



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 05:44 PM UTC

PDB ID : 8DWQ / pdb_00008dwq
BMRB ID : 31035
Title : Solution Structure of the H3 protein
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Deposited on : 2022-08-01

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

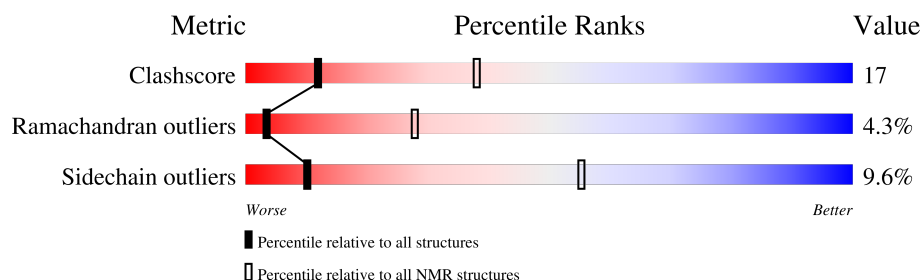
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 65%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	167	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:13-A:145, A:149-A:167 (152)	2.42	4

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

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

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

Cluster number	Models
1	1, 3, 4, 5, 7, 8, 9
2	2, 6, 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2525 atoms, of which 1238 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called H3 Protein.

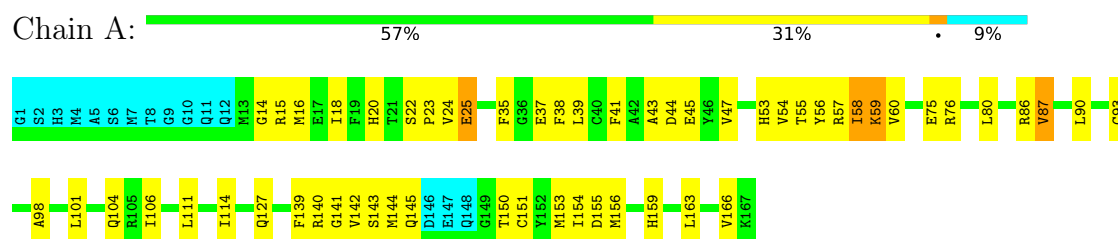
Mol	Chain	Residues	Atoms						Trace
1	A	167	Total	C	H	N	O	S	0
			2525	796	1238	216	262	13	

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: H3 Protein



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

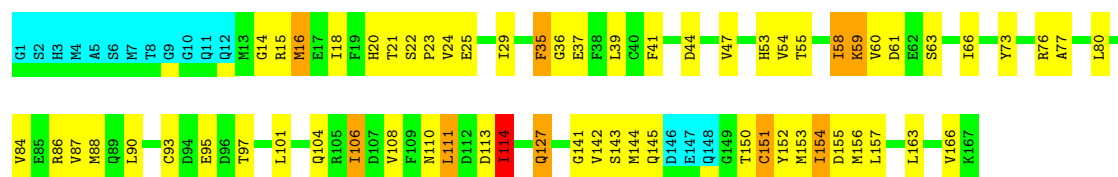
- Molecule 1: H3 Protein



4.2.2 Score per residue for model 2

- Molecule 1: H3 Protein

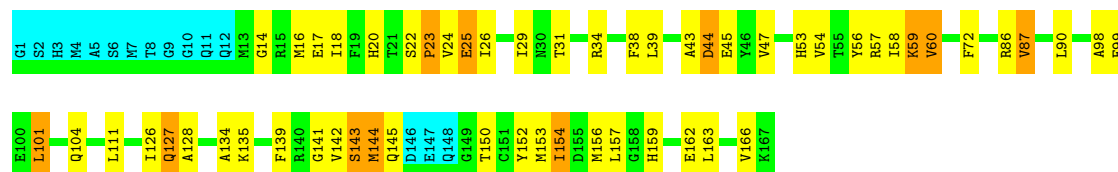




4.2.3 Score per residue for model 3

- Molecule 1: H3 Protein

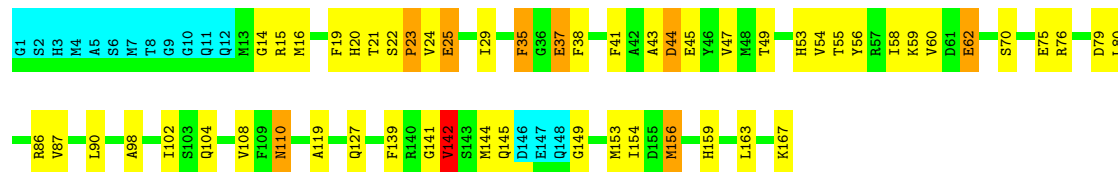
Chain A: 57% 27% 7% 9%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: H3 Protein

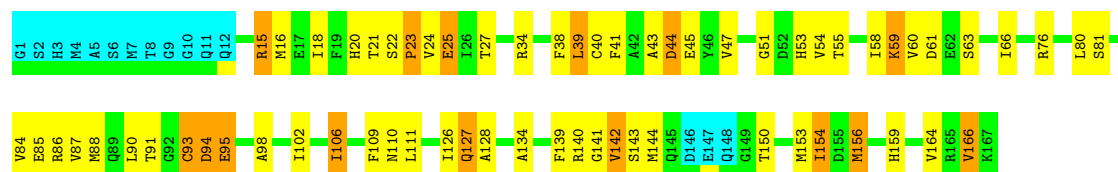
Chain A: 58% 28% 5% 9%



4.2.5 Score per residue for model 5

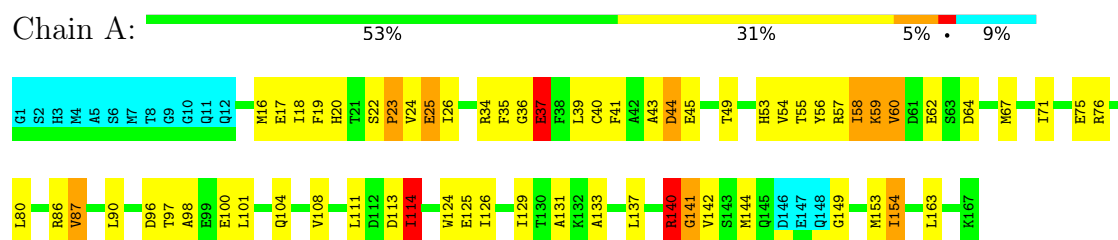
- Molecule 1: H3 Protein

Chain A: 52% 30% 9% 9%



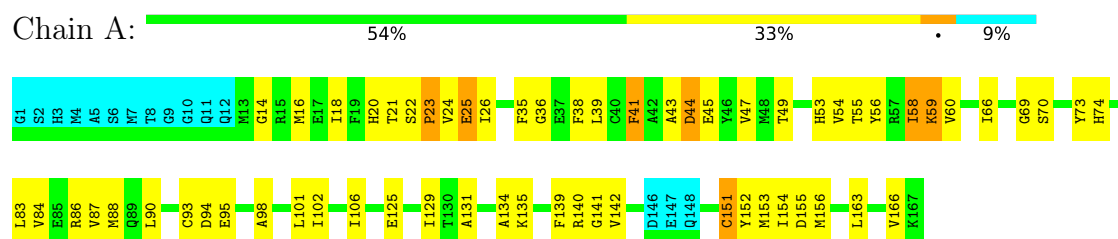
4.2.6 Score per residue for model 6

- Molecule 1: H3 Protein



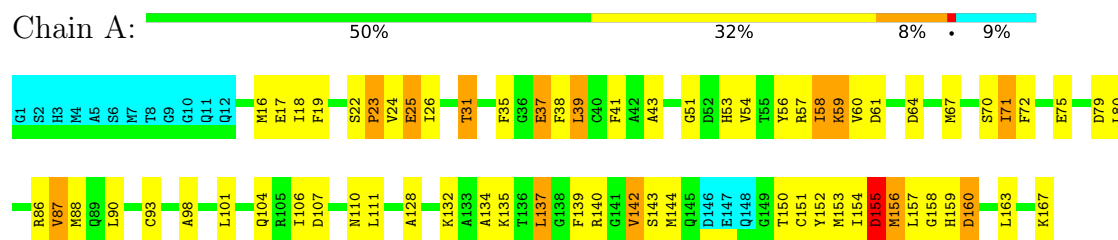
4.2.7 Score per residue for model 7

- Molecule 1: H3 Protein



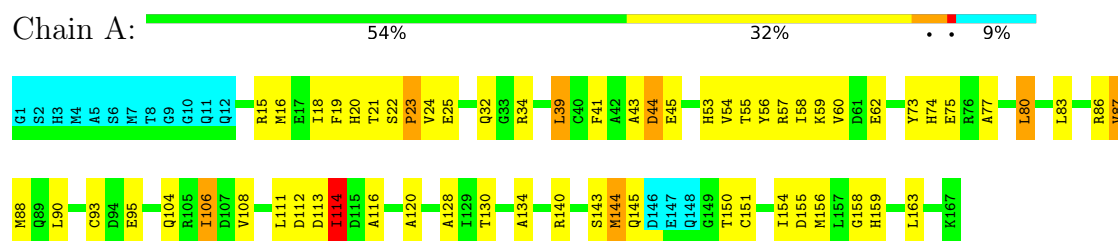
4.2.8 Score per residue for model 8

- Molecule 1: H3 Protein



4.2.9 Score per residue for model 9

- Molecule 1: H3 Protein



4.2.10 Score per residue for model 10

● Molecule 1: H3 Protein



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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
CNS	refinement	1.2

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	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.46±0.02	0±0/1198 (0.0± 0.0%)	0.76±0.04	0±0/1615 (0.0± 0.0%)
All	All	0.46	0/11980 (0.0%)	0.76	2/16150 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	140	ARG	N-CA-C	-5.73	108.08	114.62	6	1
1	A	142	VAL	CB-CA-C	-5.49	105.55	111.59	4	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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	1181	1145	1141	40±6
All	All	11810	11450	11410	403

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:MET:O	1:A:151:CYS:HB2	0.77	1.78	9	1
1:A:141:GLY:HA2	1:A:153:MET:O	0.76	1.80	4	4
1:A:25:GLU:HG2	1:A:54:VAL:HG21	0.76	1.57	9	2
1:A:24:VAL:HG23	1:A:54:VAL:HG13	0.74	1.56	2	5
1:A:156:MET:SD	1:A:159:HIS:HA	0.71	2.25	5	3
1:A:145:GLN:O	1:A:150:THR:HA	0.68	1.88	10	1
1:A:88:MET:HG3	1:A:93:CYS:SG	0.67	2.29	5	1
1:A:28:THR:O	1:A:29:ILE:HG12	0.67	1.89	10	1
1:A:22:SER:O	1:A:53:HIS:HB3	0.66	1.91	4	9
1:A:134:ALA:HB1	1:A:140:ARG:HA	0.65	1.67	8	3
1:A:108:VAL:HA	1:A:111:LEU:HD13	0.65	1.68	6	3
1:A:141:GLY:HA3	1:A:154:ILE:HD13	0.64	1.67	3	3
1:A:76:ARG:O	1:A:80:LEU:HB2	0.64	1.92	2	6
1:A:55:THR:HB	1:A:166:VAL:HG12	0.64	1.67	5	1
1:A:86:ARG:O	1:A:90:LEU:HG	0.64	1.92	6	9
1:A:71:ILE:HA	1:A:74:HIS:CE1	0.63	2.28	1	1
1:A:24:VAL:HG23	1:A:54:VAL:CG1	0.63	2.23	2	1
1:A:145:GLN:HA	1:A:149:GLY:O	0.63	1.93	1	1
1:A:104:GLN:HG3	1:A:144:MET:SD	0.62	2.34	4	2
1:A:104:GLN:HB3	1:A:143:SER:O	0.62	1.94	8	1
1:A:16:MET:CE	1:A:62:GLU:HB2	0.62	2.24	6	2
1:A:75:GLU:O	1:A:79:ASP:HB2	0.62	1.94	8	2
1:A:18:ILE:HB	1:A:41:PHE:CD1	0.62	2.29	7	3
1:A:18:ILE:O	1:A:57:ARG:HA	0.62	1.95	10	4
1:A:72:PHE:HA	1:A:75:GLU:OE1	0.61	1.95	1	1
1:A:145:GLN:HB2	1:A:150:THR:HA	0.61	1.70	2	1
1:A:144:MET:O	1:A:145:GLN:HG3	0.60	1.96	2	1
1:A:35:PHE:CD2	1:A:124:TRP:HB3	0.60	2.31	6	1
1:A:41:PHE:CE2	1:A:152:TYR:HB2	0.60	2.31	1	1
1:A:18:ILE:HB	1:A:41:PHE:CG	0.60	2.32	7	2
1:A:143:SER:HB3	1:A:152:TYR:CE1	0.60	2.31	3	1
1:A:134:ALA:HA	1:A:139:PHE:CD1	0.59	2.32	5	1
1:A:19:PHE:HA	1:A:56:TYR:O	0.59	1.97	8	5
1:A:24:VAL:HG22	1:A:25:GLU:H	0.59	1.57	5	7
1:A:23:PRO:O	1:A:54:VAL:HG22	0.58	1.98	9	8
1:A:86:ARG:O	1:A:90:LEU:HD13	0.58	1.98	10	1
1:A:63:SER:O	1:A:66:ILE:HG12	0.58	1.99	5	2
1:A:26:ILE:O	1:A:27:THR:HG23	0.58	1.99	10	1
1:A:144:MET:CE	1:A:153:MET:HG3	0.57	2.29	1	1
1:A:141:GLY:O	1:A:142:VAL:HG23	0.57	1.98	6	1
1:A:38:PHE:CZ	1:A:131:ALA:HB1	0.57	2.34	7	1
1:A:41:PHE:CD2	1:A:152:TYR:HB2	0.57	2.34	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:THR:HG23	1:A:47:VAL:HA	0.57	1.77	7	4
1:A:37:GLU:HG3	1:A:155:ASP:N	0.56	2.15	2	1
1:A:88:MET:HA	1:A:93:CYS:O	0.56	2.01	2	3
1:A:35:PHE:CD1	1:A:38:PHE:HB2	0.56	2.35	7	2
1:A:141:GLY:HA3	1:A:154:ILE:CD1	0.56	2.31	3	3
1:A:38:PHE:HA	1:A:156:MET:SD	0.56	2.41	8	1
1:A:16:MET:O	1:A:59:LYS:HA	0.56	2.01	6	4
1:A:17:GLU:HG3	1:A:59:LYS:HD2	0.55	1.78	8	2
1:A:159:HIS:O	1:A:162:GLU:HG2	0.55	2.00	10	1
1:A:20:HIS:O	1:A:55:THR:HA	0.55	2.02	9	6
1:A:60:VAL:HG21	1:A:154:ILE:HG12	0.55	1.78	2	1
1:A:127:GLN:O	1:A:130:THR:HG22	0.55	2.02	1	1
1:A:33:GLY:HA3	1:A:35:PHE:CE1	0.55	2.37	10	1
1:A:75:GLU:OE2	1:A:133:ALA:HA	0.54	2.02	6	1
1:A:16:MET:O	1:A:60:VAL:HG12	0.54	2.02	9	1
1:A:41:PHE:CB	1:A:152:TYR:HB2	0.54	2.33	8	1
1:A:41:PHE:HB3	1:A:152:TYR:HB2	0.54	1.78	8	1
1:A:20:HIS:NE2	1:A:56:TYR:HB2	0.53	2.18	7	1
1:A:127:GLN:HG2	1:A:153:MET:SD	0.53	2.44	5	1
1:A:126:ILE:O	1:A:129:ILE:HG13	0.53	2.03	6	1
1:A:145:GLN:HG3	1:A:150:THR:C	0.53	2.29	9	1
1:A:55:THR:HB	1:A:166:VAL:HG23	0.53	1.80	2	1
1:A:16:MET:HG2	1:A:60:VAL:HG12	0.53	1.81	5	3
1:A:41:PHE:O	1:A:151:CYS:HA	0.53	2.03	7	3
1:A:16:MET:HG2	1:A:60:VAL:O	0.53	2.04	4	2
1:A:17:GLU:HG3	1:A:59:LYS:CD	0.53	2.33	6	2
1:A:34:ARG:CG	1:A:128:ALA:HB2	0.53	2.34	5	1
1:A:59:LYS:N	1:A:59:LYS:HD2	0.52	2.19	1	8
1:A:127:GLN:HG3	1:A:153:MET:SD	0.52	2.44	1	3
1:A:142:VAL:HG21	1:A:153:MET:SD	0.52	2.44	6	1
1:A:39:LEU:HD22	1:A:39:LEU:O	0.52	2.04	8	1
1:A:60:VAL:HG21	1:A:154:ILE:HD12	0.52	1.80	4	1
1:A:19:PHE:CZ	1:A:57:ARG:HD3	0.52	2.40	9	1
1:A:86:ARG:NE	1:A:90:LEU:HD11	0.52	2.19	5	2
1:A:158:GLY:C	1:A:160:ASP:H	0.52	2.13	8	2
1:A:98:ALA:O	1:A:102:ILE:HG12	0.52	2.05	7	3
1:A:62:GLU:O	1:A:67:MET:HB2	0.51	2.04	6	1
1:A:159:HIS:O	1:A:163:LEU:HD23	0.51	2.05	3	2
1:A:135:LYS:HA	1:A:140:ARG:CZ	0.51	2.35	7	1
1:A:156:MET:SD	1:A:156:MET:N	0.51	2.81	4	2
1:A:93:CYS:SG	1:A:94:ASP:N	0.51	2.81	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ARG:HG3	1:A:128:ALA:HB2	0.51	1.83	1	2
1:A:16:MET:HE2	1:A:62:GLU:HB2	0.51	1.81	9	2
1:A:39:LEU:HD23	1:A:156:MET:CG	0.51	2.36	10	1
1:A:15:ARG:HA	1:A:60:VAL:O	0.51	2.05	2	2
1:A:87:VAL:CG1	1:A:98:ALA:HB1	0.51	2.36	1	4
1:A:20:HIS:NE2	1:A:39:LEU:HD21	0.51	2.21	7	1
1:A:142:VAL:CG1	1:A:153:MET:HB2	0.50	2.36	10	3
1:A:43:ALA:HB3	1:A:150:THR:HB	0.50	1.81	5	3
1:A:21:THR:HG22	1:A:55:THR:OG1	0.50	2.07	2	2
1:A:87:VAL:HG11	1:A:98:ALA:HB1	0.50	1.81	3	2
1:A:72:PHE:HB2	1:A:75:GLU:OE1	0.50	2.06	8	1
1:A:104:GLN:O	1:A:144:MET:HA	0.50	2.07	3	1
1:A:38:PHE:CZ	1:A:40:CYS:HB3	0.50	2.42	5	1
1:A:16:MET:HG2	1:A:18:ILE:CG2	0.50	2.36	1	1
1:A:55:THR:O	1:A:165:ARG:HA	0.50	2.07	1	1
1:A:106:ILE:CD1	1:A:110:ASN:HB3	0.50	2.37	5	3
1:A:142:VAL:HB	1:A:144:MET:CE	0.50	2.37	8	3
1:A:145:GLN:HG2	1:A:151:CYS:SG	0.49	2.47	9	1
1:A:141:GLY:CA	1:A:154:ILE:HD13	0.49	2.37	4	3
1:A:16:MET:SD	1:A:18:ILE:HG23	0.49	2.47	6	2
1:A:69:GLY:O	1:A:73:TYR:HB3	0.49	2.07	7	1
1:A:44:ASP:CG	1:A:45:GLU:H	0.49	2.16	9	5
1:A:144:MET:SD	1:A:144:MET:N	0.49	2.86	3	1
1:A:159:HIS:O	1:A:163:LEU:HD12	0.49	2.08	9	1
1:A:16:MET:HG3	1:A:18:ILE:HG23	0.48	1.86	5	1
1:A:72:PHE:CE2	1:A:99:GLU:HA	0.48	2.42	3	1
1:A:142:VAL:HB	1:A:153:MET:HB2	0.48	1.85	6	1
1:A:17:GLU:HA	1:A:58:ILE:O	0.48	2.08	10	1
1:A:31:THR:HA	1:A:38:PHE:O	0.48	2.08	3	1
1:A:43:ALA:O	1:A:44:ASP:HB2	0.48	2.07	7	5
1:A:22:SER:HB3	1:A:23:PRO:HD2	0.48	1.85	6	5
1:A:131:ALA:HA	1:A:141:GLY:O	0.48	2.08	6	1
1:A:114:ILE:HG22	1:A:115:ASP:N	0.48	2.24	10	1
1:A:116:ALA:O	1:A:120:ALA:HB2	0.47	2.09	9	2
1:A:39:LEU:HD13	1:A:41:PHE:CZ	0.47	2.44	9	1
1:A:16:MET:SD	1:A:62:GLU:HG2	0.47	2.50	10	1
1:A:25:GLU:H	1:A:54:VAL:CG1	0.47	2.22	10	1
1:A:20:HIS:HB2	1:A:41:PHE:HA	0.47	1.83	4	3
1:A:134:ALA:CB	1:A:140:ARG:HA	0.47	2.37	8	1
1:A:84:VAL:HB	1:A:95:GLU:CG	0.47	2.39	2	1
1:A:16:MET:HG2	1:A:18:ILE:HG23	0.47	1.87	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:MET:HE3	1:A:156:MET:HA	0.47	1.85	1	1
1:A:35:PHE:HB2	1:A:128:ALA:HA	0.46	1.85	8	1
1:A:35:PHE:CE1	1:A:38:PHE:HB2	0.46	2.45	10	1
1:A:58:ILE:HG22	1:A:163:LEU:HD13	0.46	1.86	2	2
1:A:154:ILE:N	1:A:154:ILE:HD12	0.46	2.24	2	1
1:A:143:SER:C	1:A:144:MET:HE2	0.46	2.35	5	1
1:A:34:ARG:HG2	1:A:128:ALA:HB2	0.46	1.88	5	1
1:A:143:SER:HA	1:A:151:CYS:O	0.46	2.10	2	2
1:A:44:ASP:HB2	1:A:149:GLY:HA2	0.46	1.87	6	2
1:A:139:PHE:CE2	1:A:142:VAL:HG13	0.46	2.46	4	1
1:A:47:VAL:HG23	1:A:48:MET:N	0.46	2.26	1	1
1:A:88:MET:HA	1:A:93:CYS:HA	0.46	1.86	5	1
1:A:24:VAL:CG2	1:A:54:VAL:HG13	0.46	2.39	9	2
1:A:76:ARG:HD2	1:A:95:GLU:OE2	0.46	2.11	5	1
1:A:18:ILE:CG1	1:A:58:ILE:HG12	0.46	2.41	2	1
1:A:39:LEU:HD23	1:A:156:MET:HG3	0.46	1.87	10	1
1:A:142:VAL:HG12	1:A:153:MET:HB2	0.46	1.87	10	1
1:A:26:ILE:H	1:A:26:ILE:HD12	0.46	1.71	6	3
1:A:83:LEU:O	1:A:87:VAL:HG12	0.46	2.11	7	2
1:A:154:ILE:HG22	1:A:155:ASP:N	0.46	2.25	9	2
1:A:71:ILE:O	1:A:75:GLU:HB2	0.46	2.11	10	1
1:A:142:VAL:HG13	1:A:144:MET:HE1	0.45	1.88	3	1
1:A:38:PHE:HB3	1:A:154:ILE:C	0.45	2.36	4	1
1:A:34:ARG:HB3	1:A:128:ALA:HB2	0.45	1.87	9	1
1:A:16:MET:HE1	1:A:140:ARG:NH1	0.45	2.27	6	1
1:A:140:ARG:O	1:A:154:ILE:HA	0.45	2.10	6	1
1:A:43:ALA:HB3	1:A:150:THR:CB	0.45	2.41	8	1
1:A:152:TYR:HB3	1:A:154:ILE:HD11	0.45	1.86	8	1
1:A:97:THR:O	1:A:101:LEU:HD13	0.45	2.11	10	1
1:A:29:ILE:HG21	1:A:156:MET:HE3	0.45	1.88	4	1
1:A:58:ILE:HG13	1:A:59:LYS:N	0.45	2.25	8	1
1:A:15:ARG:HG2	1:A:59:LYS:HB3	0.45	1.88	9	1
1:A:113:ASP:O	1:A:114:ILE:HG23	0.45	2.12	6	3
1:A:47:VAL:CG2	1:A:48:MET:N	0.45	2.79	1	1
1:A:144:MET:O	1:A:150:THR:HA	0.45	2.12	1	1
1:A:97:THR:O	1:A:101:LEU:HG	0.45	2.11	2	2
1:A:108:VAL:HG21	1:A:119:ALA:HB3	0.45	1.86	4	1
1:A:18:ILE:HD13	1:A:60:VAL:HG11	0.45	1.87	7	1
1:A:140:ARG:NE	1:A:155:ASP:HB2	0.45	2.26	7	1
1:A:125:GLU:O	1:A:129:ILE:HG23	0.45	2.12	6	2
1:A:64:ASP:OD2	1:A:139:PHE:HA	0.45	2.12	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:TYR:CG	1:A:163:LEU:HB3	0.45	2.47	8	1
1:A:118:ASP:O	1:A:121:GLU:HG2	0.45	2.11	1	1
1:A:59:LYS:HB2	1:A:59:LYS:HZ3	0.45	1.72	8	1
1:A:66:ILE:HD13	1:A:139:PHE:O	0.44	2.12	7	1
1:A:24:VAL:O	1:A:25:GLU:C	0.44	2.61	4	3
1:A:35:PHE:C	1:A:37:GLU:N	0.44	2.75	4	1
1:A:80:LEU:O	1:A:84:VAL:HG12	0.44	2.12	5	1
1:A:145:GLN:CB	1:A:150:THR:HA	0.44	2.41	2	1
1:A:61:ASP:HB2	1:A:140:ARG:HG2	0.44	1.88	5	1
1:A:41:PHE:CD1	1:A:41:PHE:C	0.44	2.96	1	1
1:A:144:MET:SD	1:A:151:CYS:HB3	0.44	2.53	1	1
1:A:39:LEU:HD12	1:A:41:PHE:CE2	0.43	2.49	5	1
1:A:84:VAL:O	1:A:88:MET:HB2	0.43	2.13	7	1
1:A:31:THR:HG23	1:A:37:GLU:OE1	0.43	2.13	8	1
1:A:111:LEU:O	1:A:113:ASP:N	0.43	2.51	10	1
1:A:91:THR:HB	1:A:126:ILE:CG1	0.43	2.43	5	1
1:A:142:VAL:HG23	1:A:153:MET:HB2	0.43	1.89	8	1
1:A:24:VAL:HA	1:A:54:VAL:HG22	0.43	1.90	3	2
1:A:101:LEU:O	1:A:104:GLN:HG2	0.43	2.13	2	1
1:A:81:SER:O	1:A:85:GLU:HG3	0.43	2.13	5	1
1:A:34:ARG:O	1:A:34:ARG:HD2	0.43	2.13	6	1
1:A:68:ALA:O	1:A:71:ILE:HG22	0.43	2.14	10	1
1:A:38:PHE:HB3	1:A:154:ILE:O	0.43	2.13	4	1
1:A:145:GLN:HA	1:A:150:THR:HG23	0.43	1.89	3	1
1:A:39:LEU:HD22	1:A:39:LEU:C	0.43	2.38	8	1
1:A:114:ILE:HG22	1:A:115:ASP:H	0.43	1.73	10	1
1:A:20:HIS:CE1	1:A:56:TYR:HB2	0.43	2.49	3	1
1:A:142:VAL:O	1:A:152:TYR:HA	0.43	2.14	8	2
1:A:37:GLU:O	1:A:37:GLU:HG2	0.43	2.12	10	1
1:A:18:ILE:HD11	1:A:58:ILE:HG12	0.43	1.91	7	1
1:A:39:LEU:HA	1:A:153:MET:HA	0.43	1.91	8	1
1:A:134:ALA:HB1	1:A:139:PHE:HB2	0.42	1.91	3	1
1:A:35:PHE:CE2	1:A:124:TRP:HB3	0.42	2.49	6	1
1:A:16:MET:SD	1:A:18:ILE:CG2	0.42	3.07	6	1
1:A:73:TYR:C	1:A:75:GLU:H	0.42	2.23	9	1
1:A:25:GLU:O	1:A:27:THR:HG23	0.42	2.15	5	1
1:A:29:ILE:HG21	1:A:156:MET:HB3	0.42	1.90	2	1
1:A:132:LYS:O	1:A:135:LYS:HB3	0.42	2.14	8	1
1:A:34:ARG:CB	1:A:128:ALA:HB2	0.42	2.45	9	1
1:A:58:ILE:CG2	1:A:163:LEU:HD13	0.42	2.44	2	1
1:A:41:PHE:HB3	1:A:152:TYR:H	0.42	1.74	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:HB2	1:A:162:GLU:OE2	0.42	2.15	10	1
1:A:61:ASP:OD1	1:A:64:ASP:HB3	0.42	2.15	8	1
1:A:135:LYS:HG3	1:A:140:ARG:NH2	0.42	2.29	8	1
1:A:142:VAL:HG11	1:A:144:MET:HE2	0.41	1.92	6	1
1:A:39:LEU:HB3	1:A:156:MET:CG	0.41	2.45	7	1
1:A:16:MET:HG2	1:A:60:VAL:CG1	0.41	2.45	5	1
1:A:58:ILE:CG2	1:A:163:LEU:HD23	0.41	2.46	6	1
1:A:107:ASP:O	1:A:111:LEU:HD13	0.41	2.16	8	1
1:A:134:ALA:HA	1:A:137:LEU:CD2	0.41	2.45	8	1
1:A:101:LEU:HD11	1:A:126:ILE:HD13	0.41	1.92	3	1
1:A:67:MET:SD	1:A:67:MET:N	0.41	2.92	6	1
1:A:35:PHE:O	1:A:35:PHE:CG	0.41	2.72	8	1
1:A:77:ALA:O	1:A:80:LEU:HB2	0.41	2.15	9	1
1:A:18:ILE:HB	1:A:41:PHE:HB2	0.41	1.92	10	1
1:A:144:MET:HB2	1:A:151:CYS:HB3	0.41	1.91	1	1
1:A:35:PHE:C	1:A:37:GLU:H	0.41	2.24	4	2
1:A:70:SER:HB2	1:A:139:PHE:CE1	0.41	2.50	4	1
1:A:20:HIS:HB3	1:A:40:CYS:O	0.41	2.16	6	1
1:A:39:LEU:HD22	1:A:156:MET:HE3	0.41	1.93	2	1
1:A:43:ALA:O	1:A:44:ASP:HB3	0.41	2.16	5	1
1:A:36:GLY:O	1:A:37:GLU:C	0.41	2.63	6	1
1:A:96:ASP:O	1:A:100:GLU:HG2	0.41	2.15	6	1
1:A:139:PHE:HA	1:A:155:ASP:OD1	0.41	2.15	8	1
1:A:139:PHE:CG	1:A:140:ARG:N	0.41	2.89	10	1
1:A:157:LEU:O	1:A:162:GLU:HG3	0.41	2.15	3	1
1:A:67:MET:HA	1:A:71:ILE:HD11	0.41	1.91	8	1
1:A:73:TYR:O	1:A:77:ALA:HB2	0.40	2.17	2	1
1:A:16:MET:HE2	1:A:62:GLU:CB	0.40	2.46	4	1
1:A:71:ILE:N	1:A:137:LEU:HD21	0.40	2.31	6	1
1:A:20:HIS:HB3	1:A:41:PHE:HA	0.40	1.93	7	1
1:A:38:PHE:CE1	1:A:40:CYS:HB2	0.40	2.51	10	1
1:A:70:SER:HA	1:A:74:HIS:CD2	0.40	2.51	7	1
1:A:72:PHE:CZ	1:A:99:GLU:HA	0.40	2.51	3	1
1:A:96:ASP:CG	1:A:97:THR:N	0.40	2.80	6	1
1:A:70:SER:O	1:A:137:LEU:HD11	0.40	2.15	8	1
1:A:17:GLU:CD	1:A:57:ARG:HD3	0.40	2.41	3	1
1:A:154:ILE:HD12	1:A:154:ILE:N	0.40	2.31	8	1
1:A:158:GLY:C	1:A:160:ASP:N	0.40	2.80	8	1
1:A:144:MET:HG2	1:A:151:CYS:O	0.40	2.17	10	1
1:A:24:VAL:H	1:A:54:VAL:HG22	0.40	1.76	1	1
1:A:163:LEU:N	1:A:163:LEU:HD22	0.40	2.31	7	1

6.3 Torsion angles

6.3.1 Protein backbone

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	151/167 (90%)	123±4 (82±3%)	21±4 (14±3%)	6±2 (4±1%)	3	28
All	All	1510/1670 (90%)	1234 (82%)	211 (14%)	65 (4%)	3	28

All 26 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	44	ASP	8
1	A	23	PRO	7
1	A	14	GLY	6
1	A	25	GLU	6
1	A	141	GLY	3
1	A	160	ASP	3
1	A	114	ILE	3
1	A	51	GLY	3
1	A	106	ILE	2
1	A	36	GLY	2
1	A	93	CYS	2
1	A	94	ASP	2
1	A	95	GLU	2
1	A	37	GLU	2
1	A	80	LEU	2
1	A	112	ASP	2
1	A	24	VAL	1
1	A	26	ILE	1
1	A	64	ASP	1
1	A	71	ILE	1
1	A	155	ASP	1
1	A	159	HIS	1
1	A	74	HIS	1
1	A	158	GLY	1
1	A	29	ILE	1
1	A	115	ASP	1

6.3.2 Protein sidechains ⓘ

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	126/137 (92%)	114±2 (90±1%)	12±2 (10±1%)	10	55
All	All	1260/1370 (92%)	1139 (90%)	121 (10%)	10	55

All 44 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	58	ILE	10
1	A	87	VAL	9
1	A	39	LEU	7
1	A	154	ILE	7
1	A	59	LYS	7
1	A	156	MET	5
1	A	166	VAL	5
1	A	106	ILE	5
1	A	127	GLN	5
1	A	144	MET	3
1	A	35	PHE	3
1	A	111	LEU	3
1	A	114	ILE	3
1	A	60	VAL	3
1	A	101	LEU	3
1	A	49	THR	3
1	A	142	VAL	3
1	A	16	MET	2
1	A	41	PHE	2
1	A	104	GLN	2
1	A	151	CYS	2
1	A	157	LEU	2
1	A	47	VAL	2
1	A	15	ARG	2
1	A	37	GLU	2
1	A	167	LYS	2
1	A	164	VAL	2
1	A	75	GLU	1
1	A	105	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	29	ILE	1
1	A	135	LYS	1
1	A	143	SER	1
1	A	62	GLU	1
1	A	110	ASN	1
1	A	145	GLN	1
1	A	45	GLU	1
1	A	140	ARG	1
1	A	31	THR	1
1	A	137	LEU	1
1	A	155	ASP	1
1	A	32	GLN	1
1	A	95	GLU	1
1	A	130	THR	1
1	A	150	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 65% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1420
Number of shifts mapped to atoms	1420
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 $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	151	-0.49 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	139	0.10 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	147	0.49 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 65%, i.e. 1323 atoms were assigned a chemical shift out of a possible 2021. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	545/769 (71%)	272/314 (87%)	137/304 (45%)	136/151 (90%)
Sidechain	778/1102 (71%)	523/720 (73%)	255/347 (73%)	0/35 (0%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	0/150 (0%)	0/73 (0%)	0/68 (0%)	0/9 (0%)
Overall	1323/2021 (65%)	795/1107 (72%)	392/719 (55%)	136/195 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 1420 atoms were assigned a chemical shift out of a possible 2187. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	594/847 (70%)	296/347 (85%)	151/334 (45%)	147/166 (89%)
Sidechain	826/1182 (70%)	553/771 (72%)	273/373 (73%)	0/38 (0%)
Aromatic	0/158 (0%)	0/77 (0%)	0/70 (0%)	0/11 (0%)
Overall	1420/2187 (65%)	849/1195 (71%)	424/777 (55%)	147/215 (68%)

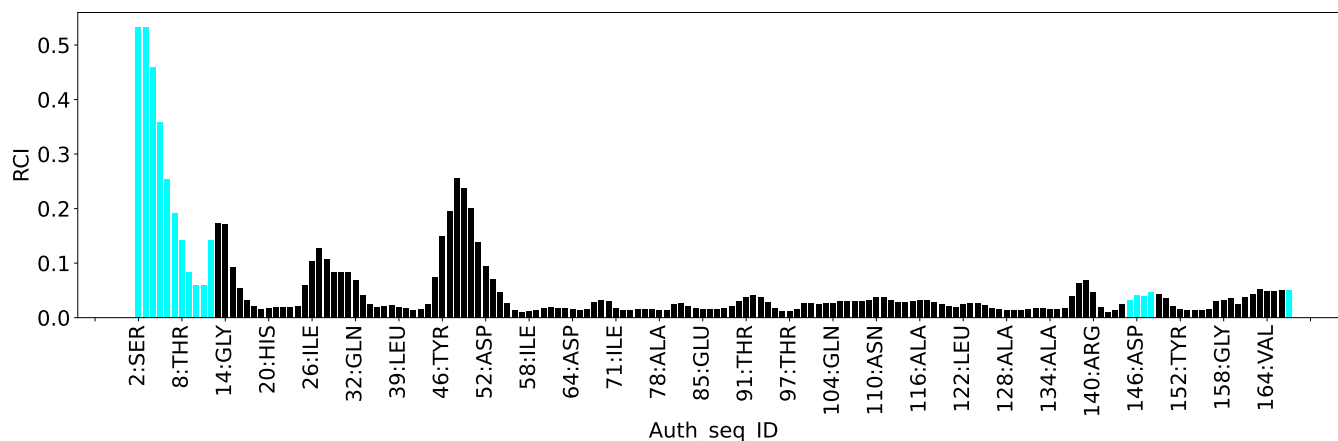
7.1.4 Statistically unusual chemical shifts [i](#)

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	2335
Intra-residue ($ i-j =0$)	703
Sequential ($ i-j =1$)	565
Medium range ($ i-j >1$ and $ i-j <5$)	438
Long range ($ i-j \geq 5$)	574
Inter-chain	0
Hydrogen bond restraints	55
Disulfide bond restraints	0
Total dihedral-angle restraints	300
Number of unmapped restraints	0
Number of restraints per residue	15.8
Number of long range restraints per residue ¹	3.6

¹Long 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)	60.6	0.2
0.2-0.5 (Medium)	60.0	0.5
>0.5 (Large)	116.3	7.99

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)	36.2	10.0
10.0-20.0 (Medium)	6.4	19.58
>20.0 (Large)	0.3	28.21

9 Distance violation analysis ⓘ

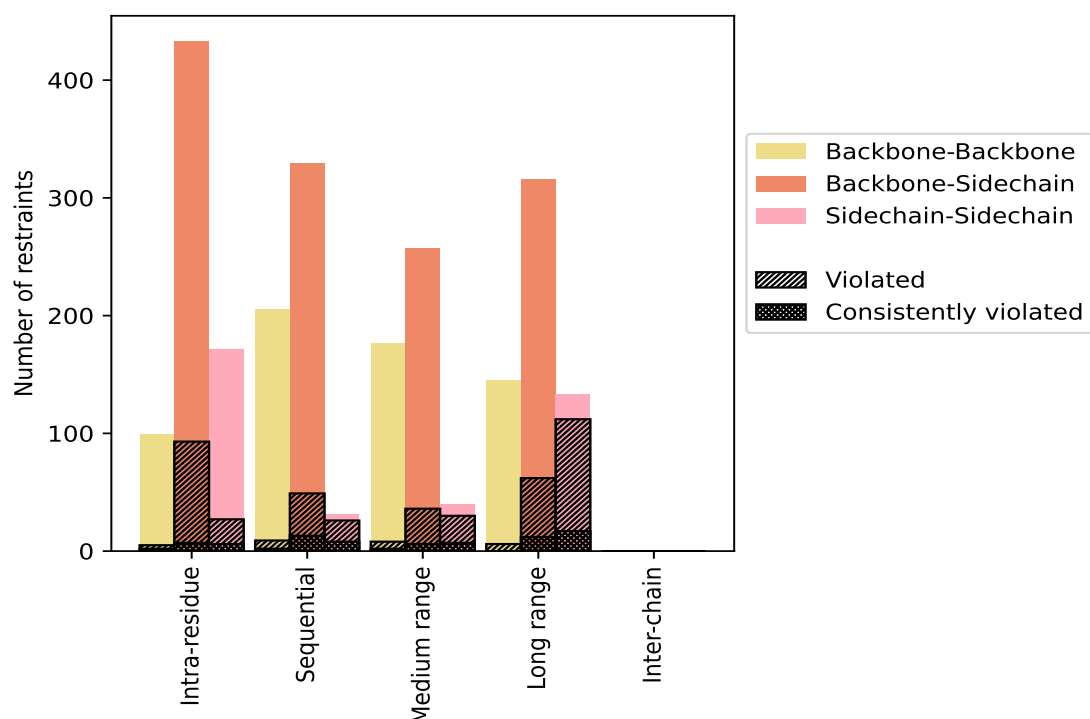
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	703	30.1	125	17.8	5.4	15	2.1	0.6
Backbone-Backbone	99	4.2	5	5.1	0.2	2	2.0	0.1
Backbone-Sidechain	433	18.5	93	21.5	4.0	7	1.6	0.3
Sidechain-Sidechain	171	7.3	27	15.8	1.2	6	3.5	0.3
Sequential (i-j =1)	565	24.2	84	14.9	3.6	23	4.1	1.0
Backbone-Backbone	205	8.8	9	4.4	0.4	2	1.0	0.1
Backbone-Sidechain	329	14.1	49	14.9	2.1	13	4.0	0.6
Sidechain-Sidechain	31	1.3	26	83.9	1.1	8	25.8	0.3
Medium range (i-j >1 & i-j <5)	438	18.8	61	13.9	2.6	15	3.4	0.6
Backbone-Backbone	176	7.5	8	4.5	0.3	2	1.1	0.1
Backbone-Sidechain	222	9.5	23	10.4	1.0	6	2.7	0.3
Sidechain-Sidechain	40	1.7	30	75.0	1.3	7	17.5	0.3
Long range (i-j ≥5)	574	24.6	172	30.0	7.4	29	5.1	1.2
Backbone-Backbone	145	6.2	6	4.1	0.3	0	0.0	0.0
Backbone-Sidechain	296	12.7	54	18.2	2.3	12	4.1	0.5
Sidechain-Sidechain	133	5.7	112	84.2	4.8	17	12.8	0.7
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	55	2.4	21	38.2	0.9	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2335	100.0	463	19.8	19.8	82	3.5	3.5
Backbone-Backbone	625	26.8	28	4.5	1.2	6	1.0	0.3
Backbone-Sidechain	1335	57.2	240	18.0	10.3	38	2.8	1.6
Sidechain-Sidechain	375	16.1	195	52.0	8.4	38	10.1	1.6

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 [i](#)



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

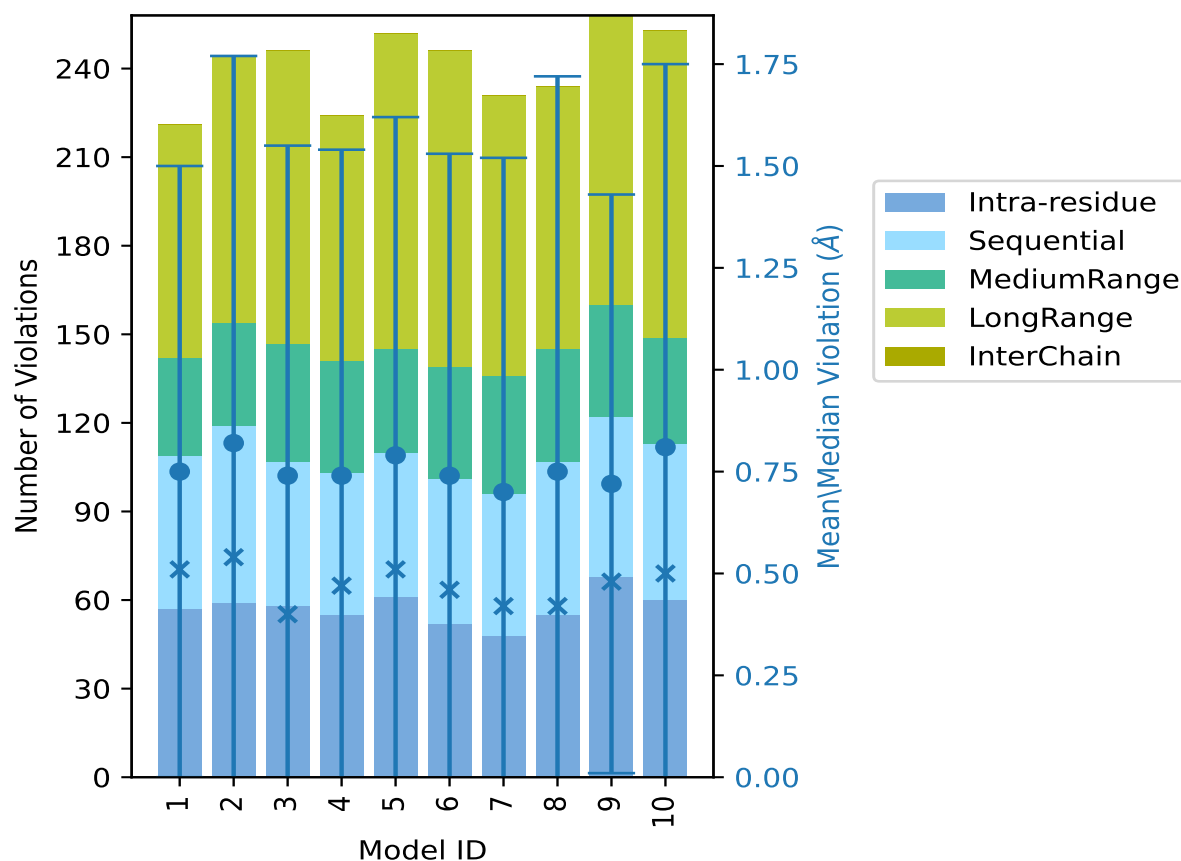
9.2 Distance violation statistics for each model [i](#)

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	57	52	33	79	0	221	0.75	4.92	0.75	0.51
2	59	60	35	90	0	244	0.82	6.74	0.95	0.54
3	58	49	40	99	0	246	0.74	4.43	0.81	0.4
4	55	48	38	83	0	224	0.74	7.0	0.8	0.47
5	61	49	35	107	0	252	0.79	5.68	0.83	0.51
6	52	49	38	107	0	246	0.74	6.15	0.79	0.46
7	48	48	40	95	0	231	0.7	7.99	0.82	0.42
8	55	52	38	89	0	234	0.75	7.26	0.97	0.42
9	68	54	38	98	0	258	0.72	3.9	0.71	0.48
10	60	53	36	104	0	253	0.81	7.44	0.94	0.5

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

9.2.1 Bar graph : Distance 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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1838(IR:578, SQ:481, MR:377, LR:402, 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	%
32	13	7	19	0	71	1	10.0
19	10	9	21	0	59	2	20.0
11	7	9	19	0	46	3	30.0

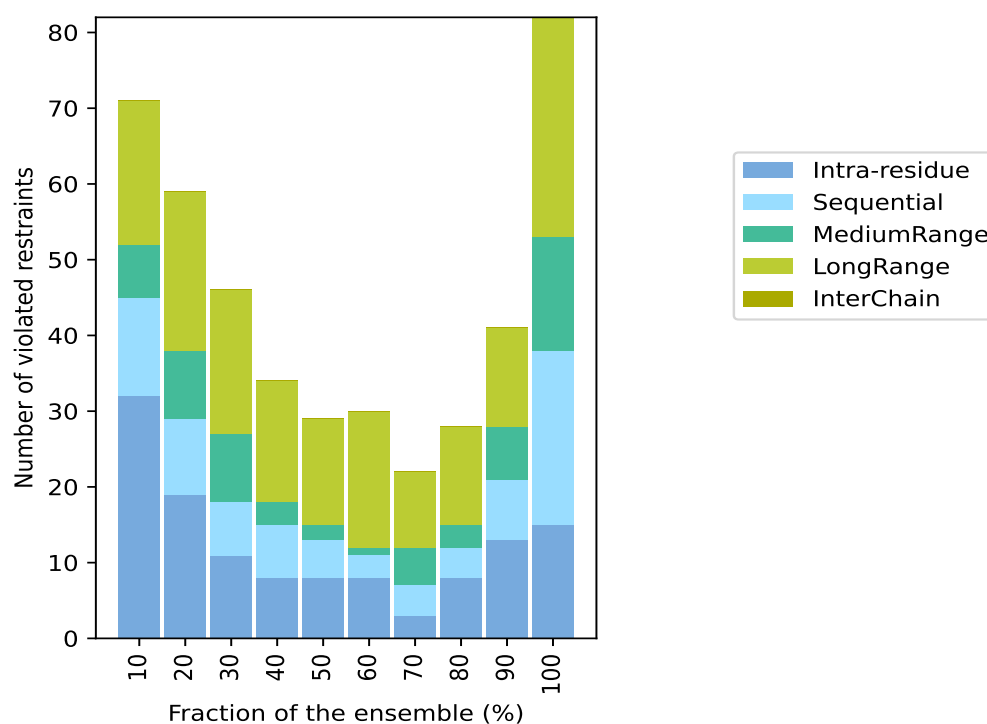
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
8	7	3	16	0	34	4	40.0
8	5	2	14	0	29	5	50.0
8	3	1	18	0	30	6	60.0
3	4	5	10	0	22	7	70.0
8	4	3	13	0	28	8	80.0
13	8	7	13	0	41	9	90.0
15	23	15	29	0	82	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)

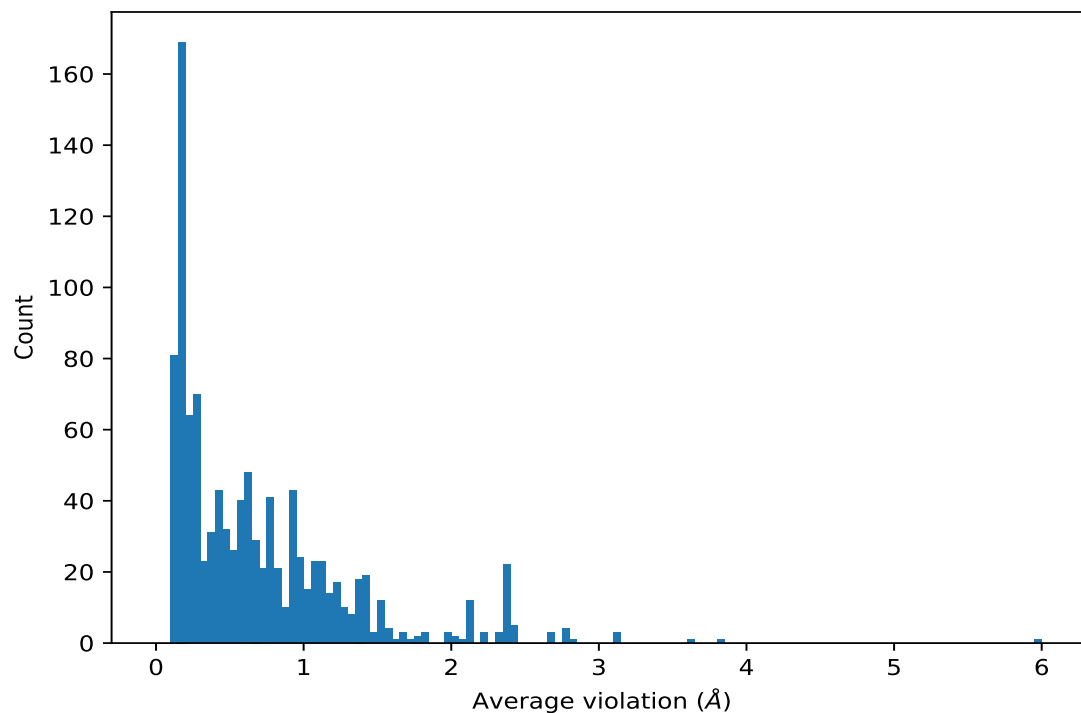


9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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 [i](#)

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)
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	10	5.96	1.53	6.41
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	10	3.84	0.11	3.85
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	10	3.64	1.5	3.48
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	10	3.13	0.25	3.18
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	10	3.13	0.25	3.18
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	10	3.13	0.25	3.18
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	10	2.81	1.48	3.36
(2,139)	1:154:A:ILE:HG22	1:18:A:ILE:HG12	10	2.43	0.31	2.46
(2,139)	1:154:A:ILE:HG23	1:18:A:ILE:HG12	10	2.43	0.31	2.46
(2,139)	1:154:A:ILE:HG21	1:18:A:ILE:HG12	10	2.43	0.31	2.46
(2,139)	1:142:A:VAL:HG21	1:154:A:ILE:HG21	10	2.43	0.31	2.46
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	10	2.39	0.57	2.77
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	10	2.39	0.57	2.77
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	10	2.39	0.57	2.77
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	10	2.14	0.97	2.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	10	2.14	0.97	2.32
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	10	2.14	0.97	2.32
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	10	2.14	1.28	1.38
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	10	2.14	1.28	1.38
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	10	2.09	0.79	1.76
(2,204)	1:90:A:LEU:H	1:86:A:ARG:HD3	10	2.04	0.08	2.08
(2,204)	1:86:A:ARG:HD3	1:89:A:GLN:H	10	2.04	0.08	2.08
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	10	1.82	0.28	1.86
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	10	1.82	0.28	1.86
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	10	1.82	0.28	1.86
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE3	10	1.76	0.32	1.79
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	10	1.76	0.32	1.79
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	10	1.7	0.3	1.82
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	10	1.62	0.85	1.66
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	10	1.56	0.33	1.62
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	10	1.52	0.79	1.6
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	10	1.52	0.79	1.6
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	10	1.5	0.15	1.46
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	10	1.5	0.15	1.46
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	10	1.5	0.15	1.46
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	10	1.44	0.17	1.5
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	10	1.38	0.32	1.46
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	10	1.38	0.32	1.46
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	10	1.36	0.46	1.25
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD13	10	1.32	0.83	0.94
(2,191)	1:57:A:ARG:H	1:163:A:LEU:HD11	10	1.32	0.83	0.94
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD11	10	1.32	0.83	0.94
(2,191)	1:57:A:ARG:H	1:163:A:LEU:HD13	10	1.32	0.83	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD12	10	1.32	0.83	0.94
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	10	1.25	0.17	1.19
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	10	1.25	0.17	1.19
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	10	1.25	0.17	1.19
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG23	10	1.22	0.12	1.19
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG22	10	1.22	0.12	1.19
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG21	10	1.22	0.12	1.19
(2,277)	1:58:A:ILE:HG22	1:163:A:LEU:HG	10	1.21	0.25	1.3
(2,277)	1:58:A:ILE:HG23	1:163:A:LEU:HG	10	1.21	0.25	1.3
(2,277)	1:58:A:ILE:HG21	1:163:A:LEU:HG	10	1.21	0.25	1.3
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	10	1.14	0.49	1.02
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	10	1.14	0.49	1.02
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	10	1.14	0.49	1.02
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	10	1.13	0.33	0.94
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	10	1.13	0.33	0.94
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	10	1.13	0.33	0.94
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	10	1.11	0.54	0.96
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	10	1.11	0.54	0.96
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	10	1.11	0.54	0.96
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	10	1.1	0.62	1.18
(2,216)	1:113:A:ASP:HB2	1:114:A:ILE:HG12	10	1.07	0.58	0.99
(2,216)	1:160:A:ASP:HB2	1:161:A:ALA:HB2	10	1.07	0.58	0.99
(2,216)	1:160:A:ASP:HB2	1:161:A:ALA:HB3	10	1.07	0.58	0.99
(2,216)	1:160:A:ASP:HB2	1:161:A:ALA:HB1	10	1.07	0.58	0.99
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	10	1.07	0.09	1.06
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	10	1.07	0.09	1.06
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	10	1.07	0.09	1.06
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	10	0.99	0.7	1.08
(2,254)	1:152:A:TYR:H	1:43:A:ALA:HB3	10	0.98	0.19	0.98
(2,254)	1:43:A:ALA:HB2	1:151:A:CYS:H	10	0.98	0.19	0.98
(2,254)	1:43:A:ALA:HB1	1:151:A:CYS:H	10	0.98	0.19	0.98
(2,254)	1:152:A:TYR:H	1:43:A:ALA:HB2	10	0.98	0.19	0.98
(2,254)	1:43:A:ALA:HB3	1:151:A:CYS:H	10	0.98	0.19	0.98
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	10	0.98	0.24	0.86
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	10	0.98	0.24	0.86
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	10	0.98	0.24	0.86
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	10	0.98	0.55	1.08
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	10	0.96	0.08	0.96
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	10	0.95	0.2	0.93
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	10	0.95	0.2	0.93
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	10	0.95	0.2	0.93
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	10	0.95	0.37	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	10	0.95	0.37	1.04
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	10	0.95	0.37	1.04
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	10	0.94	0.13	0.96
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	10	0.94	0.13	0.96
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	10	0.94	0.13	0.96
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	10	0.93	0.21	0.92
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	10	0.93	0.21	0.92
(2,207)	1:161:A:ALA:HB2	1:159:A:HIS:HB3	10	0.91	0.58	0.62
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB2	10	0.91	0.58	0.62
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB3	10	0.91	0.58	0.62
(2,207)	1:161:A:ALA:HB3	1:159:A:HIS:HB3	10	0.91	0.58	0.62
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	10	0.9	0.31	0.86
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	10	0.9	0.31	0.86
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	10	0.9	0.31	0.86
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	10	0.89	0.39	0.98
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	10	0.89	0.39	0.98
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	10	0.89	0.39	0.98
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	10	0.89	0.24	0.9
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	10	0.89	0.24	0.9
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	10	0.89	0.24	0.9
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	10	0.86	0.27	0.88
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	10	0.74	0.02	0.74
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB3	10	0.66	0.12	0.62
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB1	10	0.66	0.12	0.62
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB2	10	0.66	0.12	0.62
(2,171)	1:98:A:ALA:HB2	1:102:A:ILE:H	10	0.66	0.12	0.62
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	10	0.65	0.43	0.79
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	10	0.65	0.43	0.79
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	10	0.65	0.43	0.79
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	10	0.65	0.8	0.28
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	10	0.65	0.8	0.28
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	10	0.65	0.8	0.28
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	10	0.64	0.08	0.62
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	10	0.64	0.08	0.62
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	10	0.64	0.08	0.62
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	10	0.63	0.02	0.63
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	10	0.62	0.15	0.65
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	10	0.62	0.15	0.65
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	10	0.62	0.15	0.65
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB2	10	0.62	0.13	0.64
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB1	10	0.62	0.13	0.64
(2,271)	1:117:A:SER:HB3	1:116:A:ALA:HB2	10	0.62	0.13	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,271)	1:117:A:SER:HB2	1:116:A:ALA:HB2	10	0.62	0.13	0.64
(2,271)	1:117:A:SER:HB3	1:116:A:ALA:HB3	10	0.62	0.13	0.64
(2,271)	1:117:A:SER:HB2	1:116:A:ALA:HB3	10	0.62	0.13	0.64
(2,271)	1:117:A:SER:HB3	1:116:A:ALA:HB1	10	0.62	0.13	0.64
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB3	10	0.62	0.13	0.64
(2,93)	1:146:A:ASP:HB3	1:42:A:ALA:HB1	10	0.61	0.44	0.36
(2,93)	1:42:A:ALA:HB2	1:151:A:CYS:HB3	10	0.61	0.44	0.36
(2,93)	1:42:A:ALA:HB3	1:151:A:CYS:HB3	10	0.61	0.44	0.36
(2,93)	1:42:A:ALA:HB1	1:151:A:CYS:HB3	10	0.61	0.44	0.36
(2,93)	1:146:A:ASP:HB3	1:42:A:ALA:HB3	10	0.61	0.44	0.36
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	10	0.6	0.28	0.48
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	10	0.6	0.28	0.48
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	10	0.6	0.28	0.48
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	10	0.58	0.23	0.51
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	10	0.58	0.23	0.51
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	10	0.58	0.23	0.51
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	10	0.57	0.21	0.61
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	10	0.56	0.24	0.6
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	10	0.56	0.17	0.57
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	10	0.55	0.26	0.76
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	10	0.54	0.15	0.5
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	10	0.44	0.02	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	10	0.44	0.02	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	10	0.44	0.02	0.46
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	10	0.43	0.28	0.3
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	10	0.43	0.28	0.3
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	10	0.43	0.28	0.3
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	10	0.4	0.39	0.18
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	10	0.4	0.39	0.18
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	10	0.4	0.39	0.18
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	10	0.4	0.16	0.43
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	10	0.4	0.16	0.43
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	10	0.39	0.02	0.39
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	10	0.37	0.09	0.34
(2,154)	1:26:A:ILE:HA	1:27:A:THR:HA	10	0.37	0.09	0.34
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	10	0.36	0.27	0.28
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	10	0.36	0.27	0.28
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	10	0.36	0.27	0.28
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	10	0.35	0.07	0.34
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	10	0.32	0.06	0.32
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	10	0.27	0.08	0.26
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	10	0.27	0.08	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	10	0.26	0.04	0.27
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	10	0.24	0.04	0.24
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	10	0.24	0.04	0.24
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	10	0.24	0.04	0.24
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	10	0.23	0.06	0.24
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	10	0.23	0.06	0.24
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	10	0.23	0.06	0.24
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	10	0.23	0.0	0.23
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HB2	10	0.23	0.17	0.17
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HG3	10	0.23	0.17	0.17
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	10	0.19	0.04	0.18
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	10	0.19	0.04	0.18
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	10	0.19	0.04	0.18
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	10	0.17	0.04	0.18
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	10	0.17	0.02	0.18
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	10	0.17	0.02	0.18
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	10	0.17	0.02	0.18
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	10	0.16	0.03	0.17
(2,144)	1:75:A:GLU:H	1:74:A:HIS:HA	10	0.16	0.03	0.17
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	10	0.15	0.06	0.14
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	10	0.15	0.06	0.14
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	10	0.15	0.06	0.14
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	10	0.15	0.01	0.15
(2,212)	1:23:A:PRO:HD3	1:24:A:VAL:HG13	9	2.77	0.48	2.64
(2,212)	1:24:A:VAL:HG13	1:26:A:ILE:HA	9	2.77	0.48	2.64
(2,212)	1:24:A:VAL:HG12	1:26:A:ILE:HA	9	2.77	0.48	2.64
(2,212)	1:24:A:VAL:HG11	1:26:A:ILE:HA	9	2.77	0.48	2.64
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	9	2.39	0.86	1.89
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	9	2.35	0.58	2.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	9	2.35	0.58	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	9	2.35	0.58	2.41
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	9	2.2	1.65	1.6
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	9	2.2	1.65	1.6
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	9	2.2	1.65	1.6
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	9	1.98	0.45	2.14
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	9	1.98	0.45	2.14
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	9	1.98	0.45	2.14
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	9	1.41	0.69	1.18
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	9	1.41	0.69	1.18
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	9	1.41	0.69	1.18
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	9	1.38	0.46	1.47
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	9	1.38	0.46	1.47
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	9	1.23	0.26	1.28
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	9	1.23	0.26	1.28
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	9	1.23	0.26	1.28
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	9	1.09	0.4	1.21
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	9	1.09	0.4	1.21
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	9	1.09	0.4	1.21
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	9	1.03	0.14	1.07
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	9	1.03	0.14	1.07
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	9	1.03	0.14	1.07
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	9	0.99	0.09	0.93
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	9	0.91	0.29	0.86
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	9	0.91	0.29	0.86
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	9	0.86	0.26	0.93
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	9	0.86	0.26	0.93
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	9	0.86	0.26	0.93
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	9	0.84	0.26	0.83
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	9	0.84	0.26	0.83
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	9	0.84	0.26	0.83
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	9	0.83	0.61	0.69
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	9	0.83	0.61	0.69
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	9	0.83	0.61	0.69
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	9	0.78	0.13	0.75
(2,107)	1:47:A:VAL:HG12	1:55:A:THR:HG23	9	0.77	0.42	0.59
(2,107)	1:126:A:ILE:HG23	1:130:A:THR:HG21	9	0.77	0.42	0.59
(2,107)	1:47:A:VAL:HG13	1:55:A:THR:HG22	9	0.77	0.42	0.59
(2,107)	1:47:A:VAL:HG12	1:55:A:THR:HG22	9	0.77	0.42	0.59
(2,107)	1:47:A:VAL:HG13	1:55:A:THR:HG21	9	0.77	0.42	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,107)	1:126:A:ILE:HG22	1:130:A:THR:HG21	9	0.77	0.42	0.59
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	9	0.75	0.27	0.75
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	9	0.75	0.27	0.75
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	9	0.75	0.27	0.75
(2,162)	1:166:A:VAL:HG13	1:57:A:ARG:HA	9	0.74	0.09	0.75
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG13	9	0.74	0.09	0.75
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG11	9	0.74	0.09	0.75
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG12	9	0.74	0.09	0.75
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	9	0.74	0.25	0.71
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	9	0.74	0.25	0.71
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	9	0.74	0.25	0.71
(2,61)	1:166:A:VAL:HG23	1:165:A:ARG:HA	9	0.66	0.08	0.65
(2,61)	1:166:A:VAL:HG22	1:165:A:ARG:HA	9	0.66	0.08	0.65
(2,61)	1:166:A:VAL:HG21	1:165:A:ARG:HA	9	0.66	0.08	0.65
(2,61)	1:166:A:VAL:HG22	1:166:A:VAL:HA	9	0.66	0.08	0.65
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	9	0.66	0.21	0.68
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	9	0.66	0.21	0.68
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	9	0.66	0.21	0.68
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	9	0.62	0.1	0.62
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	9	0.57	0.24	0.54
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	9	0.53	0.01	0.53
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	9	0.53	0.01	0.53
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	9	0.53	0.01	0.53
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	9	0.51	0.0	0.51
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	9	0.48	0.19	0.47
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	9	0.48	0.19	0.47
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	9	0.48	0.19	0.47
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	9	0.47	0.03	0.47
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	9	0.45	0.74	0.2
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	9	0.45	0.3	0.38
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	9	0.39	0.02	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	9	0.39	0.02	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	9	0.39	0.02	0.4
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	9	0.39	0.17	0.48
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	9	0.36	0.17	0.36
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	9	0.34	0.29	0.15
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	9	0.27	0.1	0.28
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	9	0.27	0.1	0.28
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	9	0.27	0.1	0.28
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	9	0.27	0.1	0.28
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	9	0.27	0.1	0.28
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	9	0.27	0.1	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	9	0.19	0.02	0.2
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	9	0.19	0.01	0.19
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	9	0.19	0.08	0.14
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	9	0.19	0.08	0.14
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	9	0.17	0.06	0.14
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	9	0.17	0.06	0.14
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	9	0.17	0.06	0.14
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	9	0.16	0.02	0.15
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	9	0.16	0.02	0.15
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	9	0.16	0.02	0.15
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	9	0.15	0.03	0.15
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	9	0.14	0.02	0.14
(2,32)	1:40:A:CYS:HB3	1:153:A:MET:HG2	8	2.33	1.02	1.94
(2,32)	1:40:A:CYS:HB2	1:153:A:MET:HG2	8	2.33	1.02	1.94
(2,32)	1:48:A:MET:HG2	1:19:A:PHE:HB2	8	2.33	1.02	1.94
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	8	1.66	0.42	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	8	1.66	0.42	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	8	1.66	0.42	1.83
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	8	1.42	0.34	1.38
(2,316)	1:150:A:THR:HG21	1:144:A:MET:HB3	8	1.22	0.76	0.94
(2,316)	1:150:A:THR:HG21	1:145:A:GLN:HB2	8	1.22	0.76	0.94
(2,316)	1:150:A:THR:HG23	1:145:A:GLN:HB2	8	1.22	0.76	0.94
(2,316)	1:150:A:THR:HG23	1:144:A:MET:HB3	8	1.22	0.76	0.94
(2,316)	1:150:A:THR:HG22	1:145:A:GLN:HB2	8	1.22	0.76	0.94
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	8	1.2	0.67	1.12
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	8	1.2	0.67	1.12
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	8	1.2	0.67	1.12
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	8	1.17	0.58	1.03
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	8	1.17	0.58	1.03
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	8	1.17	0.58	1.03
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	8	1.17	0.58	1.03
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	8	1.17	0.58	1.03
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	8	1.17	0.58	1.03
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	8	0.99	0.41	1.18
(2,170)	1:142:A:VAL:HG21	1:144:A:MET:HG2	8	0.9	0.26	0.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,170)	1:142:A:VAL:HG21	1:144:A:MET:HG3	8	0.9	0.26	0.84
(2,170)	1:150:A:THR:HG23	1:144:A:MET:HG2	8	0.9	0.26	0.84
(2,170)	1:142:A:VAL:HG23	1:144:A:MET:HG3	8	0.9	0.26	0.84
(2,170)	1:142:A:VAL:HG23	1:144:A:MET:HG2	8	0.9	0.26	0.84
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	8	0.76	0.26	0.78
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	8	0.76	0.26	0.78
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	8	0.64	0.69	0.2
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	8	0.64	0.69	0.2
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	8	0.63	0.4	0.57
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	8	0.63	0.4	0.57
(2,108)	1:102:A:ILE:HG23	1:133:A:ALA:HB1	8	0.6	0.22	0.68
(2,108)	1:102:A:ILE:HG22	1:133:A:ALA:HB1	8	0.6	0.22	0.68
(2,108)	1:102:A:ILE:HG21	1:133:A:ALA:HB1	8	0.6	0.22	0.68
(2,108)	1:102:A:ILE:HG22	1:133:A:ALA:HB3	8	0.6	0.22	0.68
(2,108)	1:71:A:ILE:HB	1:102:A:ILE:HG22	8	0.6	0.22	0.68
(2,108)	1:102:A:ILE:HG23	1:133:A:ALA:HB3	8	0.6	0.22	0.68
(2,18)	1:42:A:ALA:HB3	1:41:A:PHE:HA	8	0.55	0.12	0.5
(2,18)	1:18:A:ILE:HB	1:41:A:PHE:HA	8	0.55	0.12	0.5
(2,18)	1:42:A:ALA:HB1	1:41:A:PHE:HA	8	0.55	0.12	0.5
(2,18)	1:42:A:ALA:HB2	1:41:A:PHE:HA	8	0.55	0.12	0.5
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	8	0.54	0.13	0.59
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	8	0.54	0.13	0.59
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD3	8	0.5	0.11	0.54
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD2	8	0.5	0.11	0.54
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	8	0.48	0.34	0.43
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	8	0.44	0.39	0.24
(2,294)	1:140:A:ARG:HB2	1:140:A:ARG:HA	8	0.42	0.15	0.5
(2,294)	1:32:A:GLN:HA	1:32:A:GLN:HB3	8	0.42	0.15	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	8	0.35	0.2	0.3
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	8	0.27	0.09	0.24
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	8	0.27	0.09	0.24
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	8	0.27	0.09	0.24
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	8	0.27	0.01	0.27
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	8	0.25	0.13	0.23
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	8	0.22	0.06	0.22
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	8	0.22	0.06	0.22
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	8	0.22	0.06	0.22
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	8	0.22	0.06	0.22
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	8	0.21	0.08	0.2
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	8	0.21	0.08	0.2
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	8	0.21	0.08	0.2
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	8	0.2	0.07	0.21
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	8	0.2	0.07	0.21
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	8	0.2	0.07	0.21
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	8	0.2	0.07	0.21
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	8	0.2	0.07	0.21
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	8	0.2	0.07	0.21
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	8	0.18	0.02	0.18
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	8	0.18	0.02	0.18
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	8	0.18	0.02	0.18
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	8	0.17	0.01	0.18
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	8	0.17	0.01	0.18
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	8	0.17	0.01	0.18
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	7	2.67	1.26	2.49
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	7	2.67	1.26	2.49
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	7	2.67	1.26	2.49
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	7	2.4	0.73	1.91
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	7	1.55	0.54	1.69
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	7	1.55	0.54	1.69
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	7	1.55	0.54	1.69
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	7	1.41	0.19	1.48
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	7	0.92	0.56	0.73
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	7	0.92	0.56	0.73
(2,145)	1:42:A:ALA:HB2	1:46:A:TYR:HB2	7	0.77	0.26	0.81
(2,145)	1:42:A:ALA:HB1	1:46:A:TYR:HB2	7	0.77	0.26	0.81
(2,145)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	7	0.77	0.26	0.81
(2,145)	1:42:A:ALA:HB3	1:46:A:TYR:HB2	7	0.77	0.26	0.81
(2,237)	1:161:A:ALA:H	1:163:A:LEU:HD22	7	0.75	0.27	0.68
(2,237)	1:163:A:LEU:HD22	1:164:A:VAL:H	7	0.75	0.27	0.68
(2,237)	1:161:A:ALA:H	1:163:A:LEU:HD21	7	0.75	0.27	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,237)	1:163:A:LEU:HD21	1:164:A:VAL:H	7	0.75	0.27	0.68
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	7	0.75	0.43	0.82
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	7	0.75	0.43	0.82
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	7	0.75	0.43	0.82
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	7	0.5	0.23	0.57
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	7	0.44	0.18	0.41
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	7	0.44	0.18	0.41
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	7	0.44	0.18	0.41
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	7	0.44	0.31	0.27
(2,143)	1:98:A:ALA:HB2	1:95:A:GLU:HB3	7	0.35	0.11	0.36
(2,143)	1:98:A:ALA:HB1	1:95:A:GLU:HB2	7	0.35	0.11	0.36
(2,143)	1:98:A:ALA:HB3	1:95:A:GLU:HB2	7	0.35	0.11	0.36
(2,143)	1:98:A:ALA:HB3	1:95:A:GLU:HB3	7	0.35	0.11	0.36
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	7	0.3	0.27	0.2
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	7	0.26	0.08	0.3
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	7	0.2	0.06	0.21
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	7	0.2	0.06	0.21
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	7	0.2	0.06	0.21
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	7	0.19	0.12	0.13
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	7	0.18	0.05	0.17
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	7	0.18	0.05	0.17
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	7	0.18	0.05	0.17
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	7	0.17	0.06	0.14
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	7	0.17	0.02	0.16
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	7	0.15	0.04	0.16
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	7	0.13	0.01	0.13
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	7	0.12	0.01	0.12
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	7	0.11	0.01	0.12
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	7	0.11	0.01	0.12
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	7	0.11	0.01	0.12
(4,90)	1:153:A:MET:HE1	1:127:A:GLN:HG3	6	1.3	0.11	1.29
(4,90)	1:153:A:MET:HE2	1:127:A:GLN:HG3	6	1.3	0.11	1.29
(4,90)	1:153:A:MET:HE3	1:127:A:GLN:HG3	6	1.3	0.11	1.29
(4,577)	1:54:A:VAL:HG21	1:22:A:SER:HB3	6	1.25	0.19	1.28
(4,577)	1:54:A:VAL:HG22	1:22:A:SER:HB3	6	1.25	0.19	1.28
(4,577)	1:54:A:VAL:HG23	1:22:A:SER:HB3	6	1.25	0.19	1.28
(4,457)	1:150:A:THR:HG21	1:145:A:GLN:HA	6	1.03	0.7	0.74
(4,457)	1:150:A:THR:HG22	1:145:A:GLN:HA	6	1.03	0.7	0.74
(4,457)	1:150:A:THR:HG23	1:145:A:GLN:HA	6	1.03	0.7	0.74
(4,35)	1:142:A:VAL:HG21	1:153:A:MET:HG3	6	0.98	0.54	0.72
(4,35)	1:142:A:VAL:HG22	1:153:A:MET:HG3	6	0.98	0.54	0.72
(4,35)	1:142:A:VAL:HG23	1:153:A:MET:HG3	6	0.98	0.54	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD21	6	0.94	0.5	0.88
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD22	6	0.94	0.5	0.88
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD23	6	0.94	0.5	0.88
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE1	6	0.9	0.58	1.04
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE2	6	0.9	0.58	1.04
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE3	6	0.9	0.58	1.04
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG11	6	0.9	0.57	0.74
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG12	6	0.9	0.57	0.74
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG13	6	0.9	0.57	0.74
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG11	6	0.9	0.57	0.74
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG12	6	0.9	0.57	0.74
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG13	6	0.9	0.57	0.74
(4,47)	1:58:A:ILE:HD11	1:154:A:ILE:HG12	6	0.81	0.5	0.64
(4,47)	1:58:A:ILE:HD12	1:154:A:ILE:HG12	6	0.81	0.5	0.64
(4,47)	1:58:A:ILE:HD13	1:154:A:ILE:HG12	6	0.81	0.5	0.64
(4,776)	1:16:A:MET:HG3	1:16:A:MET:H	6	0.75	0.42	0.75
(4,81)	1:39:A:LEU:HD21	1:20:A:HIS:HB3	6	0.71	0.81	0.2
(4,81)	1:39:A:LEU:HD22	1:20:A:HIS:HB3	6	0.71	0.81	0.2
(4,81)	1:39:A:LEU:HD23	1:20:A:HIS:HB3	6	0.71	0.81	0.2
(2,49)	1:163:A:LEU:HD21	1:163:A:LEU:HB3	6	0.62	0.04	0.62
(2,49)	1:163:A:LEU:HD22	1:163:A:LEU:HB3	6	0.62	0.04	0.62
(2,153)	1:54:A:VAL:HG22	1:23:A:PRO:HA	6	0.57	0.39	0.54
(2,153)	1:54:A:VAL:HG21	1:25:A:GLU:HA	6	0.57	0.39	0.54
(2,153)	1:54:A:VAL:HG23	1:25:A:GLU:HA	6	0.57	0.39	0.54
(2,153)	1:54:A:VAL:HG23	1:23:A:PRO:HA	6	0.57	0.39	0.54
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG11	6	0.53	0.1	0.52
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG12	6	0.53	0.1	0.52
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG13	6	0.53	0.1	0.52
(4,96)	1:77:A:ALA:HB1	1:74:A:HIS:HB3	6	0.49	0.26	0.59
(4,96)	1:77:A:ALA:HB2	1:74:A:HIS:HB3	6	0.49	0.26	0.59
(4,96)	1:77:A:ALA:HB3	1:74:A:HIS:HB3	6	0.49	0.26	0.59
(1,5)	1:80:A:LEU:H	1:76:A:ARG:O	6	0.49	0.71	0.18
(4,147)	1:34:A:ARG:HB2	1:34:A:ARG:HD3	6	0.45	0.05	0.45
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG21	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG22	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG23	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG21	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG22	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG23	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG21	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG22	6	0.44	0.25	0.34
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG23	6	0.44	0.25	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,160)	1:165:A:ARG:HD2	1:54:A:VAL:HA	6	0.43	0.11	0.46
(2,160)	1:53:A:HIS:HB2	1:54:A:VAL:HA	6	0.43	0.11	0.46
(4,369)	1:140:A:ARG:HA	1:140:A:ARG:HG2	6	0.39	0.09	0.4
(4,565)	1:16:A:MET:HA	1:16:A:MET:HB3	6	0.39	0.19	0.38
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG21	6	0.36	0.11	0.35
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG22	6	0.36	0.11	0.35
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG23	6	0.36	0.11	0.35
(4,344)	1:34:A:ARG:HB2	1:34:A:ARG:HD2	6	0.32	0.05	0.3
(4,312)	1:151:A:CYS:HB2	1:151:A:CYS:HA	6	0.23	0.01	0.24
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG11	6	0.21	0.05	0.22
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG12	6	0.21	0.05	0.22
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG13	6	0.21	0.05	0.22
(4,767)	1:128:A:ALA:HA	1:35:A:PHE:HA	6	0.2	0.11	0.14
(4,26)	1:163:A:LEU:HD21	1:56:A:TYR:HB3	6	0.19	0.07	0.18
(4,26)	1:163:A:LEU:HD22	1:56:A:TYR:HB3	6	0.19	0.07	0.18
(4,26)	1:163:A:LEU:HD23	1:56:A:TYR:HB3	6	0.19	0.07	0.18
(4,156)	1:16:A:MET:HE1	1:16:A:MET:HG3	6	0.19	0.03	0.2
(4,156)	1:16:A:MET:HE2	1:16:A:MET:HG3	6	0.19	0.03	0.2
(4,156)	1:16:A:MET:HE3	1:16:A:MET:HG3	6	0.19	0.03	0.2
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG21	6	0.16	0.04	0.15
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG22	6	0.16	0.04	0.15
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG23	6	0.16	0.04	0.15
(4,13)	1:54:A:VAL:H	1:23:A:PRO:HA	6	0.16	0.04	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG11	6	0.16	0.02	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG12	6	0.16	0.02	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG13	6	0.16	0.02	0.16
(4,518)	1:58:A:ILE:HB	1:163:A:LEU:HA	6	0.14	0.03	0.14
(4,57)	1:59:A:LYS:HA	1:17:A:GLU:HG2	5	1.17	0.3	1.23
(4,210)	1:12:A:GLN:HA	1:13:A:MET:HG2	5	1.17	0.07	1.19
(1,34)	1:19:A:PHE:H	1:42:A:ALA:O	5	1.14	0.74	1.44
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG2	5	1.14	0.59	1.31
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG3	5	1.14	0.59	1.31
(2,161)	1:53:A:HIS:HB2	1:54:A:VAL:HG23	5	1.09	0.25	1.11
(2,161)	1:53:A:HIS:HB2	1:54:A:VAL:HG22	5	1.09	0.25	1.11
(2,161)	1:54:A:VAL:HG22	1:165:A:ARG:HD2	5	1.09	0.25	1.11
(2,161)	1:54:A:VAL:HG21	1:165:A:ARG:HD2	5	1.09	0.25	1.11
(4,579)	1:151:A:CYS:HB2	1:144:A:MET:HB3	5	0.93	0.43	0.96
(4,277)	1:163:A:LEU:HD21	1:29:A:ILE:HG13	5	0.71	0.67	0.6
(4,277)	1:163:A:LEU:HD22	1:29:A:ILE:HG13	5	0.71	0.67	0.6
(4,277)	1:163:A:LEU:HD23	1:29:A:ILE:HG13	5	0.71	0.67	0.6
(4,484)	1:126:A:ILE:HG21	1:104:A:GLN:HG3	5	0.59	0.24	0.63
(4,484)	1:126:A:ILE:HG22	1:104:A:GLN:HG3	5	0.59	0.24	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,484)	1:126:A:ILE:HG23	1:104:A:GLN:HG3	5	0.59	0.24	0.63
(2,210)	1:152:A:TYR:HA	1:154:A:ILE:HD13	5	0.55	0.33	0.44
(2,210)	1:152:A:TYR:HA	1:154:A:ILE:HD12	5	0.55	0.33	0.44
(2,210)	1:152:A:TYR:HA	1:154:A:ILE:HD11	5	0.55	0.33	0.44
(2,210)	1:154:A:ILE:HD12	1:153:A:MET:HA	5	0.55	0.33	0.44
(2,334)	1:144:A:MET:HG2	1:151:A:CYS:HB3	5	0.5	0.24	0.49
(2,334)	1:144:A:MET:HG3	1:151:A:CYS:HB3	5	0.5	0.24	0.49
(4,385)	1:153:A:MET:HE1	1:153:A:MET:HG3	5	0.48	0.03	0.49
(4,385)	1:153:A:MET:HE2	1:153:A:MET:HG3	5	0.48	0.03	0.49
(4,385)	1:153:A:MET:HE3	1:153:A:MET:HG3	5	0.48	0.03	0.49
(4,198)	1:2:A:SER:HA	1:2:A:SER:HB2	5	0.47	0.18	0.56
(4,17)	1:59:A:LYS:HE2	1:57:A:ARG:HG2	5	0.46	0.15	0.42
(4,17)	1:59:A:LYS:HE3	1:57:A:ARG:HG2	5	0.46	0.15	0.42
(4,348)	1:165:A:ARG:HB3	1:165:A:ARG:HD2	5	0.46	0.05	0.45
(4,283)	1:62:A:GLU:HA	1:64:A:ASP:H	5	0.46	0.41	0.24
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD11	5	0.45	0.27	0.4
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD12	5	0.45	0.27	0.4
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD13	5	0.45	0.27	0.4
(4,238)	1:128:A:ALA:HB1	1:34:A:ARG:HD2	5	0.27	0.14	0.25
(4,238)	1:128:A:ALA:HB2	1:34:A:ARG:HD2	5	0.27	0.14	0.25
(4,238)	1:128:A:ALA:HB3	1:34:A:ARG:HD2	5	0.27	0.14	0.25
(4,64)	1:54:A:VAL:HG11	1:25:A:GLU:HA	5	0.26	0.11	0.27
(4,64)	1:54:A:VAL:HG12	1:25:A:GLU:HA	5	0.26	0.11	0.27
(4,64)	1:54:A:VAL:HG13	1:25:A:GLU:HA	5	0.26	0.11	0.27
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE1	5	0.25	0.11	0.17
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE2	5	0.25	0.11	0.17
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE3	5	0.25	0.11	0.17
(4,658)	1:165:A:ARG:HB2	1:165:A:ARG:HD2	5	0.19	0.03	0.21
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB1	5	0.19	0.05	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB2	5	0.19	0.05	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB3	5	0.19	0.05	0.18
(4,760)	1:153:A:MET:HE1	1:38:A:PHE:HB2	5	0.18	0.1	0.13
(4,760)	1:153:A:MET:HE2	1:38:A:PHE:HB2	5	0.18	0.1	0.13
(4,760)	1:153:A:MET:HE3	1:38:A:PHE:HB2	5	0.18	0.1	0.13
(4,128)	1:49:A:THR:HB	1:50:A:ALA:H	5	0.17	0.07	0.13
(4,644)	1:13:A:MET:HA	1:13:A:MET:HG3	5	0.17	0.01	0.16
(4,641)	1:166:A:VAL:HB	1:55:A:THR:HB	5	0.15	0.06	0.14
(4,111)	1:163:A:LEU:H	1:163:A:LEU:HG	5	0.15	0.03	0.14
(4,419)	1:20:A:HIS:HA	1:41:A:PHE:HA	5	0.15	0.03	0.16
(4,42)	1:111:A:LEU:HD11	1:110:A:ASN:HB3	5	0.15	0.03	0.14
(4,42)	1:111:A:LEU:HD12	1:110:A:ASN:HB3	5	0.15	0.03	0.14
(4,42)	1:111:A:LEU:HD13	1:110:A:ASN:HB3	5	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,634)	1:91:A:THR:HB	1:91:A:THR:HA	5	0.13	0.02	0.13
(4,519)	1:153:A:MET:HE1	1:153:A:MET:HG2	5	0.12	0.01	0.12
(4,519)	1:153:A:MET:HE2	1:153:A:MET:HG2	5	0.12	0.01	0.12
(4,519)	1:153:A:MET:HE3	1:153:A:MET:HG2	5	0.12	0.01	0.12
(4,3)	1:163:A:LEU:HD11	1:162:A:GLU:HB3	4	1.37	0.55	1.38
(4,3)	1:163:A:LEU:HD12	1:162:A:GLU:HB3	4	1.37	0.55	1.38
(4,3)	1:163:A:LEU:HD13	1:162:A:GLU:HB3	4	1.37	0.55	1.38
(4,756)	1:98:A:ALA:HB1	1:93:A:CYS:HB2	4	1.29	1.14	1.1
(4,756)	1:98:A:ALA:HB2	1:93:A:CYS:HB2	4	1.29	1.14	1.1
(4,756)	1:98:A:ALA:HB3	1:93:A:CYS:HB2	4	1.29	1.14	1.1
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD11	4	1.08	0.35	1.04
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD12	4	1.08	0.35	1.04
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD13	4	1.08	0.35	1.04
(4,426)	1:24:A:VAL:HG21	1:25:A:GLU:HG2	4	0.8	0.44	0.78
(4,426)	1:24:A:VAL:HG22	1:25:A:GLU:HG2	4	0.8	0.44	0.78
(4,426)	1:24:A:VAL:HG23	1:25:A:GLU:HG2	4	0.8	0.44	0.78
(4,759)	1:150:A:THR:H	1:149:A:GLY:HA2	4	0.71	0.04	0.72
(4,74)	1:39:A:LEU:HD21	1:156:A:MET:HB2	4	0.66	0.41	0.72
(4,74)	1:39:A:LEU:HD22	1:156:A:MET:HB2	4	0.66	0.41	0.72
(4,74)	1:39:A:LEU:HD23	1:156:A:MET:HB2	4	0.66	0.41	0.72
(4,341)	1:128:A:ALA:HB1	1:35:A:PHE:HB3	4	0.58	0.32	0.55
(4,341)	1:128:A:ALA:HB2	1:35:A:PHE:HB3	4	0.58	0.32	0.55
(4,341)	1:128:A:ALA:HB3	1:35:A:PHE:HB3	4	0.58	0.32	0.55
(4,33)	1:39:A:LEU:HD11	1:156:A:MET:HB3	4	0.57	0.48	0.4
(4,33)	1:39:A:LEU:HD12	1:156:A:MET:HB3	4	0.57	0.48	0.4
(4,33)	1:39:A:LEU:HD13	1:156:A:MET:HB3	4	0.57	0.48	0.4
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG21	4	0.47	0.19	0.46
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG22	4	0.47	0.19	0.46
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG23	4	0.47	0.19	0.46
(4,375)	1:163:A:LEU:HD11	1:156:A:MET:HG2	4	0.44	0.29	0.34
(4,375)	1:163:A:LEU:HD12	1:156:A:MET:HG2	4	0.44	0.29	0.34
(4,375)	1:163:A:LEU:HD13	1:156:A:MET:HG2	4	0.44	0.29	0.34
(4,276)	1:46:A:TYR:HA	1:46:A:TYR:HB2	4	0.41	0.01	0.41
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD11	4	0.38	0.1	0.36
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD12	4	0.38	0.1	0.36
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD13	4	0.38	0.1	0.36
(4,231)	1:59:A:LYS:HE2	1:17:A:GLU:HG2	4	0.34	0.09	0.34
(4,231)	1:59:A:LYS:HE3	1:17:A:GLU:HG2	4	0.34	0.09	0.34
(4,280)	1:140:A:ARG:HA	1:140:A:ARG:HD3	4	0.34	0.12	0.35
(2,292)	1:122:A:LEU:HA	1:91:A:THR:HG23	4	0.29	0.12	0.28
(2,292)	1:122:A:LEU:HA	1:91:A:THR:HG22	4	0.29	0.12	0.28
(2,292)	1:91:A:THR:HG21	1:90:A:LEU:HA	4	0.29	0.12	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG2	4	0.27	0.12	0.22
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG3	4	0.27	0.12	0.22
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG2	4	0.27	0.12	0.22
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG3	4	0.27	0.12	0.22
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG2	4	0.27	0.12	0.22
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG3	4	0.27	0.12	0.22
(4,428)	1:46:A:TYR:HB3	1:46:A:TYR:H	4	0.27	0.02	0.27
(4,234)	1:155:A:ASP:HA	1:38:A:PHE:HA	4	0.26	0.1	0.26
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB1	4	0.25	0.2	0.16
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB2	4	0.25	0.2	0.16
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB3	4	0.25	0.2	0.16
(4,286)	1:26:A:ILE:HG21	1:27:A:THR:HA	4	0.24	0.07	0.25
(4,286)	1:26:A:ILE:HG22	1:27:A:THR:HA	4	0.24	0.07	0.25
(4,286)	1:26:A:ILE:HG23	1:27:A:THR:HA	4	0.24	0.07	0.25
(4,394)	1:150:A:THR:HG21	1:143:A:SER:HA	4	0.19	0.07	0.19
(4,394)	1:150:A:THR:HG22	1:143:A:SER:HA	4	0.19	0.07	0.19
(4,394)	1:150:A:THR:HG23	1:143:A:SER:HA	4	0.19	0.07	0.19
(4,73)	1:154:A:ILE:HG21	1:140:A:ARG:HA	4	0.18	0.04	0.17
(4,73)	1:154:A:ILE:HG22	1:140:A:ARG:HA	4	0.18	0.04	0.17
(4,73)	1:154:A:ILE:HG23	1:140:A:ARG:HA	4	0.18	0.04	0.17
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG21	4	0.18	0.06	0.16
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG22	4	0.18	0.06	0.16
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG23	4	0.18	0.06	0.16
(4,208)	1:13:A:MET:HA	1:13:A:MET:HG2	4	0.16	0.01	0.16
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB1	4	0.16	0.02	0.16
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB2	4	0.16	0.02	0.16
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB3	4	0.16	0.02	0.16
(4,69)	1:153:A:MET:HE1	1:153:A:MET:HB2	4	0.16	0.03	0.16
(4,69)	1:153:A:MET:HE2	1:153:A:MET:HB2	4	0.16	0.03	0.16
(4,69)	1:153:A:MET:HE3	1:153:A:MET:HB2	4	0.16	0.03	0.16
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG21	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG22	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG23	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG21	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG22	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG23	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG21	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG22	4	0.16	0.05	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG23	4	0.16	0.05	0.13
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG21	4	0.16	0.03	0.16
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG22	4	0.16	0.03	0.16
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG23	4	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG21	4	0.16	0.03	0.16
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG22	4	0.16	0.03	0.16
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG23	4	0.16	0.03	0.16
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG21	4	0.16	0.03	0.16
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG22	4	0.16	0.03	0.16
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG23	4	0.16	0.03	0.16
(1,45)	1:142:A:VAL:H	1:153:A:MET:O	4	0.13	0.02	0.12
(4,32)	1:87:A:VAL:HG21	1:90:A:LEU:HB3	4	0.13	0.01	0.12
(4,32)	1:87:A:VAL:HG22	1:90:A:LEU:HB3	4	0.13	0.01	0.12
(4,32)	1:87:A:VAL:HG23	1:90:A:LEU:HB3	4	0.13	0.01	0.12
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD11	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD12	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD13	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD21	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD22	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD23	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD11	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD12	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD13	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD21	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD22	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD23	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD11	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD12	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD13	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD21	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD22	4	0.12	0.02	0.13
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD23	4	0.12	0.02	0.13
(4,267)	1:107:A:ASP:HB2	1:109:A:PHE:HB3	4	0.12	0.01	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG11	4	0.12	0.02	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG12	4	0.12	0.02	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG13	4	0.12	0.02	0.12
(4,721)	1:109:A:PHE:H	1:109:A:PHE:HA	4	0.12	0.01	0.12
(4,197)	1:46:A:TYR:HA	1:46:A:TYR:H	4	0.11	0.0	0.11
(4,94)	1:116:A:ALA:HB1	1:111:A:LEU:HB3	3	1.4	0.05	1.41
(4,94)	1:116:A:ALA:HB2	1:111:A:LEU:HB3	3	1.4	0.05	1.41
(4,94)	1:116:A:ALA:HB3	1:111:A:LEU:HB3	3	1.4	0.05	1.41
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD21	3	1.37	0.58	1.36
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD22	3	1.37	0.58	1.36
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD23	3	1.37	0.58	1.36
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD21	3	1.37	0.58	1.36
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD22	3	1.37	0.58	1.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD23	3	1.37	0.58	1.36
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD21	3	1.37	0.58	1.36
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD22	3	1.37	0.58	1.36
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD23	3	1.37	0.58	1.36
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD11	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD12	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD13	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD11	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD12	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD13	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD11	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD12	3	1.13	0.85	1.0
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD13	3	1.13	0.85	1.0
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD21	3	0.93	0.55	1.16
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD22	3	0.93	0.55	1.16
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD23	3	0.93	0.55	1.16
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG11	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG12	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG13	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG11	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG12	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG13	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG11	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG12	3	0.82	0.89	0.24
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG13	3	0.82	0.89	0.24
(4,437)	1:29:A:ILE:HG21	1:156:A:MET:HB3	3	0.72	0.33	0.6
(4,437)	1:29:A:ILE:HG22	1:156:A:MET:HB3	3	0.72	0.33	0.6
(4,437)	1:29:A:ILE:HG23	1:156:A:MET:HB3	3	0.72	0.33	0.6
(4,323)	1:32:A:GLN:HA	1:32:A:GLN:HG3	3	0.61	0.43	0.55
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD21	3	0.6	0.48	0.46
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD22	3	0.6	0.48	0.46
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD23	3	0.6	0.48	0.46
(4,695)	1:16:A:MET:HG2	1:16:A:MET:H	3	0.59	0.22	0.44
(2,138)	1:60:A:VAL:HG12	1:16:A:MET:HG3	3	0.55	0.13	0.56
(2,138)	1:60:A:VAL:HG13	1:16:A:MET:HG3	3	0.55	0.13	0.56
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE1	3	0.52	0.55	0.16
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE2	3	0.52	0.55	0.16
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE3	3	0.52	0.55	0.16
(4,301)	1:137:A:LEU:HD11	1:137:A:LEU:HA	3	0.51	0.05	0.51
(4,301)	1:137:A:LEU:HD12	1:137:A:LEU:HA	3	0.51	0.05	0.51
(4,301)	1:137:A:LEU:HD13	1:137:A:LEU:HA	3	0.51	0.05	0.51
(4,683)	1:150:A:THR:HG21	1:143:A:SER:HB2	3	0.48	0.44	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,683)	1:150:A:THR:HG22	1:143:A:SER:HB2	3	0.48	0.44	0.23
(4,683)	1:150:A:THR:HG23	1:143:A:SER:HB2	3	0.48	0.44	0.23
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG11	3	0.45	0.2	0.34
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG12	3	0.45	0.2	0.34
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG13	3	0.45	0.2	0.34
(2,217)	1:54:A:VAL:HG11	1:165:A:ARG:HD3	3	0.38	0.09	0.34
(2,217)	1:54:A:VAL:HG12	1:165:A:ARG:HD3	3	0.38	0.09	0.34
(2,217)	1:54:A:VAL:HG13	1:165:A:ARG:HD3	3	0.38	0.09	0.34
(4,349)	1:29:A:ILE:HD11	1:156:A:MET:HB3	3	0.35	0.05	0.35
(4,349)	1:29:A:ILE:HD12	1:156:A:MET:HB3	3	0.35	0.05	0.35
(4,349)	1:29:A:ILE:HD13	1:156:A:MET:HB3	3	0.35	0.05	0.35
(2,175)	1:54:A:VAL:HG11	1:25:A:GLU:HA	3	0.33	0.05	0.36
(2,175)	1:54:A:VAL:HG12	1:25:A:GLU:HA	3	0.33	0.05	0.36
(2,175)	1:54:A:VAL:HG13	1:25:A:GLU:HA	3	0.33	0.05	0.36
(2,175)	1:54:A:VAL:HG21	1:25:A:GLU:HA	3	0.33	0.05	0.36
(2,175)	1:54:A:VAL:HG22	1:25:A:GLU:HA	3	0.33	0.05	0.36
(2,175)	1:54:A:VAL:HG23	1:25:A:GLU:HA	3	0.33	0.05	0.36
(2,234)	1:50:A:ALA:HB1	1:51:A:GLY:HA2	3	0.33	0.17	0.25
(2,234)	1:50:A:ALA:HB2	1:51:A:GLY:HA2	3	0.33	0.17	0.25
(2,200)	1:114:A:ILE:HG13	1:114:A:ILE:HA	3	0.29	0.02	0.3
(4,89)	1:58:A:ILE:HG21	1:162:A:GLU:HB3	3	0.28	0.06	0.25
(4,89)	1:58:A:ILE:HG22	1:162:A:GLU:HB3	3	0.28	0.06	0.25
(4,89)	1:58:A:ILE:HG23	1:162:A:GLU:HB3	3	0.28	0.06	0.25
(4,82)	1:146:A:ASP:HB3	1:146:A:ASP:H	3	0.28	0.03	0.28
(4,596)	1:47:A:VAL:HG21	1:48:A:MET:HA	3	0.28	0.14	0.25
(4,596)	1:47:A:VAL:HG22	1:48:A:MET:HA	3	0.28	0.14	0.25
(4,596)	1:47:A:VAL:HG23	1:48:A:MET:HA	3	0.28	0.14	0.25
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE1	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE2	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE3	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE1	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE2	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE3	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE1	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE2	3	0.27	0.06	0.28
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE3	3	0.27	0.06	0.28
(4,217)	1:73:A:TYR:H	1:73:A:TYR:HB3	3	0.27	0.09	0.22
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE1	3	0.26	0.04	0.27
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE2	3	0.26	0.04	0.27
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE3	3	0.26	0.04	0.27
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE1	3	0.26	0.04	0.27
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE2	3	0.26	0.04	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE3	3	0.26	0.04	0.27
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE1	3	0.26	0.04	0.27
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE2	3	0.26	0.04	0.27
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE3	3	0.26	0.04	0.27
(4,164)	1:114:A:ILE:HG13	1:114:A:ILE:HA	3	0.24	0.02	0.26
(4,640)	1:163:A:LEU:HD21	1:156:A:MET:HG2	3	0.24	0.05	0.27
(4,640)	1:163:A:LEU:HD22	1:156:A:MET:HG2	3	0.24	0.05	0.27
(4,640)	1:163:A:LEU:HD23	1:156:A:MET:HG2	3	0.24	0.05	0.27
(4,514)	1:144:A:MET:H	1:144:A:MET:HE1	3	0.23	0.09	0.21
(4,514)	1:144:A:MET:H	1:144:A:MET:HE2	3	0.23	0.09	0.21
(4,514)	1:144:A:MET:H	1:144:A:MET:HE3	3	0.23	0.09	0.21
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE1	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE2	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE3	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE1	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE2	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE3	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE1	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE2	3	0.22	0.09	0.22
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE3	3	0.22	0.09	0.22
(4,203)	1:17:A:GLU:H	1:16:A:MET:HG3	3	0.21	0.03	0.2
(4,481)	1:118:A:ASP:H	1:115:A:ASP:HB2	3	0.2	0.03	0.22
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG21	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG22	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG23	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG21	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG22	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG23	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG21	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG22	3	0.19	0.05	0.16
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG23	3	0.19	0.05	0.16
(4,688)	1:105:A:ARG:HD3	1:105:A:ARG:H	3	0.18	0.02	0.19
(4,87)	1:91:A:THR:HG21	1:125:A:GLU:H	3	0.18	0.05	0.17
(4,87)	1:91:A:THR:HG22	1:125:A:GLU:H	3	0.18	0.05	0.17
(4,87)	1:91:A:THR:HG23	1:125:A:GLU:H	3	0.18	0.05	0.17
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG21	3	0.18	0.07	0.15
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG22	3	0.18	0.07	0.15
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG23	3	0.18	0.07	0.15
(1,8)	1:85:A:GLU:H	1:81:A:SER:O	3	0.18	0.05	0.17
(4,278)	1:162:A:GLU:HG3	1:162:A:GLU:H	3	0.17	0.04	0.14
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG21	3	0.15	0.01	0.16
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG22	3	0.15	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG23	3	0.15	0.01	0.16
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD21	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD22	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD23	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD21	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD22	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD23	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD21	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD22	3	0.15	0.04	0.14
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD23	3	0.15	0.04	0.14
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG21	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG22	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG23	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG21	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG22	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG23	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG21	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG22	3	0.15	0.04	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG23	3	0.15	0.04	0.12
(4,409)	1:167:A:LYS:H	1:165:A:ARG:HA	3	0.14	0.02	0.14
(4,303)	1:129:A:ILE:HG21	1:126:A:ILE:HA	3	0.13	0.01	0.13
(4,303)	1:129:A:ILE:HG22	1:126:A:ILE:HA	3	0.13	0.01	0.13
(4,303)	1:129:A:ILE:HG23	1:126:A:ILE:HA	3	0.13	0.01	0.13
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD11	3	0.13	0.03	0.13
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD12	3	0.13	0.03	0.13
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD13	3	0.13	0.03	0.13
(4,550)	1:127:A:GLN:HA	1:127:A:GLN:HG3	3	0.13	0.0	0.13
(4,779)	1:130:A:THR:H	1:127:A:GLN:HA	3	0.13	0.02	0.13
(4,501)	1:105:A:ARG:HA	1:106:A:ILE:H	3	0.12	0.02	0.11
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG21	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG22	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG23	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG21	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG22	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG23	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG21	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG22	3	0.11	0.01	0.11
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG23	3	0.11	0.01	0.11
(4,246)	1:163:A:LEU:HD11	1:56:A:TYR:HB2	2	1.46	0.16	1.46
(4,246)	1:163:A:LEU:HD12	1:56:A:TYR:HB2	2	1.46	0.16	1.46
(4,246)	1:163:A:LEU:HD13	1:56:A:TYR:HB2	2	1.46	0.16	1.46
(4,656)	1:59:A:LYS:HG3	1:17:A:GLU:HG2	2	1.44	0.07	1.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD11	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD12	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD13	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD11	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD12	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD13	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD11	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD12	2	1.42	0.55	1.42
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD13	2	1.42	0.55	1.42
(1,7)	1:84:A:VAL:H	1:80:A:LEU:O	2	1.39	1.11	1.39
(1,33)	1:74:A:HIS:H	1:70:A:SER:O	2	1.27	1.11	1.27
(4,649)	1:154:A:ILE:HD11	1:141:A:GLY:HA2	2	1.18	0.01	1.18
(4,649)	1:154:A:ILE:HD11	1:141:A:GLY:HA3	2	1.18	0.01	1.18
(4,649)	1:154:A:ILE:HD12	1:141:A:GLY:HA2	2	1.18	0.01	1.18
(4,649)	1:154:A:ILE:HD12	1:141:A:GLY:HA3	2	1.18	0.01	1.18
(4,649)	1:154:A:ILE:HD13	1:141:A:GLY:HA2	2	1.18	0.01	1.18
(4,649)	1:154:A:ILE:HD13	1:141:A:GLY:HA3	2	1.18	0.01	1.18
(4,249)	1:100:A:GLU:HG3	1:97:A:THR:HA	2	1.14	0.12	1.14
(4,212)	1:163:A:LEU:HD11	1:163:A:LEU:HA	2	1.09	0.01	1.09
(4,212)	1:163:A:LEU:HD12	1:163:A:LEU:HA	2	1.09	0.01	1.09
(4,212)	1:163:A:LEU:HD13	1:163:A:LEU:HA	2	1.09	0.01	1.09
(4,681)	1:84:A:VAL:HG11	1:85:A:GLU:HA	2	1.08	0.96	1.08
(4,681)	1:84:A:VAL:HG12	1:85:A:GLU:HA	2	1.08	0.96	1.08
(4,681)	1:84:A:VAL:HG13	1:85:A:GLU:HA	2	1.08	0.96	1.08
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB1	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB2	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB3	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB1	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB2	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB3	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB1	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB2	2	1.02	0.85	1.02
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB3	2	1.02	0.85	1.02
(2,115)	1:145:A:GLN:H	1:145:A:GLN:HG2	2	0.98	0.21	0.98
(2,115)	1:145:A:GLN:H	1:145:A:GLN:HG3	2	0.98	0.21	0.98
(4,386)	1:47:A:VAL:HG21	1:47:A:VAL:H	2	0.91	0.05	0.91
(4,386)	1:47:A:VAL:HG22	1:47:A:VAL:H	2	0.91	0.05	0.91
(4,386)	1:47:A:VAL:HG23	1:47:A:VAL:H	2	0.91	0.05	0.91
(4,177)	1:163:A:LEU:HD11	1:56:A:TYR:HB3	2	0.9	0.25	0.9
(4,177)	1:163:A:LEU:HD12	1:56:A:TYR:HB3	2	0.9	0.25	0.9
(4,177)	1:163:A:LEU:HD13	1:56:A:TYR:HB3	2	0.9	0.25	0.9
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG21	2	0.79	0.03	0.79

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG22	2	0.79	0.03	0.79
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG23	2	0.79	0.03	0.79
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG21	2	0.79	0.03	0.79
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG22	2	0.79	0.03	0.79
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG23	2	0.79	0.03	0.79
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG21	2	0.79	0.03	0.79
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG22	2	0.79	0.03	0.79
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG23	2	0.79	0.03	0.79
(4,750)	1:105:A:ARG:HA	1:105:A:ARG:HD3	2	0.75	0.02	0.75
(4,475)	1:47:A:VAL:HG21	1:48:A:MET:HG2	2	0.7	0.4	0.7
(4,475)	1:47:A:VAL:HG22	1:48:A:MET:HG2	2	0.7	0.4	0.7
(4,475)	1:47:A:VAL:HG23	1:48:A:MET:HG2	2	0.7	0.4	0.7
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG11	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG12	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG13	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG11	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG12	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG13	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG11	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG12	2	0.68	0.45	0.68
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG13	2	0.68	0.45	0.68
(4,40)	1:122:A:LEU:HA	1:122:A:LEU:HG	2	0.63	0.02	0.63
(4,570)	1:17:A:GLU:HB2	1:57:A:ARG:HD2	2	0.57	0.18	0.57
(4,570)	1:17:A:GLU:HB2	1:57:A:ARG:HD3	2	0.57	0.18	0.57
(4,28)	1:166:A:VAL:HG11	1:57:A:ARG:HD2	2	0.55	0.39	0.55
(4,28)	1:166:A:VAL:HG11	1:57:A:ARG:HD3	2	0.55	0.39	0.55
(4,28)	1:166:A:VAL:HG12	1:57:A:ARG:HD2	2	0.55	0.39	0.55
(4,28)	1:166:A:VAL:HG12	1:57:A:ARG:HD3	2	0.55	0.39	0.55
(4,28)	1:166:A:VAL:HG13	1:57:A:ARG:HD2	2	0.55	0.39	0.55
(4,28)	1:166:A:VAL:HG13	1:57:A:ARG:HD3	2	0.55	0.39	0.55
(2,326)	1:143:A:SER:HA	1:144:A:MET:HG2	2	0.5	0.36	0.5
(2,326)	1:143:A:SER:HA	1:144:A:MET:HG3	2	0.5	0.36	0.5
(4,774)	1:164:A:VAL:HG11	1:164:A:VAL:HA	2	0.5	0.0	0.5
(4,774)	1:164:A:VAL:HG12	1:164:A:VAL:HA	2	0.5	0.0	0.5
(4,774)	1:164:A:VAL:HG13	1:164:A:VAL:HA	2	0.5	0.0	0.5
(4,235)	1:122:A:LEU:HA	1:125:A:GLU:HG3	2	0.44	0.34	0.44
(4,455)	1:108:A:VAL:HB	1:108:A:VAL:H	2	0.44	0.01	0.44
(4,761)	1:130:A:THR:H	1:130:A:THR:HG21	2	0.41	0.05	0.41
(4,761)	1:130:A:THR:H	1:130:A:THR:HG22	2	0.41	0.05	0.41
(4,761)	1:130:A:THR:H	1:130:A:THR:HG23	2	0.41	0.05	0.41
(2,276)	1:24:A:VAL:HG13	1:25:A:GLU:HB2	2	0.4	0.2	0.4
(2,276)	1:54:A:VAL:HG23	1:25:A:GLU:HB3	2	0.4	0.2	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,86)	1:106:A:ILE:HG21	1:100:A:GLU:HG3	2	0.4	0.24	0.4
(4,86)	1:106:A:ILE:HG22	1:100:A:GLU:HG3	2	0.4	0.24	0.4
(4,86)	1:106:A:ILE:HG23	1:100:A:GLU:HG3	2	0.4	0.24	0.4
(2,186)	1:144:A:MET:HG2	1:151:A:CYS:HB2	2	0.34	0.04	0.34
(2,186)	1:144:A:MET:HG3	1:151:A:CYS:HB2	2	0.34	0.04	0.34
(4,526)	1:140:A:ARG:HB3	1:140:A:ARG:HD2	2	0.32	0.14	0.32
(4,722)	1:49:A:THR:HA	1:50:A:ALA:H	2	0.32	0.16	0.32
(4,62)	1:103:A:SER:HB2	1:105:A:ARG:HD3	2	0.3	0.08	0.3
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG21	2	0.3	0.16	0.3
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG22	2	0.3	0.16	0.3
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG23	2	0.3	0.16	0.3
(2,321)	1:41:A:PHE:H	1:40:A:CYS:HB2	2	0.28	0.11	0.28
(2,321)	1:41:A:PHE:H	1:40:A:CYS:HB3	2	0.28	0.11	0.28
(2,255)	1:55:A:THR:H	1:21:A:THR:HG21	2	0.26	0.11	0.26
(2,255)	1:55:A:THR:H	1:21:A:THR:HG22	2	0.26	0.11	0.26
(4,777)	1:83:A:LEU:HG	1:83:A:LEU:HA	2	0.26	0.02	0.26
(2,289)	1:75:A:GLU:HA	1:75:A:GLU:HG2	2	0.24	0.04	0.24
(2,289)	1:75:A:GLU:HA	1:75:A:GLU:HG3	2	0.24	0.04	0.24
(4,740)	1:87:A:VAL:HA	1:90:A:LEU:HB3	2	0.24	0.01	0.24
(4,300)	1:118:A:ASP:HB2	1:118:A:ASP:H	2	0.22	0.01	0.22
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE1	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE2	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE3	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE1	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE2	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE3	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE1	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE2	2	0.2	0.0	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE3	2	0.2	0.0	0.2
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE1	2	0.18	0.08	0.18
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE2	2	0.18	0.08	0.18
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE3	2	0.18	0.08	0.18
(4,113)	1:91:A:THR:H	1:91:A:THR:HB	2	0.17	0.0	0.17
(4,587)	1:111:A:LEU:H	1:111:A:LEU:HB3	2	0.17	0.05	0.17
(4,710)	1:61:A:ASP:HB2	1:64:A:ASP:H	2	0.17	0.05	0.17
(1,50)	1:153:A:MET:H	1:142:A:VAL:O	2	0.16	0.02	0.16
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB1	2	0.16	0.01	0.16
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB2	2	0.16	0.01	0.16
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB3	2	0.16	0.01	0.16
(4,657)	1:22:A:SER:HA	1:23:A:PRO:HD3	2	0.16	0.01	0.16
(2,215)	1:24:A:VAL:HG21	1:25:A:GLU:HB2	2	0.15	0.01	0.15
(2,215)	1:24:A:VAL:HG21	1:25:A:GLU:HB3	2	0.15	0.01	0.15

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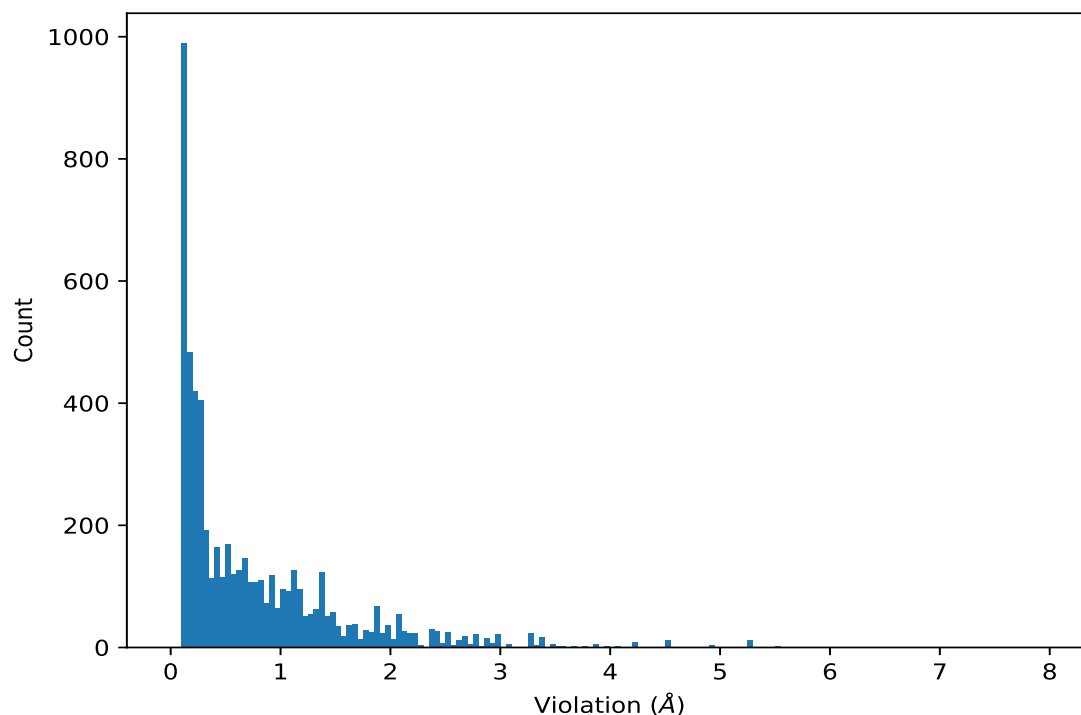
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,215)	1:24:A:VAL:HG22	1:25:A:GLU:HB2	2	0.15	0.01	0.15
(2,215)	1:24:A:VAL:HG22	1:25:A:GLU:HB3	2	0.15	0.01	0.15
(2,215)	1:24:A:VAL:HG23	1:25:A:GLU:HB2	2	0.15	0.01	0.15
(2,215)	1:24:A:VAL:HG23	1:25:A:GLU:HB3	2	0.15	0.01	0.15
(4,460)	1:153:A:MET:HE1	1:35:A:PHE:HB2	2	0.15	0.02	0.15
(4,460)	1:153:A:MET:HE2	1:35:A:PHE:HB2	2	0.15	0.02	0.15
(4,460)	1:153:A:MET:HE3	1:35:A:PHE:HB2	2	0.15	0.02	0.15
(4,272)	1:109:A:PHE:HB2	1:110:A:ASN:H	2	0.15	0.02	0.15
(4,324)	1:34:A:ARG:HB3	1:34:A:ARG:HD3	2	0.15	0.0	0.15
(4,739)	1:59:A:LYS:HE2	1:17:A:GLU:HG3	2	0.15	0.0	0.15
(4,739)	1:59:A:LYS:HE3	1:17:A:GLU:HG3	2	0.15	0.0	0.15
(4,630)	1:153:A:MET:H	1:143:A:SER:HA	2	0.14	0.02	0.14
(1,15)	1:96:A:ASP:O	1:100:A:GLU:H	2	0.14	0.04	0.14
(2,41)	1:100:A:GLU:H	1:97:A:THR:HA	2	0.14	0.02	0.14
(4,279)	1:34:A:ARG:HD2	1:34:A:ARG:HA	2	0.13	0.0	0.13
(4,411)	1:113:A:ASP:HB3	1:114:A:ILE:H	2	0.13	0.01	0.13
(4,694)	1:105:A:ARG:HD2	1:105:A:ARG:H	2	0.13	0.02	0.13
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG21	2	0.12	0.01	0.12
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG22	2	0.12	0.01	0.12
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG23	2	0.12	0.01	0.12
(4,287)	1:21:A:THR:HG21	1:55:A:THR:HA	2	0.12	0.02	0.12
(4,287)	1:21:A:THR:HG22	1:55:A:THR:HA	2	0.12	0.02	0.12
(4,287)	1:21:A:THR:HG23	1:55:A:THR:HA	2	0.12	0.02	0.12
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB1	2	0.12	0.01	0.12
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB2	2	0.12	0.01	0.12
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB3	2	0.12	0.01	0.12
(1,17)	1:117:A:SER:O	1:121:A:GLU:H	2	0.12	0.0	0.12
(4,478)	1:49:A:THR:HG21	1:49:A:THR:HA	2	0.12	0.0	0.12
(4,478)	1:49:A:THR:HG22	1:49:A:THR:HA	2	0.12	0.0	0.12
(4,478)	1:49:A:THR:HG23	1:49:A:THR:HA	2	0.12	0.0	0.12
(4,757)	1:137:A:LEU:H	1:134:A:ALA:HA	2	0.11	0.0	0.11
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG21	2	0.11	0.0	0.11
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG22	2	0.11	0.0	0.11
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG23	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	7	7.99
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	10	7.44
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	8	7.26
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	4	7.0
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	2	6.74
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	8	6.67
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	6	6.15
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	5	5.68
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	2	5.52
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	2	5.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	2	5.52
(4,240)	1:123:A:SER:HB2	1:108:A:VAL:HG11	10	5.3
(4,240)	1:123:A:SER:HB2	1:108:A:VAL:HG12	10	5.3
(4,240)	1:123:A:SER:HB2	1:108:A:VAL:HG13	10	5.3
(4,240)	1:123:A:SER:HB2	1:108:A:VAL:HG21	10	5.3
(4,240)	1:123:A:SER:HB2	1:108:A:VAL:HG22	10	5.3
(4,240)	1:123:A:SER:HB2	1:108:A:VAL:HG23	10	5.3
(4,240)	1:123:A:SER:HB3	1:108:A:VAL:HG11	10	5.3
(4,240)	1:123:A:SER:HB3	1:108:A:VAL:HG12	10	5.3
(4,240)	1:123:A:SER:HB3	1:108:A:VAL:HG13	10	5.3
(4,240)	1:123:A:SER:HB3	1:108:A:VAL:HG21	10	5.3
(4,240)	1:123:A:SER:HB3	1:108:A:VAL:HG22	10	5.3
(4,240)	1:123:A:SER:HB3	1:108:A:VAL:HG23	10	5.3
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	1	4.92
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	2	4.91
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	2	4.91
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	2	4.91
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	10	4.59
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	10	4.53
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	10	4.53
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	10	4.53
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	10	4.53
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	10	4.53
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	10	4.53
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	10	4.53
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	10	4.53
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	10	4.53
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	5	4.51
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	8	4.5
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	8	4.5
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	8	4.5
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	10	4.49
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	3	4.43
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	2	4.39
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	2	4.21
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	2	4.21
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	2	4.21
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	2	4.21
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	2	4.21
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	2	4.21
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	2	4.21
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	2	4.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	2	4.21
(1,6)	1:83:A:LEU:H	1:79:A:ASP:O	3	4.17
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	5	4.11
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	7	4.05
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	1	4.05
(2,32)	1:48:A:MET:HG2	1:19:A:PHE:HB2	8	4.04
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	5	3.96
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	8	3.96
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	9	3.9
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	8	3.9
(2,212)	1:23:A:PRO:HD3	1:24:A:VAL:HG13	2	3.89
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	1	3.87
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	3	3.86
(2,32)	1:40:A:CYS:HB2	1:153:A:MET:HG2	3	3.85
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	5	3.84
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	2	3.79
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	4	3.77
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	10	3.73
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	8	3.69
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	3	3.68
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	10	3.66
(4,227)	1:11:A:GLN:HG3	1:12:A:GLN:HB3	6	3.63
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	3	3.57
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	10	3.56
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	3	3.53
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	3	3.53
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	3	3.53
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	7	3.49
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	7	3.49
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	7	3.49
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	6	3.49
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	6	3.49
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	6	3.49
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	2	3.4
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	2	3.37
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	2	3.37
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	2	3.37
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	9	3.35
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	9	3.35
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	9	3.35
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	9	3.35
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	9	3.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	9	3.35
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	9	3.35
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	9	3.35
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	9	3.35
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	8	3.35
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	8	3.35
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	8	3.35
(2,212)	1:24:A:VAL:HG13	1:26:A:ILE:HA	9	3.35
(2,191)	1:57:A:ARG:H	1:163:A:LEU:HD13	6	3.33
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	4	3.31
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	4	3.31
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	4	3.31
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	5	3.3
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	5	3.3
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	5	3.3
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	6	3.3
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	6	3.3
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	6	3.3
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	6	3.3
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	6	3.3
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	6	3.3
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	6	3.3
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	6	3.3
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	6	3.3
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	6	3.3
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	6	3.3
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	6	3.3
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	6	3.3
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	6	3.3
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	6	3.3
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	6	3.3
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	6	3.3
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	6	3.3
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	1	3.26
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	1	3.26
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	1	3.26
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	9	3.1
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	6	3.09
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	6	3.09
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	6	3.09
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	1	3.09
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	1	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	1	3.09
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	6	3.03
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	9	2.98
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	5	2.97
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	5	2.97
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	5	2.97
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	5	2.97
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	5	2.97
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	5	2.97
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	5	2.97
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	5	2.97
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	5	2.97
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	5	2.97
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	5	2.97
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	5	2.97
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	5	2.97
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	5	2.97
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	5	2.97
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	5	2.97
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	5	2.97
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	5	2.97
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	3	2.95
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	3	2.95
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	3	2.95
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	2	2.94
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	4	2.92
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	4	2.92
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	4	2.92
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	2	2.92
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	2	2.92
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	2	2.92
(2,139)	1:154:A:ILE:HG22	1:18:A:ILE:HG12	1	2.91
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	9	2.9
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	9	2.9
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	9	2.9
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	10	2.9
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	10	2.9
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	10	2.9
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	3	2.88
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	3	2.88
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	3	2.88
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	3	2.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	3	2.88
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	3	2.88
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	3	2.88
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	3	2.88
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	3	2.88
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	2	2.88
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	3	2.83
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	3	2.83
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	3	2.83
(4,756)	1:98:A:ALA:HB1	1:93:A:CYS:HB2	5	2.8
(4,756)	1:98:A:ALA:HB2	1:93:A:CYS:HB2	5	2.8
(4,756)	1:98:A:ALA:HB3	1:93:A:CYS:HB2	5	2.8
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	8	2.8
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	8	2.8
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	8	2.8
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	8	2.8
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	8	2.8
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	8	2.8
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	1	2.79
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	1	2.79
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	1	2.79
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	4	2.78
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	4	2.78
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	4	2.78
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	5	2.78
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	5	2.78
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	5	2.78
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	7	2.76
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	7	2.76
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	7	2.76
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	6	2.75
(2,139)	1:154:A:ILE:HG22	1:18:A:ILE:HG12	7	2.74
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	8	2.72
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	7	2.7
(4,51)	1:114:A:ILE:HD11	1:115:A:ASP:HB3	7	2.7
(4,51)	1:114:A:ILE:HD12	1:115:A:ASP:HB3	7	2.7
(4,51)	1:114:A:ILE:HD13	1:115:A:ASP:HB3	7	2.7
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	2	2.67
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	2	2.67
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	2	2.67
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	2	2.67
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	2	2.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	2	2.67
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	2	2.67
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	2	2.67
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	2	2.67
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	2	2.67
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	2	2.67
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	2	2.67
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	2	2.67
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	2	2.67
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	2	2.67
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	2	2.67
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	2	2.67
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	2	2.67
(2,212)	1:24:A:VAL:HG13	1:26:A:ILE:HA	3	2.65
(2,212)	1:24:A:VAL:HG13	1:26:A:ILE:HA	10	2.65
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	6	2.64
(2,212)	1:24:A:VAL:HG12	1:26:A:ILE:HA	5	2.64
(2,139)	1:154:A:ILE:HG21	1:18:A:ILE:HG12	9	2.64
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	10	2.61
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	10	2.61
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	10	2.61
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	6	2.6
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	6	2.6
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	6	2.6
(4,44)	1:83:A:LEU:HG	1:77:A:ALA:HA	9	2.6
(4,457)	1:150:A:THR:HG21	1:145:A:GLN:HA	9	2.58
(4,457)	1:150:A:THR:HG22	1:145:A:GLN:HA	9	2.58
(4,457)	1:150:A:THR:HG23	1:145:A:GLN:HA	9	2.58
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	4	2.57
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	5	2.54
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	5	2.54
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	5	2.54
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	9	2.53
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	9	2.53
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	9	2.53
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	9	2.53
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	9	2.53
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	9	2.53
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	9	2.53
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	9	2.53
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	9	2.53
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	9	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	9	2.53
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	9	2.53
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	9	2.53
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	9	2.53
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	9	2.53
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	9	2.53
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	9	2.53
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	9	2.53
(2,191)	1:57:A:ARG:H	1:163:A:LEU:HD13	9	2.53
(2,139)	1:154:A:ILE:HG22	1:18:A:ILE:HG12	2	2.53
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	1	2.53
(1,7)	1:84:A:VAL:H	1:80:A:LEU:O	3	2.5
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	10	2.49
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	10	2.49
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	10	2.49
(2,212)	1:24:A:VAL:HG11	1:26:A:ILE:HA	7	2.47
(2,212)	1:24:A:VAL:HG13	1:26:A:ILE:HA	6	2.46
(2,139)	1:154:A:ILE:HG21	1:18:A:ILE:HG12	5	2.46
(2,139)	1:154:A:ILE:HG22	1:18:A:ILE:HG12	6	2.46
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	3	2.44
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	3	2.44
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	3	2.44
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	10	2.44
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	10	2.44
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	10	2.44
(2,32)	1:40:A:CYS:HB3	1:153:A:MET:HG2	9	2.44
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	7	2.43
(2,212)	1:24:A:VAL:HG13	1:26:A:ILE:HA	8	2.43
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	7	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	7	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	7	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	7	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	7	2.41
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	7	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	7	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	7	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	7	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	7	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	7	2.41
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	7	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	7	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	7	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	7	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	7	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	7	2.41
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	7	2.41
(2,212)	1:24:A:VAL:HG12	1:26:A:ILE:HA	4	2.4
(2,139)	1:154:A:ILE:HG23	1:18:A:ILE:HG12	10	2.4
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	10	2.39
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	10	2.39
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	10	2.39
(1,33)	1:74:A:HIS:H	1:70:A:SER:O	8	2.38
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	1	2.37
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	1	2.37
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	1	2.37
(4,81)	1:39:A:LEU:HD21	1:20:A:HIS:HB3	5	2.35
(4,81)	1:39:A:LEU:HD22	1:20:A:HIS:HB3	5	2.35
(4,81)	1:39:A:LEU:HD23	1:20:A:HIS:HB3	5	2.35
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	9	2.35
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	3	2.35
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	3	2.35
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	3	2.35
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	3	2.35
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	3	2.35
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	3	2.35
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	3	2.35
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	3	2.35
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	3	2.35
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	3	2.35
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	3	2.35
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	3	2.35
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	3	2.35
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	3	2.35
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	3	2.35
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	3	2.35
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	3	2.35
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	3	2.35
(2,139)	1:154:A:ILE:HG22	1:18:A:ILE:HG12	3	2.28
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	8	2.26
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	8	2.26
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	8	2.26
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	5	2.24
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	5	2.24
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	5	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	10	2.24
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	10	2.24
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	10	2.24
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD11	10	2.23
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD12	10	2.23
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD13	10	2.23
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD11	10	2.23
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD12	10	2.23
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD13	10	2.23
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD11	10	2.23
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD12	10	2.23
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD13	10	2.23
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	9	2.23
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	9	2.23
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	9	2.23
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	5	2.23
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	5	2.23
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	5	2.23
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	7	2.21
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	7	2.21
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	7	2.21
(2,316)	1:150:A:THR:HG23	1:144:A:MET:HB3	8	2.19
(2,139)	1:142:A:VAL:HG21	1:154:A:ILE:HG21	8	2.19
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	3	2.16
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	3	2.16
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	3	2.16
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	6	2.16
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	4	2.16
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	4	2.16
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	4	2.16
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	4	2.16
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	4	2.16
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	4	2.16
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	4	2.16
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	4	2.16
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	4	2.16
(2,316)	1:150:A:THR:HG21	1:144:A:MET:HB3	1	2.16
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	2	2.15
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	2	2.15
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	2	2.15
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	4	2.15
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	5	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	5	2.15
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	5	2.15
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	6	2.14
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	6	2.14
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	6	2.14
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	5	2.13
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	5	2.13
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	5	2.13
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	6	2.13
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	6	2.13
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	6	2.13
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	6	2.13
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	6	2.13
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	6	2.13
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	6	2.13
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	6	2.13
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	6	2.13
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	2	2.12
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	2	2.12
(2,204)	1:90:A:LEU:H	1:86:A:ARG:HD3	3	2.12
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	10	2.11
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	9	2.11
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	9	2.11
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	9	2.11
(2,204)	1:90:A:LEU:H	1:86:A:ARG:HD3	4	2.11
(4,35)	1:142:A:VAL:HG21	1:153:A:MET:HG3	3	2.1
(4,35)	1:142:A:VAL:HG22	1:153:A:MET:HG3	3	2.1
(4,35)	1:142:A:VAL:HG23	1:153:A:MET:HG3	3	2.1
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	9	2.1
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD21	4	2.09
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD22	4	2.09
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD23	4	2.09
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD21	4	2.09
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD22	4	2.09
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD23	4	2.09
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD21	4	2.09
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD22	4	2.09
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD23	4	2.09
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	9	2.09
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	10	2.09
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	10	2.09
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	10	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,316)	1:150:A:THR:HG23	1:144:A:MET:HB3	5	2.09
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG11	9	2.08
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG12	9	2.08
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG13	9	2.08
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG11	9	2.08
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG12	9	2.08
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG13	9	2.08
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG11	9	2.08
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG12	9	2.08
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG13	9	2.08
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	10	2.08
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	10	2.08
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	10	2.08
(2,204)	1:86:A:ARG:HD3	1:89:A:GLN:H	2	2.08
(2,204)	1:86:A:ARG:HD3	1:89:A:GLN:H	8	2.08
(2,204)	1:90:A:LEU:H	1:86:A:ARG:HD3	10	2.08
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	9	2.07
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	9	2.07
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	9	2.07
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	9	2.07
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	9	2.07
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	9	2.07
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	9	2.07
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	9	2.07
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	9	2.07
(2,204)	1:90:A:LEU:H	1:86:A:ARG:HD3	9	2.07
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	4	2.07
(1,5)	1:80:A:LEU:H	1:76:A:ARG:O	3	2.07
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	4	2.06
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	4	2.06
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	4	2.06
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	5	2.06
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	5	2.06
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	5	2.06
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	5	2.06
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	5	2.06
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	5	2.06
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	5	2.06
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	5	2.06
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	5	2.06
(2,204)	1:90:A:LEU:H	1:86:A:ARG:HD3	1	2.06
(2,204)	1:90:A:LEU:H	1:86:A:ARG:HD3	6	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,681)	1:84:A:VAL:HG11	1:85:A:GLU:HA	2	2.05
(4,681)	1:84:A:VAL:HG12	1:85:A:GLU:HA	2	2.05
(4,681)	1:84:A:VAL:HG13	1:85:A:GLU:HA	2	2.05
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE3	8	2.05
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	5	2.03
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	5	2.03
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	5	2.03
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	8	2.03
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	8	2.03
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	8	2.03
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	4	2.0
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	4	2.0
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	4	2.0
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	4	2.0
(4,277)	1:163:A:LEU:HD21	1:29:A:ILE:HG13	6	1.99
(4,277)	1:163:A:LEU:HD22	1:29:A:ILE:HG13	6	1.99
(4,277)	1:163:A:LEU:HD23	1:29:A:ILE:HG13	6	1.99
(4,756)	1:98:A:ALA:HB1	1:93:A:CYS:HB2	7	1.98
(4,756)	1:98:A:ALA:HB2	1:93:A:CYS:HB2	7	1.98
(4,756)	1:98:A:ALA:HB3	1:93:A:CYS:HB2	7	1.98
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	5	1.98
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	5	1.98
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	5	1.98
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	4	1.98
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	4	1.98
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	4	1.98
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD11	9	1.97
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD12	9	1.97
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD13	9	1.97
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD11	9	1.97
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD12	9	1.97
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD13	9	1.97
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD11	9	1.97
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD12	9	1.97
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD13	9	1.97
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	2	1.97
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	2	1.97
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	2	1.97
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	1	1.97
(2,32)	1:40:A:CYS:HB3	1:153:A:MET:HG2	2	1.97
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	4	1.96
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	2	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	2	1.96
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	2	1.96
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	1	1.96
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	1	1.96
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	1	1.96
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	1	1.96
(4,3)	1:163:A:LEU:HD11	1:162:A:GLU:HB3	6	1.96
(4,3)	1:163:A:LEU:HD12	1:162:A:GLU:HB3	6	1.96
(4,3)	1:163:A:LEU:HD13	1:162:A:GLU:HB3	6	1.96
(4,248)	1:55:A:THR:HG21	1:166:A:VAL:HG21	5	1.95
(4,248)	1:55:A:THR:HG21	1:166:A:VAL:HG22	5	1.95
(4,248)	1:55:A:THR:HG21	1:166:A:VAL:HG23	5	1.95
(4,248)	1:55:A:THR:HG22	1:166:A:VAL:HG21	5	1.95
(4,248)	1:55:A:THR:HG22	1:166:A:VAL:HG22	5	1.95
(4,248)	1:55:A:THR:HG22	1:166:A:VAL:HG23	5	1.95
(4,248)	1:55:A:THR:HG23	1:166:A:VAL:HG21	5	1.95
(4,248)	1:55:A:THR:HG23	1:166:A:VAL:HG22	5	1.95
(4,248)	1:55:A:THR:HG23	1:166:A:VAL:HG23	5	1.95
(4,78)	1:74:A:HIS:HB3	1:137:A:LEU:HG	6	1.95
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG2	6	1.94
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG3	6	1.94
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	9	1.93
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	9	1.93
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	7	1.92
(1,34)	1:19:A:PHE:H	1:42:A:ALA:O	10	1.92
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	5	1.91
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	5	1.91
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	5	1.91
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	5	1.91
(2,207)	1:161:A:ALA:HB2	1:159:A:HIS:HB3	1	1.91
(2,32)	1:40:A:CYS:HB3	1:153:A:MET:HG2	5	1.91
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	3	1.91
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	7	1.9
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD21	9	1.9
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD22	9	1.9
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD23	9	1.9
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	3	1.89
(2,204)	1:86:A:ARG:HD3	1:89:A:GLN:H	5	1.89
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	10	1.88
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	10	1.88
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	10	1.88
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	10	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	10	1.88
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	10	1.88
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	10	1.87
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	10	1.87
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	10	1.87
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB1	3	1.87
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB2	3	1.87
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB3	3	1.87
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB1	3	1.87
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB2	3	1.87
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB3	3	1.87
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB1	3	1.87
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB2	3	1.87
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB3	3	1.87
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	10	1.87
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	4	1.87
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	4	1.87
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	4	1.87
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	4	1.87
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	4	1.87
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	4	1.87
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	4	1.87
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	4	1.87
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	4	1.87
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	4	1.87
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	4	1.87
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	4	1.87
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	4	1.87
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	4	1.87
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	4	1.87
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	4	1.87
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	4	1.87
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	4	1.87
(2,204)	1:86:A:ARG:HD3	1:89:A:GLN:H	7	1.87
(4,3)	1:163:A:LEU:HD11	1:162:A:GLU:HB3	9	1.86
(4,3)	1:163:A:LEU:HD12	1:162:A:GLU:HB3	9	1.86
(4,3)	1:163:A:LEU:HD13	1:162:A:GLU:HB3	9	1.86
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	3	1.86
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	3	1.86
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	3	1.86
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	3	1.86
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	3	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	3	1.86
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	1	1.85
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	1	1.85
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	1	1.85
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	5	1.85
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	5	1.85
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	5	1.85
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	2	1.85
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	2	1.85
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	2	1.85
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	2	1.85
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	2	1.85
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	2	1.85
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	2	1.85
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	2	1.85
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	2	1.85
(1,34)	1:19:A:PHE:H	1:42:A:ALA:O	2	1.84
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	7	1.83
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	9	1.83
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	9	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	2	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	2	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	2	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	8	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	8	1.83
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	8	1.83
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	2	1.82
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	2	1.82
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	2	1.82
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	10	1.82
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE3	1	1.82
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	2	1.81
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	5	1.81
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	2	1.81
(2,216)	1:113:A:ASP:HB2	1:114:A:ILE:HG12	5	1.81
(2,32)	1:40:A:CYS:HB3	1:153:A:MET:HG2	6	1.81
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	1	1.8
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	1	1.8
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	1	1.8
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	1	1.8
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	1	1.8
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	1	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	1	1.79
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	1	1.79
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	1	1.79
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	4	1.79
(2,216)	1:113:A:ASP:HB2	1:114:A:ILE:HG12	1	1.79
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	2	1.79
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	5	1.79
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	4	1.78
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	6	1.78
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	2	1.78
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	2	1.78
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	2	1.78
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	10	1.78
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	7	1.78
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	7	1.77
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	7	1.77
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	7	1.77
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	1	1.76
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	1	1.76
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	4	1.76
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	2	1.76
(2,216)	1:113:A:ASP:HB2	1:114:A:ILE:HG12	8	1.76
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	9	1.75
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	4	1.75
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	4	1.75
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	7	1.75
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	4	1.75
(1,47)	1:146:A:ASP:H	1:149:A:GLY:O	6	1.75
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG11	5	1.74
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG12	5	1.74
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG13	5	1.74
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG11	5	1.74
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG12	5	1.74
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG13	5	1.74
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	1	1.74
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	7	1.74
(2,139)	1:154:A:ILE:HG23	1:18:A:ILE:HG12	4	1.74
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE2	3	1.74
(1,1)	1:69:A:GLY:H	1:65:A:ILE:O	6	1.74
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	1	1.72
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	10	1.71
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	7	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	1	1.7
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	1	1.7
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	1	1.7
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	1	1.7
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	1	1.7
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	1	1.7
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	1	1.7
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	1	1.7
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	1	1.7
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	9	1.7
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	2	1.7
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	2	1.7
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	5	1.7
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	3	1.69
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	3	1.69
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	8	1.69
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	4	1.69
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	4	1.69
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	4	1.69
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	10	1.69
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	10	1.69
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	10	1.69
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	10	1.69
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	10	1.69
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	10	1.69
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	10	1.69
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	10	1.69
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	10	1.69
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	10	1.69
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	10	1.69
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	10	1.69
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	10	1.69
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	10	1.69
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	10	1.69
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	10	1.69
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	10	1.69
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	10	1.69
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	4	1.66
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	4	1.66
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	7	1.65
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	7	1.65
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	7	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB2	7	1.65
(2,32)	1:40:A:CYS:HB3	1:153:A:MET:HG2	4	1.65
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	4	1.64
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	9	1.63
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	9	1.63
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	9	1.63
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	7	1.63
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	5	1.63
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	5	1.63
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	5	1.63
(4,49)	1:90:A:LEU:HA	1:90:A:LEU:HD21	10	1.63
(4,49)	1:90:A:LEU:HA	1:90:A:LEU:HD22	10	1.63
(4,49)	1:90:A:LEU:HA	1:90:A:LEU:HD23	10	1.63
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	6	1.63
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	6	1.62
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	6	1.62
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	6	1.62
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE1	5	1.62
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE2	5	1.62
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE3	5	1.62
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	2	1.62
(4,246)	1:163:A:LEU:HD11	1:56:A:TYR:HB2	6	1.62
(4,246)	1:163:A:LEU:HD12	1:56:A:TYR:HB2	6	1.62
(4,246)	1:163:A:LEU:HD13	1:56:A:TYR:HB2	6	1.62
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	1	1.62
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	1	1.62
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB3	3	1.61
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	7	1.6
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	1	1.6
(4,57)	1:59:A:LYS:HA	1:17:A:GLU:HG2	6	1.6
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	6	1.6
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	6	1.6
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	6	1.6
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	6	1.59
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	8	1.59
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	6	1.59
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	6	1.59
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	6	1.59
(2,107)	1:126:A:ILE:HG23	1:130:A:THR:HG21	3	1.59
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	4	1.59
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG11	7	1.57
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG12	7	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG13	7	1.57
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG11	7	1.57
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG12	7	1.57
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG13	7	1.57
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	9	1.57
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	5	1.56
(4,579)	1:151:A:CYS:HB2	1:144:A:MET:HB3	2	1.55
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	9	1.55
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	9	1.55
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	9	1.55
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	6	1.54
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	1	1.54
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	1	1.54
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	1	1.54
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	2	1.53
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	3	1.53
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	3	1.53
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	3	1.53
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	4	1.53
(4,47)	1:58:A:ILE:HD11	1:154:A:ILE:HG12	1	1.53
(4,47)	1:58:A:ILE:HD12	1:154:A:ILE:HG12	1	1.53
(4,47)	1:58:A:ILE:HD13	1:154:A:ILE:HG12	1	1.53
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	9	1.53
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	9	1.53
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	9	1.53
(4,656)	1:59:A:LYS:HG3	1:17:A:GLU:HG2	6	1.52
(4,90)	1:153:A:MET:HE1	1:127:A:GLN:HG3	4	1.52
(4,90)	1:153:A:MET:HE2	1:127:A:GLN:HG3	4	1.52
(4,90)	1:153:A:MET:HE3	1:127:A:GLN:HG3	4	1.52
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD11	10	1.51
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD12	10	1.51
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD13	10	1.51
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	3	1.51
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	7	1.51
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	7	1.51
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	8	1.5
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	2	1.5
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	2	1.5
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	2	1.5
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	3	1.5
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	3	1.5
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	3	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	4	1.5
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	4	1.5
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	4	1.5
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	1	1.49
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	1	1.49
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	1	1.49
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	4	1.49
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	7	1.49
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	7	1.49
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	7	1.49
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	10	1.49
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	9	1.49
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	9	1.49
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	9	1.49
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	10	1.49
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	10	1.49
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	4	1.49
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	4	1.49
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	4	1.49
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG23	5	1.49
(2,277)	1:58:A:ILE:HG23	1:163:A:LEU:HG	4	1.49
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	6	1.48
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	6	1.48
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	10	1.48
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	10	1.48
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	10	1.48
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	4	1.48
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	2	1.48
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	8	1.48
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD21	3	1.47
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD22	3	1.47
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD23	3	1.47
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	8	1.47
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	4	1.47
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	4	1.47
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	3	1.47
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	3	1.47
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	3	1.47
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	6	1.47
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	6	1.47
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	6	1.47
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	1	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	1	1.47
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	1	1.47
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	10	1.47
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	9	1.46
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	10	1.46
(4,94)	1:116:A:ALA:HB1	1:111:A:LEU:HB3	6	1.46
(4,94)	1:116:A:ALA:HB2	1:111:A:LEU:HB3	6	1.46
(4,94)	1:116:A:ALA:HB3	1:111:A:LEU:HB3	6	1.46
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	7	1.46
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	7	1.46
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	7	1.46
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	10	1.46
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	10	1.46
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	10	1.46
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	3	1.46
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	3	1.46
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	3	1.46
(2,216)	1:113:A:ASP:HB2	1:114:A:ILE:HG12	4	1.46
(2,93)	1:146:A:ASP:HB3	1:42:A:ALA:HB3	8	1.46
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	1	1.45
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	4	1.45
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	4	1.45
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	4	1.45
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	6	1.45
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	6	1.45
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	6	1.45
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	8	1.45
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	8	1.45
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	8	1.45
(4,577)	1:54:A:VAL:HG21	1:22:A:SER:HB3	8	1.44
(4,577)	1:54:A:VAL:HG22	1:22:A:SER:HB3	8	1.44
(4,577)	1:54:A:VAL:HG23	1:22:A:SER:HB3	8	1.44
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	9	1.44
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	9	1.44
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	9	1.44
(4,21)	1:114:A:ILE:HD11	1:115:A:ASP:HA	2	1.44
(4,21)	1:114:A:ILE:HD12	1:115:A:ASP:HA	2	1.44
(4,21)	1:114:A:ILE:HD13	1:115:A:ASP:HA	2	1.44
(1,34)	1:19:A:PHE:H	1:42:A:ALA:O	8	1.44
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	6	1.43
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	6	1.43
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	6	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	3	1.43
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	3	1.43
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	3	1.43
(2,277)	1:58:A:ILE:HG23	1:163:A:LEU:HG	5	1.43
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	8	1.42
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	8	1.42
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	8	1.42
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	3	1.42
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	3	1.42
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	3	1.42
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	3	1.42
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	3	1.42
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	3	1.42
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	3	1.42
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	1	1.42
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	1	1.42
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	1	1.42
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	1	1.42
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	1	1.42
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	8	1.42
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	8	1.42
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	8	1.42
(4,94)	1:116:A:ALA:HB1	1:111:A:LEU:HB3	2	1.41
(4,94)	1:116:A:ALA:HB2	1:111:A:LEU:HB3	2	1.41
(4,94)	1:116:A:ALA:HB3	1:111:A:LEU:HB3	2	1.41
(4,47)	1:58:A:ILE:HD11	1:154:A:ILE:HG12	7	1.41
(4,47)	1:58:A:ILE:HD12	1:154:A:ILE:HG12	7	1.41
(4,47)	1:58:A:ILE:HD13	1:154:A:ILE:HG12	7	1.41
(2,277)	1:58:A:ILE:HG23	1:163:A:LEU:HG	3	1.41
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	1	1.4
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	1	1.4
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	1	1.4
(4,577)	1:54:A:VAL:HG21	1:22:A:SER:HB3	5	1.4
(4,577)	1:54:A:VAL:HG22	1:22:A:SER:HB3	5	1.4
(4,577)	1:54:A:VAL:HG23	1:22:A:SER:HB3	5	1.4
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	10	1.4
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	6	1.39
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	6	1.39
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	6	1.39
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	3	1.39
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD11	1	1.39
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD12	1	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD13	1	1.39
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD21	1	1.39
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD22	1	1.39
(2,257)	1:163:A:LEU:HD21	1:157:A:LEU:HD23	1	1.39
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD11	1	1.39
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD12	1	1.39
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD13	1	1.39
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD21	1	1.39
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD22	1	1.39
(2,257)	1:163:A:LEU:HD22	1:157:A:LEU:HD23	1	1.39
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD11	1	1.39
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD12	1	1.39
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD13	1	1.39
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD21	1	1.39
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD22	1	1.39
(2,257)	1:163:A:LEU:HD23	1:157:A:LEU:HD23	1	1.39
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	7	1.38
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	7	1.38
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	7	1.38
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	7	1.38
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	7	1.38
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	7	1.38
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	7	1.38
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	7	1.38
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	7	1.38
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	10	1.38
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	10	1.38
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	10	1.38
(4,95)	1:155:A:ASP:HB2	1:140:A:ARG:HA	5	1.38
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	6	1.38
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	6	1.38
(2,277)	1:58:A:ILE:HG21	1:163:A:LEU:HG	8	1.38
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	6	1.37
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	6	1.37
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	6	1.37
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	6	1.37
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	6	1.37
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	6	1.37
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	6	1.37
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	6	1.37
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	6	1.37
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	10	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	4	1.37
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	4	1.37
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	4	1.37
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	4	1.37
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	4	1.37
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	4	1.37
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	4	1.37
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	4	1.37
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	4	1.37
(4,656)	1:59:A:LYS:HG3	1:17:A:GLU:HG2	8	1.37
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	3	1.37
(4,268)	1:166:A:VAL:HG21	1:55:A:THR:HB	5	1.37
(4,268)	1:166:A:VAL:HG22	1:55:A:THR:HB	5	1.37
(4,268)	1:166:A:VAL:HG23	1:55:A:THR:HB	5	1.37
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	8	1.37
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	8	1.37
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	8	1.37
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	2	1.37
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	2	1.37
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	2	1.37
(2,161)	1:53:A:HIS:HB2	1:54:A:VAL:HG23	1	1.37
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD21	9	1.36
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD22	9	1.36
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD23	9	1.36
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD21	9	1.36
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD22	9	1.36
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD23	9	1.36
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD21	9	1.36
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD22	9	1.36
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD23	9	1.36
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	5	1.36
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	5	1.36
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	5	1.36
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	5	1.36
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	5	1.36
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	5	1.36
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	5	1.36
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	5	1.36
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	5	1.36
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	5	1.36
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	5	1.36
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	5	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	3	1.36
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG2	1	1.36
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG3	1	1.36
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	4	1.35
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	4	1.35
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	4	1.35
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	4	1.35
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	4	1.35
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	4	1.35
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	4	1.35
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	4	1.35
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	4	1.35
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE1	2	1.35
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE2	2	1.35
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE3	2	1.35
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	9	1.35
(4,57)	1:59:A:LYS:HA	1:17:A:GLU:HG2	10	1.35
(4,33)	1:39:A:LEU:HD11	1:156:A:MET:HB3	5	1.35
(4,33)	1:39:A:LEU:HD12	1:156:A:MET:HB3	5	1.35
(4,33)	1:39:A:LEU:HD13	1:156:A:MET:HB3	5	1.35
(2,277)	1:58:A:ILE:HG23	1:163:A:LEU:HG	7	1.35
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	7	1.35
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	7	1.35
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	7	1.35
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	7	1.35
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	7	1.35
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	7	1.35
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	3	1.34
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD11	3	1.34
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD12	3	1.34
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD13	3	1.34
(4,577)	1:54:A:VAL:HG21	1:22:A:SER:HB3	4	1.34
(4,577)	1:54:A:VAL:HG22	1:22:A:SER:HB3	4	1.34
(4,577)	1:54:A:VAL:HG23	1:22:A:SER:HB3	4	1.34
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	8	1.34
(4,94)	1:116:A:ALA:HB1	1:111:A:LEU:HB3	9	1.34
(4,94)	1:116:A:ALA:HB2	1:111:A:LEU:HB3	9	1.34
(4,94)	1:116:A:ALA:HB3	1:111:A:LEU:HB3	9	1.34
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG22	7	1.34
(2,161)	1:53:A:HIS:HB2	1:54:A:VAL:HG22	9	1.34
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	3	1.33
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	3	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	3	1.33
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE1	10	1.33
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE2	10	1.33
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE3	10	1.33
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	7	1.33
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	7	1.33
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	7	1.33
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	10	1.32
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	10	1.32
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	10	1.32
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	10	1.32
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	7	1.32
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	5	1.32
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	5	1.32
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	5	1.32
(4,90)	1:153:A:MET:HE1	1:127:A:GLN:HG3	7	1.32
(4,90)	1:153:A:MET:HE2	1:127:A:GLN:HG3	7	1.32
(4,90)	1:153:A:MET:HE3	1:127:A:GLN:HG3	7	1.32
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	5	1.32
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	5	1.32
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	5	1.32
(2,170)	1:142:A:VAL:HG21	1:144:A:MET:HG3	3	1.32
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	10	1.32
(2,93)	1:42:A:ALA:HB2	1:151:A:CYS:HB3	2	1.32
(4,748)	1:60:A:VAL:HG11	1:61:A:ASP:HB3	8	1.31
(4,748)	1:60:A:VAL:HG12	1:61:A:ASP:HB3	8	1.31
(4,748)	1:60:A:VAL:HG13	1:61:A:ASP:HB3	8	1.31
(4,426)	1:24:A:VAL:HG21	1:25:A:GLU:HG2	1	1.31
(4,426)	1:24:A:VAL:HG22	1:25:A:GLU:HG2	1	1.31
(4,426)	1:24:A:VAL:HG23	1:25:A:GLU:HG2	1	1.31
(4,246)	1:163:A:LEU:HD11	1:56:A:TYR:HB2	9	1.31
(4,246)	1:163:A:LEU:HD12	1:56:A:TYR:HB2	9	1.31
(4,246)	1:163:A:LEU:HD13	1:56:A:TYR:HB2	9	1.31
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	5	1.31
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	5	1.31
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	10	1.31
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	10	1.31
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	10	1.31
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG2	10	1.31
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG3	10	1.31
(2,107)	1:126:A:ILE:HG22	1:130:A:THR:HG21	10	1.31
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	3	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,90)	1:153:A:MET:HE1	1:127:A:GLN:HG3	8	1.3
(4,90)	1:153:A:MET:HE2	1:127:A:GLN:HG3	8	1.3
(4,90)	1:153:A:MET:HE3	1:127:A:GLN:HG3	8	1.3
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	2	1.3
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG22	8	1.3
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	7	1.3
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE1	6	1.29
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE2	6	1.29
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE3	6	1.29
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	9	1.29
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	9	1.29
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	9	1.29
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	7	1.29
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	7	1.29
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	7	1.29
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	2	1.28
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	2	1.28
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	2	1.28
(4,90)	1:153:A:MET:HE1	1:127:A:GLN:HG3	6	1.28
(4,90)	1:153:A:MET:HE2	1:127:A:GLN:HG3	6	1.28
(4,90)	1:153:A:MET:HE3	1:127:A:GLN:HG3	6	1.28
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	1	1.28
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	1	1.28
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	1	1.28
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	6	1.28
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	8	1.27
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	8	1.27
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	8	1.27
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	8	1.27
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	8	1.27
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	8	1.27
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	8	1.27
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	8	1.27
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	8	1.27
(4,85)	1:164:A:VAL:HG21	1:57:A:ARG:HB2	10	1.27
(4,85)	1:164:A:VAL:HG22	1:57:A:ARG:HB2	10	1.27
(4,85)	1:164:A:VAL:HG23	1:57:A:ARG:HB2	10	1.27
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	5	1.27
(2,254)	1:152:A:TYR:H	1:43:A:ALA:HB3	1	1.27
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	4	1.26
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	4	1.26
(4,283)	1:62:A:GLU:HA	1:64:A:ASP:H	7	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,249)	1:100:A:GLU:HG3	1:97:A:THR:HA	4	1.26
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	3	1.25
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	3	1.25
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	3	1.25
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	3	1.25
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	3	1.25
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	3	1.25
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	3	1.25
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	3	1.25
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	3	1.25
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD21	5	1.25
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD22	5	1.25
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD23	5	1.25
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	2	1.25
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	7	1.25
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	7	1.25
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	7	1.25
(2,277)	1:58:A:ILE:HG22	1:163:A:LEU:HG	1	1.25
(4,776)	1:16:A:MET:HG3	1:16:A:MET:H	9	1.24
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	9	1.24
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	9	1.24
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	9	1.24
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	5	1.24
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	3	1.24
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	3	1.24
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	3	1.24
(4,210)	1:12:A:GLN:HA	1:13:A:MET:HG2	6	1.24
(4,210)	1:12:A:GLN:HA	1:13:A:MET:HG2	9	1.24
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	3	1.24
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	3	1.24
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	3	1.24
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	4	1.24
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	4	1.24
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	4	1.24
(4,90)	1:153:A:MET:HE1	1:127:A:GLN:HG3	9	1.24
(4,90)	1:153:A:MET:HE2	1:127:A:GLN:HG3	9	1.24
(4,90)	1:153:A:MET:HE3	1:127:A:GLN:HG3	9	1.24
(2,316)	1:150:A:THR:HG23	1:144:A:MET:HB3	10	1.24
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	10	1.23
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	10	1.23
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	1	1.23
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	1	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,244)	1:100:A:GLU:HA	1:105:A:ARG:HD2	8	1.23
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	7	1.23
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	7	1.23
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	7	1.23
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	8	1.23
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	8	1.23
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	8	1.23
(4,57)	1:59:A:LYS:HA	1:17:A:GLU:HG2	1	1.23
(4,577)	1:54:A:VAL:HG21	1:22:A:SER:HB3	7	1.22
(4,577)	1:54:A:VAL:HG22	1:22:A:SER:HB3	7	1.22
(4,577)	1:54:A:VAL:HG23	1:22:A:SER:HB3	7	1.22
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	8	1.22
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	8	1.22
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	8	1.22
(1,53)	1:154:A:ILE:H	1:39:A:LEU:O	8	1.22
(4,577)	1:54:A:VAL:HG21	1:22:A:SER:HB3	6	1.21
(4,577)	1:54:A:VAL:HG22	1:22:A:SER:HB3	6	1.21
(4,577)	1:54:A:VAL:HG23	1:22:A:SER:HB3	6	1.21
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	7	1.21
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	7	1.21
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	7	1.21
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	4	1.21
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	4	1.21
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	4	1.21
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	2	1.21
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	2	1.21
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG23	1	1.21
(2,137)	1:166:A:VAL:HG22	1:57:A:ARG:HA	5	1.21
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	2	1.2
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	2	1.2
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	2	1.2
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	9	1.2
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	8	1.2
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	8	1.2
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	5	1.2
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	5	1.2
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	5	1.2
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	6	1.2
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	6	1.2
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	6	1.2
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG21	4	1.2
(2,254)	1:152:A:TYR:H	1:43:A:ALA:HB2	7	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:145:A:GLN:H	1:145:A:GLN:HG2	9	1.2
(2,115)	1:145:A:GLN:H	1:145:A:GLN:HG3	9	1.2
(4,649)	1:154:A:ILE:HD11	1:141:A:GLY:HA2	10	1.19
(4,649)	1:154:A:ILE:HD11	1:141:A:GLY:HA3	10	1.19
(4,649)	1:154:A:ILE:HD12	1:141:A:GLY:HA2	10	1.19
(4,649)	1:154:A:ILE:HD12	1:141:A:GLY:HA3	10	1.19
(4,649)	1:154:A:ILE:HD13	1:141:A:GLY:HA2	10	1.19
(4,649)	1:154:A:ILE:HD13	1:141:A:GLY:HA3	10	1.19
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	2	1.19
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	2	1.19
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	2	1.19
(4,210)	1:12:A:GLN:HA	1:13:A:MET:HG2	2	1.19
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	8	1.19
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	5	1.19
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	9	1.18
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	9	1.18
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	9	1.18
(4,649)	1:154:A:ILE:HD11	1:141:A:GLY:HA2	6	1.18
(4,649)	1:154:A:ILE:HD11	1:141:A:GLY:HA3	6	1.18
(4,649)	1:154:A:ILE:HD12	1:141:A:GLY:HA2	6	1.18
(4,649)	1:154:A:ILE:HD12	1:141:A:GLY:HA3	6	1.18
(4,649)	1:154:A:ILE:HD13	1:141:A:GLY:HA2	6	1.18
(4,649)	1:154:A:ILE:HD13	1:141:A:GLY:HA3	6	1.18
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	1	1.18
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	1	1.18
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	1	1.18
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	2	1.18
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	2	1.18
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	2	1.18
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	8	1.18
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	8	1.18
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	8	1.18
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	9	1.18
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	9	1.18
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	8	1.18
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	8	1.18
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG22	3	1.18
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	5	1.17
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	5	1.17
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	5	1.17
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	1	1.17
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	1	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	1	1.17
(4,437)	1:29:A:ILE:HG21	1:156:A:MET:HB3	7	1.17
(4,437)	1:29:A:ILE:HG22	1:156:A:MET:HB3	7	1.17
(4,437)	1:29:A:ILE:HG23	1:156:A:MET:HB3	7	1.17
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	3	1.17
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	3	1.17
(4,90)	1:153:A:MET:HE1	1:127:A:GLN:HG3	5	1.17
(4,90)	1:153:A:MET:HE2	1:127:A:GLN:HG3	5	1.17
(4,90)	1:153:A:MET:HE3	1:127:A:GLN:HG3	5	1.17
(2,170)	1:142:A:VAL:HG23	1:144:A:MET:HG2	8	1.17
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD21	9	1.16
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD22	9	1.16
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD23	9	1.16
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	5	1.16
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	10	1.16
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	10	1.16
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	10	1.16
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	10	1.16
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	10	1.16
(4,323)	1:32:A:GLN:HA	1:32:A:GLN:HG3	9	1.16
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	10	1.16
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	10	1.16
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	10	1.16
(4,177)	1:163:A:LEU:HD11	1:56:A:TYR:HB3	6	1.16
(4,177)	1:163:A:LEU:HD12	1:56:A:TYR:HB3	6	1.16
(4,177)	1:163:A:LEU:HD13	1:56:A:TYR:HB3	6	1.16
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	6	1.16
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	6	1.16
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	6	1.16
(4,81)	1:39:A:LEU:HD21	1:20:A:HIS:HB3	10	1.16
(4,81)	1:39:A:LEU:HD22	1:20:A:HIS:HB3	10	1.16
(4,81)	1:39:A:LEU:HD23	1:20:A:HIS:HB3	10	1.16
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	4	1.16
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	4	1.16
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	4	1.16
(4,35)	1:142:A:VAL:HG21	1:153:A:MET:HG3	9	1.16
(4,35)	1:142:A:VAL:HG22	1:153:A:MET:HG3	9	1.16
(4,35)	1:142:A:VAL:HG23	1:153:A:MET:HG3	9	1.16
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG23	2	1.16
(4,776)	1:16:A:MET:HG3	1:16:A:MET:H	2	1.15
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	9	1.15
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	9	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	9	1.15
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	10	1.15
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	10	1.15
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	10	1.15
(4,426)	1:24:A:VAL:HG21	1:25:A:GLU:HG2	10	1.15
(4,426)	1:24:A:VAL:HG22	1:25:A:GLU:HG2	10	1.15
(4,426)	1:24:A:VAL:HG23	1:25:A:GLU:HG2	10	1.15
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	4	1.15
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	4	1.15
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	4	1.15
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	6	1.15
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	8	1.15
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	8	1.15
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	7	1.15
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	7	1.15
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	7	1.15
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	7	1.15
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	7	1.15
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	7	1.15
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	7	1.15
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	7	1.15
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	7	1.15
(2,277)	1:58:A:ILE:HG22	1:163:A:LEU:HG	10	1.15
(2,237)	1:161:A:ALA:H	1:163:A:LEU:HD21	8	1.15
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	6	1.14
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	6	1.14
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	6	1.14
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	1	1.14
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	4	1.14
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	4	1.14
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	4	1.14
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	10	1.14
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	10	1.14
(2,320)	1:59:A:LYS:HA	1:18:A:ILE:HG13	8	1.14
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	4	1.13
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	4	1.13
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	4	1.13
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	6	1.13
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	6	1.13
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	6	1.13
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	1	1.13
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	10	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	10	1.13
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	10	1.13
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG21	10	1.13
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	6	1.12
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	6	1.12
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	6	1.12
(4,776)	1:16:A:MET:HG3	1:16:A:MET:H	1	1.12
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG11	10	1.12
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG12	10	1.12
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG13	10	1.12
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG11	10	1.12
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG12	10	1.12
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG13	10	1.12
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG11	10	1.12
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG12	10	1.12
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG13	10	1.12
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	9	1.12
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	1	1.12
(4,210)	1:12:A:GLN:HA	1:13:A:MET:HG2	8	1.12
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	7	1.12
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	7	1.12
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	7	1.12
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	7	1.12
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	7	1.12
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	7	1.12
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	3	1.12
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	3	1.12
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	3	1.12
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG23	9	1.12
(2,237)	1:161:A:ALA:H	1:163:A:LEU:HD21	5	1.12
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB2	2	1.12
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	8	1.11
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	8	1.11
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	8	1.11
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	2	1.11
(4,579)	1:151:A:CYS:HB2	1:144:A:MET:HB3	8	1.11
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	5	1.11
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	5	1.11
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	5	1.11
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	5	1.11
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	5	1.11
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	5	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	5	1.11
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	5	1.11
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	5	1.11
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	4	1.11
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	10	1.11
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	2	1.11
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	2	1.11
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	2	1.11
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	3	1.11
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	3	1.11
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	3	1.11
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	1	1.11
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	1	1.11
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	1	1.11
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	2	1.11
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	2	1.11
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	2	1.11
(2,161)	1:53:A:HIS:HB2	1:54:A:VAL:HG22	2	1.11
(4,683)	1:150:A:THR:HG21	1:143:A:SER:HB2	5	1.1
(4,683)	1:150:A:THR:HG22	1:143:A:SER:HB2	5	1.1
(4,683)	1:150:A:THR:HG23	1:143:A:SER:HB2	5	1.1
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	6	1.1
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	2	1.1
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	2	1.1
(4,475)	1:47:A:VAL:HG21	1:48:A:MET:HG2	3	1.1
(4,475)	1:47:A:VAL:HG22	1:48:A:MET:HG2	3	1.1
(4,475)	1:47:A:VAL:HG23	1:48:A:MET:HG2	3	1.1
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	7	1.1
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	7	1.1
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	7	1.1
(4,212)	1:163:A:LEU:HD11	1:163:A:LEU:HA	9	1.1
(4,212)	1:163:A:LEU:HD12	1:163:A:LEU:HA	9	1.1
(4,212)	1:163:A:LEU:HD13	1:163:A:LEU:HA	9	1.1
(4,74)	1:39:A:LEU:HD21	1:156:A:MET:HB2	8	1.1
(4,74)	1:39:A:LEU:HD22	1:156:A:MET:HB2	8	1.1
(4,74)	1:39:A:LEU:HD23	1:156:A:MET:HB2	8	1.1
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	6	1.1
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	6	1.1
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	6	1.1
(2,145)	1:42:A:ALA:HB1	1:46:A:TYR:HB2	5	1.1
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	6	1.09
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	6	1.09
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	7	1.09
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	7	1.09
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	7	1.09
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	1	1.09
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	1	1.09
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	1	1.09
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	1	1.09
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	1	1.09
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	1	1.09
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	2	1.09
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	2	1.09
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	2	1.09
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	10	1.09
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	10	1.09
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	10	1.09
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	1	1.09
(2,277)	1:58:A:ILE:HG22	1:163:A:LEU:HG	2	1.09
(4,653)	1:166:A:VAL:HG21	1:166:A:VAL:H	5	1.08
(4,653)	1:166:A:VAL:HG22	1:166:A:VAL:H	5	1.08
(4,653)	1:166:A:VAL:HG23	1:166:A:VAL:H	5	1.08
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	9	1.08
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	9	1.08
(4,212)	1:163:A:LEU:HD11	1:163:A:LEU:HA	6	1.08
(4,212)	1:163:A:LEU:HD12	1:163:A:LEU:HA	6	1.08
(4,212)	1:163:A:LEU:HD13	1:163:A:LEU:HA	6	1.08
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	10	1.08
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	10	1.08
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	10	1.08
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	6	1.08
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	6	1.08
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	6	1.08
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	2	1.08
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	2	1.08
(2,170)	1:150:A:THR:HG23	1:144:A:MET:HG2	4	1.08
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	9	1.07
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	9	1.07
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	9	1.07
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	3	1.07
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	3	1.07
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	3	1.07
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	1	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	2	1.07
(4,210)	1:12:A:GLN:HA	1:13:A:MET:HG2	1	1.07
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	1	1.07
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	6	1.07
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	6	1.07
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	6	1.07
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	7	1.07
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	7	1.07
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	7	1.07
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	7	1.07
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	7	1.07
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	7	1.07
(4,341)	1:128:A:ALA:HB1	1:35:A:PHE:HB3	5	1.06
(4,341)	1:128:A:ALA:HB2	1:35:A:PHE:HB3	5	1.06
(4,341)	1:128:A:ALA:HB3	1:35:A:PHE:HB3	5	1.06
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	8	1.06
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	8	1.06
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	8	1.06
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	10	1.06
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	10	1.06
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	10	1.06
(2,307)	1:92:A:GLY:H	1:91:A:THR:HG22	6	1.06
(2,254)	1:43:A:ALA:HB1	1:151:A:CYS:H	6	1.06
(2,254)	1:152:A:TYR:H	1:43:A:ALA:HB2	9	1.06
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	2	1.05
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	2	1.05
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	2	1.05
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	6	1.05
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	6	1.05
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	6	1.05
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	1	1.05
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	1	1.05
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	1	1.05
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	1	1.05
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	1	1.05
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	1	1.05
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	1	1.05
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	1	1.05
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	1	1.05
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	7	1.05
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	5	1.05
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	5	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	5	1.05
(4,61)	1:111:A:LEU:HD11	1:110:A:ASN:HB2	9	1.05
(4,61)	1:111:A:LEU:HD12	1:110:A:ASN:HB2	9	1.05
(4,61)	1:111:A:LEU:HD13	1:110:A:ASN:HB2	9	1.05
(2,216)	1:113:A:ASP:HB2	1:114:A:ILE:HG12	9	1.05
(2,210)	1:152:A:TYR:HA	1:154:A:ILE:HD13	1	1.05
(2,105)	1:125:A:GLU:HA	1:34:A:ARG:HG2	9	1.05
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	7	1.04
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	10	1.04
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	10	1.04
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	10	1.04
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	4	1.04
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	4	1.04
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	4	1.04
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD21	10	1.04
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD22	10	1.04
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD23	10	1.04
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD11	4	1.04
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	5	1.03
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	5	1.03
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	5	1.03
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	8	1.03
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	8	1.03
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	8	1.03
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	9	1.03
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	9	1.03
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	9	1.03
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	6	1.03
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	6	1.03
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	5	1.03
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	5	1.03
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	5	1.03
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	7	1.03
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	7	1.03
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	7	1.03
(4,249)	1:100:A:GLU:HG3	1:97:A:THR:HA	1	1.03
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	9	1.03
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	9	1.03
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	9	1.03
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	3	1.03
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	3	1.03
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	3	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD21	3	1.03
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD22	3	1.03
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD23	3	1.03
(2,153)	1:54:A:VAL:HG22	1:23:A:PRO:HA	2	1.03
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	2	1.02
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	2	1.02
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	2	1.02
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	4	1.02
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG21	5	1.01
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG22	5	1.01
(4,782)	1:24:A:VAL:HG11	1:27:A:THR:HG23	5	1.01
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG21	5	1.01
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG22	5	1.01
(4,782)	1:24:A:VAL:HG12	1:27:A:THR:HG23	5	1.01
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG21	5	1.01
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG22	5	1.01
(4,782)	1:24:A:VAL:HG13	1:27:A:THR:HG23	5	1.01
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	7	1.01
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	7	1.01
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	7	1.01
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	4	1.01
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	4	1.01
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	4	1.01
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	4	1.01
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	4	1.01
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	4	1.01
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	3	1.01
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	3	1.01
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	3	1.01
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	8	1.01
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	10	1.01
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	10	1.01
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	10	1.01
(4,74)	1:39:A:LEU:HD21	1:156:A:MET:HB2	4	1.01
(4,74)	1:39:A:LEU:HD22	1:156:A:MET:HB2	4	1.01
(4,74)	1:39:A:LEU:HD23	1:156:A:MET:HB2	4	1.01
(2,153)	1:54:A:VAL:HG23	1:23:A:PRO:HA	10	1.01
(2,107)	1:47:A:VAL:HG12	1:55:A:THR:HG22	5	1.01
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD11	5	1.0
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD12	5	1.0
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD13	5	1.0
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD11	5	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD12	5	1.0
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD13	5	1.0
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD11	5	1.0
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD12	5	1.0
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD13	5	1.0
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	5	1.0
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	10	1.0
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	10	1.0
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	10	1.0
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	3	1.0
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	3	1.0
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	3	1.0
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	2	1.0
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	2	1.0
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	2	1.0
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	2	1.0
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	10	1.0
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	10	1.0
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	10	1.0
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	2	0.99
(4,601)	1:56:A:TYR:HA	1:166:A:VAL:HG21	5	0.99
(4,601)	1:56:A:TYR:HA	1:166:A:VAL:HG22	5	0.99
(4,601)	1:56:A:TYR:HA	1:166:A:VAL:HG23	5	0.99
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	6	0.99
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	6	0.99
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	6	0.99
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	4	0.99
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	4	0.99
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	5	0.99
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	5	0.99
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	5	0.99
(2,254)	1:43:A:ALA:HB2	1:151:A:CYS:H	2	0.99
(4,778)	1:53:A:HIS:HB2	1:23:A:PRO:HA	1	0.98
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	3	0.98
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	3	0.98
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	3	0.98
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	3	0.98
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	5	0.98
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	4	0.98
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	4	0.98
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	4	0.98
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	10	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	10	0.98
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	10	0.98
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	6	0.97
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	6	0.97
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	6	0.97
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	5	0.97
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG21	1	0.97
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG22	1	0.97
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG23	1	0.97
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG21	1	0.97
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG22	1	0.97
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG23	1	0.97
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG21	1	0.97
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG22	1	0.97
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG23	1	0.97
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	4	0.97
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	4	0.97
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	4	0.97
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	7	0.97
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	7	0.97
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	7	0.97
(2,254)	1:43:A:ALA:HB2	1:151:A:CYS:H	8	0.97
(2,170)	1:142:A:VAL:HG21	1:144:A:MET:HG2	7	0.97
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	5	0.96
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	5	0.96
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	5	0.96
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	4	0.96
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	4	0.96
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	4	0.96
(4,579)	1:151:A:CYS:HB2	1:144:A:MET:HB3	9	0.96
(4,386)	1:47:A:VAL:HG21	1:47:A:VAL:H	3	0.96
(4,386)	1:47:A:VAL:HG22	1:47:A:VAL:H	3	0.96
(4,386)	1:47:A:VAL:HG23	1:47:A:VAL:H	3	0.96
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	4	0.96
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	4	0.96
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	4	0.96
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	4	0.96
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	4	0.96
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	4	0.96
(2,254)	1:43:A:ALA:HB1	1:151:A:CYS:H	3	0.96
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD12	8	0.96
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	4	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	10	0.95
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	10	0.95
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	10	0.95
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	3	0.95
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	1	0.95
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	1	0.95
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	1	0.95
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	6	0.95
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	9	0.95
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	9	0.95
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	9	0.95
(4,91)	1:103:A:SER:H	1:100:A:GLU:HB3	9	0.95
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	6	0.95
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	6	0.95
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	6	0.95
(2,191)	1:57:A:ARG:H	1:163:A:LEU:HD11	7	0.95
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	10	0.94
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	1	0.94
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	1	0.94
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	1	0.94
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	2	0.94
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	2	0.94
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	2	0.94
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	2	0.94
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	2	0.94
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	2	0.94
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	2	0.94
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	2	0.94
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	2	0.94
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	7	0.94
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	1	0.94
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	1	0.94
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	1	0.94
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	6	0.94
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	6	0.94
(4,28)	1:166:A:VAL:HG11	1:57:A:ARG:HD2	5	0.94
(4,28)	1:166:A:VAL:HG11	1:57:A:ARG:HD3	5	0.94
(4,28)	1:166:A:VAL:HG12	1:57:A:ARG:HD2	5	0.94
(4,28)	1:166:A:VAL:HG12	1:57:A:ARG:HD3	5	0.94
(4,28)	1:166:A:VAL:HG13	1:57:A:ARG:HD2	5	0.94
(4,28)	1:166:A:VAL:HG13	1:57:A:ARG:HD3	5	0.94
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	10	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	10	0.93
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	10	0.93
(4,602)	1:54:A:VAL:HG11	1:55:A:THR:H	7	0.93
(4,602)	1:54:A:VAL:HG12	1:55:A:THR:H	7	0.93
(4,602)	1:54:A:VAL:HG13	1:55:A:THR:H	7	0.93
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	4	0.93
(4,375)	1:163:A:LEU:HD11	1:156:A:MET:HG2	3	0.93
(4,375)	1:163:A:LEU:HD12	1:156:A:MET:HG2	3	0.93
(4,375)	1:163:A:LEU:HD13	1:156:A:MET:HG2	3	0.93
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	5	0.93
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	1	0.93
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	1	0.93
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	1	0.93
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	1	0.93
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	1	0.93
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	1	0.93
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	4	0.93
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	4	0.93
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	4	0.93
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG2	2	0.93
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG3	2	0.93
(2,191)	1:57:A:ARG:H	1:163:A:LEU:HD13	10	0.93
(2,32)	1:40:A:CYS:HB3	1:153:A:MET:HG2	7	0.93
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	5	0.92
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	1	0.92
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	3	0.92
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	8	0.92
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	1	0.92
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	6	0.92
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	6	0.92
(4,452)	1:57:A:ARG:HB3	1:166:A:VAL:HG11	5	0.92
(4,452)	1:57:A:ARG:HB3	1:166:A:VAL:HG12	5	0.92
(4,452)	1:57:A:ARG:HB3	1:166:A:VAL:HG13	5	0.92
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	2	0.92
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	2	0.92
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	2	0.92
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	8	0.92
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	8	0.92
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	8	0.92
(2,216)	1:113:A:ASP:HB2	1:114:A:ILE:HG12	6	0.92
(2,145)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	8	0.92
(4,695)	1:16:A:MET:HG2	1:16:A:MET:H	9	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,580)	1:115:A:ASP:HB3	1:115:A:ASP:H	5	0.91
(4,457)	1:150:A:THR:HG21	1:145:A:GLN:HA	10	0.91
(4,457)	1:150:A:THR:HG22	1:145:A:GLN:HA	10	0.91
(4,457)	1:150:A:THR:HG23	1:145:A:GLN:HA	10	0.91
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	6	0.91
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	6	0.91
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	6	0.91
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	5	0.91
(4,57)	1:59:A:LYS:HA	1:17:A:GLU:HG2	9	0.91
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	3	0.91
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	3	0.91
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	3	0.91
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	5	0.91
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	5	0.91
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	5	0.91
(2,191)	1:57:A:ARG:H	1:163:A:LEU:HD11	2	0.91
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD13	5	0.91
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG13	2	0.91
(4,484)	1:126:A:ILE:HG21	1:104:A:GLN:HG3	10	0.9
(4,484)	1:126:A:ILE:HG22	1:104:A:GLN:HG3	10	0.9
(4,484)	1:126:A:ILE:HG23	1:104:A:GLN:HG3	10	0.9
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	9	0.9
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	9	0.9
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	9	0.9
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	9	0.9
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	9	0.9
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	9	0.9
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	9	0.9
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	9	0.9
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	9	0.9
(4,3)	1:163:A:LEU:HD11	1:162:A:GLU:HB3	10	0.9
(4,3)	1:163:A:LEU:HD12	1:162:A:GLU:HB3	10	0.9
(4,3)	1:163:A:LEU:HD13	1:162:A:GLU:HB3	10	0.9
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD11	3	0.9
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	2	0.89
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	3	0.89
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	3	0.89
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	3	0.89
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	6	0.89
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	6	0.89
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	6	0.89
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	9	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	9	0.89
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	9	0.89
(2,171)	1:98:A:ALA:HB2	1:102:A:ILE:H	5	0.89
(2,145)	1:42:A:ALA:HB3	1:46:A:TYR:HB2	10	0.89
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	1	0.88
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	1	0.88
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	1	0.88
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	9	0.88
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	9	0.88
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	9	0.88
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	9	0.88
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	9	0.88
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	9	0.88
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	9	0.88
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	9	0.88
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	9	0.88
(4,577)	1:54:A:VAL:HG21	1:22:A:SER:HB3	3	0.88
(4,577)	1:54:A:VAL:HG22	1:22:A:SER:HB3	3	0.88
(4,577)	1:54:A:VAL:HG23	1:22:A:SER:HB3	3	0.88
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	2	0.88
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	2	0.88
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	2	0.88
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	8	0.88
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	7	0.88
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	7	0.88
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	7	0.88
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD11	6	0.88
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD12	6	0.88
(4,107)	1:58:A:ILE:HD11	1:163:A:LEU:HD13	6	0.88
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD11	6	0.88
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD12	6	0.88
(4,107)	1:58:A:ILE:HD12	1:163:A:LEU:HD13	6	0.88
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD11	6	0.88
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD12	6	0.88
(4,107)	1:58:A:ILE:HD13	1:163:A:LEU:HD13	6	0.88
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	3	0.87
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	3	0.87
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	3	0.87
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	9	0.87
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	9	0.87
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	9	0.87
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	1	0.87
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	1	0.87
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	1	0.87
(2,277)	1:58:A:ILE:HG21	1:163:A:LEU:HG	9	0.87
(2,216)	1:160:A:ASP:HB2	1:161:A:ALA:HB1	10	0.87
(2,93)	1:42:A:ALA:HB3	1:151:A:CYS:HB3	7	0.87
(4,386)	1:47:A:VAL:HG21	1:47:A:VAL:H	10	0.86
(4,386)	1:47:A:VAL:HG22	1:47:A:VAL:H	10	0.86
(4,386)	1:47:A:VAL:HG23	1:47:A:VAL:H	10	0.86
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	8	0.86
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	8	0.86
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	8	0.86
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	6	0.86
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	6	0.86
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	6	0.86
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	5	0.86
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	5	0.86
(2,326)	1:143:A:SER:HA	1:144:A:MET:HG2	3	0.86
(2,326)	1:143:A:SER:HA	1:144:A:MET:HG3	3	0.86
(2,254)	1:43:A:ALA:HB3	1:151:A:CYS:H	10	0.86
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	7	0.86
(2,123)	1:58:A:ILE:HG13	1:59:A:LYS:HE3	6	0.86
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	5	0.85
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	5	0.85
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	5	0.85
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	6	0.85
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	6	0.85
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	6	0.85
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	9	0.85
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	8	0.85
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	8	0.85
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	6	0.85
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	6	0.85
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	6	0.85
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	8	0.84
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	8	0.84
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	8	0.84
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	10	0.84
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	10	0.84
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	10	0.84
(4,191)	1:11:A:GLN:HG2	1:12:A:GLN:H	4	0.84
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	1	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	3	0.84
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	3	0.84
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	3	0.84
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	6	0.83
(4,586)	1:166:A:VAL:HG11	1:166:A:VAL:HA	5	0.83
(4,586)	1:166:A:VAL:HG12	1:166:A:VAL:HA	5	0.83
(4,586)	1:166:A:VAL:HG13	1:166:A:VAL:HA	5	0.83
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	3	0.83
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	3	0.83
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	3	0.83
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	5	0.83
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	5	0.83
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	5	0.83
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	8	0.83
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	8	0.83
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	8	0.83
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	7	0.83
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	7	0.83
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	7	0.83
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	2	0.83
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	2	0.83
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	2	0.83
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	5	0.83
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	5	0.83
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	5	0.83
(2,161)	1:54:A:VAL:HG22	1:165:A:ARG:HD2	5	0.83
(2,108)	1:102:A:ILE:HG22	1:133:A:ALA:HB1	5	0.83
(4,646)	1:7:A:MET:HB2	1:8:A:THR:HA	2	0.82
(4,579)	1:151:A:CYS:HB2	1:144:A:MET:HB3	7	0.82
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	5	0.82
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	1	0.82
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	1	0.82
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	1	0.82
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG21	3	0.82
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG22	3	0.82
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG23	3	0.82
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG21	3	0.82
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG22	3	0.82
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG23	3	0.82
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG21	3	0.82
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG22	3	0.82
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG23	3	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	4	0.82
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	4	0.82
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	4	0.82
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	6	0.82
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	6	0.82
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	6	0.82
(4,47)	1:58:A:ILE:HD11	1:154:A:ILE:HG12	6	0.82
(4,47)	1:58:A:ILE:HD12	1:154:A:ILE:HG12	6	0.82
(4,47)	1:58:A:ILE:HD13	1:154:A:ILE:HG12	6	0.82
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	3	0.82
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	3	0.82
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	3	0.82
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	6	0.82
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	6	0.82
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	6	0.82
(2,254)	1:43:A:ALA:HB1	1:151:A:CYS:H	4	0.82
(2,108)	1:102:A:ILE:HG22	1:133:A:ALA:HB1	3	0.82
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	10	0.81
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	10	0.81
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	10	0.81
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	2	0.81
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	3	0.81
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	3	0.81
(2,334)	1:144:A:MET:HG2	1:151:A:CYS:HB3	3	0.81
(2,334)	1:144:A:MET:HG3	1:151:A:CYS:HB3	3	0.81
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB3	3	0.81
(2,153)	1:54:A:VAL:HG23	1:25:A:GLU:HA	9	0.81
(2,145)	1:42:A:ALA:HB2	1:46:A:TYR:HB2	1	0.81
(2,107)	1:47:A:VAL:HG12	1:55:A:THR:HG22	9	0.81
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	2	0.8
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	3	0.8
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	3	0.8
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	3	0.8
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	9	0.8
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	9	0.8
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	9	0.8
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	8	0.8
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	8	0.8
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	8	0.8
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	8	0.8
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	8	0.8
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	8	0.8
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	8	0.8
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	8	0.8
(2,210)	1:152:A:TYR:HA	1:154:A:ILE:HD11	7	0.8
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG11	4	0.8
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG12	7	0.8
(2,61)	1:166:A:VAL:HG22	1:166:A:VAL:HA	4	0.8
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD11	7	0.79
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD12	7	0.79
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD13	7	0.79
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	4	0.79
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	4	0.79
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	4	0.79
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB1	2	0.79
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG11	10	0.79
(4,719)	1:27:A:THR:HG21	1:25:A:GLU:HG3	9	0.78
(4,719)	1:27:A:THR:HG22	1:25:A:GLU:HG3	9	0.78
(4,719)	1:27:A:THR:HG23	1:25:A:GLU:HG3	9	0.78
(4,679)	1:85:A:GLU:HG2	1:84:A:VAL:HG11	2	0.78
(4,679)	1:85:A:GLU:HG2	1:84:A:VAL:HG12	2	0.78
(4,679)	1:85:A:GLU:HG2	1:84:A:VAL:HG13	2	0.78
(4,679)	1:85:A:GLU:HG3	1:84:A:VAL:HG11	2	0.78
(4,679)	1:85:A:GLU:HG3	1:84:A:VAL:HG12	2	0.78
(4,679)	1:85:A:GLU:HG3	1:84:A:VAL:HG13	2	0.78
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	9	0.78
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	9	0.78
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG11	6	0.78
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG12	6	0.78
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG13	6	0.78
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG11	6	0.78
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG12	6	0.78
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG13	6	0.78
(4,365)	1:151:A:CYS:HB3	1:144:A:MET:HB3	2	0.78
(4,235)	1:122:A:LEU:HA	1:125:A:GLU:HG3	3	0.78
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	2	0.78
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	2	0.78
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	2	0.78
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	5	0.78
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	5	0.78
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	5	0.78
(4,57)	1:59:A:LYS:HA	1:17:A:GLU:HG2	8	0.78
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	3	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	3	0.78
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	3	0.78
(2,161)	1:54:A:VAL:HG21	1:165:A:ARG:HD2	10	0.78
(2,145)	1:42:A:ALA:HB3	1:46:A:TYR:HB2	9	0.78
(4,750)	1:105:A:ARG:HA	1:105:A:ARG:HD3	3	0.77
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	5	0.77
(4,275)	1:22:A:SER:H	1:21:A:THR:HG21	10	0.77
(4,275)	1:22:A:SER:H	1:21:A:THR:HG22	10	0.77
(4,275)	1:22:A:SER:H	1:21:A:THR:HG23	10	0.77
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	5	0.77
(4,96)	1:77:A:ALA:HB1	1:74:A:HIS:HB3	10	0.77
(4,96)	1:77:A:ALA:HB2	1:74:A:HIS:HB3	10	0.77
(4,96)	1:77:A:ALA:HB3	1:74:A:HIS:HB3	10	0.77
(2,115)	1:145:A:GLN:H	1:145:A:GLN:HG2	2	0.77
(2,115)	1:145:A:GLN:H	1:145:A:GLN:HG3	2	0.77
(4,759)	1:150:A:THR:H	1:149:A:GLY:HA2	9	0.76
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE1	1	0.76
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE2	1	0.76
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE3	1	0.76
(4,570)	1:17:A:GLU:HB2	1:57:A:ARG:HD2	2	0.76
(4,570)	1:17:A:GLU:HB2	1:57:A:ARG:HD3	2	0.76
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	5	0.76
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	7	0.76
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	10	0.76
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	5	0.76
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	5	0.76
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	1	0.76
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	2	0.76
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	6	0.76
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	8	0.76
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	9	0.76
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG21	10	0.76
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG22	10	0.76
(4,151)	1:47:A:VAL:HG11	1:55:A:THR:HG23	10	0.76
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG21	10	0.76
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG22	10	0.76
(4,151)	1:47:A:VAL:HG12	1:55:A:THR:HG23	10	0.76
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG21	10	0.76
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG22	10	0.76
(4,151)	1:47:A:VAL:HG13	1:55:A:THR:HG23	10	0.76
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB2	3	0.76
(4,46)	1:89:A:GLN:HG3	1:85:A:GLU:HB3	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,271)	1:117:A:SER:HB2	1:116:A:ALA:HB2	4	0.76
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	4	0.75
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	2	0.75
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	9	0.75
(4,457)	1:150:A:THR:HG21	1:145:A:GLN:HA	1	0.75
(4,457)	1:150:A:THR:HG22	1:145:A:GLN:HA	1	0.75
(4,457)	1:150:A:THR:HG23	1:145:A:GLN:HA	1	0.75
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	4	0.75
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	9	0.75
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	9	0.75
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	9	0.75
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	2	0.75
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	2	0.75
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	2	0.75
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	3	0.75
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	3	0.75
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	9	0.75
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	9	0.75
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	9	0.75
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	2	0.75
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	2	0.75
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	2	0.75
(4,3)	1:163:A:LEU:HD11	1:162:A:GLU:HB3	2	0.75
(4,3)	1:163:A:LEU:HD12	1:162:A:GLU:HB3	2	0.75
(4,3)	1:163:A:LEU:HD13	1:162:A:GLU:HB3	2	0.75
(2,271)	1:117:A:SER:HB3	1:116:A:ALA:HB1	8	0.75
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	2	0.75
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	9	0.75
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG11	8	0.75
(2,61)	1:166:A:VAL:HG22	1:165:A:ARG:HA	6	0.75
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD11	5	0.74
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD12	5	0.74
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD13	5	0.74
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	7	0.74
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	7	0.74
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	7	0.74
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	6	0.74
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	8	0.74
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	8	0.74
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	8	0.74
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	6	0.74
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	6	0.74
(4,161)	1:29:A:ILE:HD11	1:156:A:MET:HA	1	0.74
(4,161)	1:29:A:ILE:HD12	1:156:A:MET:HA	1	0.74
(4,161)	1:29:A:ILE:HD13	1:156:A:MET:HA	1	0.74
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD11	3	0.74
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD12	3	0.74
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD13	3	0.74
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	10	0.74
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	10	0.74
(4,35)	1:142:A:VAL:HG21	1:153:A:MET:HG3	10	0.74
(4,35)	1:142:A:VAL:HG22	1:153:A:MET:HG3	10	0.74
(4,35)	1:142:A:VAL:HG23	1:153:A:MET:HG3	10	0.74
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD11	7	0.74
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD12	7	0.74
(4,34)	1:91:A:THR:HB	1:122:A:LEU:HD13	7	0.74
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD21	8	0.74
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD22	8	0.74
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD23	8	0.74
(2,237)	1:163:A:LEU:HD21	1:164:A:VAL:H	10	0.74
(2,93)	1:146:A:ASP:HB3	1:42:A:ALA:HB1	1	0.74
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD11	7	0.73
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD12	7	0.73
(4,773)	1:156:A:MET:HG2	1:39:A:LEU:HD13	7	0.73
(4,759)	1:150:A:THR:H	1:149:A:GLY:HA2	5	0.73
(4,750)	1:105:A:ARG:HA	1:105:A:ARG:HD3	1	0.73
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	4	0.73
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	4	0.73
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	4	0.73
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	4	0.73
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD21	9	0.73
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD22	9	0.73
(4,274)	1:121:A:GLU:HG3	1:122:A:LEU:HD23	9	0.73
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG11	2	0.73
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG12	2	0.73
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG13	2	0.73
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	2	0.73
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	7	0.73
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	7	0.73
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	7	0.73
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	2	0.73
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	2	0.73
(2,271)	1:117:A:SER:HB3	1:116:A:ALA:HB2	3	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG11	3	0.73
(4,759)	1:150:A:THR:H	1:149:A:GLY:HA2	8	0.72
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	6	0.72
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	6	0.72
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	6	0.72
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	1	0.72
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	8	0.72
(4,457)	1:150:A:THR:HG21	1:145:A:GLN:HA	2	0.72
(4,457)	1:150:A:THR:HG22	1:145:A:GLN:HA	2	0.72
(4,457)	1:150:A:THR:HG23	1:145:A:GLN:HA	2	0.72
(4,96)	1:77:A:ALA:HB1	1:74:A:HIS:HB3	1	0.72
(4,96)	1:77:A:ALA:HB2	1:74:A:HIS:HB3	1	0.72
(4,96)	1:77:A:ALA:HB3	1:74:A:HIS:HB3	1	0.72
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	1	0.72
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	1	0.72
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	1	0.72
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	8	0.72
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	8	0.72
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	8	0.72
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB1	6	0.72
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	1	0.72
(2,170)	1:142:A:VAL:HG21	1:144:A:MET:HG2	2	0.72
(2,18)	1:42:A:ALA:HB3	1:41:A:PHE:HA	1	0.72
(4,496)	1:86:A:ARG:HB3	1:86:A:ARG:HD2	3	0.71
(4,484)	1:126:A:ILE:HG21	1:104:A:GLN:HG3	3	0.71
(4,484)	1:126:A:ILE:HG22	1:104:A:GLN:HG3	3	0.71
(4,484)	1:126:A:ILE:HG23	1:104:A:GLN:HG3	3	0.71
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	8	0.71
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	8	0.71
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	8	0.71
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	9	0.71
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	10	0.71
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	10	0.71
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	10	0.71
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	5	0.71
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	5	0.71
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	5	0.71
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	6	0.71
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	6	0.71
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	6	0.71
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	8	0.71
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	8	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	8	0.71
(2,191)	1:56:A:TYR:H	1:163:A:LEU:HD13	1	0.71
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB2	4	0.71
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	4	0.71
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	4	0.71
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	4	0.71
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	4	0.71
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	4	0.71
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	4	0.71
(2,108)	1:102:A:ILE:HG23	1:133:A:ALA:HB3	10	0.71
(2,61)	1:166:A:VAL:HG21	1:165:A:ARG:HA	8	0.71
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG11	4	0.7
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG12	4	0.7
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG13	4	0.7
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG11	4	0.7
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG12	4	0.7
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG13	4	0.7
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	9	0.7
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	9	0.7
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	9	0.7
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	4	0.7
(4,37)	1:153:A:MET:H	1:130:A:THR:HG21	1	0.7
(4,37)	1:153:A:MET:H	1:130:A:THR:HG22	1	0.7
(4,37)	1:153:A:MET:H	1:130:A:THR:HG23	1	0.7
(4,35)	1:142:A:VAL:HG21	1:153:A:MET:HG3	2	0.7
(4,35)	1:142:A:VAL:HG22	1:153:A:MET:HG3	2	0.7
(4,35)	1:142:A:VAL:HG23	1:153:A:MET:HG3	2	0.7
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	9	0.7
(2,138)	1:60:A:VAL:HG12	1:16:A:MET:HG3	9	0.7
(2,49)	1:163:A:LEU:HD21	1:163:A:LEU:HB3	1	0.7
(4,781)	1:31:A:THR:HG21	1:32:A:GLN:HB3	4	0.69
(4,781)	1:31:A:THR:HG22	1:32:A:GLN:HB3	4	0.69
(4,781)	1:31:A:THR:HG23	1:32:A:GLN:HB3	4	0.69
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	1	0.69
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	1	0.69
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	1	0.69
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	5	0.69
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	5	0.69
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	5	0.69
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	9	0.69
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	9	0.69
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:154:A:ILE:HD11	1:18:A:ILE:HG12	9	0.69
(4,41)	1:154:A:ILE:HD12	1:18:A:ILE:HG12	9	0.69
(4,41)	1:154:A:ILE:HD13	1:18:A:ILE:HG12	9	0.69
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	10	0.69
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	10	0.69
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	10	0.69
(2,334)	1:144:A:MET:HG2	1:151:A:CYS:HB3	6	0.69
(2,334)	1:144:A:MET:HG3	1:151:A:CYS:HB3	6	0.69
(2,170)	1:142:A:VAL:HG21	1:144:A:MET:HG2	9	0.69
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	2	0.69
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	2	0.69
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	2	0.69
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	2	0.69
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	2	0.69
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	2	0.69
(2,61)	1:166:A:VAL:HG21	1:165:A:ARG:HA	3	0.69
(2,18)	1:42:A:ALA:HB3	1:41:A:PHE:HA	7	0.69
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG21	5	0.68
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG22	5	0.68
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG23	5	0.68
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	4	0.68
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	4	0.68
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	4	0.68
(4,457)	1:150:A:THR:HG21	1:145:A:GLN:HA	5	0.68
(4,457)	1:150:A:THR:HG22	1:145:A:GLN:HA	5	0.68
(4,457)	1:150:A:THR:HG23	1:145:A:GLN:HA	5	0.68
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	10	0.68
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	2	0.68
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	2	0.68
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	2	0.68
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	9	0.68
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	9	0.68
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	9	0.68
(2,237)	1:161:A:ALA:H	1:163:A:LEU:HD22	1	0.68
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG12	9	0.68
(2,108)	1:102:A:ILE:HG21	1:133:A:ALA:HB1	4	0.68
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HB2	4	0.68
(2,18)	1:42:A:ALA:HB2	1:41:A:PHE:HA	9	0.68
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	7	0.67
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	7	0.67
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	3	0.67
(4,471)	1:87:A:VAL:HG11	1:93:A:CYS:HB3	9	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,471)	1:87:A:VAL:HG12	1:93:A:CYS:HB3	9	0.67
(4,471)	1:87:A:VAL:HG13	1:93:A:CYS:HB3	9	0.67
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	7	0.67
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	4	0.67
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	7	0.67
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	6	0.67
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	7	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	2	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	2	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	2	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	3	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	3	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	3	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	5	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	5	0.67
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	5	0.67
(4,35)	1:142:A:VAL:HG21	1:153:A:MET:HG3	7	0.67
(4,35)	1:142:A:VAL:HG22	1:153:A:MET:HG3	7	0.67
(4,35)	1:142:A:VAL:HG23	1:153:A:MET:HG3	7	0.67
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	7	0.67
(2,277)	1:58:A:ILE:HG22	1:163:A:LEU:HG	6	0.67
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	5	0.67
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD3	9	0.67
(2,108)	1:102:A:ILE:HG23	1:133:A:ALA:HB1	2	0.67
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	7	0.66
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	7	0.66
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	7	0.66
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD21	5	0.66
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD22	5	0.66
(4,590)	1:71:A:ILE:HD11	1:137:A:LEU:HD23	5	0.66
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD21	5	0.66
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD22	5	0.66
(4,590)	1:71:A:ILE:HD12	1:137:A:LEU:HD23	5	0.66
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD21	5	0.66
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD22	5	0.66
(4,590)	1:71:A:ILE:HD13	1:137:A:LEU:HD23	5	0.66
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	2	0.66
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	10	0.66
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	8	0.66
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	8	0.66
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	8	0.66
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	4	0.66
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	4	0.66
(2,170)	1:142:A:VAL:HG23	1:144:A:MET:HG2	10	0.66
(2,162)	1:166:A:VAL:HG13	1:57:A:ARG:HA	1	0.66
(2,145)	1:42:A:ALA:HB1	1:46:A:TYR:HB2	7	0.66
(4,759)	1:150:A:THR:H	1:149:A:GLY:HA2	1	0.65
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	10	0.65
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	6	0.65
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	10	0.65
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	3	0.65
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	3	0.65
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	3	0.65
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	3	0.65
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	3	0.65
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	3	0.65
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	3	0.65
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	3	0.65
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	3	0.65
(4,177)	1:163:A:LEU:HD11	1:56:A:TYR:HB3	9	0.65
(4,177)	1:163:A:LEU:HD12	1:56:A:TYR:HB3	9	0.65
(4,177)	1:163:A:LEU:HD13	1:56:A:TYR:HB3	9	0.65
(4,40)	1:122:A:LEU:HA	1:122:A:LEU:HG	9	0.65
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	2	0.65
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	2	0.65
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	2	0.65
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG11	5	0.65
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG12	5	0.65
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG13	5	0.65
(2,271)	1:117:A:SER:HB3	1:116:A:ALA:HB3	5	0.65
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB3	9	0.65
(2,61)	1:166:A:VAL:HG22	1:165:A:ARG:HA	7	0.65
(2,49)	1:163:A:LEU:HD21	1:163:A:LEU:HB3	7	0.65
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	5	0.64
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	8	0.64
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	8	0.64
(4,86)	1:106:A:ILE:HG21	1:100:A:GLU:HG3	5	0.64
(4,86)	1:106:A:ILE:HG22	1:100:A:GLU:HG3	5	0.64
(4,86)	1:106:A:ILE:HG23	1:100:A:GLU:HG3	5	0.64
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	1	0.64
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	1	0.64
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	1	0.64
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	3	0.64
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	3	0.64
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	6	0.64
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	6	0.64
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	6	0.64
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	7	0.64
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	7	0.64
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	7	0.64
(2,316)	1:150:A:THR:HG21	1:145:A:GLN:HB2	6	0.64
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB1	2	0.64
(2,237)	1:163:A:LEU:HD22	1:164:A:VAL:H	2	0.64
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	7	0.63
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	7	0.63
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG21	3	0.63
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG22	3	0.63
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG23	3	0.63
(4,484)	1:126:A:ILE:HG21	1:104:A:GLN:HG3	4	0.63
(4,484)	1:126:A:ILE:HG22	1:104:A:GLN:HG3	4	0.63
(4,484)	1:126:A:ILE:HG23	1:104:A:GLN:HG3	4	0.63
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	1	0.63
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	4	0.63
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	9	0.63
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	8	0.63
(4,277)	1:163:A:LEU:HD21	1:29:A:ILE:HG13	10	0.63
(4,277)	1:163:A:LEU:HD22	1:29:A:ILE:HG13	10	0.63
(4,277)	1:163:A:LEU:HD23	1:29:A:ILE:HG13	10	0.63
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	1	0.63
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	1	0.63
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	1	0.63
(4,17)	1:59:A:LYS:HE2	1:57:A:ARG:HG2	10	0.63
(4,17)	1:59:A:LYS:HE3	1:57:A:ARG:HG2	10	0.63
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG11	2	0.63
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG12	2	0.63
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG13	2	0.63
(2,61)	1:166:A:VAL:HG23	1:165:A:ARG:HA	1	0.63
(2,61)	1:166:A:VAL:HG22	1:165:A:ARG:HA	9	0.63
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	1	0.62
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	1	0.62
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	1	0.62
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	9	0.62
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	9	0.62
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,565)	1:16:A:MET:HA	1:16:A:MET:HB3	9	0.62
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	2	0.62
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD2	3	0.62
(4,492)	1:58:A:ILE:H	1:57:A:ARG:HD3	3	0.62
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	2	0.62
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	7	0.62
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	7	0.62
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	7	0.62
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	1	0.62
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	1	0.62
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	1	0.62
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	1	0.62
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	5	0.62
(4,96)	1:77:A:ALA:HB1	1:74:A:HIS:HB3	3	0.62
(4,96)	1:77:A:ALA:HB2	1:74:A:HIS:HB3	3	0.62
(4,96)	1:77:A:ALA:HB3	1:74:A:HIS:HB3	3	0.62
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	8	0.62
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	8	0.62
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	8	0.62
(4,79)	1:106:A:ILE:HG21	1:97:A:THR:HA	8	0.62
(4,79)	1:106:A:ILE:HG22	1:97:A:THR:HA	8	0.62
(4,79)	1:106:A:ILE:HG23	1:97:A:THR:HA	8	0.62
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	9	0.62
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	2	0.62
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	2	0.62
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	2	0.62
(4,17)	1:59:A:LYS:HE2	1:57:A:ARG:HG2	6	0.62
(4,17)	1:59:A:LYS:HE3	1:57:A:ARG:HG2	6	0.62
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD21	2	0.62
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD22	2	0.62
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD23	2	0.62
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB2	1	0.62
(2,237)	1:161:A:ALA:H	1:163:A:LEU:HD21	7	0.62
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB1	6	0.62
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB2	10	0.62
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	8	0.62
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	8	0.62
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	8	0.62
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	8	0.62
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	8	0.62
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	8	0.62
(2,49)	1:163:A:LEU:HD22	1:163:A:LEU:HB3	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	1	0.61
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	3	0.61
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	4	0.61
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	6	0.61
(4,341)	1:128:A:ALA:HB1	1:35:A:PHE:HB3	3	0.61
(4,341)	1:128:A:ALA:HB2	1:35:A:PHE:HB3	3	0.61
(4,341)	1:128:A:ALA:HB3	1:35:A:PHE:HB3	3	0.61
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	4	0.61
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	4	0.61
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	4	0.61
(4,93)	1:98:A:ALA:HB1	1:96:A:ASP:HA	8	0.61
(4,93)	1:98:A:ALA:HB2	1:96:A:ASP:HA	8	0.61
(4,93)	1:98:A:ALA:HB3	1:96:A:ASP:HA	8	0.61
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	5	0.61
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	5	0.61
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	1	0.61
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	1	0.61
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	1	0.61
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	1	0.61
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	1	0.61
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	1	0.61
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	1	0.61
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	1	0.61
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	1	0.61
(4,40)	1:122:A:LEU:HA	1:122:A:LEU:HG	5	0.61
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	9	0.61
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	9	0.61
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	9	0.61
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	6	0.61
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	6	0.61
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	3	0.61
(2,108)	1:71:A:ILE:HB	1:102:A:ILE:HG22	8	0.61
(2,49)	1:163:A:LEU:HD21	1:163:A:LEU:HB3	4	0.61
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	6	0.6
(4,730)	1:71:A:ILE:HD11	1:103:A:SER:HA	7	0.6
(4,730)	1:71:A:ILE:HD12	1:103:A:SER:HA	7	0.6
(4,730)	1:71:A:ILE:HD13	1:103:A:SER:HA	7	0.6
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	3	0.6
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	3	0.6
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	5	0.6
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	5	0.6
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	10	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	10	0.6
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	3	0.6
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	3	0.6
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	3	0.6
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	10	0.6
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	10	0.6
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	2	0.6
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	2	0.6
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	2	0.6
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	5	0.6
(4,437)	1:29:A:ILE:HG21	1:156:A:MET:HB3	8	0.6
(4,437)	1:29:A:ILE:HG22	1:156:A:MET:HB3	8	0.6
(4,437)	1:29:A:ILE:HG23	1:156:A:MET:HB3	8	0.6
(4,277)	1:163:A:LEU:HD21	1:29:A:ILE:HG13	9	0.6
(4,277)	1:163:A:LEU:HD22	1:29:A:ILE:HG13	9	0.6
(4,277)	1:163:A:LEU:HD23	1:29:A:ILE:HG13	9	0.6
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	4	0.6
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	4	0.6
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	4	0.6
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	4	0.6
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	4	0.6
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	4	0.6
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	4	0.6
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	4	0.6
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	4	0.6
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	9	0.6
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB1	6	0.6
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB2	6	0.6
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB3	6	0.6
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	5	0.6
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	5	0.6
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	5	0.6
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	9	0.6
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	9	0.6
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	9	0.6
(2,276)	1:24:A:VAL:HG13	1:25:A:GLU:HB2	1	0.6
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	3	0.6
(4,474)	1:86:A:ARG:HB3	1:86:A:ARG:HD3	7	0.59
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	6	0.59
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	8	0.59
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	8	0.59
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	1	0.59
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	10	0.59
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB2	4	0.59
(2,107)	1:47:A:VAL:HG12	1:55:A:THR:HG23	2	0.59
(2,49)	1:163:A:LEU:HD21	1:163:A:LEU:HB3	8	0.59
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	2	0.58
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	2	0.58
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	9	0.58
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	9	0.58
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	10	0.58
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	7	0.58
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	7	0.58
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	7	0.58
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	7	0.58
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	8	0.58
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	9	0.58
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	9	0.58
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	9	0.58
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	2	0.58
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	2	0.58
(2,316)	1:150:A:THR:HG22	1:145:A:GLN:HB2	7	0.58
(2,254)	1:43:A:ALA:HB1	1:151:A:CYS:H	5	0.58
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	5	0.58
(2,207)	1:161:A:ALA:HB3	1:159:A:HIS:HB3	6	0.58
(2,162)	1:56:A:TYR:HA	1:166:A:VAL:HG12	6	0.58
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	4	0.57
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	5	0.57
(4,301)	1:137:A:LEU:HD11	1:137:A:LEU:HA	4	0.57
(4,301)	1:137:A:LEU:HD12	1:137:A:LEU:HA	4	0.57
(4,301)	1:137:A:LEU:HD13	1:137:A:LEU:HA	4	0.57
(2,316)	1:150:A:THR:HG23	1:145:A:GLN:HB2	4	0.57
(2,234)	1:50:A:ALA:HB2	1:51:A:GLY:HA2	7	0.57
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	2	0.57
(2,170)	1:142:A:VAL:HG23	1:144:A:MET:HG3	6	0.57
(4,565)	1:16:A:MET:HA	1:16:A:MET:HB3	2	0.56
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	4	0.56
(4,348)	1:165:A:ARG:HB3	1:165:A:ARG:HD2	9	0.56
(4,198)	1:2:A:SER:HA	1:2:A:SER:HB2	2	0.56
(4,198)	1:2:A:SER:HA	1:2:A:SER:HB2	5	0.56
(4,198)	1:2:A:SER:HA	1:2:A:SER:HB2	6	0.56
(4,198)	1:2:A:SER:HA	1:2:A:SER:HB2	9	0.56
(4,159)	1:145:A:GLN:HB3	1:145:A:GLN:H	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	2	0.56
(4,96)	1:77:A:ALA:HB1	1:74:A:HIS:HB3	7	0.56
(4,96)	1:77:A:ALA:HB2	1:74:A:HIS:HB3	7	0.56
(4,96)	1:77:A:ALA:HB3	1:74:A:HIS:HB3	7	0.56
(4,33)	1:39:A:LEU:HD11	1:156:A:MET:HB3	10	0.56
(4,33)	1:39:A:LEU:HD12	1:156:A:MET:HB3	10	0.56
(4,33)	1:39:A:LEU:HD13	1:156:A:MET:HB3	10	0.56
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB1	7	0.56
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB2	7	0.56
(4,23)	1:157:A:LEU:HB2	1:161:A:ALA:HB3	7	0.56
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD3	3	0.56
(2,171)	1:98:A:ALA:HB2	1:102:A:ILE:H	7	0.56
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB1	8	0.56
(2,138)	1:60:A:VAL:HG13	1:16:A:MET:HG3	2	0.56
(2,49)	1:163:A:LEU:HD21	1:163:A:LEU:HB3	5	0.56
(4,565)	1:16:A:MET:HA	1:16:A:MET:HB3	1	0.55
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	9	0.55
(4,323)	1:32:A:GLN:HA	1:32:A:GLN:HG3	4	0.55
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	5	0.55
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	5	0.55
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	5	0.55
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG11	7	0.55
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG12	7	0.55
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG13	7	0.55
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD2	6	0.55
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD3	10	0.55
(2,61)	1:166:A:VAL:HG22	1:165:A:ARG:HA	2	0.55
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	2	0.54
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	5	0.54
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	5	0.54
(4,484)	1:126:A:ILE:HG21	1:104:A:GLN:HG3	2	0.54
(4,484)	1:126:A:ILE:HG22	1:104:A:GLN:HG3	2	0.54
(4,484)	1:126:A:ILE:HG23	1:104:A:GLN:HG3	2	0.54
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	1	0.54
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	1	0.54
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	1	0.54
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	10	0.54
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	7	0.54
(2,61)	1:166:A:VAL:HG23	1:165:A:ARG:HA	10	0.54
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	4	0.53
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	4	0.53
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	6	0.53
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	9	0.53
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	9	0.53
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	9	0.53
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	1	0.53
(4,457)	1:150:A:THR:HG21	1:145:A:GLN:HA	8	0.53
(4,457)	1:150:A:THR:HG22	1:145:A:GLN:HA	8	0.53
(4,457)	1:150:A:THR:HG23	1:145:A:GLN:HA	8	0.53
(4,238)	1:128:A:ALA:HB1	1:34:A:ARG:HD2	5	0.53
(4,238)	1:128:A:ALA:HB2	1:34:A:ARG:HD2	5	0.53
(4,238)	1:128:A:ALA:HB3	1:34:A:ARG:HD2	5	0.53
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	2	0.53
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	2	0.53
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	2	0.53
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	3	0.53
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	3	0.53
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	3	0.53
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	4	0.53
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	4	0.53
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	4	0.53
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	5	0.53
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	5	0.53
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	5	0.53
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	10	0.53
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	10	0.53
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	10	0.53
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	3	0.53
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	3	0.53
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	3	0.53
(4,196)	1:116:A:ALA:HB1	1:117:A:SER:HA	5	0.53
(4,196)	1:116:A:ALA:HB2	1:117:A:SER:HA	5	0.53
(4,196)	1:116:A:ALA:HB3	1:117:A:SER:HA	5	0.53
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	10	0.53
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	10	0.53
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	7	0.53
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	7	0.53
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	7	0.53
(2,294)	1:32:A:GLN:HA	1:32:A:GLN:HB3	3	0.53
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	2	0.53
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD2	4	0.53
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB2	9	0.53
(2,160)	1:165:A:ARG:HD2	1:54:A:VAL:HA	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,160)	1:53:A:HIS:HB2	1:54:A:VAL:HA	8	0.53
(2,154)	1:26:A:ILE:HA	1:27:A:THR:HA	2	0.53
(2,18)	1:18:A:ILE:HB	1:41:A:PHE:HA	3	0.53
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	8	0.52
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	6	0.52
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	6	0.52
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	6	0.52
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	6	0.52
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	10	0.52
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	10	0.52
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	10	0.52
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	10	0.52
(4,385)	1:153:A:MET:HE1	1:153:A:MET:HG3	5	0.52
(4,385)	1:153:A:MET:HE2	1:153:A:MET:HG3	5	0.52
(4,385)	1:153:A:MET:HE3	1:153:A:MET:HG3	5	0.52
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	6	0.52
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	6	0.52
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	6	0.52
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	7	0.52
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	7	0.52
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	7	0.52
(4,211)	1:71:A:ILE:HG21	1:71:A:ILE:HG13	9	0.52
(4,211)	1:71:A:ILE:HG22	1:71:A:ILE:HG13	9	0.52
(4,211)	1:71:A:ILE:HG23	1:71:A:ILE:HG13	9	0.52
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	8	0.52
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	8	0.52
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	8	0.52
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	1	0.52
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	1	0.52
(2,294)	1:32:A:GLN:HA	1:32:A:GLN:HB3	10	0.52
(2,271)	1:117:A:SER:HB2	1:116:A:ALA:HB3	7	0.52
(2,216)	1:160:A:ASP:HB2	1:161:A:ALA:HB3	3	0.52
(2,171)	1:88:A:MET:H	1:98:A:ALA:HB3	1	0.52
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	2	0.51
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	1	0.51
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	1	0.51
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	1	0.51
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	5	0.51
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	5	0.51
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	5	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	1	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	3	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	4	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	5	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	6	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	8	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	9	0.51
(4,410)	1:113:A:ASP:HB3	1:113:A:ASP:HA	10	0.51
(4,385)	1:153:A:MET:HE1	1:153:A:MET:HG3	1	0.51
(4,385)	1:153:A:MET:HE2	1:153:A:MET:HG3	1	0.51
(4,385)	1:153:A:MET:HE3	1:153:A:MET:HG3	1	0.51
(4,369)	1:140:A:ARG:HA	1:140:A:ARG:HG2	10	0.51
(4,301)	1:137:A:LEU:HD11	1:137:A:LEU:HA	5	0.51
(4,301)	1:137:A:LEU:HD12	1:137:A:LEU:HA	5	0.51
(4,301)	1:137:A:LEU:HD13	1:137:A:LEU:HA	5	0.51
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	10	0.51
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	10	0.51
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	10	0.51
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	10	0.51
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	10	0.51
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	10	0.51
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	10	0.51
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	10	0.51
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	10	0.51
(4,147)	1:34:A:ARG:HB2	1:34:A:ARG:HD3	10	0.51
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG21	7	0.51
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG22	7	0.51
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG23	7	0.51
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG21	7	0.51
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG22	7	0.51
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG23	7	0.51
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG21	7	0.51
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG22	7	0.51
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG23	7	0.51
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	5	0.51
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	5	0.51
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	5	0.51
(2,294)	1:140:A:ARG:HB2	1:140:A:ARG:HA	1	0.51
(2,294)	1:140:A:ARG:HB2	1:140:A:ARG:HA	7	0.51
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	1	0.51
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	9	0.51
(2,107)	1:126:A:ILE:HG22	1:130:A:THR:HG21	7	0.51
(2,107)	1:47:A:VAL:HG12	1:55:A:THR:HG22	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,774)	1:164:A:VAL:HG11	1:164:A:VAL:HA	5	0.5
(4,774)	1:164:A:VAL:HG12	1:164:A:VAL:HA	5	0.5
(4,774)	1:164:A:VAL:HG13	1:164:A:VAL:HA	5	0.5
(4,774)	1:164:A:VAL:HG11	1:164:A:VAL:HA	10	0.5
(4,774)	1:164:A:VAL:HG12	1:164:A:VAL:HA	10	0.5
(4,774)	1:164:A:VAL:HG13	1:164:A:VAL:HA	10	0.5
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	7	0.5
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	2	0.5
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	7	0.5
(4,549)	1:122:A:LEU:HB3	1:123:A:SER:H	5	0.5
(4,341)	1:128:A:ALA:HB1	1:35:A:PHE:HB3	9	0.5
(4,341)	1:128:A:ALA:HB2	1:35:A:PHE:HB3	9	0.5
(4,341)	1:128:A:ALA:HB3	1:35:A:PHE:HB3	9	0.5
(4,280)	1:140:A:ARG:HA	1:140:A:ARG:HD3	10	0.5
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	4	0.5
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD11	6	0.5
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD12	6	0.5
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD13	6	0.5
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG21	7	0.5
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG22	7	0.5
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG23	7	0.5
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	7	0.5
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG11	6	0.5
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG12	6	0.5
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG13	6	0.5
(2,217)	1:54:A:VAL:HG13	1:165:A:ARG:HD3	6	0.5
(2,160)	1:165:A:ARG:HD2	1:54:A:VAL:HA	6	0.5
(2,143)	1:98:A:ALA:HB1	1:95:A:GLU:HB2	4	0.5
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	6	0.49
(4,385)	1:153:A:MET:HE1	1:153:A:MET:HG3	2	0.49
(4,385)	1:153:A:MET:HE2	1:153:A:MET:HG3	2	0.49
(4,385)	1:153:A:MET:HE3	1:153:A:MET:HG3	2	0.49
(4,369)	1:140:A:ARG:HA	1:140:A:ARG:HG2	9	0.49
(4,316)	1:71:A:ILE:HA	1:71:A:ILE:HG13	8	0.49
(4,147)	1:34:A:ARG:HB2	1:34:A:ARG:HD3	2	0.49
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	6	0.49
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	9	0.49
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	9	0.49
(4,35)	1:142:A:VAL:HG21	1:153:A:MET:HG3	1	0.49
(4,35)	1:142:A:VAL:HG22	1:153:A:MET:HG3	1	0.49
(4,35)	1:142:A:VAL:HG23	1:153:A:MET:HG3	1	0.49
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG11	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG12	4	0.49
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG13	4	0.49
(2,334)	1:144:A:MET:HG2	1:151:A:CYS:HB3	5	0.49
(2,334)	1:144:A:MET:HG3	1:151:A:CYS:HB3	5	0.49
(4,722)	1:49:A:THR:HA	1:50:A:ALA:H	1	0.48
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	4	0.48
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	8	0.48
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	2	0.48
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	8	0.48
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	9	0.48
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	4	0.48
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	4	0.48
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	4	0.48
(4,188)	1:15:A:ARG:HG2	1:16:A:MET:H	9	0.48
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG21	5	0.48
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG22	5	0.48
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG23	5	0.48
(4,77)	1:117:A:SER:HB2	1:115:A:ASP:HB2	4	0.48
(4,77)	1:117:A:SER:HB3	1:115:A:ASP:HB2	4	0.48
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	6	0.48
(2,294)	1:140:A:ARG:HB2	1:140:A:ARG:HA	8	0.48
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD3	2	0.48
(2,18)	1:18:A:ILE:HB	1:41:A:PHE:HA	2	0.48
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	1	0.47
(4,147)	1:34:A:ARG:HB2	1:34:A:ARG:HD3	4	0.47
(4,19)	1:61:A:ASP:HB2	1:15:A:ARG:HD2	4	0.47
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	10	0.47
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	10	0.47
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	10	0.47
(2,294)	1:32:A:GLN:HA	1:32:A:GLN:HB3	9	0.47
(2,143)	1:98:A:ALA:HB3	1:95:A:GLU:HB2	6	0.47
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG2	2	0.47
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG3	2	0.47
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG2	2	0.47
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG3	2	0.47
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG2	2	0.47
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG3	2	0.47
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD21	4	0.46
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD22	4	0.46
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD23	4	0.46
(4,761)	1:130:A:THR:H	1:130:A:THR:HG21	5	0.46
(4,761)	1:130:A:THR:H	1:130:A:THR:HG22	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,761)	1:130:A:THR:H	1:130:A:THR:HG23	5	0.46
(4,596)	1:47:A:VAL:HG21	1:48:A:MET:HA	1	0.46
(4,596)	1:47:A:VAL:HG22	1:48:A:MET:HA	1	0.46
(4,596)	1:47:A:VAL:HG23	1:48:A:MET:HA	1	0.46
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	5	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	1	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	1	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	1	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	2	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	2	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	2	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	5	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	5	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	5	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	6	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	6	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	6	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	7	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	7	0.46
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	7	0.46
(4,526)	1:140:A:ARG:HB3	1:140:A:ARG:HD2	6	0.46
(4,385)	1:153:A:MET:HE1	1:153:A:MET:HG3	10	0.46
(4,385)	1:153:A:MET:HE2	1:153:A:MET:HG3	10	0.46
(4,385)	1:153:A:MET:HE3	1:153:A:MET:HG3	10	0.46
(4,231)	1:59:A:LYS:HE2	1:17:A:GLU:HG2	6	0.46
(4,231)	1:59:A:LYS:HE3	1:17:A:GLU:HG2	6	0.46
(4,47)	1:58:A:ILE:HD11	1:154:A:ILE:HG12	5	0.46
(4,47)	1:58:A:ILE:HD12	1:154:A:ILE:HG12	5	0.46
(4,47)	1:58:A:ILE:HD13	1:154:A:ILE:HG12	5	0.46
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG21	6	0.45
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG22	6	0.45
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG23	6	0.45
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	2	0.45
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	9	0.45
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	4	0.45
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	4	0.45
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	4	0.45
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	8	0.45
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	8	0.45
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	8	0.45
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	9	0.45
(4,348)	1:165:A:ARG:HB3	1:165:A:ARG:HD2	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,348)	1:165:A:ARG:HB3	1:165:A:ARG:HD2	8	0.45
(4,301)	1:137:A:LEU:HD11	1:137:A:LEU:HA	9	0.45
(4,301)	1:137:A:LEU:HD12	1:137:A:LEU:HA	9	0.45
(4,301)	1:137:A:LEU:HD13	1:137:A:LEU:HA	9	0.45
(4,47)	1:58:A:ILE:HD11	1:154:A:ILE:HG12	3	0.45
(4,47)	1:58:A:ILE:HD12	1:154:A:ILE:HG12	3	0.45
(4,47)	1:58:A:ILE:HD13	1:154:A:ILE:HG12	3	0.45
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	7	0.45
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	7	0.45
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	7	0.45
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	4	0.45
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	4	0.45
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	4	0.45
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	8	0.45
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	8	0.45
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	8	0.45
(2,292)	1:122:A:LEU:HA	1:91:A:THR:HG23	8	0.45
(2,154)	1:26:A:ILE:HA	1:27:A:THR:HA	10	0.45
(4,695)	1:16:A:MET:HG2	1:16:A:MET:H	1	0.44
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	4	0.44
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	10	0.44
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	10	0.44
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	10	0.44
(4,455)	1:108:A:VAL:HB	1:108:A:VAL:H	5	0.44
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	4	0.44
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	4	0.44
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	4	0.44
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG11	9	0.44
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG12	9	0.44
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG13	9	0.44
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG11	9	0.44
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG12	9	0.44
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG13	9	0.44
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	8	0.44
(4,147)	1:34:A:ARG:HB2	1:34:A:ARG:HD3	9	0.44
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD11	9	0.44
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD12	9	0.44
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD13	9	0.44
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	4	0.44
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	4	0.44
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	4	0.44
(2,210)	1:154:A:ILE:HD12	1:153:A:MET:HA	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:42:A:ALA:HB1	1:41:A:PHE:HA	4	0.44
(4,695)	1:16:A:MET:HG2	1:16:A:MET:H	2	0.43
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	8	0.43
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	10	0.43
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	9	0.43
(4,455)	1:108:A:VAL:HB	1:108:A:VAL:H	6	0.43
(4,385)	1:153:A:MET:HE1	1:153:A:MET:HG3	6	0.43
(4,385)	1:153:A:MET:HE2	1:153:A:MET:HG3	6	0.43
(4,385)	1:153:A:MET:HE3	1:153:A:MET:HG3	6	0.43
(4,369)	1:140:A:ARG:HA	1:140:A:ARG:HG2	8	0.43
(4,348)	1:165:A:ARG:HB3	1:165:A:ARG:HD2	2	0.43
(4,276)	1:46:A:TYR:HA	1:46:A:TYR:HB2	6	0.43
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	6	0.43
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	6	0.43
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	6	0.43
(4,74)	1:39:A:LEU:HD21	1:156:A:MET:HB2	7	0.43
(4,74)	1:39:A:LEU:HD22	1:156:A:MET:HB2	7	0.43
(4,74)	1:39:A:LEU:HD23	1:156:A:MET:HB2	7	0.43
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	1	0.43
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	1	0.43
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	4	0.43
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	4	0.43
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	6	0.43
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD3	5	0.43
(2,160)	1:53:A:HIS:HB2	1:54:A:VAL:HA	5	0.43
(4,767)	1:128:A:ALA:HA	1:35:A:PHE:HA	8	0.42
(4,674)	1:90:A:LEU:H	1:90:A:LEU:HG	10	0.42
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	8	0.42
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE1	4	0.42
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE2	4	0.42
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE3	4	0.42
(4,349)	1:29:A:ILE:HD11	1:156:A:MET:HB3	8	0.42
(4,349)	1:29:A:ILE:HD12	1:156:A:MET:HB3	8	0.42
(4,349)	1:29:A:ILE:HD13	1:156:A:MET:HB3	8	0.42
(4,344)	1:34:A:ARG:HB2	1:34:A:ARG:HD2	8	0.42
(4,147)	1:34:A:ARG:HB2	1:34:A:ARG:HD3	7	0.42
(4,17)	1:59:A:LYS:HE2	1:57:A:ARG:HG2	8	0.42
(4,17)	1:59:A:LYS:HE3	1:57:A:ARG:HG2	8	0.42
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	9	0.42
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	9	0.42
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	10	0.42
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	10	0.42
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	10	0.42
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	10	0.42
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	10	0.42
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	5	0.42
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	4	0.42
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB2	6	0.42
(2,135)	1:122:A:LEU:HD21	1:121:A:GLU:HB3	6	0.42
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB2	6	0.42
(2,135)	1:122:A:LEU:HD22	1:121:A:GLU:HB3	6	0.42
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB2	6	0.42
(2,135)	1:122:A:LEU:HD23	1:121:A:GLU:HB3	6	0.42
(2,18)	1:42:A:ALA:HB3	1:41:A:PHE:HA	5	0.42
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	3	0.41
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	3	0.41
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	3	0.41
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	5	0.41
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	9	0.41
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	9	0.41
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	9	0.41
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	3	0.41
(4,426)	1:24:A:VAL:HG21	1:25:A:GLU:HG2	2	0.41
(4,426)	1:24:A:VAL:HG22	1:25:A:GLU:HG2	2	0.41
(4,426)	1:24:A:VAL:HG23	1:25:A:GLU:HG2	2	0.41
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	6	0.41
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	6	0.41
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	6	0.41
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	8	0.41
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	8	0.41
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	8	0.41
(4,348)	1:165:A:ARG:HB3	1:165:A:ARG:HD2	5	0.41
(4,276)	1:46:A:TYR:HA	1:46:A:TYR:HB2	1	0.41
(4,276)	1:46:A:TYR:HA	1:46:A:TYR:HB2	3	0.41
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	10	0.41
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	10	0.41
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	10	0.41
(4,168)	1:116:A:ALA:HA	1:118:A:ASP:H	6	0.41
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	2	0.41
(4,17)	1:59:A:LYS:HE2	1:57:A:ARG:HG2	4	0.41
(4,17)	1:59:A:LYS:HE3	1:57:A:ARG:HG2	4	0.41
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	5	0.41
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,334)	1:144:A:MET:HG2	1:151:A:CYS:HB3	9	0.41
(2,334)	1:144:A:MET:HG3	1:151:A:CYS:HB3	9	0.41
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB1	9	0.41
(2,271)	1:120:A:ALA:HA	1:116:A:ALA:HB3	10	0.41
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	8	0.41
(2,18)	1:18:A:ILE:HB	1:41:A:PHE:HA	6	0.41
(1,49)	1:151:A:CYS:H	1:144:A:MET:O	10	0.41
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB1	7	0.4
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB2	7	0.4
(4,753)	1:94:A:ASP:H	1:98:A:ALA:HB3	7	0.4
(4,563)	1:115:A:ASP:HB2	1:116:A:ALA:H	3	0.4
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG21	3	0.4
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG22	3	0.4
(4,562)	1:29:A:ILE:HG12	1:29:A:ILE:HG23	3	0.4
(4,476)	1:90:A:LEU:HB3	1:90:A:LEU:HD11	10	0.4
(4,476)	1:90:A:LEU:HB3	1:90:A:LEU:HD12	10	0.4
(4,476)	1:90:A:LEU:HB3	1:90:A:LEU:HD13	10	0.4
(4,437)	1:29:A:ILE:HG21	1:156:A:MET:HB3	10	0.4
(4,437)	1:29:A:ILE:HG22	1:156:A:MET:HB3	10	0.4
(4,437)	1:29:A:ILE:HG23	1:156:A:MET:HB3	10	0.4
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	2	0.4
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	2	0.4
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	2	0.4
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	3	0.4
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	3	0.4
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	3	0.4
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	1	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	1	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	1	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	1	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	2	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	2	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	2	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	3	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	3	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	3	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	4	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	4	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	4	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	10	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	10	0.4
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,217)	1:73:A:TYR:H	1:73:A:TYR:HB3	8	0.4
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD11	5	0.4
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD12	5	0.4
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD13	5	0.4
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	2	0.4
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	2	0.4
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	2	0.4
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG21	3	0.4
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG22	3	0.4
(4,71)	1:153:A:MET:HB3	1:130:A:THR:HG23	3	0.4
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	8	0.4
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	8	0.4
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	3	0.4
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	6	0.4
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	8	0.4
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB2	5	0.39
(4,589)	1:94:A:ASP:HB2	1:95:A:GLU:HB3	5	0.39
(4,570)	1:17:A:GLU:HB2	1:57:A:ARG:HD2	4	0.39
(4,570)	1:17:A:GLU:HB2	1:57:A:ARG:HD3	4	0.39
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	7	0.39
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	9	0.39
(4,276)	1:46:A:TYR:HA	1:46:A:TYR:HB2	4	0.39
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	3	0.39
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	3	0.39
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	3	0.39
(4,62)	1:103:A:SER:HB2	1:105:A:ARG:HD3	10	0.39
(2,321)	1:41:A:PHE:H	1:40:A:CYS:HB2	8	0.39
(2,321)	1:41:A:PHE:H	1:40:A:CYS:HB3	8	0.39
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	2	0.39
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	7	0.39
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	10	0.39
(2,207)	1:161:A:ALA:HB3	1:159:A:HIS:HB3	10	0.39
(2,143)	1:98:A:ALA:HB1	1:95:A:GLU:HB2	10	0.39
(2,138)	1:60:A:VAL:HG12	1:16:A:MET:HG3	1	0.39
(2,93)	1:42:A:ALA:HB3	1:151:A:CYS:HB3	3	0.39
(4,776)	1:16:A:MET:HG3	1:16:A:MET:H	3	0.38
(4,760)	1:153:A:MET:HE1	1:38:A:PHE:HB2	6	0.38
(4,760)	1:153:A:MET:HE2	1:38:A:PHE:HB2	6	0.38
(4,760)	1:153:A:MET:HE3	1:38:A:PHE:HB2	6	0.38
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	3	0.38
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	5	0.38
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG21	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG22	6	0.38
(4,517)	1:71:A:ILE:HG13	1:102:A:ILE:HG23	6	0.38
(4,231)	1:59:A:LYS:HE2	1:17:A:GLU:HG2	9	0.38
(4,231)	1:59:A:LYS:HE3	1:17:A:GLU:HG2	9	0.38
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	2	0.38
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	2	0.38
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	2	0.38
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	6	0.38
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	6	0.38
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	6	0.38
(4,64)	1:54:A:VAL:HG11	1:25:A:GLU:HA	2	0.38
(4,64)	1:54:A:VAL:HG12	1:25:A:GLU:HA	2	0.38
(4,64)	1:54:A:VAL:HG13	1:25:A:GLU:HA	2	0.38
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	4	0.38
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	8	0.38
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	8	0.38
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	8	0.38
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	8	0.38
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	8	0.38
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	8	0.38
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	10	0.38
(2,186)	1:144:A:MET:HG2	1:151:A:CYS:HB2	8	0.38
(2,186)	1:144:A:MET:HG3	1:151:A:CYS:HB2	8	0.38
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	1	0.38
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HB2	9	0.38
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	1	0.37
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	1	0.37
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	1	0.37
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	7	0.37
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	7	0.37
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	7	0.37
(4,283)	1:62:A:GLU:HA	1:64:A:ASP:H	8	0.37
(4,234)	1:155:A:ASP:HA	1:38:A:PHE:HA	2	0.37
(4,147)	1:34:A:ARG:HB2	1:34:A:ARG:HD3	8	0.37
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG21	9	0.37
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG22	9	0.37
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG23	9	0.37
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG21	9	0.37
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG22	9	0.37
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG23	9	0.37
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG21	9	0.37
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG22	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG23	9	0.37
(4,89)	1:58:A:ILE:HG21	1:162:A:GLU:HB3	10	0.37
(4,89)	1:58:A:ILE:HG22	1:162:A:GLU:HB3	10	0.37
(4,89)	1:58:A:ILE:HG23	1:162:A:GLU:HB3	10	0.37
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG21	8	0.37
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG22	8	0.37
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG23	8	0.37
(4,64)	1:54:A:VAL:HG11	1:25:A:GLU:HA	9	0.37
(4,64)	1:54:A:VAL:HG12	1:25:A:GLU:HA	9	0.37
(4,64)	1:54:A:VAL:HG13	1:25:A:GLU:HA	9	0.37
(2,292)	1:122:A:LEU:HA	1:91:A:THR:HG22	10	0.37
(2,255)	1:55:A:THR:H	1:21:A:THR:HG21	1	0.37
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	1	0.37
(2,219)	1:16:A:MET:HA	1:15:A:ARG:HB3	7	0.37
(2,175)	1:54:A:VAL:HG11	1:25:A:GLU:HA	10	0.37
(2,175)	1:54:A:VAL:HG12	1:25:A:GLU:HA	10	0.37
(2,175)	1:54:A:VAL:HG13	1:25:A:GLU:HA	10	0.37
(2,175)	1:54:A:VAL:HG21	1:25:A:GLU:HA	10	0.37
(2,175)	1:54:A:VAL:HG22	1:25:A:GLU:HA	10	0.37
(2,175)	1:54:A:VAL:HG23	1:25:A:GLU:HA	10	0.37
(4,776)	1:16:A:MET:HG3	1:16:A:MET:H	5	0.36
(4,761)	1:130:A:THR:H	1:130:A:THR:HG21	9	0.36
(4,761)	1:130:A:THR:H	1:130:A:THR:HG22	9	0.36
(4,761)	1:130:A:THR:H	1:130:A:THR:HG23	9	0.36
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	9	0.36
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	5	0.36
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	5	0.36
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	5	0.36
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	7	0.36
(4,369)	1:140:A:ARG:HA	1:140:A:ARG:HG2	5	0.36
(4,280)	1:140:A:ARG:HA	1:140:A:ARG:HD3	8	0.36
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	5	0.36
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	5	0.36
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	5	0.36
(2,207)	1:160:A:ASP:HB3	1:161:A:ALA:HB3	5	0.36
(2,175)	1:54:A:VAL:HG11	1:25:A:GLU:HA	2	0.36
(2,175)	1:54:A:VAL:HG12	1:25:A:GLU:HA	2	0.36
(2,175)	1:54:A:VAL:HG13	1:25:A:GLU:HA	2	0.36
(2,175)	1:54:A:VAL:HG21	1:25:A:GLU:HA	2	0.36
(2,175)	1:54:A:VAL:HG22	1:25:A:GLU:HA	2	0.36
(2,175)	1:54:A:VAL:HG23	1:25:A:GLU:HA	2	0.36
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,143)	1:98:A:ALA:HB2	1:95:A:GLU:HB3	3	0.36
(2,107)	1:47:A:VAL:HG13	1:55:A:THR:HG22	4	0.36
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	6	0.35
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	10	0.35
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	1	0.35
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD11	5	0.35
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD12	5	0.35
(4,400)	1:122:A:LEU:HB3	1:122:A:LEU:HD13	5	0.35
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	5	0.35
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	5	0.35
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	5	0.35
(4,349)	1:29:A:ILE:HD11	1:156:A:MET:HB3	3	0.35
(4,349)	1:29:A:ILE:HD12	1:156:A:MET:HB3	3	0.35
(4,349)	1:29:A:ILE:HD13	1:156:A:MET:HB3	3	0.35
(4,170)	1:26:A:ILE:HG13	1:26:A:ILE:HG21	5	0.35
(4,170)	1:26:A:ILE:HG13	1:26:A:ILE:HG22	5	0.35
(4,170)	1:26:A:ILE:HG13	1:26:A:ILE:HG23	5	0.35
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB1	9	0.35
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB2	9	0.35
(4,133)	1:152:A:TYR:H	1:42:A:ALA:HB3	9	0.35
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	3	0.35
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	3	0.35
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG11	10	0.35
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG12	10	0.35
(4,9)	1:95:A:GLU:HG3	1:84:A:VAL:HG13	10	0.35
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	9	0.35
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	1	0.34
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	7	0.34
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG21	2	0.34
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG22	2	0.34
(4,533)	1:53:A:HIS:HB3	1:21:A:THR:HG23	2	0.34
(4,514)	1:144:A:MET:H	1:144:A:MET:HE1	6	0.34
(4,514)	1:144:A:MET:H	1:144:A:MET:HE2	6	0.34
(4,514)	1:144:A:MET:H	1:144:A:MET:HE3	6	0.34
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE1	9	0.34
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE2	9	0.34
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE3	9	0.34
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	3	0.34
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	2	0.34
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	10	0.34
(4,375)	1:163:A:LEU:HD11	1:156:A:MET:HG2	10	0.34
(4,375)	1:163:A:LEU:HD12	1:156:A:MET:HG2	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,375)	1:163:A:LEU:HD13	1:156:A:MET:HG2	10	0.34
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	10	0.34
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	10	0.34
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	10	0.34
(4,280)	1:140:A:ARG:HA	1:140:A:ARG:HD3	9	0.34
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	8	0.34
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	8	0.34
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	8	0.34
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG11	9	0.34
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG12	9	0.34
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG13	9	0.34
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	7	0.34
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	7	0.34
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	7	0.34
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE1	6	0.34
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE2	6	0.34
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE3	6	0.34
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE1	6	0.34
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE2	6	0.34
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE3	6	0.34
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE1	6	0.34
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE2	6	0.34
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE3	6	0.34
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	5	0.34
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	5	0.34
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	5	0.34
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	5	0.34
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	5	0.34
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	5	0.34
(2,251)	1:88:A:MET:HA	1:89:A:GLN:HA	4	0.34
(2,217)	1:54:A:VAL:HG11	1:165:A:ARG:HD3	3	0.34
(2,93)	1:42:A:ALA:HB1	1:151:A:CYS:HB3	6	0.34
(1,34)	1:19:A:PHE:H	1:42:A:ALA:O	7	0.34
(4,592)	1:47:A:VAL:HG11	1:21:A:THR:HG21	3	0.33
(4,592)	1:47:A:VAL:HG11	1:21:A:THR:HG22	3	0.33
(4,592)	1:47:A:VAL:HG11	1:21:A:THR:HG23	3	0.33
(4,592)	1:47:A:VAL:HG12	1:21:A:THR:HG21	3	0.33
(4,592)	1:47:A:VAL:HG12	1:21:A:THR:HG22	3	0.33
(4,592)	1:47:A:VAL:HG12	1:21:A:THR:HG23	3	0.33
(4,592)	1:47:A:VAL:HG13	1:21:A:THR:HG21	3	0.33
(4,592)	1:47:A:VAL:HG13	1:21:A:THR:HG22	3	0.33
(4,592)	1:47:A:VAL:HG13	1:21:A:THR:HG23	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,543)	1:39:A:LEU:HD11	1:39:A:LEU:H	1	0.33
(4,543)	1:39:A:LEU:HD12	1:39:A:LEU:H	1	0.33
(4,543)	1:39:A:LEU:HD13	1:39:A:LEU:H	1	0.33
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE1	5	0.33
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE2	5	0.33
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE3	5	0.33
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE1	5	0.33
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE2	5	0.33
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE3	5	0.33
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE1	5	0.33
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE2	5	0.33
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE3	5	0.33
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	10	0.33
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	10	0.33
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	10	0.33
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	7	0.33
(4,375)	1:163:A:LEU:HD11	1:156:A:MET:HG2	7	0.33
(4,375)	1:163:A:LEU:HD12	1:156:A:MET:HG2	7	0.33
(4,375)	1:163:A:LEU:HD13	1:156:A:MET:HG2	7	0.33
(4,234)	1:155:A:ASP:HA	1:38:A:PHE:HA	10	0.33
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	5	0.33
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	5	0.33
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	5	0.33
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG21	4	0.33
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG22	4	0.33
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG23	4	0.33
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	6	0.33
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	6	0.33
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	10	0.32
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	10	0.32
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	4	0.32
(4,344)	1:34:A:ARG:HB2	1:34:A:ARG:HD2	4	0.32
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG21	6	0.32
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG22	6	0.32
(4,261)	1:126:A:ILE:HG21	1:130:A:THR:HG23	6	0.32
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG21	6	0.32
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG22	6	0.32
(4,261)	1:126:A:ILE:HG22	1:130:A:THR:HG23	6	0.32
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG21	6	0.32
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG22	6	0.32
(4,261)	1:126:A:ILE:HG23	1:130:A:THR:HG23	6	0.32
(4,7)	1:155:A:ASP:HB2	1:140:A:ARG:HB3	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	7	0.32
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	7	0.32
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	7	0.32
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	7	0.32
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	7	0.32
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	7	0.32
(2,237)	1:161:A:ALA:H	1:163:A:LEU:HD22	3	0.32
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	5	0.32
(2,216)	1:160:A:ASP:HB2	1:161:A:ALA:HB2	7	0.32
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	3	0.32
(2,143)	1:98:A:ALA:HB3	1:95:A:GLU:HB2	8	0.32
(2,93)	1:42:A:ALA:HB1	1:151:A:CYS:HB3	4	0.32
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	10	0.31
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	10	0.31
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	10	0.31
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	3	0.31
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	1	0.31
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	1	0.31
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	1	0.31
(4,475)	1:47:A:VAL:HG21	1:48:A:MET:HG2	10	0.31
(4,475)	1:47:A:VAL:HG22	1:48:A:MET:HG2	10	0.31
(4,475)	1:47:A:VAL:HG23	1:48:A:MET:HG2	10	0.31
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	7	0.31
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	7	0.31
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	7	0.31
(4,426)	1:24:A:VAL:HG21	1:25:A:GLU:HG2	9	0.31
(4,426)	1:24:A:VAL:HG22	1:25:A:GLU:HG2	9	0.31
(4,426)	1:24:A:VAL:HG23	1:25:A:GLU:HG2	9	0.31
(4,415)	1:87:A:VAL:HA	1:90:A:LEU:HG	10	0.31
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	9	0.31
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	4	0.31
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	7	0.31
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	10	0.31
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	7	0.31
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	7	0.31
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	7	0.31
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	8	0.31
(4,344)	1:34:A:ARG:HB2	1:34:A:ARG:HD2	7	0.31
(4,286)	1:26:A:ILE:HG21	1:27:A:THR:HA	10	0.31
(4,286)	1:26:A:ILE:HG22	1:27:A:THR:HA	10	0.31
(4,286)	1:26:A:ILE:HG23	1:27:A:THR:HA	10	0.31
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	5	0.31
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	5	0.31
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	6	0.31
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	6	0.31
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	6	0.31
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	6	0.31
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	6	0.31
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	6	0.31
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	6	0.31
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	6	0.31
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	6	0.31
(4,82)	1:146:A:ASP:HB3	1:146:A:ASP:H	7	0.31
(4,26)	1:163:A:LEU:HD21	1:56:A:TYR:HB3	10	0.31
(4,26)	1:163:A:LEU:HD22	1:56:A:TYR:HB3	10	0.31
(4,26)	1:163:A:LEU:HD23	1:56:A:TYR:HB3	10	0.31
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	7	0.31
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	7	0.31
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	7	0.31
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	7	0.31
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	7	0.31
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	7	0.31
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	1	0.31
(2,186)	1:144:A:MET:HG2	1:151:A:CYS:HB2	1	0.31
(2,186)	1:144:A:MET:HG3	1:151:A:CYS:HB2	1	0.31
(2,160)	1:53:A:HIS:HB2	1:54:A:VAL:HA	4	0.31
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	4	0.31
(1,32)	1:133:A:ALA:O	1:137:A:LEU:H	8	0.31
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	9	0.3
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	8	0.3
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	8	0.3
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	8	0.3
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG21	7	0.3
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG22	7	0.3
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG23	7	0.3
(4,433)	1:50:A:ALA:HB1	1:51:A:GLY:HA3	9	0.3
(4,433)	1:50:A:ALA:HB2	1:51:A:GLY:HA3	9	0.3
(4,433)	1:50:A:ALA:HB3	1:51:A:GLY:HA3	9	0.3
(4,428)	1:46:A:TYR:HB3	1:46:A:TYR:H	6	0.3
(4,417)	1:127:A:GLN:HG2	1:127:A:GLN:H	2	0.3
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	2	0.3
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	8	0.3
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	8	0.3
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	8	0.3
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE1	6	0.3
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE2	6	0.3
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE3	6	0.3
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE1	6	0.3
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE2	6	0.3
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE3	6	0.3
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE1	6	0.3
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE2	6	0.3
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE3	6	0.3
(4,231)	1:59:A:LYS:HE2	1:17:A:GLU:HG2	1	0.3
(4,231)	1:59:A:LYS:HE3	1:17:A:GLU:HG2	1	0.3
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	6	0.3
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	6	0.3
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	6	0.3
(4,202)	1:39:A:LEU:HD21	1:39:A:LEU:H	10	0.3
(4,202)	1:39:A:LEU:HD22	1:39:A:LEU:H	10	0.3
(4,202)	1:39:A:LEU:HD23	1:39:A:LEU:H	10	0.3
(4,128)	1:49:A:THR:HB	1:50:A:ALA:H	2	0.3
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG21	10	0.3
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG22	10	0.3
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG23	10	0.3
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG21	10	0.3
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG22	10	0.3
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG23	10	0.3
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG21	10	0.3
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG22	10	0.3
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG23	10	0.3
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	4	0.3
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	5	0.3
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD21	6	0.3
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD22	6	0.3
(4,10)	1:91:A:THR:HA	1:122:A:LEU:HD23	6	0.3
(2,217)	1:54:A:VAL:HG12	1:165:A:ARG:HD3	4	0.3
(2,200)	1:114:A:ILE:HG13	1:114:A:ILE:HA	6	0.3
(2,200)	1:114:A:ILE:HG13	1:114:A:ILE:HA	9	0.3
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	5	0.3
(2,93)	1:42:A:ALA:HB2	1:151:A:CYS:HB3	9	0.3
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	9	0.29
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	9	0.29
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	1	0.29
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	2	0.29
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	2	0.29
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	2	0.29
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	5	0.29
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	5	0.29
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	5	0.29
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	6	0.29
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	6	0.29
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	6	0.29
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	5	0.29
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	6	0.29
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	6	0.29
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	6	0.29
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	6	0.29
(4,371)	1:26:A:ILE:HD11	1:26:A:ILE:HA	5	0.29
(4,371)	1:26:A:ILE:HD12	1:26:A:ILE:HA	5	0.29
(4,371)	1:26:A:ILE:HD13	1:26:A:ILE:HA	5	0.29
(4,369)	1:140:A:ARG:HA	1:140:A:ARG:HG2	2	0.29
(4,349)	1:29:A:ILE:HD11	1:156:A:MET:HB3	9	0.29
(4,349)	1:29:A:ILE:HD12	1:156:A:MET:HB3	9	0.29
(4,349)	1:29:A:ILE:HD13	1:156:A:MET:HB3	9	0.29
(4,344)	1:34:A:ARG:HB2	1:34:A:ARG:HD2	2	0.29
(4,238)	1:128:A:ALA:HB1	1:34:A:ARG:HD2	1	0.29
(4,238)	1:128:A:ALA:HB2	1:34:A:ARG:HD2	1	0.29
(4,238)	1:128:A:ALA:HB3	1:34:A:ARG:HD2	1	0.29
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	6	0.29
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	6	0.29
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	6	0.29
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	3	0.29
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	3	0.29
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	3	0.29
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD11	2	0.29
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD12	2	0.29
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD13	2	0.29
(4,55)	1:12:A:GLN:HA	1:15:A:ARG:HD3	3	0.29
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	8	0.29
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	8	0.29
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	1	0.29
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	1	0.29
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	10	0.29
(2,108)	1:102:A:ILE:HG22	1:133:A:ALA:HB3	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,767)	1:128:A:ALA:HA	1:35:A:PHE:HA	1	0.28
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	4	0.28
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	3	0.28
(4,640)	1:163:A:LEU:HD21	1:156:A:MET:HG2	8	0.28
(4,640)	1:163:A:LEU:HD22	1:156:A:MET:HG2	8	0.28
(4,640)	1:163:A:LEU:HD23	1:156:A:MET:HG2	8	0.28
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	4	0.28
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	4	0.28
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	4	0.28
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	2	0.28
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	2	0.28
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	2	0.28
(4,428)	1:46:A:TYR:HB3	1:46:A:TYR:H	3	0.28
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	1	0.28
(4,344)	1:34:A:ARG:HB2	1:34:A:ARG:HD2	10	0.28
(4,286)	1:26:A:ILE:HG21	1:27:A:THR:HA	9	0.28
(4,286)	1:26:A:ILE:HG22	1:27:A:THR:HA	9	0.28
(4,286)	1:26:A:ILE:HG23	1:27:A:THR:HA	9	0.28
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG21	8	0.28
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG22	8	0.28
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG23	8	0.28
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	8	0.28
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	8	0.28
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	8	0.28
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	5	0.28
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	5	0.28
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	5	0.28
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG11	10	0.28
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG12	10	0.28
(4,184)	1:25:A:GLU:H	1:24:A:VAL:HG13	10	0.28
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG21	2	0.28
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG22	2	0.28
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG23	2	0.28
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG21	2	0.28
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG22	2	0.28
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG23	2	0.28
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG21	2	0.28
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG22	2	0.28
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG23	2	0.28
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG21	6	0.28
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG22	6	0.28
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG23	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,82)	1:146:A:ASP:HB3	1:146:A:ASP:H	10	0.28
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	2	0.28
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	3	0.28
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	10	0.28
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE1	3	0.28
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE2	3	0.28
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE3	3	0.28
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE1	3	0.28
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE2	3	0.28
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE3	3	0.28
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE1	3	0.28
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE2	3	0.28
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE3	3	0.28
(4,30)	1:29:A:ILE:HD11	1:156:A:MET:H	10	0.28
(4,30)	1:29:A:ILE:HD12	1:156:A:MET:H	10	0.28
(4,30)	1:29:A:ILE:HD13	1:156:A:MET:H	10	0.28
(4,29)	1:39:A:LEU:HD21	1:30:A:ASN:HB3	5	0.28
(4,29)	1:39:A:LEU:HD22	1:30:A:ASN:HB3	5	0.28
(4,29)	1:39:A:LEU:HD23	1:30:A:ASN:HB3	5	0.28
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	6	0.28
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	2	0.28
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	2	0.28
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	2	0.28
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	2	0.28
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	2	0.28
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	2	0.28
(2,289)	1:75:A:GLU:HA	1:75:A:GLU:HG2	3	0.28
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	3	0.28
(2,207)	1:161:A:ALA:HB2	1:159:A:HIS:HB3	8	0.28
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	7	0.28
(2,143)	1:98:A:ALA:HB1	1:95:A:GLU:HB2	9	0.28
(1,7)	1:84:A:VAL:H	1:80:A:LEU:O	8	0.28
(4,777)	1:83:A:LEU:HG	1:83:A:LEU:HA	1	0.27
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	2	0.27
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	2	0.27
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	2	0.27
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	1	0.27
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	2	0.27
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	5	0.27
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	9	0.27
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	10	0.27
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG21	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG22	1	0.27
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG23	1	0.27
(4,641)	1:166:A:VAL:HB	1:55:A:THR:HB	5	0.27
(4,640)	1:163:A:LEU:HD21	1:156:A:MET:HG2	10	0.27
(4,640)	1:163:A:LEU:HD22	1:156:A:MET:HG2	10	0.27
(4,640)	1:163:A:LEU:HD23	1:156:A:MET:HG2	10	0.27
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	1	0.27
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	1	0.27
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	1	0.27
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	8	0.27
(4,553)	1:22:A:SER:HB3	1:23:A:PRO:HA	3	0.27
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	6	0.27
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	6	0.27
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	6	0.27
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	3	0.27
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	3	0.27
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	3	0.27
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	8	0.27
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	8	0.27
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	8	0.27
(4,394)	1:150:A:THR:HG21	1:143:A:SER:HA	3	0.27
(4,394)	1:150:A:THR:HG22	1:143:A:SER:HA	3	0.27
(4,394)	1:150:A:THR:HG23	1:143:A:SER:HA	3	0.27
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	1	0.27
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	1	0.27
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	1	0.27
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	4	0.27
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	4	0.27
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	4	0.27
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	9	0.27
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	9	0.27
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	9	0.27
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	10	0.27
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	10	0.27
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	10	0.27
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE1	3	0.27
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE2	3	0.27
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE3	3	0.27
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE1	3	0.27
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE2	3	0.27
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE3	3	0.27
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE1	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE2	3	0.27
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE3	3	0.27
(4,344)	1:34:A:ARG:HB2	1:34:A:ARG:HD2	9	0.27
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	9	0.27
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	9	0.27
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	9	0.27
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	3	0.27
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	3	0.27
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	3	0.27
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	1	0.27
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	1	0.27
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	1	0.27
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	1	0.27
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	1	0.27
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	1	0.27
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	1	0.27
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	1	0.27
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	1	0.27
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	2	0.27
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	2	0.27
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	2	0.27
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	2	0.27
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	2	0.27
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	2	0.27
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	2	0.27
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	2	0.27
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	2	0.27
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD11	10	0.27
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD12	10	0.27
(4,103)	1:163:A:LEU:H	1:163:A:LEU:HD13	10	0.27
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	3	0.27
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	3	0.27
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	3	0.27
(4,64)	1:54:A:VAL:HG11	1:25:A:GLU:HA	10	0.27
(4,64)	1:54:A:VAL:HG12	1:25:A:GLU:HA	10	0.27
(4,64)	1:54:A:VAL:HG13	1:25:A:GLU:HA	10	0.27
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	8	0.27
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	9	0.27
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	2	0.27
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	2	0.27
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	2	0.27
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	2	0.27
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	5	0.27
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	5	0.27
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	5	0.27
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	5	0.27
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	5	0.27
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	5	0.27
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG2	10	0.27
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG3	10	0.27
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG2	10	0.27
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG3	10	0.27
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG2	10	0.27
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG3	10	0.27
(4,776)	1:16:A:MET:HG3	1:16:A:MET:H	6	0.26
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	6	0.26
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	3	0.26
(4,717)	1:59:A:LYS:HD2	1:59:A:LYS:HG2	7	0.26
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	2	0.26
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG21	9	0.26
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG22	9	0.26
(4,603)	1:156:A:MET:HG2	1:29:A:ILE:HG23	9	0.26
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	2	0.26
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	2	0.26
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	2	0.26
(4,428)	1:46:A:TYR:HB3	1:46:A:TYR:H	1	0.26
(4,394)	1:150:A:THR:HG21	1:143:A:SER:HA	10	0.26
(4,394)	1:150:A:THR:HG22	1:143:A:SER:HA	10	0.26
(4,394)	1:150:A:THR:HG23	1:143:A:SER:HA	10	0.26
(4,369)	1:140:A:ARG:HA	1:140:A:ARG:HG2	6	0.26
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	5	0.26
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG21	6	0.26
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG22	6	0.26
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG23	6	0.26
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG21	6	0.26
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG22	6	0.26
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG23	6	0.26
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG21	6	0.26
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG22	6	0.26
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG23	6	0.26
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	3	0.26
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	3	0.26
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	5	0.26
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	5	0.26
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	5	0.26
(4,164)	1:114:A:ILE:HG13	1:114:A:ILE:HA	6	0.26
(4,164)	1:114:A:ILE:HG13	1:114:A:ILE:HA	9	0.26
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG11	7	0.26
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG12	7	0.26
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG13	7	0.26
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	10	0.26
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	10	0.26
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	10	0.26
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	10	0.26
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	10	0.26
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	10	0.26
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	10	0.26
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	10	0.26
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	10	0.26
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	1	0.26
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	6	0.26
(4,26)	1:163:A:LEU:HD21	1:56:A:TYR:HB3	5	0.26
(4,26)	1:163:A:LEU:HD22	1:56:A:TYR:HB3	5	0.26
(4,26)	1:163:A:LEU:HD23	1:56:A:TYR:HB3	5	0.26
(4,4)	1:113:A:ASP:HB2	1:113:A:ASP:H	7	0.26
(2,316)	1:150:A:THR:HG21	1:145:A:GLN:HB2	3	0.26
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	9	0.26
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	9	0.26
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	9	0.26
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	9	0.26
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	9	0.26
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	9	0.26
(2,200)	1:114:A:ILE:HG13	1:114:A:ILE:HA	2	0.26
(2,175)	1:54:A:VAL:HG11	1:25:A:GLU:HA	9	0.26
(2,175)	1:54:A:VAL:HG12	1:25:A:GLU:HA	9	0.26
(2,175)	1:54:A:VAL:HG13	1:25:A:GLU:HA	9	0.26
(2,175)	1:54:A:VAL:HG21	1:25:A:GLU:HA	9	0.26
(2,175)	1:54:A:VAL:HG22	1:25:A:GLU:HA	9	0.26
(2,175)	1:54:A:VAL:HG23	1:25:A:GLU:HA	9	0.26
(2,174)	1:60:A:VAL:H	1:15:A:ARG:HD2	8	0.26
(2,160)	1:53:A:HIS:HB2	1:54:A:VAL:HA	7	0.26
(2,154)	1:26:A:ILE:HA	1:25:A:GLU:HA	8	0.26
(2,153)	1:54:A:VAL:HG21	1:25:A:GLU:HA	6	0.26
(2,107)	1:47:A:VAL:HG13	1:55:A:THR:HG21	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:80:A:LEU:H	1:76:A:ARG:O	8	0.26
(4,740)	1:87:A:VAL:HA	1:90:A:LEU:HB3	5	0.25
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	7	0.25
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	7	0.25
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	7	0.25
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	4	0.25
(4,596)	1:47:A:VAL:HG21	1:48:A:MET:HA	3	0.25
(4,596)	1:47:A:VAL:HG22	1:48:A:MET:HA	3	0.25
(4,596)	1:47:A:VAL:HG23	1:48:A:MET:HA	3	0.25
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	7	0.25
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	7	0.25
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	7	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	1	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	1	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	1	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	4	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	4	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	4	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD21	9	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD22	9	0.25
(4,432)	1:86:A:ARG:HD3	1:90:A:LEU:HD23	9	0.25
(4,266)	1:118:A:ASP:H	1:115:A:ASP:HB3	7	0.25
(4,238)	1:128:A:ALA:HB1	1:34:A:ARG:HD2	3	0.25
(4,238)	1:128:A:ALA:HB2	1:34:A:ARG:HD2	3	0.25
(4,238)	1:128:A:ALA:HB3	1:34:A:ARG:HD2	3	0.25
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	1	0.25
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	1	0.25
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	1	0.25
(4,203)	1:17:A:GLU:H	1:16:A:MET:HG3	7	0.25
(4,139)	1:60:A:VAL:HG21	1:16:A:MET:HG2	4	0.25
(4,139)	1:60:A:VAL:HG22	1:16:A:MET:HG2	4	0.25
(4,139)	1:60:A:VAL:HG23	1:16:A:MET:HG2	4	0.25
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG11	5	0.25
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG12	5	0.25
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG13	5	0.25
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG11	8	0.25
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG12	8	0.25
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG13	8	0.25
(4,89)	1:58:A:ILE:HG21	1:162:A:GLU:HB3	6	0.25
(4,89)	1:58:A:ILE:HG22	1:162:A:GLU:HB3	6	0.25
(4,89)	1:58:A:ILE:HG23	1:162:A:GLU:HB3	6	0.25
(4,87)	1:91:A:THR:HG21	1:125:A:GLU:H	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,87)	1:91:A:THR:HG22	1:125:A:GLU:H	8	0.25
(4,87)	1:91:A:THR:HG23	1:125:A:GLU:H	8	0.25
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE1	10	0.25
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE2	10	0.25
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE3	10	0.25
(4,31)	1:165:A:ARG:HB3	1:165:A:ARG:HD3	9	0.25
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	4	0.25
(4,13)	1:54:A:VAL:H	1:23:A:PRO:HA	6	0.25
(2,234)	1:50:A:ALA:HB2	1:51:A:GLY:HA2	6	0.25
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	7	0.25
(2,210)	1:152:A:TYR:HA	1:154:A:ILE:HD12	6	0.25
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	5	0.25
(4,777)	1:83:A:LEU:HG	1:83:A:LEU:HA	9	0.24
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	5	0.24
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	5	0.24
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	5	0.24
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	10	0.24
(4,643)	1:109:A:PHE:HA	1:110:A:ASN:H	6	0.24
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	4	0.24
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	5	0.24
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	8	0.24
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE1	6	0.24
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE2	6	0.24
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE3	6	0.24
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	6	0.24
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	9	0.24
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	9	0.24
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	9	0.24
(4,428)	1:46:A:TYR:HB3	1:46:A:TYR:H	4	0.24
(4,391)	1:47:A:VAL:HG11	1:47:A:VAL:HA	2	0.24
(4,391)	1:47:A:VAL:HG12	1:47:A:VAL:HA	2	0.24
(4,391)	1:47:A:VAL:HG13	1:47:A:VAL:HA	2	0.24
(4,390)	1:140:A:ARG:HA	1:140:A:ARG:HD2	6	0.24
(4,312)	1:151:A:CYS:HB2	1:151:A:CYS:HA	3	0.24
(4,312)	1:151:A:CYS:HB2	1:151:A:CYS:HA	5	0.24
(4,312)	1:151:A:CYS:HB2	1:151:A:CYS:HA	10	0.24
(4,283)	1:62:A:GLU:HA	1:64:A:ASP:H	9	0.24
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	7	0.24
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	9	0.24
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	2	0.24
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	2	0.24
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	1	0.24
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	1	0.24
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	1	0.24
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	7	0.24
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	7	0.24
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	7	0.24
(4,154)	1:144:A:MET:H	1:150:A:THR:HG21	9	0.24
(4,154)	1:144:A:MET:H	1:150:A:THR:HG22	9	0.24
(4,154)	1:144:A:MET:H	1:150:A:THR:HG23	9	0.24
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG21	2	0.24
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG22	2	0.24
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG23	2	0.24
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG21	2	0.24
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG22	2	0.24
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG23	2	0.24
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG21	2	0.24
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG22	2	0.24
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG23	2	0.24
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG21	6	0.24
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG22	6	0.24
(4,105)	1:58:A:ILE:HD11	1:154:A:ILE:HG23	6	0.24
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG21	6	0.24
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG22	6	0.24
(4,105)	1:58:A:ILE:HD12	1:154:A:ILE:HG23	6	0.24
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG21	6	0.24
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG22	6	0.24
(4,105)	1:58:A:ILE:HD13	1:154:A:ILE:HG23	6	0.24
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	4	0.24
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	4	0.24
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	4	0.24
(4,88)	1:54:A:VAL:HG11	1:165:A:ARG:HG3	7	0.24
(4,88)	1:54:A:VAL:HG12	1:165:A:ARG:HG3	7	0.24
(4,88)	1:54:A:VAL:HG13	1:165:A:ARG:HG3	7	0.24
(4,82)	1:146:A:ASP:HB3	1:146:A:ASP:H	9	0.24
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG11	6	0.24
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG12	6	0.24
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG13	6	0.24
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG11	6	0.24
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG12	6	0.24
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG13	6	0.24
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG11	6	0.24
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG12	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG13	6	0.24
(4,33)	1:39:A:LEU:HD11	1:156:A:MET:HB3	7	0.24
(4,33)	1:39:A:LEU:HD12	1:156:A:MET:HB3	7	0.24
(4,33)	1:39:A:LEU:HD13	1:156:A:MET:HB3	7	0.24
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB1	2	0.24
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB2	2	0.24
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB3	2	0.24
(4,17)	1:59:A:LYS:HE2	1:57:A:ARG:HG2	2	0.24
(4,17)	1:59:A:LYS:HE3	1:57:A:ARG:HG2	2	0.24
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	10	0.24
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	10	0.24
(2,216)	1:160:A:ASP:HB2	1:161:A:ALA:HB2	2	0.24
(2,93)	1:42:A:ALA:HB3	1:151:A:CYS:HB3	5	0.24
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	8	0.24
(1,8)	1:85:A:GLU:H	1:81:A:SER:O	9	0.24
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG11	6	0.23
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG12	6	0.23
(4,763)	1:134:A:ALA:HB1	1:142:A:VAL:HG13	6	0.23
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG11	6	0.23
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG12	6	0.23
(4,763)	1:134:A:ALA:HB2	1:142:A:VAL:HG13	6	0.23
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG11	6	0.23
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG12	6	0.23
(4,763)	1:134:A:ALA:HB3	1:142:A:VAL:HG13	6	0.23
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	3	0.23
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	3	0.23
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	3	0.23
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	3	0.23
(4,740)	1:87:A:VAL:HA	1:90:A:LEU:HB3	7	0.23
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	8	0.23
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	8	0.23
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	8	0.23
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	8	0.23
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	8	0.23
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	8	0.23
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	8	0.23
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	8	0.23
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	8	0.23
(4,702)	1:107:A:ASP:HB3	1:108:A:VAL:HG11	2	0.23
(4,702)	1:107:A:ASP:HB3	1:108:A:VAL:HG12	2	0.23
(4,702)	1:107:A:ASP:HB3	1:108:A:VAL:HG13	2	0.23
(4,702)	1:107:A:ASP:HB3	1:108:A:VAL:HG21	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,702)	1:107:A:ASP:HB3	1:108:A:VAL:HG22	2	0.23
(4,702)	1:107:A:ASP:HB3	1:108:A:VAL:HG23	2	0.23
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG21	7	0.23
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG22	7	0.23
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG23	7	0.23
(4,683)	1:150:A:THR:HG21	1:143:A:SER:HB2	6	0.23
(4,683)	1:150:A:THR:HG22	1:143:A:SER:HB2	6	0.23
(4,683)	1:150:A:THR:HG23	1:143:A:SER:HB2	6	0.23
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	1	0.23
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	2	0.23
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	3	0.23
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	6	0.23
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	7	0.23
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	9	0.23
(4,632)	1:114:A:ILE:HG12	1:114:A:ILE:HB	10	0.23
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	9	0.23
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	4	0.23
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	4	0.23
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	4	0.23
(4,366)	1:86:A:ARG:HB2	1:83:A:LEU:HA	2	0.23
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	3	0.23
(4,312)	1:151:A:CYS:HB2	1:151:A:CYS:HA	4	0.23
(4,312)	1:151:A:CYS:HB2	1:151:A:CYS:HA	6	0.23
(4,300)	1:118:A:ASP:HB2	1:118:A:ASP:H	9	0.23
(4,278)	1:162:A:GLU:HG3	1:162:A:GLU:H	4	0.23
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	2	0.23
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	4	0.23
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	4	0.23
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	4	0.23
(4,156)	1:16:A:MET:HE1	1:16:A:MET:HG3	2	0.23
(4,156)	1:16:A:MET:HE2	1:16:A:MET:HG3	2	0.23
(4,156)	1:16:A:MET:HE3	1:16:A:MET:HG3	2	0.23
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG21	5	0.23
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG22	5	0.23
(4,144)	1:142:A:VAL:HB	1:130:A:THR:HG23	5	0.23
(4,140)	1:60:A:VAL:HG11	1:16:A:MET:HB3	6	0.23
(4,140)	1:60:A:VAL:HG12	1:16:A:MET:HB3	6	0.23
(4,140)	1:60:A:VAL:HG13	1:16:A:MET:HB3	6	0.23
(4,89)	1:58:A:ILE:HG21	1:162:A:GLU:HB3	2	0.23
(4,89)	1:58:A:ILE:HG22	1:162:A:GLU:HB3	2	0.23
(4,89)	1:58:A:ILE:HG23	1:162:A:GLU:HB3	2	0.23
(4,81)	1:39:A:LEU:HD21	1:20:A:HIS:HB3	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,81)	1:39:A:LEU:HD22	1:20:A:HIS:HB3	7	0.23
(4,81)	1:39:A:LEU:HD23	1:20:A:HIS:HB3	7	0.23
(4,73)	1:154:A:ILE:HG21	1:140:A:ARG:HA	1	0.23
(4,73)	1:154:A:ILE:HG22	1:140:A:ARG:HA	1	0.23
(4,73)	1:154:A:ILE:HG23	1:140:A:ARG:HA	1	0.23
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB1	6	0.23
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB2	6	0.23
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB3	6	0.23
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	3	0.23
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	2	0.23
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	2	0.23
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	2	0.23
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	2	0.23
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	2	0.23
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	2	0.23
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	8	0.23
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	8	0.23
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	8	0.23
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	8	0.23
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	8	0.23
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	8	0.23
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	2	0.22
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	5	0.22
(4,756)	1:98:A:ALA:HB1	1:93:A:CYS:HB2	9	0.22
(4,756)	1:98:A:ALA:HB2	1:93:A:CYS:HB2	9	0.22
(4,756)	1:98:A:ALA:HB3	1:93:A:CYS:HB2	9	0.22
(4,710)	1:61:A:ASP:HB2	1:64:A:ASP:H	7	0.22
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG21	1	0.22
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG22	1	0.22
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG23	1	0.22
(4,658)	1:165:A:ARG:HB2	1:165:A:ARG:HD2	8	0.22
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	6	0.22
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	6	0.22
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	6	0.22
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	9	0.22
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	9	0.22
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	9	0.22
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	3	0.22
(4,587)	1:111:A:LEU:H	1:111:A:LEU:HB3	10	0.22
(4,579)	1:151:A:CYS:HB2	1:144:A:MET:HB3	1	0.22
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	8	0.22
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	3	0.22
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	3	0.22
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	3	0.22
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE1	8	0.22
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE2	8	0.22
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE3	8	0.22
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE1	8	0.22
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE2	8	0.22
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE3	8	0.22
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE1	8	0.22
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE2	8	0.22
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE3	8	0.22
(4,481)	1:118:A:ASP:H	1:115:A:ASP:HB2	2	0.22
(4,481)	1:118:A:ASP:H	1:115:A:ASP:HB2	9	0.22
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	9	0.22
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	9	0.22
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	9	0.22
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	9	0.22
(4,300)	1:118:A:ASP:HB2	1:118:A:ASP:H	2	0.22
(4,286)	1:26:A:ILE:HG21	1:27:A:THR:HA	2	0.22
(4,286)	1:26:A:ILE:HG22	1:27:A:THR:HA	2	0.22
(4,286)	1:26:A:ILE:HG23	1:27:A:THR:HA	2	0.22
(4,283)	1:62:A:GLU:HA	1:64:A:ASP:H	4	0.22
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	4	0.22
(4,231)	1:59:A:LYS:HE2	1:17:A:GLU:HG2	10	0.22
(4,231)	1:59:A:LYS:HE3	1:17:A:GLU:HG2	10	0.22
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	10	0.22
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	10	0.22
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	10	0.22
(4,217)	1:73:A:TYR:H	1:73:A:TYR:HB3	2	0.22
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	10	0.22
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	10	0.22
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	10	0.22
(4,156)	1:16:A:MET:HE1	1:16:A:MET:HG3	1	0.22
(4,156)	1:16:A:MET:HE2	1:16:A:MET:HG3	1	0.22
(4,156)	1:16:A:MET:HE3	1:16:A:MET:HG3	1	0.22
(4,76)	1:122:A:LEU:HG	1:91:A:THR:HA	5	0.22
(4,62)	1:103:A:SER:HB2	1:105:A:ARG:HD3	9	0.22
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	2	0.22
(4,2)	1:47:A:VAL:HB	1:55:A:THR:HG21	10	0.22
(4,2)	1:47:A:VAL:HB	1:55:A:THR:HG22	10	0.22
(4,2)	1:47:A:VAL:HB	1:55:A:THR:HG23	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	3	0.22
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	3	0.22
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	10	0.21
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	10	0.21
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	10	0.21
(4,688)	1:105:A:ARG:HD3	1:105:A:ARG:H	1	0.21
(4,658)	1:165:A:ARG:HB2	1:165:A:ARG:HD2	1	0.21
(4,658)	1:165:A:ARG:HB2	1:165:A:ARG:HD2	5	0.21
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	7	0.21
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	7	0.21
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	7	0.21
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	4	0.21
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	5	0.21
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	6	0.21
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	7	0.21
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	9	0.21
(4,565)	1:16:A:MET:HA	1:16:A:MET:HB3	3	0.21
(4,515)	1:152:A:TYR:HB2	1:154:A:ILE:HD11	6	0.21
(4,515)	1:152:A:TYR:HB2	1:154:A:ILE:HD12	6	0.21
(4,515)	1:152:A:TYR:HB2	1:154:A:ILE:HD13	6	0.21
(4,514)	1:144:A:MET:H	1:144:A:MET:HE1	9	0.21
(4,514)	1:144:A:MET:H	1:144:A:MET:HE2	9	0.21
(4,514)	1:144:A:MET:H	1:144:A:MET:HE3	9	0.21
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	3	0.21
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	3	0.21
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	3	0.21
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	3	0.21
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE1	5	0.21
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE2	5	0.21
(4,345)	1:18:A:ILE:HG21	1:16:A:MET:HE3	5	0.21
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE1	5	0.21
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE2	5	0.21
(4,345)	1:18:A:ILE:HG22	1:16:A:MET:HE3	5	0.21
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE1	5	0.21
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE2	5	0.21
(4,345)	1:18:A:ILE:HG23	1:16:A:MET:HE3	5	0.21
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	3	0.21
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	5	0.21
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	10	0.21
(4,312)	1:151:A:CYS:HB2	1:151:A:CYS:HA	9	0.21
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	3	0.21
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	7	0.21
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	7	0.21
(4,164)	1:114:A:ILE:HG13	1:114:A:ILE:HA	2	0.21
(4,111)	1:163:A:LEU:H	1:163:A:LEU:HG	8	0.21
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB1	10	0.21
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB2	10	0.21
(4,43)	1:47:A:VAL:HG21	1:42:A:ALA:HB3	10	0.21
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB1	10	0.21
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB2	10	0.21
(4,43)	1:47:A:VAL:HG22	1:42:A:ALA:HB3	10	0.21
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB1	10	0.21
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB2	10	0.21
(4,43)	1:47:A:VAL:HG23	1:42:A:ALA:HB3	10	0.21
(4,42)	1:111:A:LEU:HD11	1:110:A:ASN:HB3	2	0.21
(4,42)	1:111:A:LEU:HD12	1:110:A:ASN:HB3	2	0.21
(4,42)	1:111:A:LEU:HD13	1:110:A:ASN:HB3	2	0.21
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	4	0.21
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	4	0.21
(2,312)	1:47:A:VAL:HG21	1:19:A:PHE:HB2	1	0.21
(2,312)	1:47:A:VAL:HG21	1:19:A:PHE:HB3	1	0.21
(2,312)	1:47:A:VAL:HG22	1:19:A:PHE:HB2	1	0.21
(2,312)	1:47:A:VAL:HG22	1:19:A:PHE:HB3	1	0.21
(2,312)	1:47:A:VAL:HG23	1:19:A:PHE:HB2	1	0.21
(2,312)	1:47:A:VAL:HG23	1:19:A:PHE:HB3	1	0.21
(2,210)	1:152:A:TYR:HA	1:154:A:ILE:HD13	5	0.21
(2,145)	1:42:A:ALA:HB1	1:46:A:TYR:HB2	2	0.21
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	3	0.21
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	9	0.21
(1,5)	1:80:A:LEU:H	1:76:A:ARG:O	7	0.21
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	1	0.2
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	7	0.2
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	10	0.2
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	2	0.2
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	2	0.2
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	2	0.2
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	1	0.2
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	1	0.2
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	1	0.2
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	1	0.2
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	4	0.2
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	10	0.2
(4,700)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,700)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	6	0.2
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG21	3	0.2
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG22	3	0.2
(4,637)	1:163:A:LEU:HA	1:164:A:VAL:HG23	3	0.2
(4,565)	1:16:A:MET:HA	1:16:A:MET:HB3	5	0.2
(4,565)	1:16:A:MET:HA	1:16:A:MET:HB3	6	0.2
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	5	0.2
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	5	0.2
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	5	0.2
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	10	0.2
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	10	0.2
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	10	0.2
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	1	0.2
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	1	0.2
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	1	0.2
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	5	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE1	2	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE2	2	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE3	2	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE1	2	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE2	2	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE3	2	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE1	2	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE2	2	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE3	2	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE1	10	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE2	10	0.2
(4,523)	1:154:A:ILE:HD11	1:16:A:MET:HE3	10	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE1	10	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE2	10	0.2
(4,523)	1:154:A:ILE:HD12	1:16:A:MET:HE3	10	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE1	10	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE2	10	0.2
(4,523)	1:154:A:ILE:HD13	1:16:A:MET:HE3	10	0.2
(4,503)	1:34:A:ARG:HD3	1:34:A:ARG:HA	5	0.2
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	6	0.2
(4,326)	1:13:A:MET:HA	1:13:A:MET:HB2	7	0.2
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	2	0.2
(4,217)	1:73:A:TYR:H	1:73:A:TYR:HB3	3	0.2
(4,203)	1:17:A:GLU:H	1:16:A:MET:HG3	10	0.2
(4,156)	1:16:A:MET:HE1	1:16:A:MET:HG3	9	0.2
(4,156)	1:16:A:MET:HE2	1:16:A:MET:HG3	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,156)	1:16:A:MET:HE3	1:16:A:MET:HG3	9	0.2
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD11	9	0.2
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD12	9	0.2
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD13	9	0.2
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD21	7	0.2
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD22	7	0.2
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD23	7	0.2
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD21	7	0.2
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD22	7	0.2
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD23	7	0.2
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD21	7	0.2
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD22	7	0.2
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD23	7	0.2
(4,73)	1:154:A:ILE:HG21	1:140:A:ARG:HA	7	0.2
(4,73)	1:154:A:ILE:HG22	1:140:A:ARG:HA	7	0.2
(4,73)	1:154:A:ILE:HG23	1:140:A:ARG:HA	7	0.2
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG21	10	0.2
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG22	10	0.2
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG23	10	0.2
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG21	10	0.2
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG22	10	0.2
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG23	10	0.2
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG21	10	0.2
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG22	10	0.2
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG23	10	0.2
(4,66)	1:86:A:ARG:HD2	1:90:A:LEU:HD21	10	0.2
(4,66)	1:86:A:ARG:HD2	1:90:A:LEU:HD22	10	0.2
(4,66)	1:86:A:ARG:HD2	1:90:A:LEU:HD23	10	0.2
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE1	4	0.2
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE2	4	0.2
(4,38)	1:142:A:VAL:HG21	1:144:A:MET:HE3	4	0.2
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE1	4	0.2
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE2	4	0.2
(4,38)	1:142:A:VAL:HG22	1:144:A:MET:HE3	4	0.2
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE1	4	0.2
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE2	4	0.2
(4,38)	1:142:A:VAL:HG23	1:144:A:MET:HE3	4	0.2
(4,26)	1:163:A:LEU:HD21	1:56:A:TYR:HB3	2	0.2
(4,26)	1:163:A:LEU:HD22	1:56:A:TYR:HB3	2	0.2
(4,26)	1:163:A:LEU:HD23	1:56:A:TYR:HB3	2	0.2
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	3	0.2
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	3	0.2
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	3	0.2
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	3	0.2
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	3	0.2
(2,289)	1:75:A:GLU:HA	1:75:A:GLU:HG3	4	0.2
(2,276)	1:54:A:VAL:HG23	1:25:A:GLU:HB3	2	0.2
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	1	0.2
(2,108)	1:102:A:ILE:HG23	1:133:A:ALA:HB3	9	0.2
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HB2	1	0.2
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HB2	10	0.2
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	3	0.2
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	6	0.2
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	3	0.19
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	6	0.19
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	3	0.19
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	3	0.19
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	3	0.19
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	7	0.19
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	7	0.19
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	7	0.19
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	8	0.19
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	8	0.19
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	8	0.19
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	3	0.19
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	5	0.19
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	6	0.19
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	8	0.19
(4,688)	1:105:A:ARG:HD3	1:105:A:ARG:H	3	0.19
(4,644)	1:13:A:MET:HA	1:13:A:MET:HG3	10	0.19
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	3	0.19
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	8	0.19
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	7	0.19
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	7	0.19
(4,527)	1:87:A:VAL:HG21	1:98:A:ALA:H	8	0.19
(4,527)	1:87:A:VAL:HG22	1:98:A:ALA:H	8	0.19
(4,527)	1:87:A:VAL:HG23	1:98:A:ALA:H	8	0.19
(4,512)	1:59:A:LYS:HG2	1:17:A:GLU:HG2	7	0.19
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	2	0.19
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	2	0.19
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	2	0.19
(4,419)	1:20:A:HIS:HA	1:41:A:PHE:HA	6	0.19
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	4	0.19
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	4	0.19
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	5	0.19
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	5	0.19
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	5	0.19
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	6	0.19
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	6	0.19
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	6	0.19
(4,283)	1:62:A:GLU:HA	1:64:A:ASP:H	6	0.19
(4,277)	1:163:A:LEU:HD21	1:29:A:ILE:HG13	7	0.19
(4,277)	1:163:A:LEU:HD22	1:29:A:ILE:HG13	7	0.19
(4,277)	1:163:A:LEU:HD23	1:29:A:ILE:HG13	7	0.19
(4,234)	1:155:A:ASP:HA	1:38:A:PHE:HA	5	0.19
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	3	0.19
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	3	0.19
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	3	0.19
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	8	0.19
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	8	0.19
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	8	0.19
(4,156)	1:16:A:MET:HE1	1:16:A:MET:HG3	6	0.19
(4,156)	1:16:A:MET:HE2	1:16:A:MET:HG3	6	0.19
(4,156)	1:16:A:MET:HE3	1:16:A:MET:HG3	6	0.19
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG11	9	0.19
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG12	9	0.19
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG13	9	0.19
(4,128)	1:49:A:THR:HB	1:50:A:ALA:H	10	0.19
(4,69)	1:153:A:MET:HE1	1:153:A:MET:HB2	3	0.19
(4,69)	1:153:A:MET:HE2	1:153:A:MET:HB2	3	0.19
(4,69)	1:153:A:MET:HE3	1:153:A:MET:HB2	3	0.19
(4,47)	1:58:A:ILE:HD11	1:154:A:ILE:HG12	10	0.19
(4,47)	1:58:A:ILE:HD12	1:154:A:ILE:HG12	10	0.19
(4,47)	1:58:A:ILE:HD13	1:154:A:ILE:HG12	10	0.19
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG21	5	0.19
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG22	5	0.19
(4,25)	1:57:A:ARG:HG2	1:166:A:VAL:HG23	5	0.19
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	7	0.19
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	7	0.19
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	9	0.19
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	9	0.19
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	9	0.19
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	9	0.19
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	9	0.19
(2,153)	1:54:A:VAL:HG23	1:25:A:GLU:HA	4	0.19
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	5	0.18
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	5	0.18
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	5	0.18
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	3	0.18
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	3	0.18
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	3	0.18
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	4	0.18
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	4	0.18
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	4	0.18
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	9	0.18
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	9	0.18
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	9	0.18
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	10	0.18
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	10	0.18
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	10	0.18
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	2	0.18
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	3	0.18
(4,686)	1:111:A:LEU:HD11	1:111:A:LEU:HB2	10	0.18
(4,686)	1:111:A:LEU:HD12	1:111:A:LEU:HB2	10	0.18
(4,686)	1:111:A:LEU:HD13	1:111:A:LEU:HB2	10	0.18
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG21	9	0.18
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG22	9	0.18
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG23	9	0.18
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	5	0.18
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	1	0.18
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	1	0.18
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	1	0.18
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	3	0.18
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	3	0.18
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	3	0.18
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	5	0.18
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	5	0.18
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	5	0.18
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	7	0.18
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	7	0.18
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	7	0.18
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	8	0.18
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	8	0.18
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	8	0.18
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,532)	1:17:A:GLU:HG3	1:57:A:ARG:HD3	3	0.18
(4,526)	1:140:A:ARG:HB3	1:140:A:ARG:HD2	10	0.18
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	4	0.18
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	4	0.18
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	4	0.18
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	6	0.18
(4,524)	1:105:A:ARG:HD3	1:105:A:ARG:HB2	9	0.18
(4,518)	1:58:A:ILE:HB	1:163:A:LEU:HA	1	0.18
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	1	0.18
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	7	0.18
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	7	0.18
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	7	0.18
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	1	0.18
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	1	0.18
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	1	0.18
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	4	0.18
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	4	0.18
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	4	0.18
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB1	8	0.18
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB2	8	0.18
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB3	8	0.18
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	3	0.18
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	3	0.18
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	3	0.18
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	7	0.18
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	7	0.18
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	7	0.18
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	8	0.18
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	8	0.18
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	8	0.18
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	5	0.18
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	5	0.18
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	5	0.18
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	7	0.18
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	8	0.18
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	4	0.18
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	8	0.18
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	6	0.18
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	5	0.18
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	5	0.18
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	5	0.18
(4,232)	1:153:A:MET:HE1	1:153:A:MET:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,232)	1:153:A:MET:HE2	1:153:A:MET:HA	9	0.18
(4,232)	1:153:A:MET:HE3	1:153:A:MET:HA	9	0.18
(4,208)	1:13:A:MET:HA	1:13:A:MET:HG2	7	0.18
(4,203)	1:17:A:GLU:H	1:16:A:MET:HG3	8	0.18
(4,156)	1:16:A:MET:HE1	1:16:A:MET:HG3	3	0.18
(4,156)	1:16:A:MET:HE2	1:16:A:MET:HG3	3	0.18
(4,156)	1:16:A:MET:HE3	1:16:A:MET:HG3	3	0.18
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG21	7	0.18
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG22	7	0.18
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG23	7	0.18
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG21	7	0.18
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG22	7	0.18
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG23	7	0.18
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG21	7	0.18
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG22	7	0.18
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG23	7	0.18
(4,101)	1:154:A:ILE:HG21	1:140:A:ARG:HB3	10	0.18
(4,101)	1:154:A:ILE:HG22	1:140:A:ARG:HB3	10	0.18
(4,101)	1:154:A:ILE:HG23	1:140:A:ARG:HB3	10	0.18
(4,81)	1:39:A:LEU:HD21	1:20:A:HIS:HB3	3	0.18
(4,81)	1:39:A:LEU:HD22	1:20:A:HIS:HB3	3	0.18
(4,81)	1:39:A:LEU:HD23	1:20:A:HIS:HB3	3	0.18
(4,81)	1:39:A:LEU:HD21	1:20:A:HIS:HB3	6	0.18
(4,81)	1:39:A:LEU:HD22	1:20:A:HIS:HB3	6	0.18
(4,81)	1:39:A:LEU:HD23	1:20:A:HIS:HB3	6	0.18
(4,69)	1:153:A:MET:HE1	1:153:A:MET:HB2	4	0.18
(4,69)	1:153:A:MET:HE2	1:153:A:MET:HB2	4	0.18
(4,69)	1:153:A:MET:HE3	1:153:A:MET:HB2	4	0.18
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	5	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB1	9	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB2	9	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB3	9	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB1	10	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB2	10	0.18
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB3	10	0.18
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	9	0.18
(2,292)	1:122:A:LEU:HA	1:91:A:THR:HG22	4	0.18
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	5	0.18
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG2	9	0.18
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG3	9	0.18
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG2	9	0.18
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG3	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG2	9	0.18
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG3	9	0.18
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HG3	2	0.18
(1,52)	1:41:A:PHE:H	1:152:A:TYR:O	8	0.18
(1,48)	1:149:A:GLY:H	1:146:A:ASP:O	2	0.18
(1,34)	1:19:A:PHE:H	1:42:A:ALA:O	1	0.18
(1,4)	1:79:A:ASP:H	1:75:A:GLU:O	3	0.18
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD11	9	0.17
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD12	9	0.17
(4,768)	1:29:A:ILE:HG21	1:39:A:LEU:HD13	9	0.17
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD11	9	0.17
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD12	9	0.17
(4,768)	1:29:A:ILE:HG22	1:39:A:LEU:HD13	9	0.17
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD11	9	0.17
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD12	9	0.17
(4,768)	1:29:A:ILE:HG23	1:39:A:LEU:HD13	9	0.17
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD21	2	0.17
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD22	2	0.17
(4,765)	1:156:A:MET:HG2	1:39:A:LEU:HD23	2	0.17
(4,756)	1:98:A:ALA:HB1	1:93:A:CYS:HB2	8	0.17
(4,756)	1:98:A:ALA:HB2	1:93:A:CYS:HB2	8	0.17
(4,756)	1:98:A:ALA:HB3	1:93:A:CYS:HB2	8	0.17
(4,737)	1:115:A:ASP:HB2	1:115:A:ASP:HA	9	0.17
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	10	0.17
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	10	0.17
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	10	0.17
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	10	0.17
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	10	0.17
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	10	0.17
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	10	0.17
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	10	0.17
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	10	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG11	1	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG12	1	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG13	1	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG11	3	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG12	3	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG13	3	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG11	7	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG12	7	0.17
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG13	7	0.17
(4,644)	1:13:A:MET:HA	1:13:A:MET:HG3	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,640)	1:163:A:LEU:HD21	1:156:A:MET:HG2	7	0.17
(4,640)	1:163:A:LEU:HD22	1:156:A:MET:HG2	7	0.17
(4,640)	1:163:A:LEU:HD23	1:156:A:MET:HG2	7	0.17
(4,634)	1:91:A:THR:HB	1:91:A:THR:HA	8	0.17
(4,613)	1:9:A:GLY:H	1:11:A:GLN:HG2	1	0.17
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	8	0.17
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	4	0.17
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	4	0.17
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	4	0.17
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	2	0.17
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	6	0.17
(4,484)	1:126:A:ILE:HG21	1:104:A:GLN:HG3	5	0.17
(4,484)	1:126:A:ILE:HG22	1:104:A:GLN:HG3	5	0.17
(4,484)	1:126:A:ILE:HG23	1:104:A:GLN:HG3	5	0.17
(4,467)	1:86:A:ARG:HD3	1:86:A:ARG:HA	10	0.17
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	4	0.17
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	4	0.17
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	4	0.17
(4,460)	1:153:A:MET:HE1	1:35:A:PHE:HB2	1	0.17
(4,460)	1:153:A:MET:HE2	1:35:A:PHE:HB2	1	0.17
(4,460)	1:153:A:MET:HE3	1:35:A:PHE:HB2	1	0.17
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE1	6	0.17
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE2	6	0.17
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE3	6	0.17
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	7	0.17
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	7	0.17
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	7	0.17
(4,413)	1:29:A:ILE:HG13	1:29:A:ILE:HA	3	0.17
(4,384)	1:95:A:GLU:HG3	1:84:A:VAL:HA	5	0.17
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB1	10	0.17
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB2	10	0.17
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB3	10	0.17
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	1	0.17
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	1	0.17
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	1	0.17
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	6	0.17
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	6	0.17
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	6	0.17
(4,340)	1:100:A:GLU:HG2	1:101:A:LEU:H	2	0.17
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD11	2	0.17
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD12	2	0.17
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD13	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	3	0.17
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	10	0.17
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	9	0.17
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	9	0.17
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	9	0.17
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	2	0.17
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	2	0.17
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	2	0.17
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	6	0.17
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	6	0.17
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	6	0.17
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB1	9	0.17
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB2	9	0.17
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB3	9	0.17
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB1	1	0.17
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB2	1	0.17
(4,155)	1:47:A:VAL:HG11	1:42:A:ALA:HB3	1	0.17
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB1	1	0.17
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB2	1	0.17
(4,155)	1:47:A:VAL:HG12	1:42:A:ALA:HB3	1	0.17
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB1	1	0.17
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB2	1	0.17
(4,155)	1:47:A:VAL:HG13	1:42:A:ALA:HB3	1	0.17
(4,138)	1:147:A:GLU:HG3	1:147:A:GLU:H	3	0.17
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG11	10	0.17
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG12	10	0.17
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG13	10	0.17
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG21	4	0.17
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG22	4	0.17
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG23	4	0.17
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG21	4	0.17
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG22	4	0.17
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG23	4	0.17
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG21	4	0.17
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG22	4	0.17
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG23	4	0.17
(4,113)	1:91:A:THR:H	1:91:A:THR:HB	5	0.17
(4,113)	1:91:A:THR:H	1:91:A:THR:HB	7	0.17
(4,87)	1:91:A:THR:HG21	1:125:A:GLU:H	7	0.17
(4,87)	1:91:A:THR:HG22	1:125:A:GLU:H	7	0.17
(4,87)	1:91:A:THR:HG23	1:125:A:GLU:H	7	0.17
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG21	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG22	3	0.17
(4,84)	1:53:A:HIS:HB3	1:54:A:VAL:HG23	3	0.17
(4,81)	1:39:A:LEU:HD21	1:20:A:HIS:HB3	9	0.17
(4,81)	1:39:A:LEU:HD22	1:20:A:HIS:HB3	9	0.17
(4,81)	1:39:A:LEU:HD23	1:20:A:HIS:HB3	9	0.17
(4,52)	1:154:A:ILE:HD11	1:18:A:ILE:HB	9	0.17
(4,52)	1:154:A:ILE:HD12	1:18:A:ILE:HB	9	0.17
(4,52)	1:154:A:ILE:HD13	1:18:A:ILE:HB	9	0.17
(4,50)	1:86:A:ARG:H	1:86:A:ARG:HG2	7	0.17
(4,13)	1:54:A:VAL:H	1:23:A:PRO:HA	5	0.17
(4,13)	1:54:A:VAL:H	1:23:A:PRO:HA	8	0.17
(2,321)	1:41:A:PHE:H	1:40:A:CYS:HB2	3	0.17
(2,321)	1:41:A:PHE:H	1:40:A:CYS:HB3	3	0.17
(2,294)	1:140:A:ARG:HB2	1:140:A:ARG:HA	2	0.17
(2,234)	1:50:A:ALA:HB1	1:51:A:GLY:HA2	8	0.17
(2,226)	1:61:A:ASP:H	1:15:A:ARG:HD2	6	0.17
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	6	0.17
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	7	0.17
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	10	0.17
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG2	1	0.17
(2,76)	1:150:A:THR:HG21	1:145:A:GLN:HG3	1	0.17
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG2	1	0.17
(2,76)	1:150:A:THR:HG22	1:145:A:GLN:HG3	1	0.17
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG2	1	0.17
(2,76)	1:150:A:THR:HG23	1:145:A:GLN:HG3	1	0.17
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	4	0.17
(1,50)	1:153:A:MET:H	1:142:A:VAL:O	6	0.17
(1,15)	1:96:A:ASP:O	1:100:A:GLU:H	7	0.17
(1,8)	1:85:A:GLU:H	1:81:A:SER:O	6	0.17
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	8	0.16
(4,760)	1:153:A:MET:HE1	1:38:A:PHE:HB2	5	0.16
(4,760)	1:153:A:MET:HE2	1:38:A:PHE:HB2	5	0.16
(4,760)	1:153:A:MET:HE3	1:38:A:PHE:HB2	5	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG11	2	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG12	2	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG13	2	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG11	9	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG12	9	0.16
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG13	9	0.16
(4,672)	1:60:A:VAL:HG21	1:154:A:ILE:HG12	4	0.16
(4,672)	1:60:A:VAL:HG22	1:154:A:ILE:HG12	4	0.16
(4,672)	1:60:A:VAL:HG23	1:154:A:ILE:HG12	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	2	0.16
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	2	0.16
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	2	0.16
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	7	0.16
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	7	0.16
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	7	0.16
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG21	1	0.16
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG22	1	0.16
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG23	1	0.16
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG21	6	0.16
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG22	6	0.16
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG23	6	0.16
(4,658)	1:165:A:ARG:HB2	1:165:A:ARG:HD2	2	0.16
(4,657)	1:22:A:SER:HA	1:23:A:PRO:HD3	7	0.16
(4,644)	1:13:A:MET:HA	1:13:A:MET:HG3	5	0.16
(4,644)	1:13:A:MET:HA	1:13:A:MET:HG3	7	0.16
(4,630)	1:153:A:MET:H	1:143:A:SER:HA	5	0.16
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	2	0.16
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	10	0.16
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	10	0.16
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	10	0.16
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	4	0.16
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	3	0.16
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	4	0.16
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB1	9	0.16
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB2	9	0.16
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB3	9	0.16
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	2	0.16
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	2	0.16
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	2	0.16
(4,518)	1:58:A:ILE:HB	1:163:A:LEU:HA	4	0.16
(4,518)	1:58:A:ILE:HB	1:163:A:LEU:HA	6	0.16
(4,481)	1:118:A:ASP:H	1:115:A:ASP:HB2	6	0.16
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	2	0.16
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE1	8	0.16
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE2	8	0.16
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE3	8	0.16
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	5	0.16
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	5	0.16
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	5	0.16
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	10	0.16
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	10	0.16
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG11	10	0.16
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG12	10	0.16
(4,423)	1:95:A:GLU:HB2	1:84:A:VAL:HG13	10	0.16
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG11	10	0.16
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG12	10	0.16
(4,423)	1:95:A:GLU:HB3	1:84:A:VAL:HG13	10	0.16
(4,419)	1:20:A:HIS:HA	1:41:A:PHE:HA	4	0.16
(4,419)	1:20:A:HIS:HA	1:41:A:PHE:HA	10	0.16
(4,409)	1:167:A:LYS:H	1:165:A:ARG:HA	9	0.16
(4,378)	1:54:A:VAL:HG21	1:25:A:GLU:H	1	0.16
(4,378)	1:54:A:VAL:HG22	1:25:A:GLU:H	1	0.16
(4,378)	1:54:A:VAL:HG23	1:25:A:GLU:H	1	0.16
(4,375)	1:163:A:LEU:HD11	1:156:A:MET:HG2	8	0.16
(4,375)	1:163:A:LEU:HD12	1:156:A:MET:HG2	8	0.16
(4,375)	1:163:A:LEU:HD13	1:156:A:MET:HG2	8	0.16
(4,341)	1:128:A:ALA:HB1	1:35:A:PHE:HB3	6	0.16
(4,341)	1:128:A:ALA:HB2	1:35:A:PHE:HB3	6	0.16
(4,341)	1:128:A:ALA:HB3	1:35:A:PHE:HB3	6	0.16
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	7	0.16
(4,321)	1:25:A:GLU:HG2	1:25:A:GLU:HA	9	0.16
(4,280)	1:140:A:ARG:HA	1:140:A:ARG:HD3	2	0.16
(4,277)	1:163:A:LEU:HD21	1:29:A:ILE:HG13	3	0.16
(4,277)	1:163:A:LEU:HD22	1:29:A:ILE:HG13	3	0.16
(4,277)	1:163:A:LEU:HD23	1:29:A:ILE:HG13	3	0.16
(4,272)	1:109:A:PHE:HB2	1:110:A:ASN:H	2	0.16
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	7	0.16
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG21	2	0.16
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG22	2	0.16
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG23	2	0.16
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG21	2	0.16
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG22	2	0.16
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG23	2	0.16
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG21	2	0.16
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG22	2	0.16
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG23	2	0.16
(4,257)	1:100:A:GLU:HG3	1:100:A:GLU:H	8	0.16
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	4	0.16
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	4	0.16
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	4	0.16
(4,208)	1:13:A:MET:HA	1:13:A:MET:HG2	3	0.16
(4,208)	1:13:A:MET:HA	1:13:A:MET:HG2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,208)	1:13:A:MET:HA	1:13:A:MET:HG2	10	0.16
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE1	10	0.16
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE2	10	0.16
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE3	10	0.16
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG21	8	0.16
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG22	8	0.16
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG23	8	0.16
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG21	8	0.16
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG22	8	0.16
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG23	8	0.16
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG21	8	0.16
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG22	8	0.16
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG23	8	0.16
(4,111)	1:163:A:LEU:H	1:163:A:LEU:HG	1	0.16
(4,28)	1:166:A:VAL:HG11	1:57:A:ARG:HD2	9	0.16
(4,28)	1:166:A:VAL:HG11	1:57:A:ARG:HD3	9	0.16
(4,28)	1:166:A:VAL:HG12	1:57:A:ARG:HD2	9	0.16
(4,28)	1:166:A:VAL:HG12	1:57:A:ARG:HD3	9	0.16
(4,28)	1:166:A:VAL:HG13	1:57:A:ARG:HD2	9	0.16
(4,28)	1:166:A:VAL:HG13	1:57:A:ARG:HD3	9	0.16
(2,294)	1:140:A:ARG:HB2	1:140:A:ARG:HA	6	0.16
(2,292)	1:91:A:THR:HG21	1:90:A:LEU:HA	7	0.16
(2,215)	1:24:A:VAL:HG21	1:25:A:GLU:HB2	9	0.16
(2,215)	1:24:A:VAL:HG21	1:25:A:GLU:HB3	9	0.16
(2,215)	1:24:A:VAL:HG22	1:25:A:GLU:HB2	9	0.16
(2,215)	1:24:A:VAL:HG22	1:25:A:GLU:HB3	9	0.16
(2,215)	1:24:A:VAL:HG23	1:25:A:GLU:HB2	9	0.16
(2,215)	1:24:A:VAL:HG23	1:25:A:GLU:HB3	9	0.16
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	2	0.16
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HG3	5	0.16
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	7	0.16
(1,45)	1:142:A:VAL:H	1:153:A:MET:O	10	0.16
(1,33)	1:74:A:HIS:H	1:70:A:SER:O	9	0.16
(4,779)	1:130:A:THR:H	1:127:A:GLN:HA	7	0.15
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	6	0.15
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	6	0.15
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	6	0.15
(4,758)	1:47:A:VAL:HB	1:21:A:THR:HG21	3	0.15
(4,758)	1:47:A:VAL:HB	1:21:A:THR:HG22	3	0.15
(4,758)	1:47:A:VAL:HB	1:21:A:THR:HG23	3	0.15
(4,739)	1:59:A:LYS:HE2	1:17:A:GLU:HG3	7	0.15
(4,739)	1:59:A:LYS:HE3	1:17:A:GLU:HG3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	7	0.15
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	7	0.15
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	7	0.15
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	7	0.15
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	7	0.15
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	7	0.15
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	7	0.15
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	7	0.15
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	7	0.15
(4,722)	1:49:A:THR:HA	1:50:A:ALA:H	3	0.15
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG21	8	0.15
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG22	8	0.15
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG23	8	0.15
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	10	0.15
(4,694)	1:105:A:ARG:HD2	1:105:A:ARG:H	6	0.15
(4,691)	1:100:A:GLU:HA	1:101:A:LEU:H	5	0.15
(4,688)	1:105:A:ARG:HD3	1:105:A:ARG:H	5	0.15
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	1	0.15
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	1	0.15
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	1	0.15
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	1	0.15
(4,657)	1:22:A:SER:HA	1:23:A:PRO:HD3	4	0.15
(4,644)	1:13:A:MET:HA	1:13:A:MET:HG3	4	0.15
(4,625)	1:109:A:PHE:HA	1:108:A:VAL:HG11	6	0.15
(4,625)	1:109:A:PHE:HA	1:108:A:VAL:HG12	6	0.15
(4,625)	1:109:A:PHE:HA	1:108:A:VAL:HG13	6	0.15
(4,625)	1:109:A:PHE:HA	1:108:A:VAL:HG21	6	0.15
(4,625)	1:109:A:PHE:HA	1:108:A:VAL:HG22	6	0.15
(4,625)	1:109:A:PHE:HA	1:108:A:VAL:HG23	6	0.15
(4,569)	1:163:A:LEU:HD11	1:163:A:LEU:HB2	2	0.15
(4,569)	1:163:A:LEU:HD12	1:163:A:LEU:HB2	2	0.15
(4,569)	1:163:A:LEU:HD13	1:163:A:LEU:HB2	2	0.15
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	6	0.15
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	2	0.15
(4,546)	1:111:A:LEU:HD21	1:108:A:VAL:HA	1	0.15
(4,546)	1:111:A:LEU:HD22	1:108:A:VAL:HA	1	0.15
(4,546)	1:111:A:LEU:HD23	1:108:A:VAL:HA	1	0.15
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB1	8	0.15
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB2	8	0.15
(4,540)	1:43:A:ALA:H	1:43:A:ALA:HB3	8	0.15
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	7	0.15
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	7	0.15
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	8	0.15
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	8	0.15
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	8	0.15
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	9	0.15
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	9	0.15
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	9	0.15
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	8	0.15
(4,501)	1:105:A:ARG:HA	1:106:A:ILE:H	8	0.15
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	3	0.15
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	4	0.15
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	5	0.15
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	6	0.15
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	8	0.15
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	9	0.15
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	10	0.15
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	8	0.15
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	8	0.15
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	8	0.15
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE1	7	0.15
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE2	7	0.15
(4,449)	1:62:A:GLU:HA	1:16:A:MET:HE3	7	0.15
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG11	6	0.15
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG12	6	0.15
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG13	6	0.15
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB1	9	0.15
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB2	9	0.15
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB3	9	0.15
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	2	0.15
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	2	0.15
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	2	0.15
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	2	0.15
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	2	0.15
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	2	0.15
(4,324)	1:34:A:ARG:HB3	1:34:A:ARG:HD3	6	0.15
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	10	0.15
(4,303)	1:129:A:ILE:HG21	1:126:A:ILE:HA	7	0.15
(4,303)	1:129:A:ILE:HG22	1:126:A:ILE:HA	7	0.15
(4,303)	1:129:A:ILE:HG23	1:126:A:ILE:HA	7	0.15
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	7	0.15
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	7	0.15
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,293)	1:166:A:VAL:HA	1:166:A:VAL:HB	5	0.15
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	5	0.15
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG21	2	0.15
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG22	2	0.15
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG23	2	0.15
(4,267)	1:107:A:ASP:HB2	1:109:A:PHE:HB3	4	0.15
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	7	0.15
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	7	0.15
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	7	0.15
(4,214)	1:153:A:MET:HE1	1:128:A:ALA:HA	10	0.15
(4,214)	1:153:A:MET:HE2	1:128:A:ALA:HA	10	0.15
(4,214)	1:153:A:MET:HE3	1:128:A:ALA:HA	10	0.15
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	2	0.15
(4,108)	1:71:A:ILE:HG21	1:72:A:PHE:HA	9	0.15
(4,108)	1:71:A:ILE:HG22	1:72:A:PHE:HA	9	0.15
(4,108)	1:71:A:ILE:HG23	1:72:A:PHE:HA	9	0.15
(4,100)	1:98:A:ALA:HB1	1:84:A:VAL:HA	5	0.15
(4,100)	1:98:A:ALA:HB2	1:84:A:VAL:HA	5	0.15
(4,100)	1:98:A:ALA:HB3	1:84:A:VAL:HA	5	0.15
(4,98)	1:118:A:ASP:HB2	1:121:A:GLU:HG2	10	0.15
(4,86)	1:106:A:ILE:HG21	1:100:A:GLU:HG3	10	0.15
(4,86)	1:106:A:ILE:HG22	1:100:A:GLU:HG3	10	0.15
(4,86)	1:106:A:ILE:HG23	1:100:A:GLU:HG3	10	0.15
(4,64)	1:54:A:VAL:HG11	1:25:A:GLU:HA	6	0.15
(4,64)	1:54:A:VAL:HG12	1:25:A:GLU:HA	6	0.15
(4,64)	1:54:A:VAL:HG13	1:25:A:GLU:HA	6	0.15
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	6	0.15
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	6	0.15
(4,42)	1:111:A:LEU:HD11	1:110:A:ASN:HB3	6	0.15
(4,42)	1:111:A:LEU:HD12	1:110:A:ASN:HB3	6	0.15
(4,42)	1:111:A:LEU:HD13	1:110:A:ASN:HB3	6	0.15
(4,26)	1:163:A:LEU:HD21	1:56:A:TYR:HB3	7	0.15
(4,26)	1:163:A:LEU:HD22	1:56:A:TYR:HB3	7	0.15
(4,26)	1:163:A:LEU:HD23	1:56:A:TYR:HB3	7	0.15
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	1	0.15
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	1	0.15
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	1	0.15
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	1	0.15
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	1	0.15
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	1	0.15
(2,326)	1:143:A:SER:HA	1:144:A:MET:HG2	1	0.15
(2,326)	1:143:A:SER:HA	1:144:A:MET:HG3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG2	3	0.15
(2,323)	1:153:A:MET:HG2	1:144:A:MET:HG3	3	0.15
(2,255)	1:55:A:THR:H	1:21:A:THR:HG22	9	0.15
(2,143)	1:98:A:ALA:HB3	1:95:A:GLU:HB3	7	0.15
(2,41)	1:100:A:GLU:H	1:97:A:THR:HA	1	0.15
(4,780)	1:166:A:VAL:HA	1:165:A:ARG:HG3	4	0.14
(4,767)	1:128:A:ALA:HA	1:35:A:PHE:HA	7	0.14
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG21	5	0.14
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG22	5	0.14
(4,754)	1:104:A:GLN:HG2	1:130:A:THR:HG23	5	0.14
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	4	0.14
(4,739)	1:59:A:LYS:HE2	1:17:A:GLU:HG3	3	0.14
(4,739)	1:59:A:LYS:HE3	1:17:A:GLU:HG3	3	0.14
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	6	0.14
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	6	0.14
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	6	0.14
(4,721)	1:109:A:PHE:H	1:109:A:PHE:HA	9	0.14
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	10	0.14
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG21	10	0.14
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG22	10	0.14
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG23	10	0.14
(4,666)	1:42:A:ALA:HB1	1:151:A:CYS:HB2	8	0.14
(4,666)	1:42:A:ALA:HB2	1:151:A:CYS:HB2	8	0.14
(4,666)	1:42:A:ALA:HB3	1:151:A:CYS:HB2	8	0.14
(4,658)	1:165:A:ARG:HB2	1:165:A:ARG:HD2	9	0.14
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	7	0.14
(4,641)	1:166:A:VAL:HB	1:55:A:THR:HB	6	0.14
(4,641)	1:166:A:VAL:HB	1:55:A:THR:HB	10	0.14
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	3	0.14
(4,566)	1:95:A:GLU:HG2	1:84:A:VAL:HA	10	0.14
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	3	0.14
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	4	0.14
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	7	0.14
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	5	0.14
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	5	0.14
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	5	0.14
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	6	0.14
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	6	0.14
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	6	0.14
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	7	0.14
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	1	0.14
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	1	0.14
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	1	0.14
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	9	0.14
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	9	0.14
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	9	0.14
(4,445)	1:60:A:VAL:HG11	1:60:A:VAL:HA	8	0.14
(4,445)	1:60:A:VAL:HG12	1:60:A:VAL:HA	8	0.14
(4,445)	1:60:A:VAL:HG13	1:60:A:VAL:HA	8	0.14
(4,411)	1:113:A:ASP:HB3	1:114:A:ILE:H	7	0.14
(4,409)	1:167:A:LYS:H	1:165:A:ARG:HA	7	0.14
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB1	2	0.14
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB2	2	0.14
(4,362)	1:43:A:ALA:H	1:42:A:ALA:HB3	2	0.14
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	9	0.14
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	9	0.14
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	9	0.14
(4,355)	1:24:A:VAL:HG11	1:24:A:VAL:HA	10	0.14
(4,355)	1:24:A:VAL:HG12	1:24:A:VAL:HA	10	0.14
(4,355)	1:24:A:VAL:HG13	1:24:A:VAL:HA	10	0.14
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	8	0.14
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	8	0.14
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	8	0.14
(4,324)	1:34:A:ARG:HB3	1:34:A:ARG:HD3	1	0.14
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	1	0.14
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	1	0.14
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	1	0.14
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	4	0.14
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	4	0.14
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	4	0.14
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	6	0.14
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	6	0.14
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	6	0.14
(4,287)	1:21:A:THR:HG21	1:55:A:THR:HA	6	0.14
(4,287)	1:21:A:THR:HG22	1:55:A:THR:HA	6	0.14
(4,287)	1:21:A:THR:HG23	1:55:A:THR:HA	6	0.14
(4,278)	1:162:A:GLU:HG3	1:162:A:GLU:H	7	0.14
(4,278)	1:162:A:GLU:HG3	1:162:A:GLU:H	8	0.14
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	9	0.14
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG21	10	0.14
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG22	10	0.14
(4,269)	1:71:A:ILE:HG21	1:102:A:ILE:HG23	10	0.14
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG21	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG22	10	0.14
(4,269)	1:71:A:ILE:HG22	1:102:A:ILE:HG23	10	0.14
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG21	10	0.14
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG22	10	0.14
(4,269)	1:71:A:ILE:HG23	1:102:A:ILE:HG23	10	0.14
(4,238)	1:128:A:ALA:HB1	1:34:A:ARG:HD2	6	0.14
(4,238)	1:128:A:ALA:HB2	1:34:A:ARG:HD2	6	0.14
(4,238)	1:128:A:ALA:HB3	1:34:A:ARG:HD2	6	0.14
(4,229)	1:60:A:VAL:HG21	1:154:A:ILE:HB	1	0.14
(4,229)	1:60:A:VAL:HG22	1:154:A:ILE:HB	1	0.14
(4,229)	1:60:A:VAL:HG23	1:154:A:ILE:HB	1	0.14
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	4	0.14
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB1	3	0.14
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB2	3	0.14
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB3	3	0.14
(4,156)	1:16:A:MET:HE1	1:16:A:MET:HG3	5	0.14
(4,156)	1:16:A:MET:HE2	1:16:A:MET:HG3	5	0.14
(4,156)	1:16:A:MET:HE3	1:16:A:MET:HG3	5	0.14
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD21	4	0.14
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD22	4	0.14
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD23	4	0.14
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD21	4	0.14
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD22	4	0.14
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD23	4	0.14
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD21	4	0.14
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD22	4	0.14
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD23	4	0.14
(4,111)	1:163:A:LEU:H	1:163:A:LEU:HG	5	0.14
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	4	0.14
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	4	0.14
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	4	0.14
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	4	0.14
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	4	0.14
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	4	0.14
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	4	0.14
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	4	0.14
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	4	0.14
(4,96)	1:77:A:ALA:HB1	1:74:A:HIS:HB3	2	0.14
(4,96)	1:77:A:ALA:HB2	1:74:A:HIS:HB3	2	0.14
(4,96)	1:77:A:ALA:HB3	1:74:A:HIS:HB3	2	0.14
(4,92)	1:60:A:VAL:HG21	1:61:A:ASP:HB3	7	0.14
(4,92)	1:60:A:VAL:HG22	1:61:A:ASP:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,92)	1:60:A:VAL:HG23	1:61:A:ASP:HB3	7	0.14
(4,73)	1:154:A:ILE:HG21	1:140:A:ARG:HA	9	0.14
(4,73)	1:154:A:ILE:HG22	1:140:A:ARG:HA	9	0.14
(4,73)	1:154:A:ILE:HG23	1:140:A:ARG:HA	9	0.14
(4,69)	1:153:A:MET:HE1	1:153:A:MET:HB2	9	0.14
(4,69)	1:153:A:MET:HE2	1:153:A:MET:HB2	9	0.14
(4,69)	1:153:A:MET:HE3	1:153:A:MET:HB2	9	0.14
(4,42)	1:111:A:LEU:HD11	1:110:A:ASN:HB3	1	0.14
(4,42)	1:111:A:LEU:HD12	1:110:A:ASN:HB3	1	0.14
(4,42)	1:111:A:LEU:HD13	1:110:A:ASN:HB3	1	0.14
(4,32)	1:87:A:VAL:HG21	1:90:A:LEU:HB3	2	0.14
(4,32)	1:87:A:VAL:HG22	1:90:A:LEU:HB3	2	0.14
(4,32)	1:87:A:VAL:HG23	1:90:A:LEU:HB3	2	0.14
(4,26)	1:163:A:LEU:HD21	1:56:A:TYR:HB3	4	0.14
(4,26)	1:163:A:LEU:HD22	1:56:A:TYR:HB3	4	0.14
(4,26)	1:163:A:LEU:HD23	1:56:A:TYR:HB3	4	0.14
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	1	0.14
(4,18)	1:126:A:ILE:HB	1:125:A:GLU:H	10	0.14
(4,13)	1:54:A:VAL:H	1:23:A:PRO:HA	4	0.14
(4,12)	1:101:A:LEU:HB2	1:100:A:GLU:HB2	3	0.14
(4,12)	1:101:A:LEU:HB3	1:100:A:GLU:HB2	3	0.14
(2,346)	1:14:A:GLY:HA2	1:15:A:ARG:HD3	9	0.14
(2,346)	1:14:A:GLY:HA3	1:15:A:ARG:HD3	9	0.14
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	4	0.14
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	4	0.14
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	4	0.14
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	4	0.14
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	4	0.14
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	4	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD11	3	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD12	3	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD13	3	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD21	3	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD22	3	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD23	3	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD11	3	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD12	3	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD13	3	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD21	3	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD22	3	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD23	3	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD11	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD12	3	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD13	3	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD21	3	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD22	3	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD23	3	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD11	8	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD12	8	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD13	8	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD21	8	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD22	8	0.14
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD23	8	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD11	8	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD12	8	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD13	8	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD21	8	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD22	8	0.14
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD23	8	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD11	8	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD12	8	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD13	8	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD21	8	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD22	8	0.14
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD23	8	0.14
(2,215)	1:24:A:VAL:HG21	1:25:A:GLU:HB2	2	0.14
(2,215)	1:24:A:VAL:HG21	1:25:A:GLU:HB3	2	0.14
(2,215)	1:24:A:VAL:HG22	1:25:A:GLU:HB2	2	0.14
(2,215)	1:24:A:VAL:HG22	1:25:A:GLU:HB3	2	0.14
(2,215)	1:24:A:VAL:HG23	1:25:A:GLU:HB2	2	0.14
(2,215)	1:24:A:VAL:HG23	1:25:A:GLU:HB3	2	0.14
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	4	0.14
(2,103)	1:151:A:CYS:HB2	1:151:A:CYS:H	8	0.14
(2,93)	1:42:A:ALA:HB2	1:151:A:CYS:HB3	10	0.14
(2,66)	1:71:A:ILE:HG22	1:71:A:ILE:HG12	8	0.14
(2,31)	1:48:A:MET:HG3	1:48:A:MET:HA	8	0.14
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HG3	7	0.14
(1,50)	1:153:A:MET:H	1:142:A:VAL:O	10	0.14
(1,5)	1:80:A:LEU:H	1:76:A:ARG:O	1	0.14
(4,779)	1:130:A:THR:H	1:127:A:GLN:HA	8	0.13
(4,767)	1:128:A:ALA:HA	1:35:A:PHE:HA	4	0.13
(4,767)	1:128:A:ALA:HA	1:35:A:PHE:HA	9	0.13
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	10	0.13
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	10	0.13
(4,760)	1:153:A:MET:HE1	1:38:A:PHE:HB2	2	0.13
(4,760)	1:153:A:MET:HE2	1:38:A:PHE:HB2	2	0.13
(4,760)	1:153:A:MET:HE3	1:38:A:PHE:HB2	2	0.13
(4,760)	1:153:A:MET:HE1	1:38:A:PHE:HB2	9	0.13
(4,760)	1:153:A:MET:HE2	1:38:A:PHE:HB2	9	0.13
(4,760)	1:153:A:MET:HE3	1:38:A:PHE:HB2	9	0.13
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	1	0.13
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	1	0.13
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	1	0.13
(4,732)	1:2:A:SER:HA	1:4:A:MET:HB3	8	0.13
(4,721)	1:109:A:PHE:H	1:109:A:PHE:HA	6	0.13
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	1	0.13
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	3	0.13
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	5	0.13
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	7	0.13
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	8	0.13
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG21	9	0.13
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG22	9	0.13
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG23	9	0.13
(4,697)	1:93:A:CYS:HB2	1:97:A:THR:HB	7	0.13
(4,678)	1:114:A:ILE:HA	1:114:A:ILE:H	10	0.13
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	6	0.13
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG21	3	0.13
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG22	3	0.13
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG23	3	0.13
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG21	4	0.13
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG22	4	0.13
(4,660)	1:7:A:MET:HA	1:8:A:THR:HG23	4	0.13
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	8	0.13
(4,634)	1:91:A:THR:HB	1:91:A:THR:HA	1	0.13
(4,634)	1:91:A:THR:HB	1:91:A:THR:HA	3	0.13
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	1	0.13
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	10	0.13
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	5	0.13
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	8	0.13
(4,550)	1:127:A:GLN:HA	1:127:A:GLN:HG3	3	0.13
(4,550)	1:127:A:GLN:HA	1:127:A:GLN:HG3	10	0.13
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG21	3	0.13
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG22	3	0.13
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG23	3	0.13
(4,525)	1:58:A:ILE:HD11	1:59:A:LYS:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,525)	1:58:A:ILE:HD12	1:59:A:LYS:H	3	0.13
(4,525)	1:58:A:ILE:HD13	1:59:A:LYS:H	3	0.13
(4,519)	1:153:A:MET:HE1	1:153:A:MET:HG2	3	0.13
(4,519)	1:153:A:MET:HE2	1:153:A:MET:HG2	3	0.13
(4,519)	1:153:A:MET:HE3	1:153:A:MET:HG2	3	0.13
(4,519)	1:153:A:MET:HE1	1:153:A:MET:HG2	9	0.13
(4,519)	1:153:A:MET:HE2	1:153:A:MET:HG2	9	0.13
(4,519)	1:153:A:MET:HE3	1:153:A:MET:HG2	9	0.13
(4,514)	1:144:A:MET:H	1:144:A:MET:HE1	2	0.13
(4,514)	1:144:A:MET:H	1:144:A:MET:HE2	2	0.13
(4,514)	1:144:A:MET:H	1:144:A:MET:HE3	2	0.13
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	3	0.13
(4,479)	1:48:A:MET:HG3	1:48:A:MET:HB3	7	0.13
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	5	0.13
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	5	0.13
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	5	0.13
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	6	0.13
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	6	0.13
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	6	0.13
(4,464)	1:153:A:MET:H	1:153:A:MET:HG3	9	0.13
(4,460)	1:153:A:MET:HE1	1:35:A:PHE:HB2	8	0.13
(4,460)	1:153:A:MET:HE2	1:35:A:PHE:HB2	8	0.13
(4,460)	1:153:A:MET:HE3	1:35:A:PHE:HB2	8	0.13
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB1	5	0.13
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB2	5	0.13
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB3	5	0.13
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	1	0.13
(4,404)	1:105:A:ARG:HA	1:105:A:ARG:HB2	3	0.13
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD11	1	0.13
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD12	1	0.13
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD13	1	0.13
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	7	0.13
(4,303)	1:129:A:ILE:HG21	1:126:A:ILE:HA	8	0.13
(4,303)	1:129:A:ILE:HG22	1:126:A:ILE:HA	8	0.13
(4,303)	1:129:A:ILE:HG23	1:126:A:ILE:HA	8	0.13
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	2	0.13
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	2	0.13
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	2	0.13
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	5	0.13
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	5	0.13
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	5	0.13
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	9	0.13
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	9	0.13
(4,286)	1:26:A:ILE:HG21	1:27:A:THR:HA	5	0.13
(4,286)	1:26:A:ILE:HG22	1:27:A:THR:HA	5	0.13
(4,286)	1:26:A:ILE:HG23	1:27:A:THR:HA	5	0.13
(4,279)	1:34:A:ARG:HD2	1:34:A:ARG:HA	4	0.13
(4,279)	1:34:A:ARG:HD2	1:34:A:ARG:HA	10	0.13
(4,272)	1:109:A:PHE:HB2	1:110:A:ASN:H	6	0.13
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	2	0.13
(4,238)	1:128:A:ALA:HB1	1:34:A:ARG:HD2	9	0.13
(4,238)	1:128:A:ALA:HB2	1:34:A:ARG:HD2	9	0.13
(4,238)	1:128:A:ALA:HB3	1:34:A:ARG:HD2	9	0.13
(4,234)	1:155:A:ASP:HA	1:38:A:PHE:HA	3	0.13
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	8	0.13
(4,128)	1:49:A:THR:HB	1:50:A:ALA:H	5	0.13
(4,128)	1:49:A:THR:HB	1:50:A:ALA:H	7	0.13
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG21	9	0.13
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG22	9	0.13
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG23	9	0.13
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG21	9	0.13
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG22	9	0.13
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG23	9	0.13
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG21	9	0.13
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG22	9	0.13
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG23	9	0.13
(4,111)	1:163:A:LEU:H	1:163:A:LEU:HG	4	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG21	1	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG22	1	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG23	1	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG21	1	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG22	1	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG23	1	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG21	1	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG22	1	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG23	1	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG21	7	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG22	7	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG23	7	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG21	7	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG22	7	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG23	7	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG21	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG22	7	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG23	7	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG21	9	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG22	9	0.13
(4,106)	1:18:A:ILE:HD11	1:154:A:ILE:HG23	9	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG21	9	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG22	9	0.13
(4,106)	1:18:A:ILE:HD12	1:154:A:ILE:HG23	9	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG21	9	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG22	9	0.13
(4,106)	1:18:A:ILE:HD13	1:154:A:ILE:HG23	9	0.13
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	5	0.13
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	5	0.13
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	5	0.13
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	5	0.13
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	5	0.13
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	5	0.13
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	5	0.13
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	5	0.13
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	5	0.13
(4,73)	1:154:A:ILE:HG21	1:140:A:ARG:HA	8	0.13
(4,73)	1:154:A:ILE:HG22	1:140:A:ARG:HA	8	0.13
(4,73)	1:154:A:ILE:HG23	1:140:A:ARG:HA	8	0.13
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG12	7	0.13
(4,53)	1:126:A:ILE:HG13	1:129:A:ILE:HG13	7	0.13
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG11	7	0.13
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG12	7	0.13
(4,48)	1:102:A:ILE:HD11	1:87:A:VAL:HG13	7	0.13
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG11	7	0.13
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG12	7	0.13
(4,48)	1:102:A:ILE:HD12	1:87:A:VAL:HG13	7	0.13
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG11	7	0.13
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG12	7	0.13
(4,48)	1:102:A:ILE:HD13	1:87:A:VAL:HG13	7	0.13
(4,33)	1:39:A:LEU:HD11	1:156:A:MET:HB3	1	0.13
(4,33)	1:39:A:LEU:HD12	1:156:A:MET:HB3	1	0.13
(4,33)	1:39:A:LEU:HD13	1:156:A:MET:HB3	1	0.13
(4,32)	1:87:A:VAL:HG21	1:90:A:LEU:HB3	6	0.13
(4,32)	1:87:A:VAL:HG22	1:90:A:LEU:HB3	6	0.13
(4,32)	1:87:A:VAL:HG23	1:90:A:LEU:HB3	6	0.13
(1,45)	1:142:A:VAL:H	1:153:A:MET:O	7	0.13
(1,5)	1:80:A:LEU:H	1:76:A:ARG:O	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	8	0.12
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	8	0.12
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	8	0.12
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	8	0.12
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	9	0.12
(4,736)	1:153:A:MET:HG3	1:153:A:MET:HA	4	0.12
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	2	0.12
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	2	0.12
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	2	0.12
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	2	0.12
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	2	0.12
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	2	0.12
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	2	0.12
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	2	0.12
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	2	0.12
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD21	3	0.12
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD22	3	0.12
(4,733)	1:71:A:ILE:HG21	1:137:A:LEU:HD23	3	0.12
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD21	3	0.12
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD22	3	0.12
(4,733)	1:71:A:ILE:HG22	1:137:A:LEU:HD23	3	0.12
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD21	3	0.12
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD22	3	0.12
(4,733)	1:71:A:ILE:HG23	1:137:A:LEU:HD23	3	0.12
(4,720)	1:114:A:ILE:HA	1:114:A:ILE:HB	4	0.12
(4,710)	1:61:A:ASP:HB2	1:64:A:ASP:H	2	0.12
(4,706)	1:58:A:ILE:HD11	1:162:A:GLU:HB2	1	0.12
(4,706)	1:58:A:ILE:HD12	1:162:A:GLU:HB2	1	0.12
(4,706)	1:58:A:ILE:HD13	1:162:A:GLU:HB2	1	0.12
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG21	2	0.12
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG22	2	0.12
(4,698)	1:19:A:PHE:H	1:18:A:ILE:HG23	2	0.12
(4,681)	1:84:A:VAL:HG11	1:85:A:GLU:HA	10	0.12
(4,681)	1:84:A:VAL:HG12	1:85:A:GLU:HA	10	0.12
(4,681)	1:84:A:VAL:HG13	1:85:A:GLU:HA	10	0.12
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG21	2	0.12
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG22	2	0.12
(4,661)	1:20:A:HIS:HA	1:55:A:THR:HG23	2	0.12
(4,654)	1:106:A:ILE:HD11	1:106:A:ILE:HA	10	0.12
(4,654)	1:106:A:ILE:HD12	1:106:A:ILE:HA	10	0.12
(4,654)	1:106:A:ILE:HD13	1:106:A:ILE:HA	10	0.12
(4,634)	1:91:A:THR:HB	1:91:A:THR:HA	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,634)	1:91:A:THR:HB	1:91:A:THR:HA	4	0.12
(4,630)	1:153:A:MET:H	1:143:A:SER:HA	8	0.12
(4,596)	1:47:A:VAL:HG21	1:48:A:MET:HA	2	0.12
(4,596)	1:47:A:VAL:HG22	1:48:A:MET:HA	2	0.12
(4,596)	1:47:A:VAL:HG23	1:48:A:MET:HA	2	0.12
(4,587)	1:111:A:LEU:H	1:111:A:LEU:HB3	9	0.12
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	1	0.12
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	1	0.12
(4,550)	1:127:A:GLN:HA	1:127:A:GLN:HG3	2	0.12
(4,541)	1:126:A:ILE:HG12	1:123:A:SER:HA	5	0.12
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG21	8	0.12
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG22	8	0.12
(4,529)	1:53:A:HIS:HB2	1:21:A:THR:HG23	8	0.12
(4,519)	1:153:A:MET:HE1	1:153:A:MET:HG2	7	0.12
(4,519)	1:153:A:MET:HE2	1:153:A:MET:HG2	7	0.12
(4,519)	1:153:A:MET:HE3	1:153:A:MET:HG2	7	0.12
(4,519)	1:153:A:MET:HE1	1:153:A:MET:HG2	8	0.12
(4,519)	1:153:A:MET:HE2	1:153:A:MET:HG2	8	0.12
(4,519)	1:153:A:MET:HE3	1:153:A:MET:HG2	8	0.12
(4,518)	1:58:A:ILE:HB	1:163:A:LEU:HA	8	0.12
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	4	0.12
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE1	4	0.12
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE2	4	0.12
(4,511)	1:142:A:VAL:HG11	1:144:A:MET:HE3	4	0.12
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE1	4	0.12
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE2	4	0.12
(4,511)	1:142:A:VAL:HG12	1:144:A:MET:HE3	4	0.12
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE1	4	0.12
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE2	4	0.12
(4,511)	1:142:A:VAL:HG13	1:144:A:MET:HE3	4	0.12
(4,478)	1:49:A:THR:HG21	1:49:A:THR:HA	10	0.12
(4,478)	1:49:A:THR:HG22	1:49:A:THR:HA	10	0.12
(4,478)	1:49:A:THR:HG23	1:49:A:THR:HA	10	0.12
(4,465)	1:27:A:THR:HG21	1:26:A:ILE:HA	3	0.12
(4,465)	1:27:A:THR:HG22	1:26:A:ILE:HA	3	0.12
(4,465)	1:27:A:THR:HG23	1:26:A:ILE:HA	3	0.12
(4,419)	1:20:A:HIS:HA	1:41:A:PHE:HA	5	0.12
(4,419)	1:20:A:HIS:HA	1:41:A:PHE:HA	7	0.12
(4,411)	1:113:A:ASP:HB3	1:114:A:ILE:H	9	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG11	5	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG12	5	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG13	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG11	8	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG12	8	0.12
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG13	8	0.12
(4,394)	1:150:A:THR:HG21	1:143:A:SER:HA	6	0.12
(4,394)	1:150:A:THR:HG22	1:143:A:SER:HA	6	0.12
(4,394)	1:150:A:THR:HG23	1:143:A:SER:HA	6	0.12
(4,394)	1:150:A:THR:HG21	1:143:A:SER:HA	8	0.12
(4,394)	1:150:A:THR:HG22	1:143:A:SER:HA	8	0.12
(4,394)	1:150:A:THR:HG23	1:143:A:SER:HA	8	0.12
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG21	4	0.12
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG22	4	0.12
(4,353)	1:18:A:ILE:H	1:58:A:ILE:HG23	4	0.12
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	10	0.12
(4,323)	1:32:A:GLN:HA	1:32:A:GLN:HG3	8	0.12
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	5	0.12
(4,303)	1:129:A:ILE:HG21	1:126:A:ILE:HA	9	0.12
(4,303)	1:129:A:ILE:HG22	1:126:A:ILE:HA	9	0.12
(4,303)	1:129:A:ILE:HG23	1:126:A:ILE:HA	9	0.12
(4,288)	1:112:A:ASP:H	1:111:A:LEU:HA	10	0.12
(4,267)	1:107:A:ASP:HB2	1:109:A:PHE:HB3	2	0.12
(4,267)	1:107:A:ASP:HB2	1:109:A:PHE:HB3	8	0.12
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	3	0.12
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	3	0.12
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	3	0.12
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	5	0.12
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	5	0.12
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	5	0.12
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	7	0.12
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	7	0.12
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	7	0.12
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	8	0.12
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	8	0.12
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	8	0.12
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	9	0.12
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	9	0.12
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	9	0.12
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	5	0.12
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG11	6	0.12
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG12	6	0.12
(4,135)	1:95:A:GLU:HA	1:87:A:VAL:HG13	6	0.12
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD11	8	0.12
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,132)	1:156:A:MET:HG2	1:29:A:ILE:HD13	8	0.12
(4,128)	1:49:A:THR:HB	1:50:A:ALA:H	4	0.12
(4,111)	1:163:A:LEU:H	1:163:A:LEU:HG	7	0.12
(4,96)	1:77:A:ALA:HB1	1:74:A:HIS:HB3	4	0.12
(4,96)	1:77:A:ALA:HB2	1:74:A:HIS:HB3	4	0.12
(4,96)	1:77:A:ALA:HB3	1:74:A:HIS:HB3	4	0.12
(4,87)	1:91:A:THR:HG21	1:125:A:GLU:H	3	0.12
(4,87)	1:91:A:THR:HG22	1:125:A:GLU:H	3	0.12
(4,87)	1:91:A:THR:HG23	1:125:A:GLU:H	3	0.12
(4,69)	1:153:A:MET:HE1	1:153:A:MET:HB2	8	0.12
(4,69)	1:153:A:MET:HE2	1:153:A:MET:HB2	8	0.12
(4,69)	1:153:A:MET:HE3	1:153:A:MET:HB2	8	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG21	4	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG22	4	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG23	4	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG21	4	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG22	4	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG23	4	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG21	4	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG22	4	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG23	4	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG21	6	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG22	6	0.12
(4,68)	1:144:A:MET:HE1	1:130:A:THR:HG23	6	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG21	6	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG22	6	0.12
(4,68)	1:144:A:MET:HE2	1:130:A:THR:HG23	6	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG21	6	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG22	6	0.12
(4,68)	1:144:A:MET:HE3	1:130:A:THR:HG23	6	0.12
(4,64)	1:54:A:VAL:HG11	1:25:A:GLU:HA	5	0.12
(4,64)	1:54:A:VAL:HG12	1:25:A:GLU:HA	5	0.12
(4,64)	1:54:A:VAL:HG13	1:25:A:GLU:HA	5	0.12
(4,63)	1:57:A:ARG:H	1:166:A:VAL:HG21	5	0.12
(4,63)	1:57:A:ARG:H	1:166:A:VAL:HG22	5	0.12
(4,63)	1:57:A:ARG:H	1:166:A:VAL:HG23	5	0.12
(4,42)	1:111:A:LEU:HD11	1:110:A:ASN:HB3	4	0.12
(4,42)	1:111:A:LEU:HD12	1:110:A:ASN:HB3	4	0.12
(4,42)	1:111:A:LEU:HD13	1:110:A:ASN:HB3	4	0.12
(4,32)	1:87:A:VAL:HG21	1:90:A:LEU:HB3	4	0.12
(4,32)	1:87:A:VAL:HG22	1:90:A:LEU:HB3	4	0.12
(4,32)	1:87:A:VAL:HG23	1:90:A:LEU:HB3	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:87:A:VAL:HG21	1:90:A:LEU:HB3	9	0.12
(4,32)	1:87:A:VAL:HG22	1:90:A:LEU:HB3	9	0.12
(4,32)	1:87:A:VAL:HG23	1:90:A:LEU:HB3	9	0.12
(4,22)	1:59:A:LYS:HA	1:59:A:LYS:HD2	6	0.12
(4,15)	1:130:A:THR:HG21	1:104:A:GLN:HB3	3	0.12
(4,15)	1:130:A:THR:HG22	1:104:A:GLN:HB3	3	0.12
(4,15)	1:130:A:THR:HG23	1:104:A:GLN:HB3	3	0.12
(4,13)	1:54:A:VAL:H	1:23:A:PRO:HA	3	0.12
(4,13)	1:54:A:VAL:H	1:23:A:PRO:HA	7	0.12
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	3	0.12
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	3	0.12
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	3	0.12
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	3	0.12
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	3	0.12
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	3	0.12
(2,315)	1:47:A:VAL:HG11	1:46:A:TYR:HA	6	0.12
(2,315)	1:47:A:VAL:HG12	1:46:A:TYR:HA	6	0.12
(2,315)	1:47:A:VAL:HG13	1:46:A:TYR:HA	6	0.12
(2,315)	1:47:A:VAL:HG21	1:46:A:TYR:HA	6	0.12
(2,315)	1:47:A:VAL:HG22	1:46:A:TYR:HA	6	0.12
(2,315)	1:47:A:VAL:HG23	1:46:A:TYR:HA	6	0.12
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD11	7	0.12
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD12	7	0.12
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD13	7	0.12
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD21	7	0.12
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD22	7	0.12
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD23	7	0.12
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD11	7	0.12
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD12	7	0.12
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD13	7	0.12
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD21	7	0.12
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD22	7	0.12
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD23	7	0.12
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD11	7	0.12
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD12	7	0.12
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD13	7	0.12
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD21	7	0.12
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD22	7	0.12
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD23	7	0.12
(2,144)	1:75:A:GLU:H	1:75:A:GLU:HA	9	0.12
(2,57)	1:41:A:PHE:HB2	1:18:A:ILE:HG21	1	0.12
(2,57)	1:41:A:PHE:HB2	1:18:A:ILE:HG22	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:41:A:PHE:HB2	1:18:A:ILE:HG23	1	0.12
(2,57)	1:41:A:PHE:HB3	1:18:A:ILE:HG21	1	0.12
(2,57)	1:41:A:PHE:HB3	1:18:A:ILE:HG22	1	0.12
(2,57)	1:41:A:PHE:HB3	1:18:A:ILE:HG23	1	0.12
(2,41)	1:100:A:GLU:H	1:97:A:THR:HA	4	0.12
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HB2	6	0.12
(2,1)	1:40:A:CYS:H	1:40:A:CYS:HB2	8	0.12
(2,1)	1:40:A:CYS:H	1:40:A:CYS:HB3	8	0.12
(1,55)	1:150:A:THR:H	1:43:A:ALA:O	2	0.12
(1,45)	1:142:A:VAL:H	1:153:A:MET:O	1	0.12
(1,43)	1:164:A:VAL:H	1:57:A:ARG:O	5	0.12
(1,17)	1:117:A:SER:O	1:121:A:GLU:H	1	0.12
(1,8)	1:85:A:GLU:H	1:81:A:SER:O	10	0.12
(1,3)	1:78:A:ALA:H	1:74:A:HIS:O	9	0.12
(4,767)	1:128:A:ALA:HA	1:35:A:PHE:HA	5	0.11
(4,760)	1:153:A:MET:HE1	1:38:A:PHE:HB2	10	0.11
(4,760)	1:153:A:MET:HE2	1:38:A:PHE:HB2	10	0.11
(4,760)	1:153:A:MET:HE3	1:38:A:PHE:HB2	10	0.11
(4,757)	1:137:A:LEU:H	1:134:A:ALA:HA	3	0.11
(4,757)	1:137:A:LEU:H	1:134:A:ALA:HA	5	0.11
(4,738)	1:55:A:THR:HG21	1:166:A:VAL:HB	5	0.11
(4,738)	1:55:A:THR:HG22	1:166:A:VAL:HB	5	0.11
(4,738)	1:55:A:THR:HG23	1:166:A:VAL:HB	5	0.11
(4,721)	1:109:A:PHE:H	1:109:A:PHE:HA	2	0.11
(4,721)	1:109:A:PHE:H	1:109:A:PHE:HA	7	0.11
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG11	10	0.11
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG12	10	0.11
(4,709)	1:142:A:VAL:HA	1:142:A:VAL:HG13	10	0.11
(4,701)	1:155:A:ASP:HB3	1:154:A:ILE:HG21	8	0.11
(4,701)	1:155:A:ASP:HB3	1:154:A:ILE:HG22	8	0.11
(4,701)	1:155:A:ASP:HB3	1:154:A:ILE:HG23	8	0.11
(4,694)	1:105:A:ARG:HD2	1:105:A:ARG:H	5	0.11
(4,693)	1:23:A:PRO:HD2	1:23:A:PRO:HA	9	0.11
(4,687)	1:85:A:GLU:HG2	1:85:A:GLU:HA	9	0.11
(4,687)	1:85:A:GLU:HG3	1:85:A:GLU:HA	9	0.11
(4,673)	1:15:A:ARG:HD3	1:12:A:GLN:HB2	4	0.11
(4,671)	1:106:A:ILE:HD11	1:110:A:ASN:H	10	0.11
(4,671)	1:106:A:ILE:HD12	1:110:A:ASN:H	10	0.11
(4,671)	1:106:A:ILE:HD13	1:110:A:ASN:H	10	0.11
(4,645)	1:121:A:GLU:HG3	1:121:A:GLU:HA	4	0.11
(4,641)	1:166:A:VAL:HB	1:55:A:THR:HB	7	0.11
(4,641)	1:166:A:VAL:HB	1:55:A:THR:HB	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,605)	1:26:A:ILE:HD11	1:26:A:ILE:H	5	0.11
(4,605)	1:26:A:ILE:HD12	1:26:A:ILE:H	5	0.11
(4,605)	1:26:A:ILE:HD13	1:26:A:ILE:H	5	0.11
(4,588)	1:147:A:GLU:HA	1:147:A:GLU:H	9	0.11
(4,558)	1:129:A:ILE:H	1:129:A:ILE:HB	10	0.11
(4,555)	1:34:A:ARG:HA	1:34:A:ARG:HG3	3	0.11
(4,552)	1:29:A:ILE:HG21	1:29:A:ILE:HA	3	0.11
(4,552)	1:29:A:ILE:HG22	1:29:A:ILE:HA	3	0.11
(4,552)	1:29:A:ILE:HG23	1:29:A:ILE:HA	3	0.11
(4,519)	1:153:A:MET:HE1	1:153:A:MET:HG2	4	0.11
(4,519)	1:153:A:MET:HE2	1:153:A:MET:HG2	4	0.11
(4,519)	1:153:A:MET:HE3	1:153:A:MET:HG2	4	0.11
(4,518)	1:58:A:ILE:HB	1:163:A:LEU:HA	5	0.11
(4,501)	1:105:A:ARG:HA	1:106:A:ILE:H	5	0.11
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG21	4	0.11
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG22	4	0.11
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG23	4	0.11
(4,478)	1:49:A:THR:HG21	1:49:A:THR:HA	1	0.11
(4,478)	1:49:A:THR:HG22	1:49:A:THR:HA	1	0.11
(4,478)	1:49:A:THR:HG23	1:49:A:THR:HA	1	0.11
(4,473)	1:150:A:THR:H	1:150:A:THR:HB	1	0.11
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB1	3	0.11
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB2	3	0.11
(4,414)	1:116:A:ALA:HA	1:120:A:ALA:HB3	3	0.11
(4,409)	1:167:A:LYS:H	1:165:A:ARG:HA	3	0.11
(4,346)	1:53:A:HIS:HB3	1:21:A:THR:HB	1	0.11
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	2	0.11
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	1	0.11
(4,320)	1:166:A:VAL:HA	1:165:A:ARG:HG2	3	0.11
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	8	0.11
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	8	0.11
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	8	0.11
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	8	0.11
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG21	7	0.11
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG22	7	0.11
(4,270)	1:29:A:ILE:HB	1:31:A:THR:HG23	7	0.11
(4,267)	1:107:A:ASP:HB2	1:109:A:PHE:HB3	5	0.11
(4,235)	1:122:A:LEU:HA	1:125:A:GLU:HG3	2	0.11
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	1	0.11
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	1	0.11
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	1	0.11
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	4	0.11
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	4	0.11
(4,198)	1:2:A:SER:HA	1:2:A:SER:HB2	8	0.11
(4,197)	1:46:A:TYR:HA	1:46:A:TYR:H	1	0.11
(4,197)	1:46:A:TYR:HA	1:46:A:TYR:H	4	0.11
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	3	0.11
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	7	0.11
(4,186)	1:53:A:HIS:HB3	1:23:A:PRO:HA	9	0.11
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG21	5	0.11
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG22	5	0.11
(4,121)	1:18:A:ILE:HD11	1:60:A:VAL:HG23	5	0.11
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG21	5	0.11
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG22	5	0.11
(4,121)	1:18:A:ILE:HD12	1:60:A:VAL:HG23	5	0.11
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG21	5	0.11
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG22	5	0.11
(4,121)	1:18:A:ILE:HD13	1:60:A:VAL:HG23	5	0.11
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG21	4	0.11
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG22	4	0.11
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG23	4	0.11
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG21	4	0.11
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG22	4	0.11
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG23	4	0.11
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG21	4	0.11
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG22	4	0.11
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG23	4	0.11
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD21	3	0.11
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD22	3	0.11
(4,114)	1:58:A:ILE:HD11	1:163:A:LEU:HD23	3	0.11
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD21	3	0.11
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD22	3	0.11
(4,114)	1:58:A:ILE:HD12	1:163:A:LEU:HD23	3	0.11
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD21	3	0.11
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD22	3	0.11
(4,114)	1:58:A:ILE:HD13	1:163:A:LEU:HD23	3	0.11
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	8	0.11
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	8	0.11
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	8	0.11
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	8	0.11
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	8	0.11
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	8	0.11
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	8	0.11
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	8	0.11
(4,42)	1:111:A:LEU:HD11	1:110:A:ASN:HB3	9	0.11
(4,42)	1:111:A:LEU:HD12	1:110:A:ASN:HB3	9	0.11
(4,42)	1:111:A:LEU:HD13	1:110:A:ASN:HB3	9	0.11
(4,26)	1:163:A:LEU:HD21	1:56:A:TYR:HB3	3	0.11
(4,26)	1:163:A:LEU:HD22	1:56:A:TYR:HB3	3	0.11
(4,26)	1:163:A:LEU:HD23	1:56:A:TYR:HB3	3	0.11
(4,5)	1:127:A:GLN:HA	1:126:A:ILE:HB	8	0.11
(2,334)	1:144:A:MET:HG2	1:151:A:CYS:HB3	7	0.11
(2,334)	1:144:A:MET:HG3	1:151:A:CYS:HB3	7	0.11
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG2	6	0.11
(2,328)	1:87:A:VAL:HG11	1:86:A:ARG:HG3	6	0.11
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG2	6	0.11
(2,328)	1:87:A:VAL:HG12	1:86:A:ARG:HG3	6	0.11
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG2	6	0.11
(2,328)	1:87:A:VAL:HG13	1:86:A:ARG:HG3	6	0.11
(2,229)	1:3:A:HIS:H	1:2:A:SER:HB2	1	0.11
(2,153)	1:54:A:VAL:HG21	1:25:A:GLU:HA	3	0.11
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HG3	3	0.11
(2,27)	1:32:A:GLN:HA	1:32:A:GLN:HB2	8	0.11
(1,17)	1:117:A:SER:O	1:121:A:GLU:H	6	0.11
(1,5)	1:80:A:LEU:H	1:76:A:ARG:O	4	0.11
(4,779)	1:130:A:THR:H	1:127:A:GLN:HA	4	0.1
(4,771)	1:137:A:LEU:HG	1:137:A:LEU:HA	8	0.1
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD21	6	0.1
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD22	6	0.1
(4,770)	1:71:A:ILE:HA	1:137:A:LEU:HD23	6	0.1
(4,764)	1:18:A:ILE:HG21	1:16:A:MET:HB2	4	0.1
(4,764)	1:18:A:ILE:HG22	1:16:A:MET:HB2	4	0.1
(4,764)	1:18:A:ILE:HG23	1:16:A:MET:HB2	4	0.1
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG21	8	0.1
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG22	8	0.1
(4,755)	1:127:A:GLN:HG2	1:130:A:THR:HG23	8	0.1
(4,751)	1:167:A:LYS:H	1:54:A:VAL:HA	7	0.1
(4,724)	1:29:A:ILE:HD11	1:30:A:ASN:H	8	0.1
(4,724)	1:29:A:ILE:HD12	1:30:A:ASN:H	8	0.1
(4,724)	1:29:A:ILE:HD13	1:30:A:ASN:H	8	0.1
(4,715)	1:128:A:ALA:H	1:125:A:GLU:HA	4	0.1
(4,683)	1:150:A:THR:HG21	1:143:A:SER:HB2	2	0.1
(4,683)	1:150:A:THR:HG22	1:143:A:SER:HB2	2	0.1
(4,683)	1:150:A:THR:HG23	1:143:A:SER:HB2	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,648)	1:151:A:CYS:HB3	1:151:A:CYS:HA	8	0.1
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE1	3	0.1
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE2	3	0.1
(4,612)	1:153:A:MET:HG2	1:144:A:MET:HE3	3	0.1
(4,518)	1:58:A:ILE:HB	1:163:A:LEU:HA	3	0.1
(4,513)	1:26:A:ILE:HG12	1:26:A:ILE:H	6	0.1
(4,501)	1:105:A:ARG:HA	1:106:A:ILE:H	2	0.1
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG21	1	0.1
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG22	1	0.1
(4,483)	1:127:A:GLN:HA	1:126:A:ILE:HG23	1	0.1
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG11	9	0.1
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG12	9	0.1
(4,397)	1:57:A:ARG:H	1:166:A:VAL:HG13	9	0.1
(4,334)	1:34:A:ARG:HA	1:35:A:PHE:H	1	0.1
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD11	3	0.1
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD12	3	0.1
(4,333)	1:142:A:VAL:H	1:154:A:ILE:HD13	3	0.1
(4,299)	1:106:A:ILE:HD11	1:111:A:LEU:H	3	0.1
(4,299)	1:106:A:ILE:HD12	1:111:A:LEU:H	3	0.1
(4,299)	1:106:A:ILE:HD13	1:111:A:LEU:H	3	0.1
(4,287)	1:21:A:THR:HG21	1:55:A:THR:HA	4	0.1
(4,287)	1:21:A:THR:HG22	1:55:A:THR:HA	4	0.1
(4,287)	1:21:A:THR:HG23	1:55:A:THR:HA	4	0.1
(4,271)	1:104:A:GLN:HA	1:104:A:GLN:HG3	1	0.1
(4,230)	1:111:A:LEU:HD11	1:111:A:LEU:HB3	9	0.1
(4,230)	1:111:A:LEU:HD12	1:111:A:LEU:HB3	9	0.1
(4,230)	1:111:A:LEU:HD13	1:111:A:LEU:HB3	9	0.1
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG21	4	0.1
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG22	4	0.1
(4,205)	1:155:A:ASP:HB2	1:154:A:ILE:HG23	4	0.1
(4,197)	1:46:A:TYR:HA	1:46:A:TYR:H	3	0.1
(4,197)	1:46:A:TYR:HA	1:46:A:TYR:H	6	0.1
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB1	10	0.1
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB2	10	0.1
(4,167)	1:162:A:GLU:HG2	1:161:A:ALA:HB3	10	0.1
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE1	4	0.1
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE2	4	0.1
(4,143)	1:143:A:SER:HA	1:144:A:MET:HE3	4	0.1
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG21	8	0.1
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG22	8	0.1
(4,119)	1:58:A:ILE:HD11	1:60:A:VAL:HG23	8	0.1
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG21	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG22	8	0.1
(4,119)	1:58:A:ILE:HD12	1:60:A:VAL:HG23	8	0.1
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG21	8	0.1
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG22	8	0.1
(4,119)	1:58:A:ILE:HD13	1:60:A:VAL:HG23	8	0.1
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	3	0.1
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	3	0.1
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	3	0.1
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	3	0.1
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	3	0.1
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	3	0.1
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	3	0.1
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	3	0.1
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	3	0.1
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD11	7	0.1
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD12	7	0.1
(4,104)	1:58:A:ILE:HD11	1:154:A:ILE:HD13	7	0.1
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD11	7	0.1
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD12	7	0.1
(4,104)	1:58:A:ILE:HD12	1:154:A:ILE:HD13	7	0.1
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD11	7	0.1
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD12	7	0.1
(4,104)	1:58:A:ILE:HD13	1:154:A:ILE:HD13	7	0.1
(4,74)	1:39:A:LEU:HD21	1:156:A:MET:HB2	6	0.1
(4,74)	1:39:A:LEU:HD22	1:156:A:MET:HB2	6	0.1
(4,74)	1:39:A:LEU:HD23	1:156:A:MET:HB2	6	0.1
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE1	5	0.1
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE2	5	0.1
(4,65)	1:152:A:TYR:HA	1:144:A:MET:HE3	5	0.1
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB1	1	0.1
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB2	1	0.1
(4,27)	1:111:A:LEU:H	1:116:A:ALA:HB3	1	0.1
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD11	4	0.1
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD12	4	0.1
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD13	4	0.1
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD21	4	0.1
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD22	4	0.1
(2,228)	1:154:A:ILE:HG21	1:157:A:LEU:HD23	4	0.1
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD11	4	0.1
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD12	4	0.1
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD13	4	0.1
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD21	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD22	4	0.1
(2,228)	1:154:A:ILE:HG22	1:157:A:LEU:HD23	4	0.1
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD11	4	0.1
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD12	4	0.1
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD13	4	0.1
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD21	4	0.1
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD22	4	0.1
(2,228)	1:154:A:ILE:HG23	1:157:A:LEU:HD23	4	0.1
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	6	0.1
(2,223)	1:60:A:VAL:HA	1:15:A:ARG:HD2	8	0.1
(2,144)	1:75:A:GLU:H	1:74:A:HIS:HA	8	0.1
(2,39)	1:73:A:TYR:H	1:72:A:PHE:HA	6	0.1
(1,45)	1:142:A:VAL:H	1:153:A:MET:O	9	0.1
(1,15)	1:96:A:ASP:O	1:100:A:GLU:H	5	0.1

10 Dihedral-angle violation analysis [i](#)

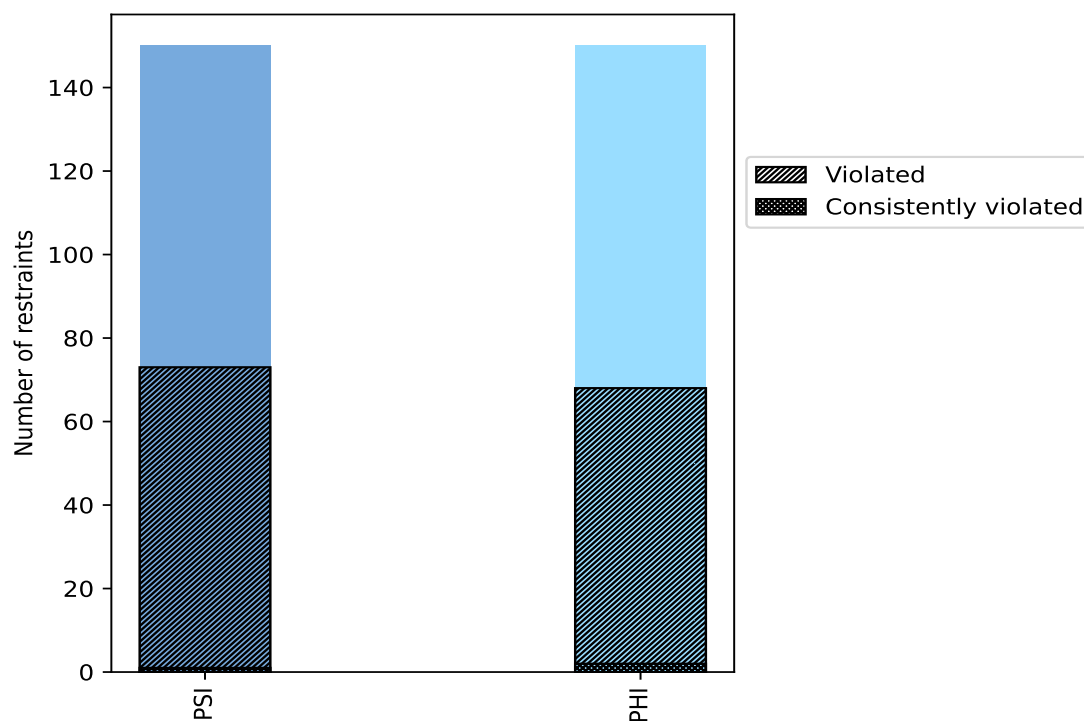
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	150	50.0	73	48.7	24.3	1	0.7	0.3
PHI	150	50.0	68	45.3	22.7	2	1.3	0.7
Total	300	100.0	141	47.0	47.0	3	1.0	1.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



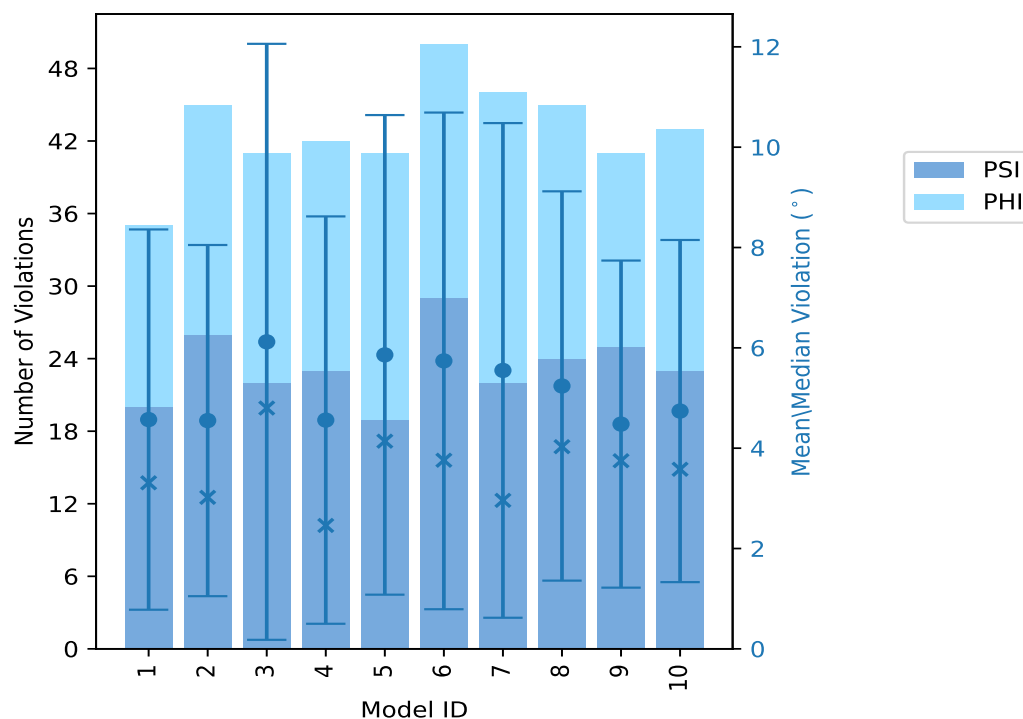
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	20	15	35	4.57	18.68	3.79	3.31
2	26	19	45	4.55	14.3	3.5	3.02
3	22	19	41	6.12	28.21	5.94	4.8
4	23	19	42	4.56	16.36	4.06	2.46
5	19	22	41	5.86	22.39	4.78	4.14
6	29	21	50	5.74	19.58	4.95	3.76
7	22	24	46	5.55	18.12	4.93	2.96
8	24	21	45	5.24	15.29	3.88	4.03
9	25	16	41	4.48	12.92	3.26	3.75
10	23	20	43	4.74	14.63	3.41	3.58

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

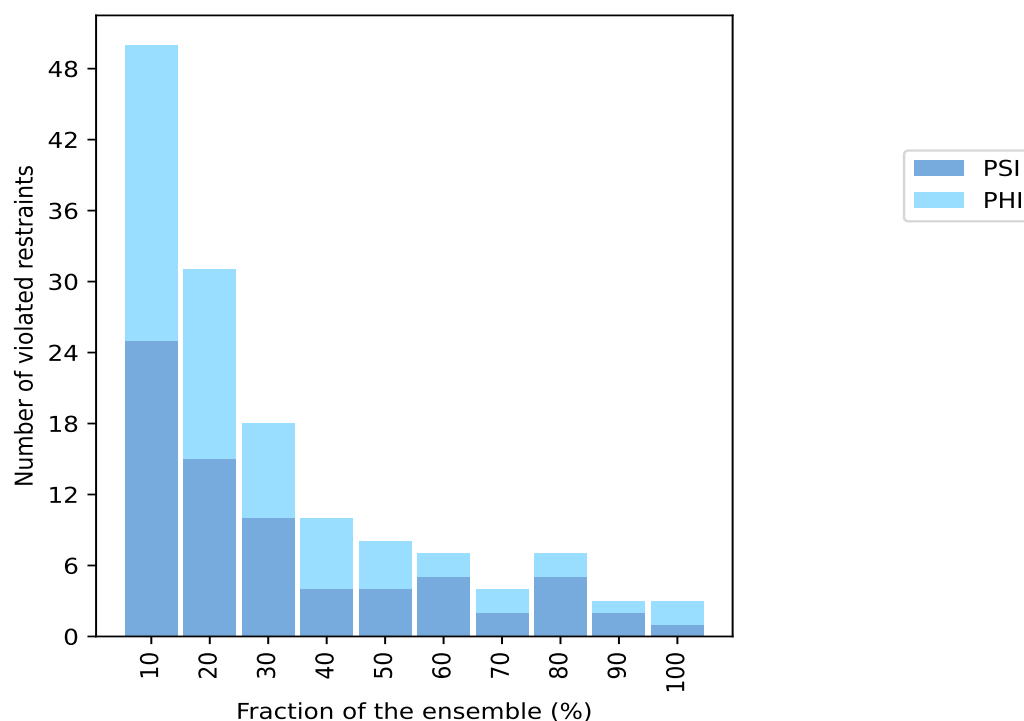
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count ¹	%
25	25	50	1	10.0
15	16	31	2	20.0
10	8	18	3	30.0
4	6	10	4	40.0
4	4	8	5	50.0
5	2	7	6	60.0
2	2	4	7	70.0
5	2	7	8	80.0
2	1	3	9	90.0
1	2	3	10	100.0

¹ Number of models with violations

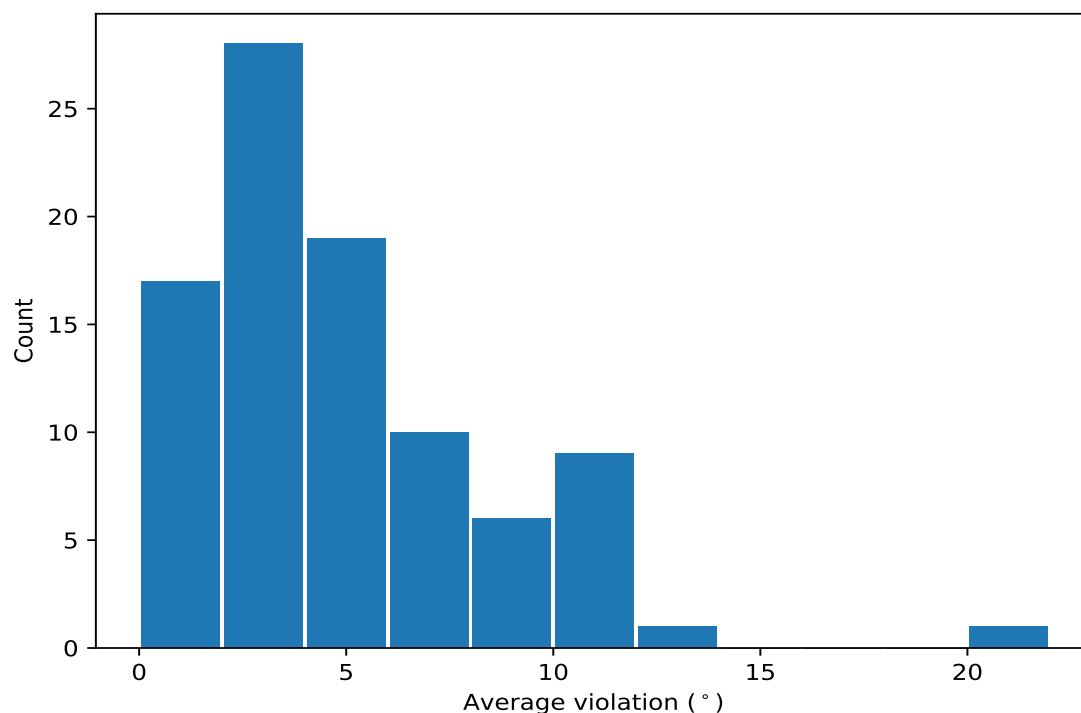
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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 [i](#)

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
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	10	10.84	2.84	11.88
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	10	10.75	2.12	11.45
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	10	5.92	3.34	5.58
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	9	7.38	3.23	6.97
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	9	6.52	2.42	6.1
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	9	5.91	2.76	6.57
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	8	9.54	6.17	7.32
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	8	8.65	2.4	7.78
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	8	7.85	3.89	8.2
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	8	5.96	3.4	5.04
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	8	5.14	1.94	6.15
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	8	3.0	0.96	3.0
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	8	2.76	1.08	2.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	7	8.92	2.82	9.18
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	7	7.2	8.81	3.05
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	7	4.58	3.86	1.95
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	7	3.02	2.35	2.23
(1,254)	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1:142:A:VAL:N	6	11.06	4.43	10.7
(1,255)	1:141:A:GLY:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	6	9.08	4.75	7.14
(1,156)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:THR:N	6	5.83	5.89	2.04
(1,262)	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	1:146:A:ASP:N	6	4.56	1.34	3.92
(1,46)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:GLY:N	6	2.43	0.95	2.24
(1,44)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	6	2.24	0.47	2.13
(1,197)	1:111:A:LEU:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	6	2.11	0.53	2.12
(1,260)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:GLN:N	5	5.97	4.43	3.21
(1,248)	1:138:A:GLY:N	1:138:A:GLY:CA	1:138:A:GLY:C	1:139:A:PHE:N	5	4.02	2.65	3.45
(1,133)	1:78:A:ALA:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	5	3.64	4.59	1.23
(1,99)	1:61:A:ASP:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	5	3.07	1.14	2.26
(1,50)	1:35:A:PHE:N	1:35:A:PHE:CA	1:35:A:PHE:C	1:36:A:GLY:N	5	2.99	0.87	2.68
(1,123)	1:73:A:TYR:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	5	2.88	2.7	1.8
(1,66)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:ASP:N	5	2.18	0.84	1.67
(1,131)	1:77:A:ALA:C	1:78:A:ALA:N	1:78:A:ALA:CA	1:78:A:ALA:C	5	1.82	0.59	1.64
(1,271)	1:149:A:GLY:C	1:150:A:THR:N	1:150:A:THR:CA	1:150:A:THR:C	4	10.41	0.96	10.65
(1,104)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:ILE:N	4	6.78	4.7	5.33
(1,251)	1:139:A:PHE:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	4	6.52	4.9	4.78
(1,289)	1:159:A:HIS:C	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	4	5.04	1.38	5.58
(1,264)	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	1:147:A:GLU:N	4	4.53	3.66	3.26
(1,278)	1:153:A:MET:N	1:153:A:MET:CA	1:153:A:MET:C	1:154:A:ILE:N	4	4.2	1.06	4.29
(1,285)	1:156:A:MET:C	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	4	4.05	1.19	4.36
(1,284)	1:156:A:MET:N	1:156:A:MET:CA	1:156:A:MET:C	1:157:A:LEU:N	4	2.62	0.86	2.92
(1,37)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	4	1.61	0.41	1.51
(1,21)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	4	1.34	0.17	1.4
(1,135)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	3	10.41	11.95	2.37
(1,105)	1:64:A:ASP:C	1:65:A:ILE:N	1:65:A:ILE:CA	1:65:A:ILE:C	3	10.22	5.86	7.33
(1,200)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:ASP:N	3	8.33	1.85	8.83
(1,201)	1:114:A:ILE:C	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	3	6.38	1.28	6.64
(1,122)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:HIS:N	3	5.52	2.87	3.75
(1,263)	1:145:A:GLN:C	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	3	5.39	0.42	5.59
(1,40)	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1:29:A:ILE:N	3	4.31	4.09	1.61
(1,202)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ALA:N	3	3.24	0.46	3.37
(1,12)	1:12:A:GLN:N	1:12:A:GLN:CA	1:12:A:GLN:C	1:13:A:MET:N	3	3.05	1.19	2.62
(1,259)	1:143:A:SER:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	3	2.93	1.21	3.47
(1,84)	1:54:A:VAL:N	1:54:A:VAL:CA	1:54:A:VAL:C	1:55:A:THR:N	3	2.51	0.17	2.39
(1,78)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:GLY:N	3	2.13	0.81	2.38
(1,148)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:VAL:N	3	2.02	1.38	1.07
(1,14)	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1:14:A:GLY:N	3	1.94	0.3	2.14
(1,25)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	3	1.88	0.76	1.57
(1,65)	1:42:A:ALA:C	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	3	1.66	0.13	1.69
(1,39)	1:27:A:THR:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	3	1.64	0.46	1.46
(1,28)	1:21:A:THR:N	1:21:A:THR:CA	1:21:A:THR:C	1:22:A:SER:N	3	1.37	0.37	1.18
(1,160)	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	1:93:A:CYS:N	2	20.26	2.13	20.26
(1,261)	1:144:A:MET:C	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	2	13.73	0.91	13.73
(1,161)	1:92:A:GLY:C	1:93:A:CYS:N	1:93:A:CYS:CA	1:93:A:CYS:C	2	11.86	1.74	11.86
(1,157)	1:90:A:LEU:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	2	11.25	1.11	11.25

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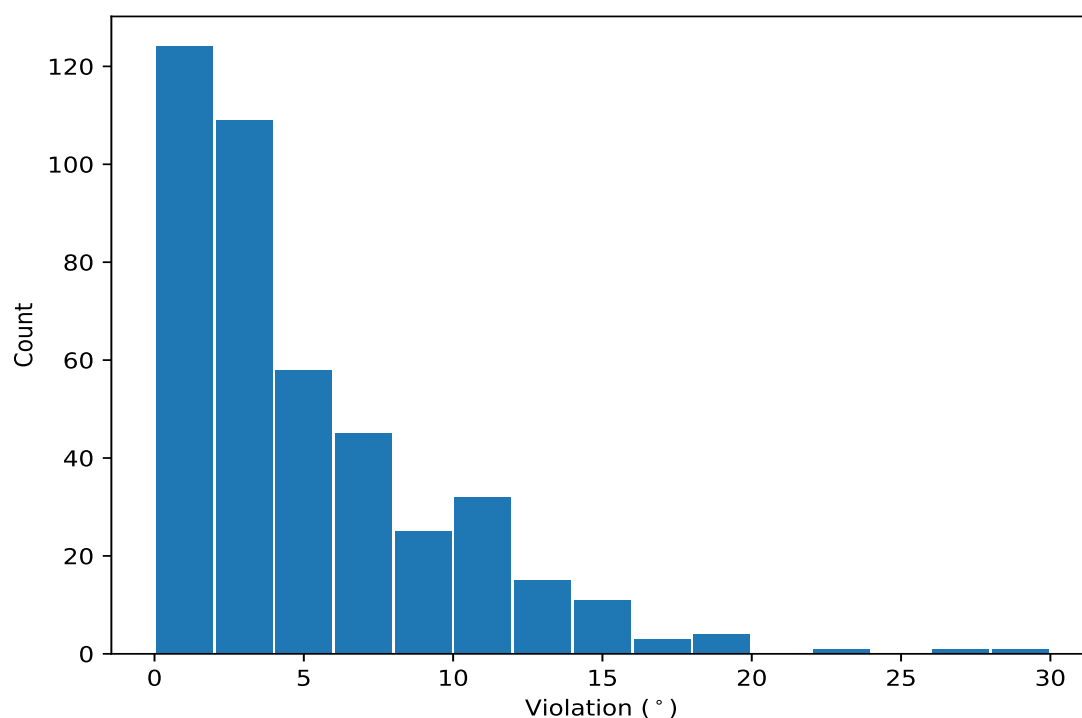
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,159)	1:91:A:THR:C	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	2	10.15	0.45	10.15
(1,250)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ARG:N	2	8.72	5.74	8.72
(1,158)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:GLY:N	2	7.24	0.35	7.24
(1,60)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	1:41:A:PHE:N	2	6.74	3.78	6.74
(1,124)	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	1:75:A:GLU:N	2	6.03	0.88	6.03
(1,59)	1:39:A:LEU:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	2	5.25	3.67	5.25
(1,38)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:THR:N	2	4.24	1.88	4.24
(1,162)	1:93:A:CYS:N	1:93:A:CYS:CA	1:93:A:CYS:C	1:94:A:ASP:N	2	4.04	2.22	4.04
(1,136)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:SER:N	2	3.56	1.36	3.56
(1,119)	1:71:A:ILE:C	1:72:A:PHE:N	1:72:A:PHE:CA	1:72:A:PHE:C	2	3.46	2.22	3.46
(1,100)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:SER:N	2	3.42	0.61	3.42
(1,57)	1:38:A:PHE:C	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	2	3.28	0.97	3.28
(1,198)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:ASP:N	2	2.92	1.2	2.92
(1,194)	1:110:A:ASN:N	1:110:A:ASN:CA	1:110:A:ASN:C	1:111:A:LEU:N	2	2.63	0.44	2.63
(1,113)	1:68:A:ALA:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	2	2.62	1.1	2.62
(1,102)	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	1:64:A:ASP:N	2	2.46	1.44	2.46
(1,205)	1:116:A:ALA:C	1:117:A:SER:N	1:117:A:SER:CA	1:117:A:SER:C	2	2.12	0.43	2.12
(1,89)	1:56:A:TYR:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	2	2.04	0.44	2.04
(1,153)	1:88:A:MET:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	2	1.84	0.66	1.84
(1,8)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:GLY:N	2	1.71	0.08	1.71
(1,137)	1:80:A:LEU:C	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	2	1.64	0.32	1.64
(1,56)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:LEU:N	2	1.63	0.37	1.63
(1,63)	1:41:A:PHE:C	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	2	1.62	0.18	1.62
(1,190)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:PHE:N	2	1.54	0.47	1.54
(1,45)	1:31:A:THR:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	2	1.5	0.15	1.5
(1,27)	1:20:A:HIS:C	1:21:A:THR:N	1:21:A:THR:CA	1:21:A:THR:C	2	1.42	0.16	1.42
(1,85)	1:54:A:VAL:C	1:55:A:THR:N	1:55:A:THR:CA	1:55:A:THR:C	2	1.33	0.01	1.33

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	3	28.21
(1,135)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	3	27.31
(1,160)	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	1:93:A:CYS:N	5	22.39
(1,254)	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1:142:A:VAL:N	6	19.58
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	1	18.68
(1,105)	1:64:A:ASP:C	1:65:A:ILE:N	1:65:A:ILE:CA	1:65:A:ILE:C	6	18.39
(1,160)	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	1:93:A:CYS:N	7	18.12
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	4	16.36
(1,255)	1:141:A:GLY:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	6	16.34
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	7	16.25
(1,156)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:THR:N	7	15.71
(1,121)	1:72:A:PHE:C	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	8	15.29
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	4	14.78
(1,251)	1:139:A:PHE:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	6	14.73
(1,261)	1:144:A:MET:C	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	10	14.63
(1,255)	1:141:A:GLY:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	10	14.52
(1,104)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:ILE:N	6	14.52
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	7	14.52
(1,250)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ARG:N	6	14.46
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	7	14.37
(1,260)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:GLN:N	2	14.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	8	13.63
(1,161)	1:92:A:GLY:C	1:93:A:CYS:N	1:93:A:CYS:CA	1:93:A:CYS:C	5	13.59
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	5	13.41
(1,120)	1:72:A:PHE:N	1:72:A:PHE:CA	1:72:A:PHE:C	1:73:A:TYR:N	8	13.33
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	6	13.05
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	9	12.92
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	7	12.88
(1,261)	1:144:A:MET:C	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	2	12.82
(1,133)	1:78:A:ALA:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	3	12.8
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	3	12.7
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	2	12.5
(1,157)	1:90:A:LEU:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	7	12.36
(1,156)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:THR:N	5	12.36
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	6	12.31
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	4	12.16
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	9	11.91
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	3	11.84
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	7	11.84
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1	11.64
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	7	11.57
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	5	11.55
(1,254)	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1:142:A:VAL:N	3	11.51
(1,271)	1:149:A:GLY:C	1:150:A:THR:N	1:150:A:THR:CA	1:150:A:THR:C	5	11.43
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	8	11.35
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	1	11.17
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	4	11.11
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	1	11.1
(1,271)	1:149:A:GLY:C	1:150:A:THR:N	1:150:A:THR:CA	1:150:A:THR:C	9	11.04
(1,254)	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1:142:A:VAL:N	10	11.01
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	2	11.01
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	8	10.86
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	4	10.86
(1,159)	1:91:A:THR:C	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	5	10.6
(1,60)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	1:41:A:PHE:N	8	10.52
(1,264)	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	1:147:A:GLU:N	9	10.49
(1,254)	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1:142:A:VAL:N	4	10.39
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	5	10.39
(1,200)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:ASP:N	9	10.31
(1,271)	1:149:A:GLY:C	1:150:A:THR:N	1:150:A:THR:CA	1:150:A:THR:C	8	10.26
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	10	10.25
(1,157)	1:90:A:LEU:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	5	10.14
(1,161)	1:92:A:GLY:C	1:93:A:CYS:N	1:93:A:CYS:CA	1:93:A:CYS:C	7	10.12
(1,106)	1:65:A:ILE:N	1:65:A:ILE:CA	1:65:A:ILE:C	1:66:A:ILE:N	6	10.1
(1,40)	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1:29:A:ILE:N	10	10.08
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	2	10.05
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	4	10.04
(1,61)	1:40:A:CYS:C	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	8	10.0
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	6	9.74
(1,159)	1:91:A:THR:C	1:92:A:GLY:N	1:92:A:GLY:CA	1:92:A:GLY:C	7	9.7
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	3	9.63
(1,122)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:HIS:N	8	9.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	2	9.56
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	5	9.52
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	2	9.5
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	9	9.38
(1,254)	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1:142:A:VAL:N	5	9.24
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	3	9.18
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	5	9.13
(1,271)	1:149:A:GLY:C	1:150:A:THR:N	1:150:A:THR:CA	1:150:A:THR:C	1	8.92
(1,59)	1:39:A:LEU:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	8	8.92
(1,200)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:ASP:N	6	8.83
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	4	8.76
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	5	8.76
(1,248)	1:138:A:GLY:N	1:138:A:GLY:CA	1:138:A:GLY:C	1:139:A:PHE:N	6	8.7
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	4	8.67
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	7	8.61
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	10	8.38
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	7	8.37
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	2	8.34
(1,123)	1:73:A:TYR:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	8	8.26
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	3	8.15
(1,107)	1:65:A:ILE:C	1:66:A:ILE:N	1:66:A:ILE:CA	1:66:A:ILE:C	6	8.14
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	5	7.92
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	3	7.83
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	6	7.83
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	10	7.81
(1,201)	1:114:A:ILE:C	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	9	7.79
(1,255)	1:141:A:GLY:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	5	7.74
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	9	7.73
(1,158)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:GLY:N	7	7.58
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	10	7.56
(1,132)	1:78:A:ALA:N	1:78:A:ALA:CA	1:78:A:ALA:C	1:79:A:ASP:N	3	7.52
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	8	7.41
(1,138)	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	1:82:A:GLY:N	3	7.37
(1,105)	1:64:A:ASP:C	1:65:A:ILE:N	1:65:A:ILE:CA	1:65:A:ILE:C	8	7.33
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	9	7.25
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	2	7.03
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	2	7.0
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	1	6.99
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	3	6.97
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	10	6.97
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1	6.91
(1,124)	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	1:75:A:GLU:N	8	6.91
(1,158)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:GLY:N	5	6.89
(1,260)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:GLN:N	10	6.78
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	5	6.76
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	10	6.69
(1,201)	1:114:A:ILE:C	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	6	6.64
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	7	6.57
(1,255)	1:141:A:GLY:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	4	6.55
(1,262)	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	1:146:A:ASP:N	2	6.46
(1,52)	1:36:A:GLY:N	1:36:A:GLY:CA	1:36:A:GLY:C	1:37:A:GLU:N	6	6.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	8	6.46
(1,255)	1:141:A:GLY:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	3	6.37
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	2	6.33
(1,262)	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	1:146:A:ASP:N	6	6.32
(1,162)	1:93:A:CYS:N	1:93:A:CYS:CA	1:93:A:CYS:C	1:94:A:ASP:N	7	6.26
(1,289)	1:159:A:HIS:C	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	4	6.23
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	10	6.23
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	3	6.22
(1,38)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:THR:N	10	6.12
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	5	6.11
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	3	6.11
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	5	6.1
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	7	6.08
(1,289)	1:159:A:HIS:C	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	9	6.07
(1,73)	1:47:A:VAL:C	1:48:A:MET:N	1:48:A:MET:CA	1:48:A:MET:C	1	6.03
(1,249)	1:138:A:GLY:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	6	5.96
(1,104)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:ILE:N	8	5.96
(1,33)	1:23:A:PRO:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	1	5.96
(1,75)	1:48:A:MET:C	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1	5.94
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	6	5.91
(1,117)	1:70:A:SER:C	1:71:A:ILE:N	1:71:A:ILE:CA	1:71:A:ILE:C	8	5.87
(1,200)	1:114:A:ILE:N	1:114:A:ILE:CA	1:114:A:ILE:C	1:115:A:ASP:N	2	5.85
(1,263)	1:145:A:GLN:C	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	4	5.77
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	9	5.77
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	6	5.71
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	10	5.7
(1,34)	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	1:25:A:GLU:N	2	5.7
(1,119)	1:71:A:ILE:C	1:72:A:PHE:N	1:72:A:PHE:CA	1:72:A:PHE:C	8	5.68
(1,74)	1:48:A:MET:N	1:48:A:MET:CA	1:48:A:MET:C	1:49:A:THR:N	1	5.63
(1,278)	1:153:A:MET:N	1:153:A:MET:CA	1:153:A:MET:C	1:154:A:ILE:N	4	5.59
(1,263)	1:145:A:GLN:C	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	6	5.59
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	10	5.56
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	3	5.51
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	10	5.44
(1,285)	1:156:A:MET:C	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	3	5.35
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	3	5.18
(1,124)	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	1:75:A:GLU:N	9	5.15
(1,41)	1:28:A:THR:C	1:29:A:ILE:N	1:29:A:ILE:CA	1:29:A:ILE:C	10	5.15
(1,289)	1:159:A:HIS:C	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	3	5.1
(1,251)	1:139:A:PHE:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	10	5.0
(1,105)	1:64:A:ASP:C	1:65:A:ILE:N	1:65:A:ILE:CA	1:65:A:ILE:C	4	4.94
(1,136)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:SER:N	8	4.92
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	9	4.88
(1,248)	1:138:A:GLY:N	1:138:A:GLY:CA	1:138:A:GLY:C	1:139:A:PHE:N	9	4.84
(1,263)	1:145:A:GLN:C	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	3	4.8
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	8	4.79
(1,99)	1:61:A:ASP:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	7	4.75
(1,201)	1:114:A:ILE:C	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	2	4.7
(1,104)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:ILE:N	4	4.7
(1,12)	1:12:A:GLN:N	1:12:A:GLN:CA	1:12:A:GLN:C	1:13:A:MET:N	5	4.68
(1,270)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:THR:N	1	4.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,254)	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	1:142:A:VAL:N	2	4.65
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	9	4.65
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	9	4.59
(1,285)	1:156:A:MET:C	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	9	4.58
(1,278)	1:153:A:MET:N	1:153:A:MET:CA	1:153:A:MET:C	1:154:A:ILE:N	6	4.58
(1,251)	1:139:A:PHE:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	2	4.55
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	4	4.54
(1,264)	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	1:147:A:GLU:N	1	4.53
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	2	4.48
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	2	4.43
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	8	4.41
(1,46)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:GLY:N	1	4.27
(1,262)	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	1:146:A:ASP:N	4	4.25
(1,57)	1:38:A:PHE:C	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1	4.25
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	9	4.18
(1,285)	1:156:A:MET:C	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	5	4.14
(1,50)	1:35:A:PHE:N	1:35:A:PHE:CA	1:35:A:PHE:C	1:36:A:GLY:N	4	4.14
(1,198)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:ASP:N	9	4.13
(1,99)	1:61:A:ASP:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	8	4.11
(1,259)	1:143:A:SER:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	6	4.06
(1,100)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:SER:N	8	4.03
(1,278)	1:153:A:MET:N	1:153:A:MET:CA	1:153:A:MET:C	1:154:A:ILE:N	3	4.0
(1,148)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:VAL:N	10	3.97
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	3	3.94
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	7	3.93
(1,269)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1	3.92
(1,102)	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	1:64:A:ASP:N	6	3.91
(1,50)	1:35:A:PHE:N	1:35:A:PHE:CA	1:35:A:PHE:C	1:36:A:GLY:N	10	3.88
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	9	3.84
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	6	3.77
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	6	3.75
(1,122)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:HIS:N	9	3.75
(1,116)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:ILE:N	8	3.75
(1,202)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ALA:N	6	3.72
(1,113)	1:68:A:ALA:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	8	3.71
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	10	3.71
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	3	3.65
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	3	3.59
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	8	3.59
(1,262)	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	1:146:A:ASP:N	10	3.58
(1,262)	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	1:146:A:ASP:N	3	3.57
(1,77)	1:49:A:THR:C	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1	3.53
(1,55)	1:37:A:GLU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	10	3.52
(1,259)	1:143:A:SER:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	10	3.47
(1,248)	1:138:A:GLY:N	1:138:A:GLY:CA	1:138:A:GLY:C	1:139:A:PHE:N	7	3.45
(1,284)	1:156:A:MET:N	1:156:A:MET:CA	1:156:A:MET:C	1:157:A:LEU:N	2	3.43
(1,202)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ALA:N	2	3.37
(1,66)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:ASP:N	10	3.37
(1,112)	1:68:A:ALA:N	1:68:A:ALA:CA	1:68:A:ALA:C	1:69:A:GLY:N	8	3.33
(1,76)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:ALA:N	1	3.31
(1,122)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:HIS:N	7	3.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,260)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:GLN:N	4	3.21
(1,260)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:GLN:N	3	3.2
(1,262)	1:145:A:GLN:N	1:145:A:GLN:CA	1:145:A:GLN:C	1:146:A:ASP:N	7	3.16
(1,126)	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1:76:A:ARG:N	8	3.15
(1,284)	1:156:A:MET:N	1:156:A:MET:CA	1:156:A:MET:C	1:157:A:LEU:N	8	3.13
(1,194)	1:110:A:ASN:N	1:110:A:ASN:CA	1:110:A:ASN:C	1:111:A:LEU:N	2	3.07
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	6	3.06
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	1	3.05
(1,66)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:ASP:N	2	3.02
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	1	2.99
(1,78)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:GLY:N	7	2.98
(1,250)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ARG:N	10	2.97
(1,255)	1:141:A:GLY:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	2	2.96
(1,60)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	1:41:A:PHE:N	10	2.96
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	4	2.95
(1,25)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	7	2.93
(1,44)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	7	2.9
(1,197)	1:111:A:LEU:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	3	2.88
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	9	2.84
(1,100)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:SER:N	2	2.82
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	6	2.79
(1,289)	1:159:A:HIS:C	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	7	2.78
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	2	2.78
(1,44)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	6	2.77
(1,6)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:MET:N	9	2.77
(1,84)	1:54:A:VAL:N	1:54:A:VAL:CA	1:54:A:VAL:C	1:55:A:THR:N	10	2.75
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:PHE:N	2	2.74
(1,284)	1:156:A:MET:N	1:156:A:MET:CA	1:156:A:MET:C	1:157:A:LEU:N	5	2.72
(1,46)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:GLY:N	9	2.71
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1	2.7
(1,50)	1:35:A:PHE:N	1:35:A:PHE:CA	1:35:A:PHE:C	1:36:A:GLY:N	2	2.68
(1,278)	1:153:A:MET:N	1:153:A:MET:CA	1:153:A:MET:C	1:154:A:ILE:N	5	2.65
(1,202)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ALA:N	9	2.62
(1,12)	1:12:A:GLN:N	1:12:A:GLN:CA	1:12:A:GLN:C	1:13:A:MET:N	2	2.62
(1,131)	1:77:A:ALA:C	1:78:A:ALA:N	1:78:A:ALA:CA	1:78:A:ALA:C	4	2.61
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	6	2.57
(1,205)	1:116:A:ALA:C	1:117:A:SER:N	1:117:A:SER:CA	1:117:A:SER:C	2	2.55
(1,197)	1:111:A:LEU:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	7	2.55
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	7	2.53
(1,153)	1:88:A:MET:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	7	2.5
(1,89)	1:56:A:TYR:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	5	2.47
(1,46)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:GLY:N	5	2.47
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	3	2.45
(1,287)	1:158:A:GLY:C	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	6	2.44
(1,156)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:THR:N	8	2.43
(1,84)	1:54:A:VAL:N	1:54:A:VAL:CA	1:54:A:VAL:C	1:55:A:THR:N	2	2.39
(1,260)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:GLN:N	6	2.38
(1,84)	1:54:A:VAL:N	1:54:A:VAL:CA	1:54:A:VAL:C	1:55:A:THR:N	1	2.38
(1,78)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:GLY:N	9	2.38
(1,135)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	5	2.37
(1,131)	1:77:A:ALA:C	1:78:A:ALA:N	1:78:A:ALA:CA	1:78:A:ALA:C	7	2.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:THR:N	9	2.36
(1,252)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:GLY:N	6	2.32
(1,57)	1:38:A:PHE:C	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	4	2.32
(1,265)	1:146:A:ASP:C	1:147:A:GLU:N	1:147:A:GLU:CA	1:147:A:GLU:C	9	2.3
(1,197)	1:111:A:LEU:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	10	2.3
(1,50)	1:35:A:PHE:N	1:35:A:PHE:CA	1:35:A:PHE:C	1:36:A:GLY:N	7	2.3
(1,39)	1:27:A:THR:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	10	2.27
(1,99)	1:61:A:ASP:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	6	2.26
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	4	2.23
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	6	2.23
(1,47)	1:33:A:GLY:C	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	8	2.23
(1,37)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	5	2.23
(1,99)	1:61:A:ASP:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	10	2.22
(1,136)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:SER:N	3	2.2
(1,194)	1:110:A:ASN:N	1:110:A:ASN:CA	1:110:A:ASN:C	1:111:A:LEU:N	6	2.19
(1,44)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	4	2.19
(1,155)	1:89:A:GLN:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	10	2.16
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	4	2.16
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	10	2.16
(1,14)	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1:14:A:GLY:N	1	2.16
(1,14)	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1:14:A:GLY:N	2	2.14
(1,285)	1:156:A:MET:C	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	2	2.12
(1,44)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	3	2.07
(1,253)	1:140:A:ARG:C	1:141:A:GLY:N	1:141:A:GLY:CA	1:141:A:GLY:C	7	2.06
(1,44)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	5	2.04
(1,190)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:PHE:N	1	2.01
(1,46)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:GLY:N	3	2.01
(1,264)	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	1:147:A:GLU:N	10	2.0
(1,56)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:LEU:N	6	2.0
(1,99)	1:61:A:ASP:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	4	1.99
(1,280)	1:154:A:ILE:N	1:154:A:ILE:CA	1:154:A:ILE:C	1:155:A:ASP:N	1	1.98
(1,137)	1:80:A:LEU:C	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	8	1.96
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	5	1.95
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1	1.95
(1,197)	1:111:A:LEU:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	5	1.94
(1,50)	1:35:A:PHE:N	1:35:A:PHE:CA	1:35:A:PHE:C	1:36:A:GLY:N	6	1.94
(1,288)	1:159:A:HIS:N	1:159:A:HIS:CA	1:159:A:HIS:C	1:160:A:ASP:N	2	1.93
(1,104)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:ILE:N	9	1.92
(1,28)	1:21:A:THR:N	1:21:A:THR:CA	1:21:A:THR:C	1:22:A:SER:N	4	1.89
(1,133)	1:78:A:ALA:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	6	1.88
(1,101)	1:62:A:GLU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	8	1.88
(1,46)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:GLY:N	8	1.87
(1,12)	1:12:A:GLN:N	1:12:A:GLN:CA	1:12:A:GLN:C	1:13:A:MET:N	7	1.86
(1,123)	1:73:A:TYR:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	7	1.83
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	9	1.83
(1,162)	1:93:A:CYS:N	1:93:A:CYS:CA	1:93:A:CYS:C	1:94:A:ASP:N	5	1.82
(1,248)	1:138:A:GLY:N	1:138:A:GLY:CA	1:138:A:GLY:C	1:139:A:PHE:N	2	1.81
(1,165)	1:94:A:ASP:C	1:95:A:GLU:N	1:95:A:GLU:CA	1:95:A:GLU:C	5	1.81
(1,65)	1:42:A:ALA:C	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	9	1.81
(1,123)	1:73:A:TYR:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	10	1.8
(1,63)	1:41:A:PHE:C	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	1	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,251)	1:139:A:PHE:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	5	1.79
(1,8)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:GLY:N	9	1.79
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	8	1.77
(1,53)	1:36:A:GLY:C	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	4	1.75
(1,198)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:ASP:N	2	1.72
(1,37)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	7	1.72
(1,83)	1:53:A:HIS:C	1:54:A:VAL:N	1:54:A:VAL:CA	1:54:A:VAL:C	1	1.71
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	10	1.7
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	9	1.69
(1,205)	1:116:A:ALA:C	1:117:A:SER:N	1:117:A:SER:CA	1:117:A:SER:C	7	1.69
(1,65)	1:42:A:ALA:C	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	5	1.69
(1,197)	1:111:A:LEU:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	8	1.68
(1,66)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:ASP:N	6	1.67
(1,203)	1:115:A:ASP:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	9	1.65
(1,156)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:THR:N	4	1.65
(1,45)	1:31:A:THR:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	2	1.65
(1,131)	1:77:A:ALA:C	1:78:A:ALA:N	1:78:A:ALA:CA	1:78:A:ALA:C	10	1.64
(1,8)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:GLY:N	3	1.63
(1,163)	1:93:A:CYS:C	1:94:A:ASP:N	1:94:A:ASP:CA	1:94:A:ASP:C	7	1.62
(1,40)	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1:29:A:ILE:N	9	1.61
(1,89)	1:56:A:TYR:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	1	1.6
(1,268)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	1	1.58
(1,59)	1:39:A:LEU:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	10	1.58
(1,27)	1:20:A:HIS:C	1:21:A:THR:N	1:21:A:THR:CA	1:21:A:THR:C	8	1.58
(1,25)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	5	1.57
(1,282)	1:155:A:ASP:N	1:155:A:ASP:CA	1:155:A:ASP:C	1:156:A:MET:N	9	1.56
(1,135)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	9	1.56
(1,66)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:ASP:N	4	1.54
(1,13)	1:12:A:GLN:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	5	1.54
(1,156)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:THR:N	6	1.53
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	5	1.53
(1,113)	1:68:A:ALA:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	6	1.52
(1,32)	1:23:A:PRO:N	1:23:A:PRO:CA	1:23:A:PRO:C	1:24:A:VAL:N	9	1.51
(1,14)	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1:14:A:GLY:N	4	1.51
(1,44)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	8	1.5
(1,21)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	3	1.5
(1,65)	1:42:A:ALA:C	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	4	1.49
(1,24)	1:19:A:PHE:N	1:19:A:PHE:CA	1:19:A:PHE:C	1:20:A:HIS:N	1	1.48
(1,21)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	7	1.47
(1,39)	1:27:A:THR:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	8	1.46
(1,134)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	2	1.45
(1,131)	1:77:A:ALA:C	1:78:A:ALA:N	1:78:A:ALA:CA	1:78:A:ALA:C	5	1.45
(1,63)	1:41:A:PHE:C	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	7	1.45
(1,108)	1:66:A:ILE:N	1:66:A:ILE:CA	1:66:A:ILE:C	1:67:A:MET:N	8	1.4
(1,123)	1:73:A:TYR:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	1	1.38
(1,68)	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	1:46:A:TYR:N	3	1.38
(1,207)	1:117:A:SER:C	1:118:A:ASP:N	1:118:A:ASP:CA	1:118:A:ASP:C	2	1.36
(1,292)	1:161:A:ALA:N	1:161:A:ALA:CA	1:161:A:ALA:C	1:162:A:GLU:N	4	1.35
(1,45)	1:31:A:THR:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	6	1.35
(1,21)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	9	1.34
(1,85)	1:54:A:VAL:C	1:55:A:THR:N	1:55:A:THR:CA	1:55:A:THR:C	6	1.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,248)	1:138:A:GLY:N	1:138:A:GLY:CA	1:138:A:GLY:C	1:139:A:PHE:N	5	1.32
(1,156)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:THR:N	10	1.32
(1,85)	1:54:A:VAL:C	1:55:A:THR:N	1:55:A:THR:CA	1:55:A:THR:C	4	1.32
(1,137)	1:80:A:LEU:C	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	3	1.31
(1,130)	1:77:A:ALA:N	1:77:A:ALA:CA	1:77:A:ALA:C	1:78:A:ALA:N	4	1.31
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	6	1.31
(1,66)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:ASP:N	7	1.3
(1,37)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	4	1.3
(1,210)	1:119:A:ALA:N	1:119:A:ALA:CA	1:119:A:ALA:C	1:120:A:ALA:N	1	1.29
(1,197)	1:111:A:LEU:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	4	1.29
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	2	1.28
(1,56)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:LEU:N	7	1.26
(1,27)	1:20:A:HIS:C	1:21:A:THR:N	1:21:A:THR:CA	1:21:A:THR:C	6	1.26
(1,259)	1:143:A:SER:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	7	1.25
(1,119)	1:71:A:ILE:C	1:72:A:PHE:N	1:72:A:PHE:CA	1:72:A:PHE:C	2	1.25
(1,90)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	1:58:A:ILE:N	1	1.24
(1,46)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:GLY:N	10	1.24
(1,133)	1:78:A:ALA:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	10	1.23
(1,40)	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1:29:A:ILE:N	2	1.23
(1,284)	1:156:A:MET:N	1:156:A:MET:CA	1:156:A:MET:C	1:157:A:LEU:N	6	1.19
(1,133)	1:78:A:ALA:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	4	1.19
(1,39)	1:27:A:THR:C	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	3	1.19
(1,37)	1:25:A:GLU:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	8	1.19
(1,28)	1:21:A:THR:N	1:21:A:THR:CA	1:21:A:THR:C	1:22:A:SER:N	5	1.18
(1,153)	1:88:A:MET:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	3	1.17
(1,139)	1:81:A:SER:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	3	1.17
(1,286)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:GLY:N	4	1.16
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LEU:N	7	1.16
(1,35)	1:24:A:VAL:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	3	1.16
(1,25)	1:19:A:PHE:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	4	1.15
(1,123)	1:73:A:TYR:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	2	1.14
(1,196)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:ASP:N	9	1.13
(1,264)	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	1:147:A:GLU:N	8	1.11
(1,247)	1:137:A:LEU:C	1:138:A:GLY:N	1:138:A:GLY:CA	1:138:A:GLY:C	2	1.11
(1,273)	1:150:A:THR:C	1:151:A:CYS:N	1:151:A:CYS:CA	1:151:A:CYS:C	8	1.1
(1,103)	1:63:A:SER:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	9	1.1
(1,133)	1:78:A:ALA:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	7	1.09
(1,190)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:PHE:N	7	1.07
(1,148)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:VAL:N	4	1.07
(1,21)	1:17:A:GLU:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	5	1.06
(1,16)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:MET:N	6	1.06
(1,214)	1:121:A:GLU:N	1:121:A:GLU:CA	1:121:A:GLU:C	1:122:A:LEU:N	3	1.05
(1,118)	1:71:A:ILE:N	1:71:A:ILE:CA	1:71:A:ILE:C	1:72:A:PHE:N	8	1.05
(1,78)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:GLY:N	10	1.04
(1,28)	1:21:A:THR:N	1:21:A:THR:CA	1:21:A:THR:C	1:22:A:SER:N	6	1.04
(1,182)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:GLN:N	10	1.03
(1,148)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:VAL:N	1	1.03
(1,115)	1:69:A:GLY:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	7	1.03
(1,131)	1:77:A:ALA:C	1:78:A:ALA:N	1:78:A:ALA:CA	1:78:A:ALA:C	2	1.02
(1,102)	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	1:64:A:ASP:N	4	1.02
(1,97)	1:60:A:VAL:C	1:61:A:ASP:N	1:61:A:ASP:CA	1:61:A:ASP:C	8	1.02