:54:A:GLN:HA	1:55:A:PHE:H	2	0.43
(6,189)	1:43:A:GLU:H	1:44:A:THR:H	2	0.43
(6,47)	1:12:A:LYS:HA	1:13:A:THR:H	1	0.43
(6,41)	1:11:A:ILE:H	1:12:A:LYS:H	2	0.43
(6,26)	1:8:A:GLN:HA	1:9:A:GLU:H	1	0.43
(4,251)	1:84:A:LYS:HA	1:87:A:ASP:H	1	0.43
(4,216)	1:74:A:HIS:HA	1:76:A:HIS:H	1	0.43
(4,83)	1:31:A:ASP:HA	1:34:A:ALA:H	1	0.43
(4,36)	1:11:A:ILE:HA	1:14:A:LEU:H	2	0.43
(7,283)	1:83:A:LEU:HG	1:83:A:LEU:H	2	0.42
(7,247)	1:73:A:PHE:HB2	1:73:A:PHE:H	2	0.42
(7,188)	1:55:A:PHE:HB2	1:55:A:PHE:H	1	0.42
(7,131)	1:36:A:SER:HB3	1:36:A:SER:H	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,122)	1:33:A:PHE:HB3	1:33:A:PHE:H	1	0.42
(7,94)	1:25:A:THR:H	1:25:A:THR:HB	2	0.42
(6,254)	1:60:A:GLU:HA	1:61:A:LYS:H	1	0.42
(6,245)	1:57:A:SER:H	1:58:A:HIS:H	1	0.42
(6,225)	1:53:A:ARG:HA	1:54:A:GLN:H	1	0.42
(6,192)	1:44:A:THR:HA	1:45:A:PHE:H	1	0.42
(6,188)	1:43:A:GLU:HA	1:44:A:THR:H	1	0.42
(6,131)	1:30:A:THR:H	1:31:A:ASP:H	1	0.42
(6,29)	1:9:A:GLU:HA	1:10:A:ILE:H	1	0.42
(6,8)	1:5:A:ILE:H	1:6:A:THR:H	2	0.42
(4,338)	1:120:A:MET:H	1:123:A:LYS:H	2	0.42
(4,116)	1:42:A:LYS:HA	1:46:A:CYS:H	2	0.42
(7,432)	1:124:A:TYR:HB3	1:124:A:TYR:H	2	0.41
(7,267)	1:80:A:ILE:HB	1:80:A:ILE:H	2	0.41
(7,116)	1:32:A:ILE:HB	1:32:A:ILE:H	1	0.41
(7,29)	1:9:A:GLU:H	1:9:A:GLU:HB3	2	0.41
(6,248)	1:58:A:HIS:H	1:59:A:HIS:H	1	0.41
(6,212)	1:48:A:ALA:H	1:49:A:ALA:H	2	0.41
(6,47)	1:12:A:LYS:HA	1:13:A:THR:H	2	0.41
(4,255)	1:85:A:ARG:HA	1:87:A:ASP:H	1	0.41
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD11	1	0.41
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD12	1	0.41
(4,38)	1:14:A:LEU:H	1:11:A:ILE:HD13	1	0.41
(7,262)	1:79:A:LEU:HB2	1:79:A:LEU:H	1	0.4
(7,200)	1:58:A:HIS:HB2	1:58:A:HIS:H	2	0.4
(7,123)	1:33:A:PHE:HB2	1:33:A:PHE:H	2	0.4
(7,117)	1:32:A:ILE:HG13	1:32:A:ILE:H	2	0.4
(7,114)	1:31:A:ASP:HB2	1:31:A:ASP:H	1	0.4
(6,351)	1:84:A:LYS:H	1:85:A:ARG:H	2	0.4
(6,329)	1:80:A:ILE:HB	1:81:A:ARG:H	1	0.4
(6,310)	1:75:A:ARG:H	1:76:A:HIS:H	2	0.4
(6,67)	1:17:A:LEU:H	1:16:A:SER:HB2	1	0.4
(6,67)	1:17:A:LEU:H	1:16:A:SER:HB3	1	0.4
(6,39)	1:11:A:ILE:H	1:10:A:ILE:HB	1	0.4
(6,22)	1:7:A:LEU:HB2	1:8:A:GLN:H	1	0.4
(6,22)	1:7:A:LEU:HB3	1:8:A:GLN:H	1	0.4
(4,114)	1:43:A:GLU:HG2	1:40:A:THR:H	2	0.4
(4,114)	1:43:A:GLU:HG3	1:40:A:THR:H	2	0.4
(4,13)	1:10:A:ILE:H	1:6:A:THR:HA	2	0.4
(7,2)	1:3:A:THR:H	1:3:A:THR:HB	1	0.39
(6,454)	1:108:A:THR:HA	1:109:A:LEU:H	1	0.39
(6,209)	1:47:A:ARG:HA	1:48:A:ALA:H	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,324)	1:115:A:ARG:HA	1:117:A:LYS:H	1	0.39
(4,155)	1:54:A:GLN:HA	1:56:A:TYR:H	1	0.39
(4,132)	1:45:A:PHE:H	1:48:A:ALA:H	2	0.39
(7,14)	1:6:A:THR:H	1:6:A:THR:HB	2	0.38
(6,490)	1:115:A:ARG:H	1:116:A:LEU:H	1	0.38
(6,475)	1:111:A:ASN:H	1:112:A:PHE:H	1	0.38
(6,224)	1:51:A:VAL:H	1:52:A:LEU:H	2	0.38
(6,206)	1:46:A:CYS:HB2	1:47:A:ARG:H	1	0.38
(6,130)	1:30:A:THR:HG21	1:31:A:ASP:H	1	0.38
(6,130)	1:30:A:THR:HG22	1:31:A:ASP:H	1	0.38
(6,130)	1:30:A:THR:HG23	1:31:A:ASP:H	1	0.38
(6,55)	1:14:A:LEU:H	1:15:A:ASN:HB3	2	0.38
(6,19)	1:7:A:LEU:H	1:6:A:THR:HG1	2	0.38
(4,249)	1:83:A:LEU:HA	1:85:A:ARG:H	1	0.38
(4,39)	1:12:A:LYS:HA	1:15:A:ASN:H	2	0.38
(4,29)	1:9:A:GLU:HA	1:12:A:LYS:H	2	0.38
(3,88)	1:107:A:SER:N	1:29:A:VAL:O	2	0.38
(7,307)	1:89:A:ASN:HB3	1:89:A:ASN:H	2	0.37
(6,160)	1:36:A:SER:HB2	1:37:A:LYS:H	2	0.37
(4,321)	1:114:A:GLU:HA	1:117:A:LYS:H	2	0.37
(4,225)	1:76:A:HIS:H	1:78:A:GLN:H	2	0.37
(7,350)	1:101:A:VAL:HB	1:101:A:VAL:H	1	0.36
(7,298)	1:87:A:ASP:HB3	1:87:A:ASP:H	2	0.36
(7,172)	1:50:A:THR:HB	1:50:A:THR:H	2	0.36
(7,116)	1:32:A:ILE:HB	1:32:A:ILE:H	2	0.36
(6,299)	1:72:A:GLN:H	1:73:A:PHE:H	1	0.36
(6,299)	1:72:A:GLN:H	1:73:A:PHE:H	2	0.36
(6,278)	1:68:A:ALA:H	1:69:A:THR:H	1	0.36
(6,199)	1:45:A:PHE:H	1:46:A:CYS:H	1	0.36
(6,175)	1:39:A:THR:HA	1:40:A:THR:H	1	0.36
(6,131)	1:30:A:THR:H	1:31:A:ASP:H	2	0.36
(6,68)	1:17:A:LEU:H	1:16:A:SER:HB2	1	0.36
(4,190)	1:72:A:GLN:HG2	1:68:A:ALA:H	1	0.36
(4,88)	1:31:A:ASP:HA	1:33:A:PHE:H	1	0.36
(3,55)	1:91:A:TRP:H	1:87:A:ASP:O	1	0.36
(6,494)	1:116:A:LEU:H	1:117:A:LYS:H	1	0.35
(6,454)	1:108:A:THR:HA	1:109:A:LEU:H	2	0.35
(6,451)	1:107:A:SER:HA	1:108:A:THR:H	1	0.35
(6,377)	1:89:A:ASN:H	1:90:A:LEU:H	2	0.35
(6,134)	1:31:A:ASP:HA	1:32:A:ILE:H	1	0.35
(6,130)	1:30:A:THR:HG21	1:31:A:ASP:H	2	0.35
(6,130)	1:30:A:THR:HG22	1:31:A:ASP:H	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,130)	1:30:A:THR:HG23	1:31:A:ASP:H	2	0.35
(6,124)	1:29:A:VAL:HA	1:30:A:THR:H	1	0.35
(6,14)	1:7:A:LEU:H	1:6:A:THR:H	2	0.35
(4,338)	1:120:A:MET:H	1:123:A:LYS:H	1	0.35
(4,71)	1:27:A:LEU:HD11	1:24:A:CYS:HB2	2	0.35
(4,71)	1:27:A:LEU:HD12	1:24:A:CYS:HB2	2	0.35
(4,71)	1:27:A:LEU:HD13	1:24:A:CYS:HB2	2	0.35
(7,37)	1:11:A:ILE:H	1:11:A:ILE:HG13	1	0.34
(6,494)	1:116:A:LEU:H	1:117:A:LYS:H	2	0.34
(6,326)	1:79:A:LEU:H	1:80:A:ILE:H	1	0.34
(6,241)	1:56:A:TYR:H	1:57:A:SER:H	2	0.34
(6,67)	1:17:A:LEU:H	1:16:A:SER:HB2	2	0.34
(6,67)	1:17:A:LEU:H	1:16:A:SER:HB3	2	0.34
(4,132)	1:45:A:PHE:H	1:48:A:ALA:H	1	0.34
(4,50)	1:14:A:LEU:H	1:16:A:SER:H	2	0.34
(7,255)	1:76:A:HIS:HB3	1:76:A:HIS:H	2	0.33
(7,109)	1:30:A:THR:HA	1:30:A:THR:H	1	0.33
(6,517)	1:121:A:ARG:H	1:122:A:GLU:H	1	0.33
(6,429)	1:102:A:LYS:HA	1:103:A:GLU:H	1	0.33
(6,349)	1:83:A:LEU:H	1:84:A:LYS:H	2	0.33
(6,291)	1:71:A:GLN:H	1:72:A:GLN:H	2	0.33
(6,269)	1:65:A:CYS:HB2	1:66:A:LEU:H	1	0.33
(6,199)	1:45:A:PHE:H	1:46:A:CYS:H	2	0.33
(6,198)	1:44:A:THR:H	1:45:A:PHE:HB2	2	0.33
(6,182)	1:42:A:LYS:H	1:43:A:GLU:H	2	0.33
(6,153)	1:34:A:ALA:HA	1:35:A:ALA:H	1	0.33
(6,21)	1:7:A:LEU:H	1:8:A:GLN:H	1	0.33
(4,307)	1:111:A:ASN:HB3	1:114:A:GLU:H	2	0.33
(4,153)	1:52:A:LEU:HA	1:55:A:PHE:H	2	0.33
(2,5)	1:31:A:ASP:H	1:106:A:GLN:HE21	2	0.33
(2,5)	1:31:A:ASP:H	1:106:A:GLN:HE22	2	0.33
(7,322)	1:91:A:TRP:HD1	1:91:A:TRP:HB3	1	0.32
(6,224)	1:51:A:VAL:H	1:52:A:LEU:H	1	0.32
(6,128)	1:30:A:THR:HA	1:31:A:ASP:H	1	0.32
(6,123)	1:29:A:VAL:HB	1:30:A:THR:H	2	0.32
(6,50)	1:13:A:THR:H	1:14:A:LEU:H	2	0.32
(6,30)	1:9:A:GLU:H	1:10:A:ILE:H	2	0.32
(4,308)	1:111:A:ASN:HB2	1:114:A:GLU:H	1	0.32
(4,155)	1:54:A:GLN:HA	1:56:A:TYR:H	2	0.32
(6,488)	1:114:A:GLU:H	1:115:A:ARG:H	2	0.31
(6,317)	1:77:A:LYS:H	1:78:A:GLN:H	2	0.31
(6,235)	1:55:A:PHE:H	1:56:A:TYR:H	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,218)	1:50:A:THR:H	1:51:A:VAL:H	1	0.31
(6,212)	1:48:A:ALA:H	1:49:A:ALA:H	1	0.31
(6,30)	1:9:A:GLU:H	1:10:A:ILE:H	1	0.31
(4,305)	1:110:A:GLU:HA	1:113:A:LEU:H	2	0.31
(4,35)	1:11:A:ILE:HA	1:13:A:THR:H	1	0.31
(4,5)	1:6:A:THR:H	1:4:A:ASP:HB2	1	0.31
(6,490)	1:115:A:ARG:H	1:116:A:LEU:H	2	0.3
(6,343)	1:82:A:PHE:H	1:83:A:LEU:H	1	0.3
(6,317)	1:77:A:LYS:H	1:78:A:GLN:H	1	0.3
(6,162)	1:36:A:SER:H	1:37:A:LYS:H	2	0.3
(6,112)	1:27:A:LEU:HA	1:28:A:THR:H	1	0.3
(4,146)	1:49:A:ALA:HA	1:51:A:VAL:H	2	0.3
(4,138)	1:46:A:CYS:HB2	1:48:A:ALA:H	1	0.3
(4,4)	1:6:A:THR:H	1:4:A:ASP:HB3	1	0.3
(3,56)	1:91:A:TRP:N	1:87:A:ASP:O	1	0.3
(3,35)	1:57:A:SER:H	1:53:A:ARG:O	1	0.3
(7,246)	1:73:A:PHE:HB3	1:73:A:PHE:H	1	0.29
(7,214)	1:62:A:ASP:HB2	1:62:A:ASP:H	2	0.29
(7,113)	1:31:A:ASP:HB3	1:31:A:ASP:H	1	0.29
(6,501)	1:118:A:THR:H	1:119:A:ILE:H	2	0.29
(6,418)	1:100:A:PRO:HD2	1:99:A:CYS:H	1	0.29
(6,189)	1:43:A:GLU:H	1:44:A:THR:H	1	0.29
(4,222)	1:75:A:ARG:HA	1:78:A:GLN:H	1	0.29
(4,28)	1:9:A:GLU:HA	1:11:A:ILE:H	2	0.29
(7,334)	1:94:A:ALA:HA	1:94:A:ALA:H	2	0.28
(7,328)	1:93:A:LEU:HA	1:93:A:LEU:H	2	0.28
(7,300)	1:88:A:ARG:HA	1:88:A:ARG:H	2	0.28
(7,275)	1:82:A:PHE:HA	1:82:A:PHE:H	2	0.28
(7,245)	1:73:A:PHE:HA	1:73:A:PHE:H	1	0.28
(7,32)	1:10:A:ILE:H	1:10:A:ILE:HA	1	0.28
(6,517)	1:121:A:ARG:H	1:122:A:GLU:H	2	0.28
(6,373)	1:88:A:ARG:H	1:89:A:ASN:H	1	0.28
(6,235)	1:55:A:PHE:H	1:56:A:TYR:H	2	0.28
(6,112)	1:27:A:LEU:HA	1:28:A:THR:H	2	0.28
(6,94)	1:21:A:LYS:HA	1:22:A:THR:H	2	0.28
(6,60)	1:15:A:ASN:H	1:16:A:SER:H	1	0.28
(6,54)	1:14:A:LEU:H	1:15:A:ASN:H	2	0.28
(4,29)	1:9:A:GLU:HA	1:12:A:LYS:H	1	0.28
(4,8)	1:5:A:ILE:HA	1:8:A:GLN:H	1	0.28
(6,94)	1:21:A:LYS:HA	1:22:A:THR:H	1	0.27
(6,8)	1:5:A:ILE:H	1:6:A:THR:H	1	0.27
(4,189)	1:72:A:GLN:HG3	1:68:A:ALA:H	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,297)	1:87:A:ASP:HA	1:87:A:ASP:H	2	0.26
(7,142)	1:39:A:THR:HB	1:39:A:THR:H	1	0.26
(7,126)	1:34:A:ALA:HA	1:34:A:ALA:H	2	0.26
(6,488)	1:114:A:GLU:H	1:115:A:ARG:H	1	0.26
(6,359)	1:85:A:ARG:H	1:86:A:LEU:H	1	0.26
(6,359)	1:85:A:ARG:H	1:86:A:LEU:H	2	0.26
(6,241)	1:56:A:TYR:H	1:57:A:SER:H	1	0.26
(6,68)	1:17:A:LEU:H	1:16:A:SER:HB2	2	0.26
(7,336)	1:95:A:GLY:HA3	1:95:A:GLY:H	1	0.25
(7,318)	1:91:A:TRP:HE3	1:91:A:TRP:HA	1	0.25
(7,109)	1:30:A:THR:HA	1:30:A:THR:H	2	0.25
(6,349)	1:83:A:LEU:H	1:84:A:LYS:H	1	0.25
(6,128)	1:30:A:THR:HA	1:31:A:ASP:H	2	0.25
(4,255)	1:85:A:ARG:HA	1:87:A:ASP:H	2	0.25
(4,226)	1:77:A:LYS:HA	1:80:A:ILE:H	1	0.25
(4,225)	1:76:A:HIS:H	1:78:A:GLN:H	1	0.25
(4,35)	1:11:A:ILE:HA	1:13:A:THR:H	2	0.25
(7,377)	1:108:A:THR:HG21	1:108:A:THR:H	2	0.24
(7,377)	1:108:A:THR:HG22	1:108:A:THR:H	2	0.24
(7,377)	1:108:A:THR:HG23	1:108:A:THR:H	2	0.24
(7,259)	1:78:A:GLN:HA	1:78:A:GLN:H	2	0.24
(7,156)	1:44:A:THR:HA	1:44:A:THR:H	1	0.24
(7,59)	1:15:A:ASN:H	1:15:A:ASN:HA	2	0.24
(7,41)	1:12:A:LYS:H	1:12:A:LYS:HA	1	0.24
(6,351)	1:84:A:LYS:H	1:85:A:ARG:H	1	0.24
(6,341)	1:82:A:PHE:HB2	1:83:A:LEU:H	1	0.24
(6,338)	1:81:A:ARG:H	1:82:A:PHE:H	1	0.24
(5,1)	1:10:A:ILE:HA	1:12:A:LYS:H	2	0.24
(3,87)	1:107:A:SER:H	1:29:A:VAL:O	1	0.24
(3,77)	1:122:A:GLU:H	1:118:A:THR:O	1	0.24
(7,205)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	1	0.23
(7,205)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	2	0.23
(7,156)	1:44:A:THR:HA	1:44:A:THR:H	2	0.23
(7,45)	1:14:A:LEU:H	1:14:A:LEU:HA	2	0.23
(7,43)	1:13:A:THR:H	1:13:A:THR:HA	1	0.23
(6,367)	1:87:A:ASP:HB2	1:88:A:ARG:H	2	0.23
(6,218)	1:50:A:THR:H	1:51:A:VAL:H	2	0.23
(6,134)	1:31:A:ASP:HA	1:32:A:ILE:H	2	0.23
(4,353)	1:126:A:LYS:HA	1:128:A:SER:H	1	0.23
(4,232)	1:79:A:LEU:HA	1:82:A:PHE:H	1	0.23
(4,162)	1:55:A:PHE:HZ	1:59:A:HIS:HD2	1	0.23
(4,123)	1:43:A:GLU:HG2	1:45:A:PHE:H	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,123)	1:43:A:GLU:HG3	1:45:A:PHE:H	1	0.23
(4,105)	1:39:A:THR:HG21	1:43:A:GLU:H	1	0.23
(4,105)	1:39:A:THR:HG22	1:43:A:GLU:H	1	0.23
(4,105)	1:39:A:THR:HG23	1:43:A:GLU:H	1	0.23
(4,23)	1:8:A:GLN:HA	1:11:A:ILE:H	2	0.23
(3,35)	1:57:A:SER:H	1:53:A:ARG:O	2	0.23
(3,13)	1:46:A:CYS:H	1:42:A:LYS:O	2	0.23
(7,292)	1:86:A:LEU:HA	1:86:A:LEU:H	1	0.22
(7,286)	1:84:A:LYS:HA	1:84:A:LYS:H	1	0.22
(7,218)	1:64:A:ARG:HA	1:64:A:ARG:H	2	0.22
(7,196)	1:57:A:SER:HB3	1:57:A:SER:H	1	0.22
(7,163)	1:46:A:CYS:HA	1:46:A:CYS:H	2	0.22
(7,36)	1:11:A:ILE:H	1:11:A:ILE:HB	1	0.22
(6,320)	1:78:A:GLN:H	1:79:A:LEU:H	2	0.22
(6,198)	1:44:A:THR:H	1:45:A:PHE:HB2	1	0.22
(6,124)	1:29:A:VAL:HA	1:30:A:THR:H	2	0.22
(6,103)	1:24:A:CYS:H	1:23:A:LEU:HG	1	0.22
(4,39)	1:12:A:LYS:HA	1:15:A:ASN:H	1	0.22
(7,409)	1:118:A:THR:HA	1:118:A:THR:H	1	0.21
(7,406)	1:117:A:LYS:HA	1:117:A:LYS:H	1	0.21
(7,287)	1:85:A:ARG:HA	1:85:A:ARG:H	2	0.21
(7,178)	1:52:A:LEU:HA	1:52:A:LEU:H	1	0.21
(7,163)	1:46:A:CYS:HA	1:46:A:CYS:H	1	0.21
(7,76)	1:20:A:GLN:H	1:20:A:GLN:HB3	2	0.21
(7,71)	1:19:A:GLU:H	1:19:A:GLU:HA	1	0.21
(7,45)	1:14:A:LEU:H	1:14:A:LEU:HA	1	0.21
(7,22)	1:8:A:GLN:HA	1:8:A:GLN:H	2	0.21
(7,7)	1:5:A:ILE:H	1:5:A:ILE:HA	1	0.21
(6,267)	1:65:A:CYS:H	1:66:A:LEU:H	2	0.21
(6,54)	1:14:A:LEU:H	1:15:A:ASN:H	1	0.21
(6,48)	1:12:A:LYS:H	1:13:A:THR:H	2	0.21
(4,114)	1:43:A:GLU:HG2	1:40:A:THR:H	1	0.21
(4,114)	1:43:A:GLU:HG3	1:40:A:THR:H	1	0.21
(3,14)	1:46:A:CYS:N	1:42:A:LYS:O	2	0.21
(3,9)	1:15:A:ASN:H	1:11:A:ILE:O	2	0.21
(7,406)	1:117:A:LYS:HA	1:117:A:LYS:H	2	0.2
(7,300)	1:88:A:ARG:HA	1:88:A:ARG:H	1	0.2
(7,272)	1:81:A:ARG:HA	1:81:A:ARG:H	1	0.2
(7,245)	1:73:A:PHE:HA	1:73:A:PHE:H	2	0.2
(6,266)	1:64:A:ARG:H	1:65:A:CYS:H	2	0.2
(6,227)	1:54:A:GLN:H	1:55:A:PHE:H	2	0.2
(6,187)	1:43:A:GLU:HG2	1:44:A:THR:H	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,187)	1:43:A:GLU:HG3	1:44:A:THR:H	1	0.2
(7,395)	1:112:A:PHE:HB2	1:112:A:PHE:H	1	0.19
(7,322)	1:91:A:TRP:HD1	1:91:A:TRP:HB3	2	0.19
(7,287)	1:85:A:ARG:HA	1:85:A:ARG:H	1	0.19
(7,272)	1:81:A:ARG:HA	1:81:A:ARG:H	2	0.19
(7,260)	1:79:A:LEU:HA	1:79:A:LEU:H	1	0.19
(7,240)	1:72:A:GLN:HA	1:72:A:GLN:H	1	0.19
(7,186)	1:55:A:PHE:HA	1:55:A:PHE:H	2	0.19
(7,183)	1:54:A:GLN:HA	1:54:A:GLN:H	1	0.19
(7,183)	1:54:A:GLN:HA	1:54:A:GLN:H	2	0.19
(7,169)	1:49:A:ALA:HA	1:49:A:ALA:H	1	0.19
(7,128)	1:35:A:ALA:HA	1:35:A:ALA:H	2	0.19
(7,41)	1:12:A:LYS:H	1:12:A:LYS:HA	2	0.19
(7,32)	1:10:A:ILE:H	1:10:A:ILE:HA	2	0.19
(6,429)	1:102:A:LYS:HA	1:103:A:GLU:H	2	0.19
(6,33)	1:10:A:ILE:H	1:11:A:ILE:H	2	0.19
(4,123)	1:43:A:GLU:HG2	1:45:A:PHE:H	2	0.19
(4,123)	1:43:A:GLU:HG3	1:45:A:PHE:H	2	0.19
(3,79)	1:123:A:LYS:H	1:119:A:ILE:O	2	0.19
(3,7)	1:14:A:LEU:H	1:10:A:ILE:O	1	0.19
(7,388)	1:111:A:ASN:HA	1:111:A:ASN:H	1	0.18
(7,258)	1:77:A:LYS:HA	1:77:A:LYS:H	1	0.18
(7,207)	1:60:A:GLU:HA	1:60:A:GLU:H	1	0.18
(7,186)	1:55:A:PHE:HA	1:55:A:PHE:H	1	0.18
(7,178)	1:52:A:LEU:HA	1:52:A:LEU:H	2	0.18
(7,171)	1:50:A:THR:HA	1:50:A:THR:H	2	0.18
(7,126)	1:34:A:ALA:HA	1:34:A:ALA:H	1	0.18
(7,59)	1:15:A:ASN:H	1:15:A:ASN:HA	1	0.18
(7,22)	1:8:A:GLN:HA	1:8:A:GLN:H	1	0.18
(6,208)	1:46:A:CYS:H	1:47:A:ARG:H	2	0.18
(3,71)	1:119:A:ILE:H	1:115:A:ARG:O	1	0.18
(1,6)	1:46:A:CYS:SG	1:99:A:CYS:SG	1	0.18
(1,6)	1:46:A:CYS:SG	1:99:A:CYS:SG	2	0.18
(1,5)	1:24:A:CYS:SG	1:65:A:CYS:SG	1	0.18
(1,5)	1:24:A:CYS:SG	1:65:A:CYS:SG	2	0.18
(1,4)	1:46:A:CYS:SG	1:99:A:CYS:SG	1	0.18
(1,4)	1:46:A:CYS:SG	1:99:A:CYS:SG	2	0.18
(1,3)	1:24:A:CYS:SG	1:65:A:CYS:SG	1	0.18
(1,3)	1:24:A:CYS:SG	1:65:A:CYS:SG	2	0.18
(1,2)	1:46:A:CYS:SG	1:99:A:CYS:SG	1	0.18
(1,2)	1:46:A:CYS:SG	1:99:A:CYS:SG	2	0.18
(1,1)	1:24:A:CYS:SG	1:65:A:CYS:SG	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:24:A:CYS:SG	1:65:A:CYS:SG	2	0.18
(7,425)	1:122:A:GLU:HA	1:122:A:GLU:H	2	0.17
(7,409)	1:118:A:THR:HA	1:118:A:THR:H	2	0.17
(7,403)	1:115:A:ARG:HA	1:115:A:ARG:H	2	0.17
(7,328)	1:93:A:LEU:HA	1:93:A:LEU:H	1	0.17
(7,174)	1:51:A:VAL:HA	1:51:A:VAL:H	1	0.17
(7,160)	1:45:A:PHE:H	1:45:A:PHE:HA	1	0.17
(7,153)	1:43:A:GLU:HA	1:43:A:GLU:H	1	0.17
(7,7)	1:5:A:ILE:H	1:5:A:ILE:HA	2	0.17
(6,315)	1:76:A:HIS:H	1:77:A:LYS:H	1	0.17
(6,231)	1:55:A:PHE:HB2	1:56:A:TYR:H	1	0.17
(6,227)	1:54:A:GLN:H	1:55:A:PHE:H	1	0.17
(6,193)	1:44:A:THR:H	1:45:A:PHE:H	2	0.17
(6,178)	1:40:A:THR:HB	1:41:A:GLU:H	2	0.17
(6,105)	1:24:A:CYS:H	1:23:A:LEU:HB2	2	0.17
(4,240)	1:81:A:ARG:HA	1:83:A:LEU:H	1	0.17
(4,51)	1:15:A:ASN:HA	1:18:A:THR:H	2	0.17
(3,55)	1:91:A:TRP:H	1:87:A:ASP:O	2	0.17
(3,5)	1:13:A:THR:H	1:9:A:GLU:O	1	0.17
(7,393)	1:112:A:PHE:HA	1:112:A:PHE:H	1	0.16
(7,393)	1:112:A:PHE:HA	1:112:A:PHE:H	2	0.16
(7,297)	1:87:A:ASP:HA	1:87:A:ASP:H	1	0.16
(7,275)	1:82:A:PHE:HA	1:82:A:PHE:H	1	0.16
(7,251)	1:75:A:ARG:HA	1:75:A:ARG:H	2	0.16
(7,249)	1:74:A:HIS:HA	1:74:A:HIS:H	2	0.16
(7,235)	1:71:A:GLN:HA	1:71:A:GLN:H	1	0.16
(7,174)	1:51:A:VAL:HA	1:51:A:VAL:H	2	0.16
(7,171)	1:50:A:THR:HA	1:50:A:THR:H	1	0.16
(7,160)	1:45:A:PHE:H	1:45:A:PHE:HA	2	0.16
(7,128)	1:35:A:ALA:HA	1:35:A:ALA:H	1	0.16
(7,121)	1:33:A:PHE:HA	1:33:A:PHE:H	1	0.16
(7,43)	1:13:A:THR:H	1:13:A:THR:HA	2	0.16
(7,28)	1:9:A:GLU:H	1:9:A:GLU:HA	2	0.16
(7,13)	1:6:A:THR:H	1:6:A:THR:HA	2	0.16
(6,326)	1:79:A:LEU:H	1:80:A:ILE:H	2	0.16
(6,51)	1:14:A:LEU:H	1:13:A:THR:HB	1	0.16
(4,308)	1:111:A:ASN:HB2	1:114:A:GLU:H	2	0.16
(4,158)	1:55:A:PHE:HE1	1:59:A:HIS:HD2	2	0.16
(4,158)	1:55:A:PHE:HE2	1:59:A:HIS:HD2	2	0.16
(4,138)	1:46:A:CYS:HB2	1:48:A:ALA:H	2	0.16
(3,57)	1:112:A:PHE:H	1:108:A:THR:O	1	0.16
(3,11)	1:17:A:LEU:H	1:13:A:THR:O	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,427)	1:123:A:LYS:HA	1:123:A:LYS:H	2	0.15
(7,388)	1:111:A:ASN:HA	1:111:A:ASN:H	2	0.15
(7,334)	1:94:A:ALA:HA	1:94:A:ALA:H	1	0.15
(7,286)	1:84:A:LYS:HA	1:84:A:LYS:H	2	0.15
(7,153)	1:43:A:GLU:HA	1:43:A:GLU:H	2	0.15
(7,96)	1:27:A:LEU:HA	1:27:A:LEU:H	2	0.15
(7,81)	1:21:A:LYS:HA	1:21:A:LYS:H	2	0.15
(7,60)	1:16:A:SER:H	1:16:A:SER:HA	1	0.15
(7,60)	1:16:A:SER:H	1:16:A:SER:HA	2	0.15
(7,35)	1:11:A:ILE:HA	1:11:A:ILE:H	1	0.15
(6,501)	1:118:A:THR:H	1:119:A:ILE:H	1	0.15
(6,210)	1:47:A:ARG:H	1:48:A:ALA:H	1	0.15
(4,232)	1:79:A:LEU:HA	1:82:A:PHE:H	2	0.15
(4,231)	1:78:A:GLN:H	1:80:A:ILE:H	2	0.15
(3,51)	1:88:A:ARG:H	1:84:A:LYS:O	2	0.15
(7,403)	1:115:A:ARG:HA	1:115:A:ARG:H	1	0.14
(7,260)	1:79:A:LEU:HA	1:79:A:LEU:H	2	0.14
(7,259)	1:78:A:GLN:HA	1:78:A:GLN:H	1	0.14
(7,195)	1:57:A:SER:HA	1:57:A:SER:H	1	0.14
(7,115)	1:32:A:ILE:HA	1:32:A:ILE:H	1	0.14
(7,102)	1:28:A:THR:HA	1:28:A:THR:H	1	0.14
(7,68)	1:18:A:THR:H	1:18:A:THR:HA	2	0.14
(6,323)	1:79:A:LEU:HB2	1:80:A:ILE:H	1	0.14
(6,311)	1:76:A:HIS:HB3	1:77:A:LYS:H	1	0.14
(4,226)	1:77:A:LYS:HA	1:80:A:ILE:H	2	0.14
(4,83)	1:31:A:ASP:HA	1:34:A:ALA:H	2	0.14
(3,79)	1:123:A:LYS:H	1:119:A:ILE:O	1	0.14
(3,72)	1:119:A:ILE:N	1:115:A:ARG:O	1	0.14
(3,29)	1:54:A:GLN:H	1:50:A:THR:O	1	0.14
(3,17)	1:48:A:ALA:H	1:44:A:THR:O	2	0.14
(3,6)	1:13:A:THR:N	1:9:A:GLU:O	1	0.14
(7,292)	1:86:A:LEU:HA	1:86:A:LEU:H	2	0.13
(7,258)	1:77:A:LYS:HA	1:77:A:LYS:H	2	0.13
(7,188)	1:55:A:PHE:HB2	1:55:A:PHE:H	2	0.13
(7,169)	1:49:A:ALA:HA	1:49:A:ALA:H	2	0.13
(7,87)	1:23:A:LEU:H	1:23:A:LEU:HA	2	0.13
(7,28)	1:9:A:GLU:H	1:9:A:GLU:HA	1	0.13
(3,43)	1:83:A:LEU:H	1:79:A:LEU:O	2	0.13
(3,37)	1:80:A:ILE:H	1:76:A:HIS:O	2	0.13
(3,21)	1:50:A:THR:H	1:46:A:CYS:O	1	0.13
(3,1)	1:8:A:GLN:H	1:4:A:ASP:O	2	0.13
(7,235)	1:71:A:GLN:HA	1:71:A:GLN:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(7,198)	1:58:A:HIS:HA	1:58:A:HIS:H	1	0.12
(7,198)	1:58:A:HIS:HA	1:58:A:HIS:H	2	0.12
(7,75)	1:20:A:GLN:HA	1:20:A:GLN:H	1	0.12
(7,35)	1:11:A:ILE:HA	1:11:A:ILE:H	2	0.12
(7,4)	1:4:A:ASP:HA	1:4:A:ASP:H	1	0.12
(6,310)	1:75:A:ARG:H	1:76:A:HIS:H	1	0.12
(6,208)	1:46:A:CYS:H	1:47:A:ARG:H	1	0.12
(6,48)	1:12:A:LYS:H	1:13:A:THR:H	1	0.12
(3,52)	1:88:A:ARG:N	1:84:A:LYS:O	2	0.12
(3,45)	1:84:A:LYS:H	1:80:A:ILE:O	2	0.12
(3,12)	1:17:A:LEU:N	1:13:A:THR:O	2	0.12
(7,304)	1:89:A:ASN:HA	1:89:A:ASN:H	1	0.11
(7,87)	1:23:A:LEU:H	1:23:A:LEU:HA	1	0.11
(7,13)	1:6:A:THR:H	1:6:A:THR:HA	1	0.11
(6,56)	1:14:A:LEU:H	1:15:A:ASN:HB2	1	0.11
(4,321)	1:114:A:GLU:HA	1:117:A:LYS:H	1	0.11
(4,295)	1:111:A:ASN:HB2	1:108:A:THR:H	2	0.11
(3,33)	1:56:A:TYR:H	1:52:A:LEU:O	1	0.11
(3,80)	1:123:A:LYS:N	1:119:A:ILE:O	1	0.1
(3,69)	1:118:A:THR:H	1:114:A:GLU:O	1	0.1
(3,53)	1:90:A:LEU:H	1:86:A:LEU:O	2	0.1
(3,5)	1:13:A:THR:H	1:9:A:GLU:O	2	0.1

10 Dihedral-angle violation analysis

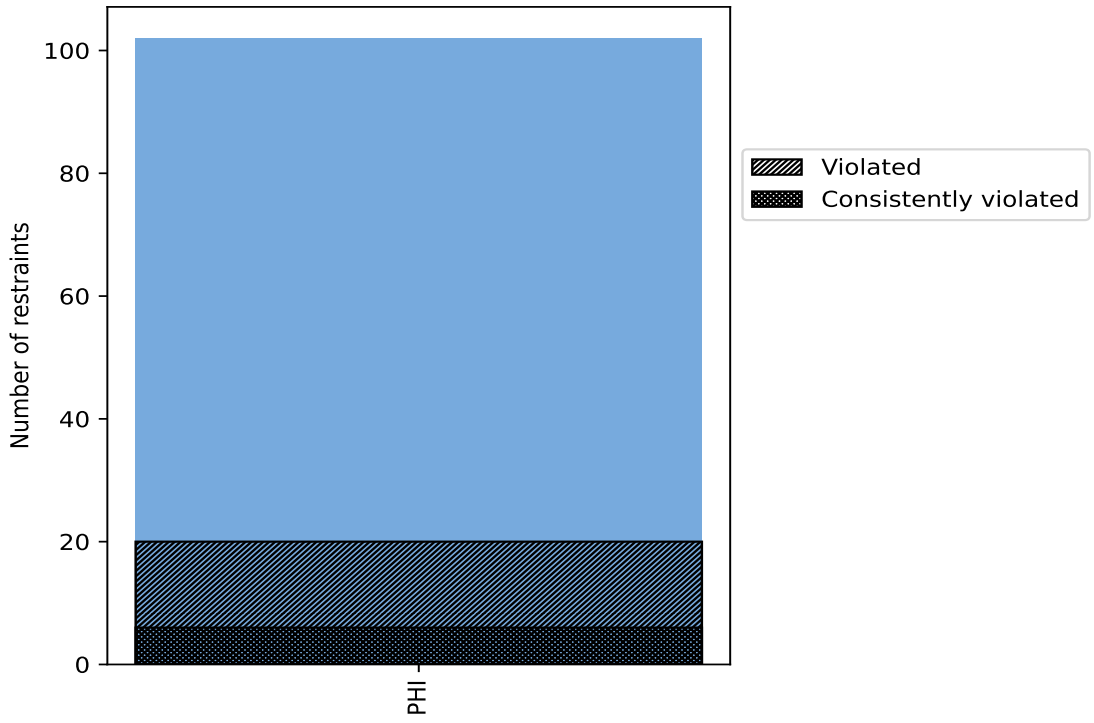
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	102	100.0	20	19.6	19.6	6	5.9	5.9
Total	102	100.0	20	19.6	19.6	6	5.9	5.9

[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



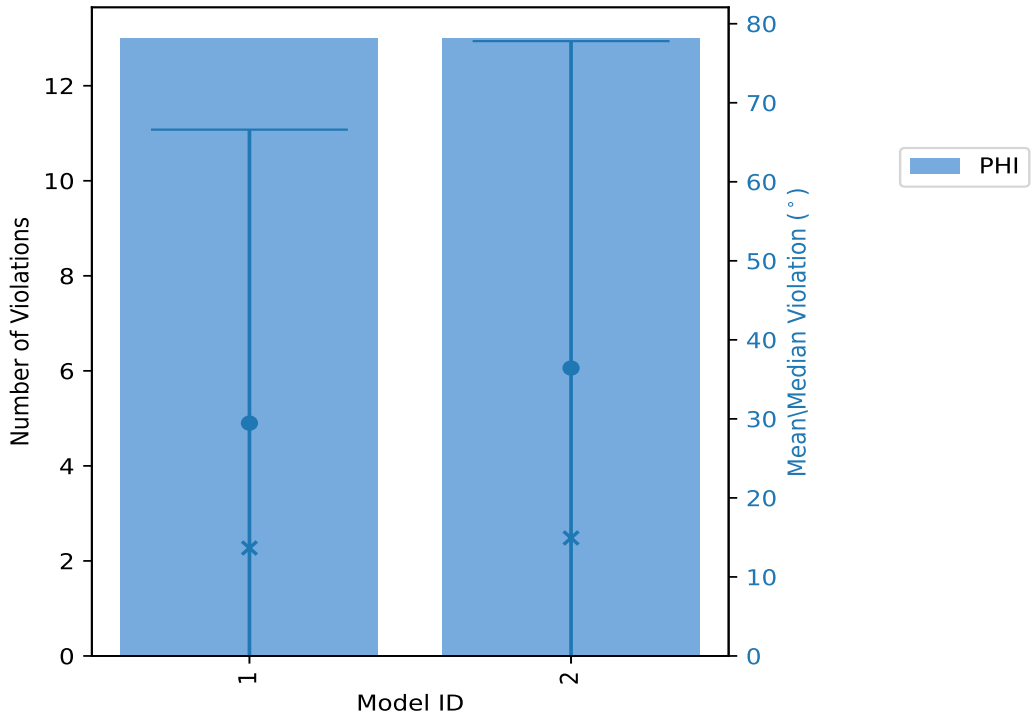
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	Total				
1	13	13	29.46	126.17	37.14	13.66
2	13	13	36.43	132.53	41.37	14.93

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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 (i)

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	Total	Count[1]	%
14	14	1	50.0

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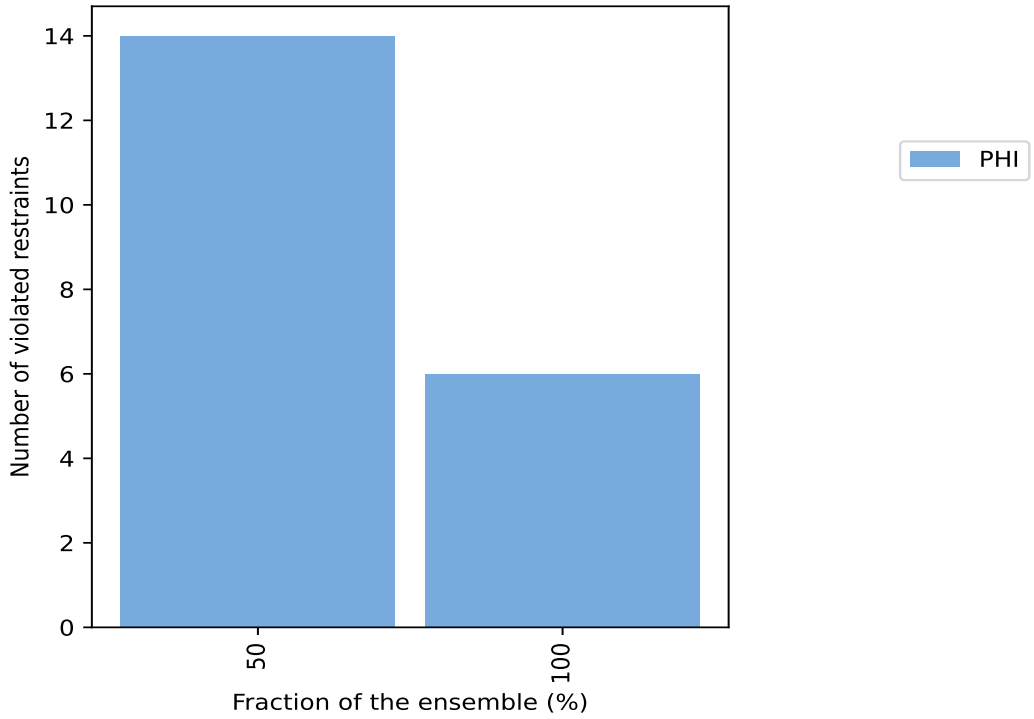
Number of violated restraints		Fraction of the ensemble	
PHI	Total	Count[1]	%
6	6	2	100.0

[1] Number of models with violations

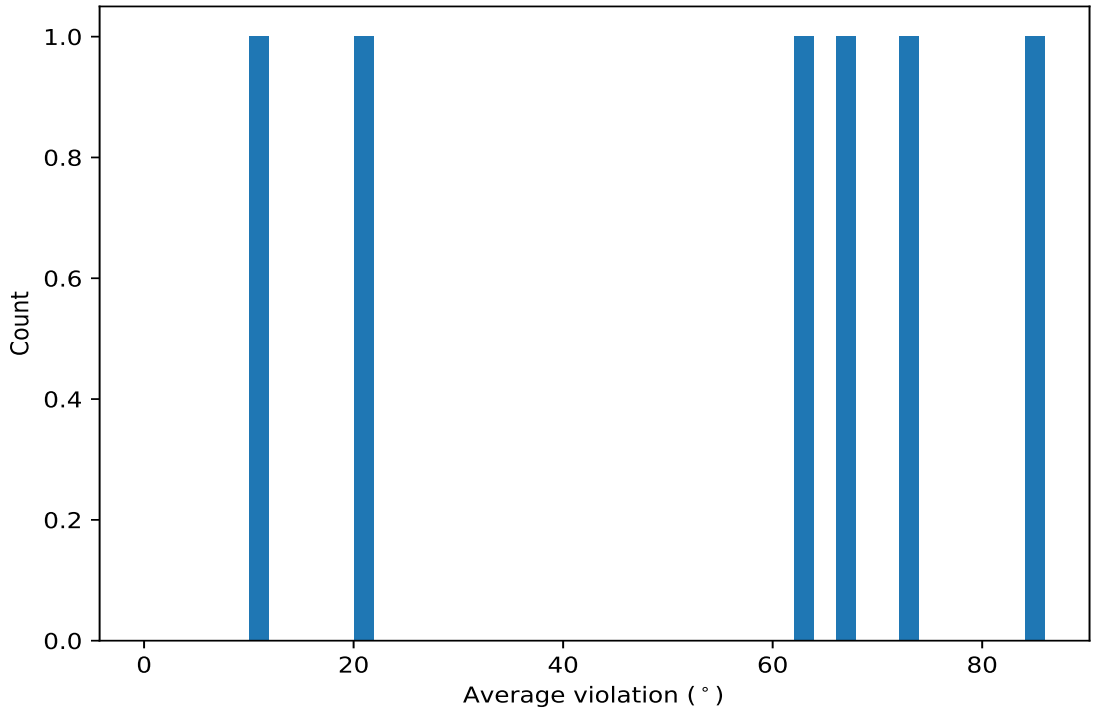
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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.

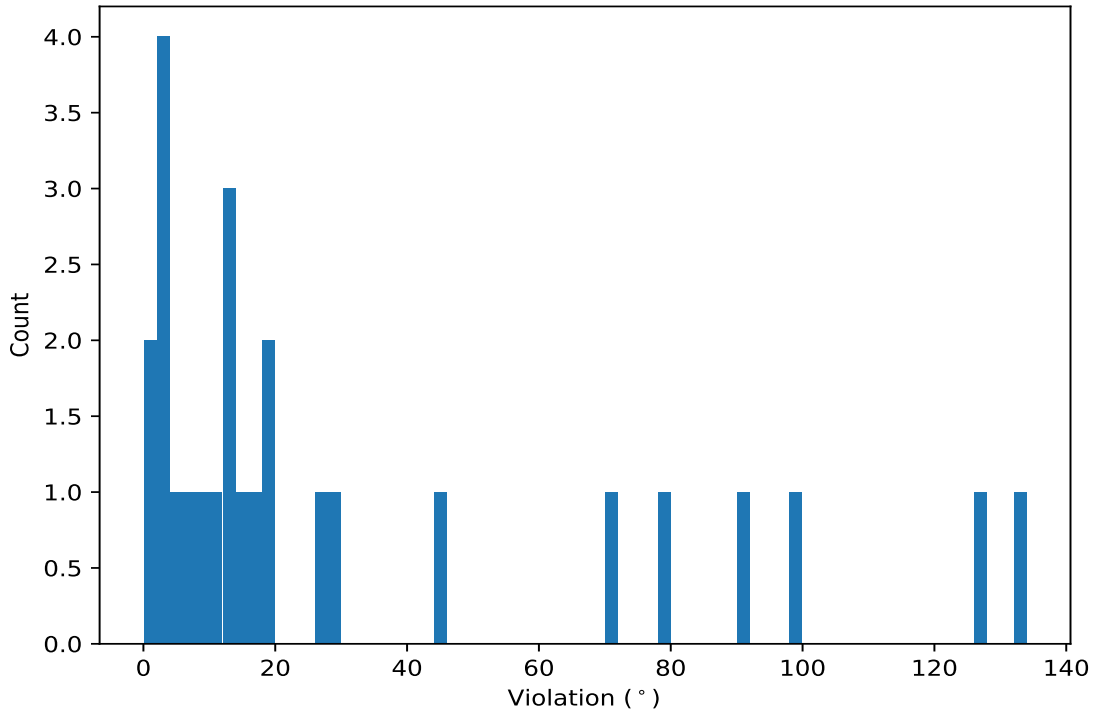
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,1)	1:3:A:THR:C	1:4:A:ASP:N	1:4:A:ASP:CA	1:4:A:ASP:C	2	85.46	13.8	85.46
(1,80)	1:59:A:HIS:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	2	72.64	59.89	72.64
(1,76)	1:20:A:GLN:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	2	67.07	59.1	67.07
(1,73)	1:126:A:LYS:C	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	2	62.57	16.62	62.57
(1,90)	1:28:A:THR:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	2	21.16	7.98	21.16
(1,91)	1:30:A:THR:C	1:31:A:ASP:N	1:31:A:ASP:CA	1:31:A:ASP:C	2	10.86	8.43	10.86

[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

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 (°)
(1,80)	1:59:A:HIS:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	2	132.53
(1,76)	1:20:A:GLN:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1	126.17
(1,1)	1:3:A:THR:C	1:4:A:ASP:N	1:4:A:ASP:CA	1:4:A:ASP:C	2	99.26
(1,74)	1:127:A:CYS:C	1:128:A:SER:N	1:128:A:SER:CA	1:128:A:SER:C	2	90.7
(1,73)	1:126:A:LYS:C	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	1	79.18
(1,1)	1:3:A:THR:C	1:4:A:ASP:N	1:4:A:ASP:CA	1:4:A:ASP:C	1	71.66
(1,73)	1:126:A:LYS:C	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	2	45.95
(1,90)	1:28:A:THR:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1	29.14
(1,99)	1:97:A:ASN:C	1:98:A:SER:N	1:98:A:SER:CA	1:98:A:SER:C	2	26.36
(1,91)	1:30:A:THR:C	1:31:A:ASP:N	1:31:A:ASP:CA	1:31:A:ASP:C	2	19.29
(1,81)	1:62:A:ASP:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1	18.32
(1,75)	1:18:A:THR:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1	17.64
(1,87)	1:19:A:GLU:C	1:20:A:GLN:N	1:20:A:GLN:CA	1:20:A:GLN:C	2	14.93
(1,82)	1:69:A:THR:C	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	1	13.66
(1,90)	1:28:A:THR:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	2	13.19
(1,80)	1:59:A:HIS:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1	12.75
(1,88)	1:21:A:LYS:C	1:22:A:THR:N	1:22:A:THR:CA	1:22:A:THR:C	2	11.92
(1,77)	1:24:A:CYS:C	1:25:A:THR:N	1:25:A:THR:CA	1:25:A:THR:C	2	8.54
(1,76)	1:20:A:GLN:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	2	7.97
(1,101)	1:105:A:ASN:C	1:106:A:GLN:N	1:106:A:GLN:CA	1:106:A:GLN:C	1	4.44
(1,16)	1:41:A:GLU:C	1:42:A:LYS:N	1:42:A:LYS:CA	1:42:A:LYS:C	1	3.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:30:A:THR:C	1:31:A:ASP:N	1:31:A:ASP:CA	1:31:A:ASP:C	1	2.44
(1,97)	1:63:A:THR:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1	2.4
(1,14)	1:16:A:SER:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1	2.13
(1,94)	1:36:A:SER:C	1:37:A:LYS:N	1:37:A:LYS:CA	1:37:A:LYS:C	2	1.57
(1,85)	1:101:A:VAL:C	1:102:A:LYS:N	1:102:A:LYS:CA	1:102:A:LYS:C	2	1.34