



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 02:16 AM UTC

PDB ID : 6U1L / pdb_00006u1l
Title : Structure of two-domain translational regulator Yih1 reveals a possible mechanism of action
Authors : Harjes, E.; Jameson, G.B.; Edwards, P.J.B.; Goroncy, A.K.; Loo, T.; Norris, G.E.
Deposited on : 2019-08-16

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

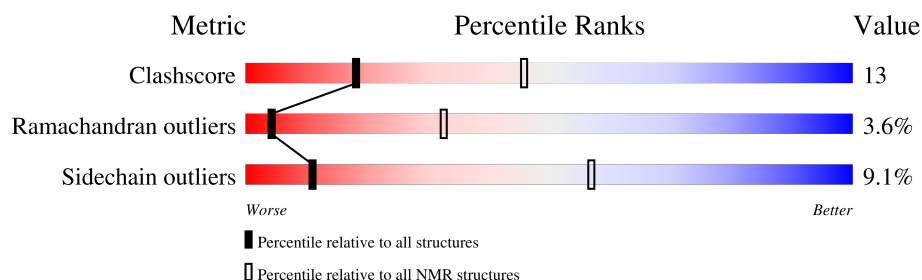
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	258	

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:68, A:76-A:93, A:97-A:112 (99)	0.89	1
2	A:126-A:258 (133)	1.01	6

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 1 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 8, 9, 10
Single-model clusters	4; 5; 7

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3995 atoms, of which 1955 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein IMPACT homolog.

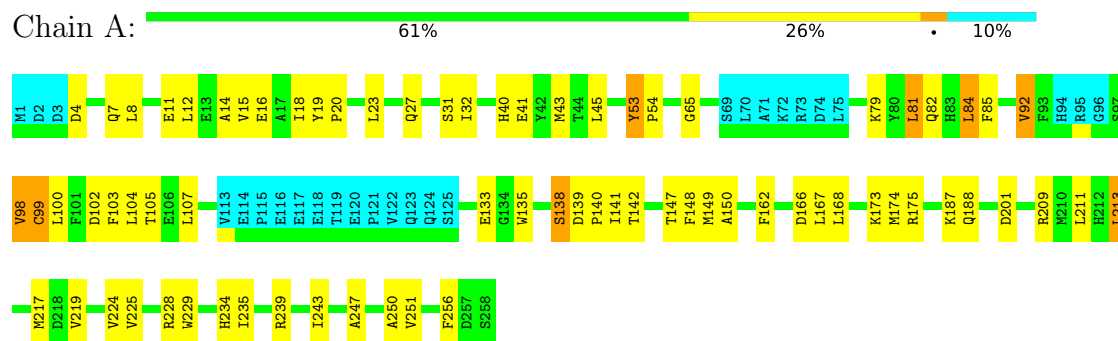
Mol	Chain	Residues	Atoms						Trace
1	A	258	Total	C	H	N	O	S	0
			3995	1286	1955	337	406	11	

4 Residue-property plots [i](#)

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: Protein IMPACT homolog

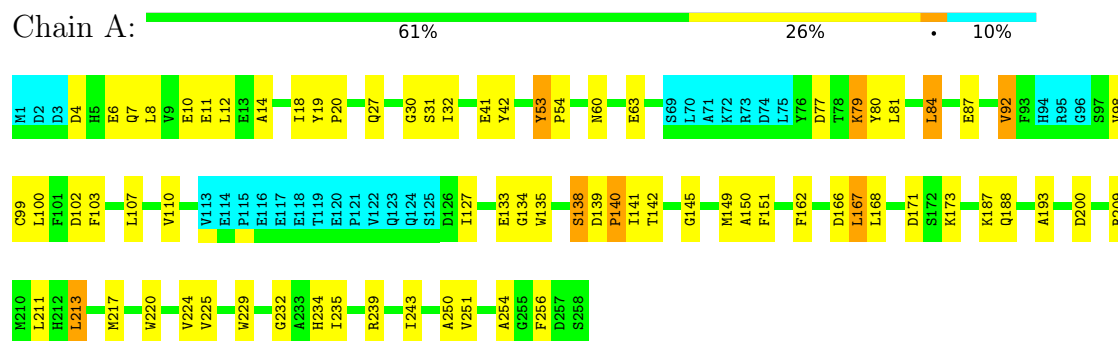


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

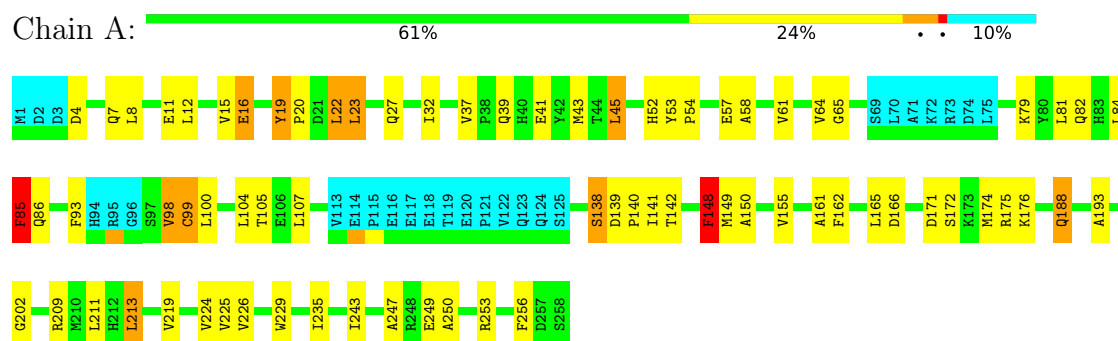
4.2.1 Score per residue for model 1

- Molecule 1: Protein IMPACT homolog



4.2.2 Score per residue for model 2

- Molecule 1: Protein IMPACT homolog



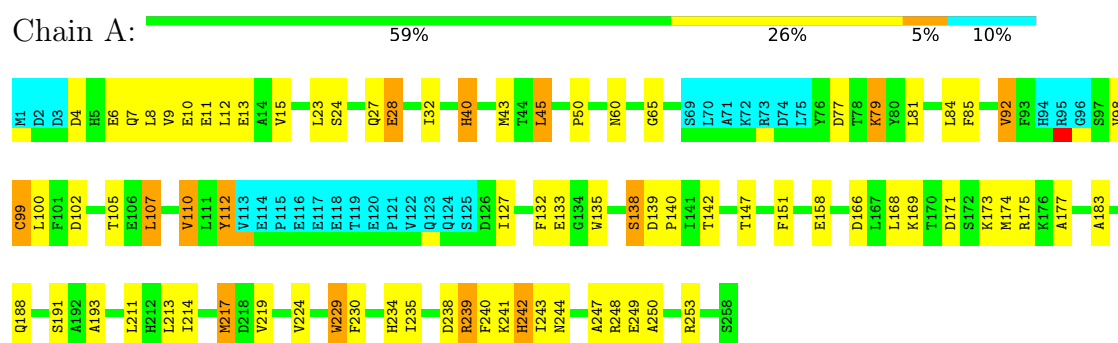
4.2.3 Score per residue for model 3

- Molecule 1: Protein IMPACT homolog



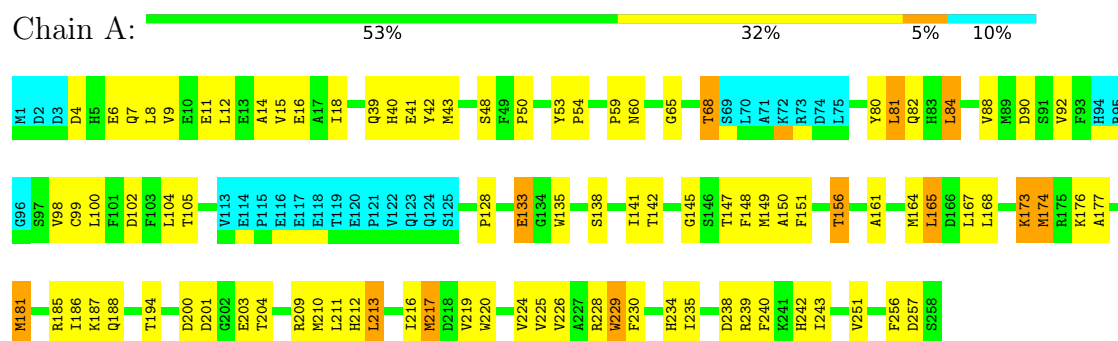
4.2.4 Score per residue for model 4

- Molecule 1: Protein IMPACT homolog



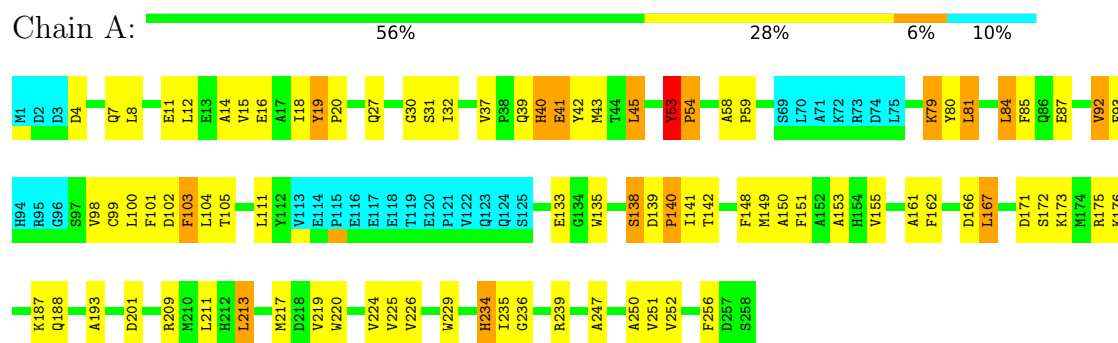
4.2.5 Score per residue for model 5

- Molecule 1: Protein IMPACT homolog



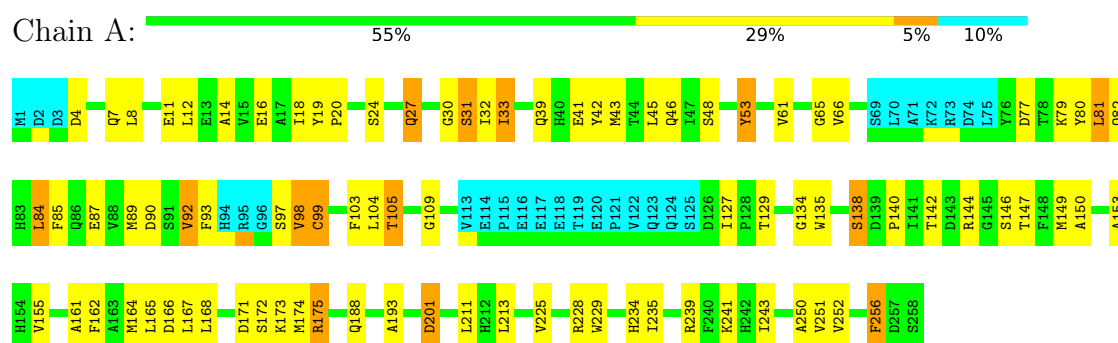
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Protein IMPACT homolog



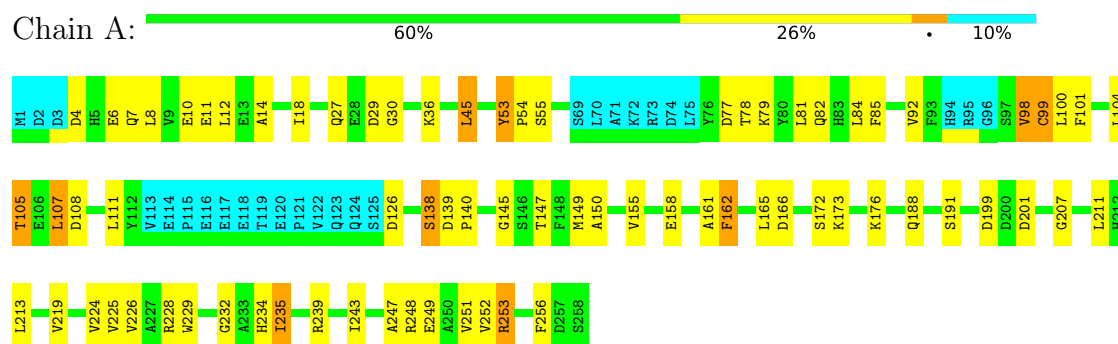
4.2.7 Score per residue for model 7

- Molecule 1: Protein IMPACT homolog



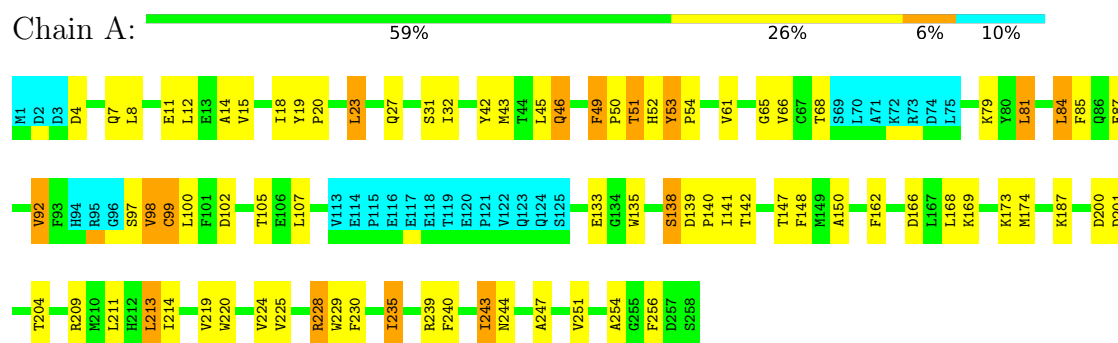
4.2.8 Score per residue for model 8

- Molecule 1: Protein IMPACT homolog



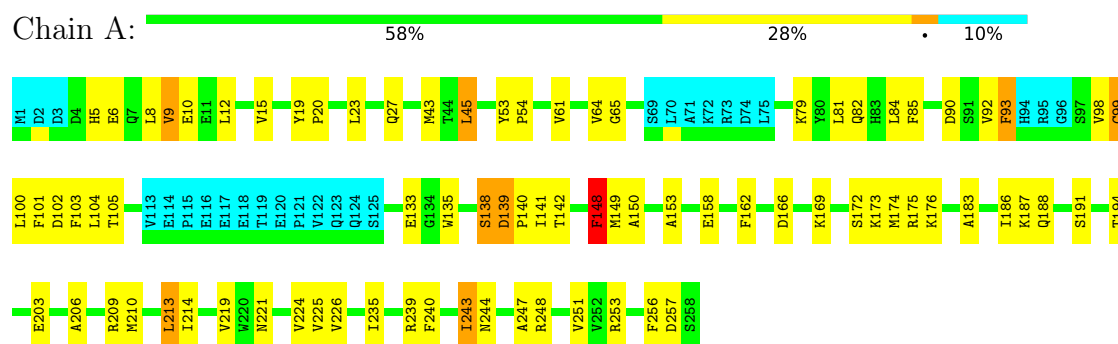
4.2.9 Score per residue for model 9

- Molecule 1: Protein IMPACT homolog



4.2.10 Score per residue for model 10

- Molecule 1: Protein IMPACT homolog



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 40 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	structure calculation	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2691
Number of shifts mapped to atoms	2691
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	0.85±0.02	0±1/1876 (0.0± 0.0%)	0.81±0.03	1±1/2551 (0.0± 0.0%)
All	All	0.85	5/18760 (0.0%)	0.81	10/25510 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	167	LEU	N-CA	-6.50	1.38	1.46	6	3
1	A	140	PRO	C-N	-6.21	1.25	1.33	6	2

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	85	PHE	CA-CB-CG	7.29	121.09	113.80	2	1
1	A	148	PHE	CA-CB-CG	6.52	120.32	113.80	2	2
1	A	49	PHE	CA-C-N	5.25	125.71	120.52	9	1
1	A	49	PHE	C-N-CA	5.25	125.71	120.52	9	1
1	A	93	PHE	N-CA-C	-5.05	107.50	113.97	6	1
1	A	53	TYR	CA-C-N	5.04	126.14	119.84	10	2
1	A	53	TYR	C-N-CA	5.04	126.14	119.84	10	2

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	1832	1760	1751	47±6
All	All	18320	17600	17510	473

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:MET:SD	1:A:81:LEU:HG	0.76	2.21	2	7
1:A:141:ILE:HB	1:A:148:PHE:CE1	0.72	2.19	10	2
1:A:142:THR:HG23	1:A:235:ILE:HD12	0.68	1.64	2	8
1:A:187:LYS:HG3	1:A:220:TRP:CD1	0.68	2.24	9	3
1:A:82:GLN:HG2	1:A:85:PHE:CE2	0.66	2.26	2	1
1:A:52:HIS:O	1:A:57:GLU:HB3	0.65	1.91	2	1
1:A:6:GLU:O	1:A:10:GLU:HB2	0.65	1.91	10	2
1:A:85:PHE:HD1	1:A:86:GLN:N	0.65	1.90	2	1
1:A:82:GLN:HA	1:A:85:PHE:CD2	0.64	2.27	2	1
1:A:4:ASP:HA	1:A:7:GLN:NE2	0.64	2.08	6	9
1:A:100:LEU:HD23	1:A:100:LEU:H	0.63	1.53	10	4
1:A:82:GLN:HA	1:A:85:PHE:CE2	0.62	2.30	2	1
1:A:102:ASP:O	1:A:105:THR:HG22	0.62	1.94	3	4
1:A:8:LEU:O	1:A:12:LEU:HG	0.60	1.97	3	10
1:A:50:PRO:C	1:A:52:HIS:H	0.60	2.04	9	1
1:A:138:SER:C	1:A:140:PRO:HD3	0.60	2.21	6	9
1:A:45:LEU:HG	1:A:85:PHE:CE1	0.60	2.31	10	3
1:A:173:LYS:HG3	1:A:174:MET:SD	0.60	2.37	4	1
1:A:240:PHE:O	1:A:244:ASN:HB2	0.59	1.97	9	2
1:A:84:LEU:O	1:A:87:GLU:HG2	0.59	1.97	7	4
1:A:206:ALA:O	1:A:210:MET:HG2	0.59	1.97	10	1
1:A:8:LEU:O	1:A:11:GLU:HG2	0.59	1.97	6	8
1:A:102:ASP:O	1:A:105:THR:HB	0.59	1.98	9	1
1:A:150:ALA:HA	1:A:225:VAL:O	0.59	1.97	7	9
1:A:171:ASP:OD1	1:A:173:LYS:HG2	0.59	1.97	1	3
1:A:147:THR:HB	1:A:229:TRP:O	0.59	1.97	4	1
1:A:133:GLU:C	1:A:135:TRP:H	0.59	2.06	5	3
1:A:213:LEU:O	1:A:217:MET:HB2	0.59	1.98	5	2
1:A:43:MET:HA	1:A:65:GLY:O	0.58	1.98	7	6
1:A:61:VAL:HG12	1:A:89:MET:SD	0.58	2.37	7	1
1:A:171:ASP:O	1:A:175:ARG:HB2	0.58	1.97	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:GLU:O	1:A:42:TYR:HB2	0.58	1.97	7	1
1:A:172:SER:O	1:A:176:LYS:HG2	0.58	1.99	2	2
1:A:188:GLN:HB2	1:A:193:ALA:O	0.58	1.99	2	1
1:A:219:VAL:HG21	1:A:256:PHE:HA	0.57	1.77	9	4
1:A:145:GLY:HA2	1:A:232:GLY:O	0.57	1.98	8	3
1:A:251:VAL:O	1:A:256:PHE:HB2	0.57	2.00	8	5
1:A:89:MET:HA	1:A:92:VAL:CG1	0.57	2.29	7	1
1:A:142:THR:HG21	1:A:234:HIS:O	0.57	1.99	1	3
1:A:176:LYS:HB2	1:A:229:TRP:CZ2	0.57	2.35	8	1
1:A:45:LEU:HG	1:A:85:PHE:CZ	0.56	2.34	6	2
1:A:140:PRO:O	1:A:243:ILE:HG21	0.56	2.00	4	1
1:A:209:ARG:O	1:A:213:LEU:HB2	0.56	2.00	10	6
1:A:155:VAL:HG21	1:A:161:ALA:HB2	0.55	1.78	6	4
1:A:30:GLY:O	1:A:32:ILE:N	0.55	2.40	3	4
1:A:239:ARG:NE	1:A:239:ARG:HA	0.55	2.17	4	1
1:A:85:PHE:CD1	1:A:86:GLN:N	0.55	2.74	2	1
1:A:107:LEU:HA	1:A:110:VAL:HG12	0.55	1.78	4	2
1:A:15:VAL:HB	1:A:100:LEU:CD1	0.54	2.31	9	3
1:A:224:VAL:HB	1:A:256:PHE:CZ	0.54	2.37	2	8
1:A:14:ALA:O	1:A:18:ILE:HG13	0.54	2.02	8	7
1:A:138:SER:O	1:A:140:PRO:HD3	0.54	2.03	3	7
1:A:162:PHE:O	1:A:166:ASP:HB2	0.54	2.02	6	8
1:A:12:LEU:O	1:A:16:GLU:HB2	0.54	2.03	6	5
1:A:140:PRO:HD2	1:A:243:ILE:HG21	0.54	1.79	4	1
1:A:173:LYS:HG2	1:A:174:MET:SD	0.54	2.43	5	1
1:A:248:ARG:O	1:A:252:VAL:HG22	0.54	2.02	8	1
1:A:200:ASP:HB2	1:A:204:THR:HA	0.53	1.79	9	1
1:A:239:ARG:O	1:A:243:ILE:HG12	0.53	2.04	3	4
1:A:151:PHE:O	1:A:224:VAL:HA	0.53	2.04	5	4
1:A:244:ASN:O	1:A:248:ARG:HG3	0.53	2.03	4	2
1:A:79:LYS:HD2	1:A:79:LYS:C	0.53	2.29	4	1
1:A:15:VAL:HG13	1:A:23:LEU:HG	0.53	1.80	4	1
1:A:77:ASP:OD1	1:A:79:LYS:HG2	0.53	2.04	8	1
1:A:92:VAL:HG12	1:A:102:ASP:HB3	0.53	1.81	6	2
1:A:183:ALA:HB1	1:A:214:ILE:HD13	0.53	1.81	4	2
1:A:199:ASP:OD2	1:A:207:GLY:HA3	0.53	2.04	8	1
1:A:139:ASP:HA	1:A:247:ALA:CB	0.53	2.34	9	5
1:A:12:LEU:O	1:A:15:VAL:HG12	0.52	2.04	5	4
1:A:138:SER:O	1:A:247:ALA:HA	0.52	2.05	2	2
1:A:147:THR:O	1:A:228:ARG:HA	0.52	2.05	9	5
1:A:42:TYR:O	1:A:66:VAL:HA	0.52	2.04	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:THR:HG23	1:A:234:HIS:O	0.52	2.04	7	1
1:A:81:LEU:O	1:A:85:PHE:HB2	0.52	2.05	4	2
1:A:61:VAL:HG22	1:A:82:GLN:OE1	0.52	2.05	10	2
1:A:128:PRO:HD3	1:A:149:MET:SD	0.51	2.45	5	1
1:A:252:VAL:HA	1:A:256:PHE:O	0.51	2.05	7	1
1:A:135:TRP:CE3	1:A:153:ALA:HB2	0.51	2.40	7	3
1:A:142:THR:HG21	1:A:234:HIS:CD2	0.51	2.41	3	1
1:A:212:HIS:O	1:A:216:ILE:HG13	0.51	2.06	5	1
1:A:133:GLU:HG3	1:A:133:GLU:O	0.51	2.04	4	1
1:A:147:THR:OG1	1:A:235:ILE:HD11	0.51	2.06	4	2
1:A:98:VAL:O	1:A:99:CYS:HB3	0.51	2.06	7	4
1:A:181:MET:CG	1:A:226:VAL:HB	0.51	2.36	5	1
1:A:84:LEU:O	1:A:88:VAL:HG23	0.50	2.05	5	1
1:A:104:LEU:HD12	1:A:105:THR:N	0.50	2.22	7	4
1:A:5:HIS:O	1:A:9:VAL:HG13	0.50	2.06	10	1
1:A:27:GLN:HG2	1:A:32:ILE:HB	0.50	1.83	1	6
1:A:238:ASP:O	1:A:242:HIS:HB2	0.50	2.06	5	2
1:A:39:GLN:O	1:A:40:HIS:HB3	0.50	2.06	5	1
1:A:50:PRO:C	1:A:52:HIS:N	0.50	2.69	9	1
1:A:229:TRP:HA	1:A:229:TRP:CE3	0.50	2.42	5	2
1:A:141:ILE:HB	1:A:148:PHE:CD1	0.49	2.42	2	2
1:A:149:MET:O	1:A:226:VAL:HA	0.49	2.07	2	5
1:A:249:GLU:O	1:A:253:ARG:HB2	0.49	2.07	8	3
1:A:39:GLN:HA	1:A:39:GLN:OE1	0.49	2.07	7	1
1:A:140:PRO:HG2	1:A:243:ILE:CD1	0.49	2.37	10	2
1:A:85:PHE:CE1	1:A:107:LEU:HD21	0.49	2.43	4	1
1:A:134:GLY:O	1:A:164:MET:HE1	0.49	2.08	7	1
1:A:79:LYS:HD3	1:A:80:TYR:N	0.49	2.23	6	2
1:A:166:ASP:O	1:A:169:LYS:HG3	0.49	2.08	4	1
1:A:241:LYS:HD3	1:A:241:LYS:C	0.49	2.32	3	1
1:A:140:PRO:HD2	1:A:243:ILE:CG2	0.48	2.38	4	1
1:A:88:VAL:O	1:A:92:VAL:HG13	0.48	2.07	5	1
1:A:51:THR:HA	1:A:53:TYR:CE1	0.48	2.43	9	1
1:A:92:VAL:HG21	1:A:99:CYS:SG	0.48	2.49	3	2
1:A:219:VAL:HG21	1:A:256:PHE:CD2	0.48	2.43	5	2
1:A:15:VAL:CG1	1:A:23:LEU:HG	0.48	2.39	9	1
1:A:61:VAL:HB	1:A:85:PHE:CE2	0.48	2.43	9	1
1:A:142:THR:H	1:A:240:PHE:HB3	0.48	1.68	4	1
1:A:251:VAL:HG22	1:A:256:PHE:CB	0.48	2.39	5	2
1:A:158:GLU:O	1:A:162:PHE:HB2	0.48	2.09	8	1
1:A:127:ILE:HD13	1:A:239:ARG:HE	0.48	1.69	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:VAL:HG11	1:A:103:PHE:CB	0.48	2.39	3	1
1:A:45:LEU:HD12	1:A:64:VAL:CG1	0.48	2.38	10	1
1:A:188:GLN:HG2	1:A:193:ALA:O	0.48	2.09	1	2
1:A:9:VAL:O	1:A:13:GLU:HG3	0.48	2.08	4	1
1:A:8:LEU:HD11	1:A:49:PHE:CD1	0.48	2.44	9	1
1:A:138:SER:HB2	1:A:250:ALA:CB	0.47	2.39	4	5
1:A:140:PRO:HD2	1:A:243:ILE:HD13	0.47	1.86	1	1
1:A:15:VAL:HG21	1:A:23:LEU:HD13	0.47	1.86	10	1
1:A:145:GLY:O	1:A:230:PHE:HA	0.47	2.10	5	1
1:A:111:LEU:O	1:A:111:LEU:HD23	0.47	2.09	6	1
1:A:100:LEU:HD23	1:A:100:LEU:N	0.47	2.23	9	4
1:A:222:VAL:HG11	1:A:255:GLY:O	0.47	2.09	3	1
1:A:171:ASP:O	1:A:175:ARG:HG3	0.47	2.08	2	1
1:A:80:TYR:O	1:A:84:LEU:HD23	0.47	2.10	3	2
1:A:50:PRO:HG3	1:A:60:ASN:OD1	0.47	2.10	4	1
1:A:188:GLN:HA	1:A:188:GLN:OE1	0.47	2.10	5	3
1:A:173:LYS:HD2	1:A:173:LYS:H	0.47	1.68	5	1
1:A:239:ARG:HA	1:A:239:ARG:CZ	0.47	2.39	4	1
1:A:54:PRO:HB3	1:A:98:VAL:O	0.47	2.10	8	2
1:A:141:ILE:HG22	1:A:142:THR:N	0.47	2.25	3	2
1:A:15:VAL:HG11	1:A:23:LEU:HG	0.47	1.87	2	1
1:A:164:MET:O	1:A:167:LEU:HG	0.47	2.10	5	1
1:A:24:SER:O	1:A:33:ILE:HB	0.47	2.09	7	1
1:A:78:THR:O	1:A:82:GLN:HB2	0.47	2.10	8	1
1:A:58:ALA:HB1	1:A:59:PRO:HD2	0.46	1.87	6	1
1:A:85:PHE:O	1:A:89:MET:HG3	0.46	2.10	7	1
1:A:85:PHE:CZ	1:A:103:PHE:CE1	0.46	3.03	3	1
1:A:139:ASP:OD1	1:A:251:VAL:HB	0.46	2.10	3	1
1:A:251:VAL:HG22	1:A:256:PHE:HB2	0.46	1.86	5	2
1:A:187:LYS:HB3	1:A:220:TRP:CD1	0.46	2.46	3	1
1:A:37:VAL:HG23	1:A:43:MET:O	0.46	2.10	2	1
1:A:132:PHE:CB	1:A:135:TRP:HB2	0.46	2.41	4	1
1:A:39:GLN:O	1:A:40:HIS:HB2	0.46	2.11	6	1
1:A:138:SER:HB2	1:A:250:ALA:HB2	0.46	1.87	7	2
1:A:90:ASP:HA	1:A:93:PHE:HB2	0.46	1.88	10	1
1:A:187:LYS:HA	1:A:194:THR:HG22	0.46	1.88	5	3
1:A:19:TYR:HB2	1:A:22:LEU:HB3	0.45	1.88	2	1
1:A:126:ASP:O	1:A:147:THR:HG21	0.45	2.11	8	2
1:A:87:GLU:O	1:A:90:ASP:HB3	0.45	2.11	7	1
1:A:132:PHE:HB3	1:A:135:TRP:HB2	0.45	1.88	4	1
1:A:39:GLN:HB3	1:A:41:GLU:OE1	0.45	2.11	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:PRO:O	1:A:141:ILE:HG12	0.45	2.11	10	2
1:A:177:ALA:HA	1:A:229:TRP:NE1	0.45	2.26	5	1
1:A:173:LYS:O	1:A:176:LYS:HG3	0.45	2.10	10	1
1:A:48:SER:O	1:A:60:ASN:HB2	0.45	2.11	5	1
1:A:219:VAL:CG2	1:A:256:PHE:HA	0.45	2.42	6	1
1:A:45:LEU:HD12	1:A:64:VAL:HG12	0.45	1.88	2	1
1:A:99:CYS:SG	1:A:100:LEU:N	0.45	2.90	2	1
1:A:148:PHE:C	1:A:148:PHE:CD1	0.45	2.95	10	1
1:A:236:GLY:O	1:A:239:ARG:HB2	0.45	2.11	6	1
1:A:151:PHE:CZ	1:A:174:MET:HE1	0.44	2.47	3	3
1:A:61:VAL:CG1	1:A:85:PHE:CD1	0.44	3.00	2	1
1:A:148:PHE:O	1:A:148:PHE:HD1	0.44	1.94	2	1
1:A:142:THR:HB	1:A:240:PHE:HB3	0.44	1.89	5	1
1:A:81:LEU:HA	1:A:84:LEU:HD21	0.44	1.90	3	2
1:A:101:PHE:O	1:A:104:LEU:HG	0.44	2.13	3	4
1:A:127:ILE:HD11	1:A:235:ILE:HD13	0.44	1.89	4	1
1:A:253:ARG:HD3	1:A:253:ARG:C	0.44	2.38	10	1
1:A:139:ASP:O	1:A:149:MET:HA	0.44	2.13	1	1
1:A:77:ASP:OD1	1:A:79:LYS:HG3	0.44	2.13	4	1
1:A:89:MET:HA	1:A:92:VAL:HG12	0.43	1.89	7	1
1:A:161:ALA:O	1:A:165:LEU:HB3	0.43	2.13	2	3
1:A:77:ASP:OD2	1:A:79:LYS:HE3	0.43	2.13	3	1
1:A:141:ILE:HB	1:A:148:PHE:HB2	0.43	1.90	9	1
1:A:133:GLU:C	1:A:135:TRP:N	0.43	2.76	5	5
1:A:188:GLN:HB3	1:A:191:SER:HB2	0.43	1.90	4	2
1:A:172:SER:HA	1:A:175:ARG:HB2	0.43	1.90	10	3
1:A:127:ILE:HG12	1:A:149:MET:HE2	0.43	1.90	7	1
1:A:100:LEU:H	1:A:100:LEU:CD2	0.43	2.24	10	1
1:A:28:GLU:H	1:A:28:GLU:CD	0.43	2.21	4	1
1:A:11:GLU:OE1	1:A:100:LEU:HD22	0.43	2.13	3	1
1:A:187:LYS:CG	1:A:220:TRP:CD1	0.43	3.01	6	1
1:A:140:PRO:HB2	1:A:239:ARG:NH2	0.43	2.28	1	1
1:A:144:ARG:C	1:A:146:SER:H	0.42	2.22	3	2
1:A:248:ARG:HH11	1:A:252:VAL:CG2	0.42	2.27	3	1
1:A:141:ILE:N	1:A:148:PHE:O	0.42	2.52	5	2
1:A:169:LYS:HB3	1:A:169:LYS:HZ3	0.42	1.74	9	1
1:A:100:LEU:N	1:A:100:LEU:HD23	0.42	2.29	2	2
1:A:188:GLN:CB	1:A:191:SER:HB2	0.42	2.45	10	1
1:A:156:THR:O	1:A:186:ILE:HD12	0.42	2.14	5	1
1:A:107:LEU:O	1:A:111:LEU:HB2	0.42	2.15	8	1
1:A:77:ASP:OD2	1:A:79:LYS:HG3	0.42	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TYR:HB3	1:A:54:PRO:HD2	0.42	1.92	3	1
1:A:98:VAL:O	1:A:99:CYS:HB2	0.42	2.14	3	1
1:A:54:PRO:HA	1:A:58:ALA:HA	0.42	1.91	3	1
1:A:84:LEU:HA	1:A:87:GLU:HG2	0.42	1.92	3	1
1:A:181:MET:HA	1:A:200:ASP:O	0.42	2.15	5	1
1:A:142:THR:OG1	1:A:239:ARG:HB3	0.42	2.14	7	1
1:A:188:GLN:HG3	1:A:193:ALA:HB3	0.42	1.92	7	2
1:A:6:GLU:O	1:A:9:VAL:HG12	0.42	2.14	5	1
1:A:210:MET:HA	1:A:213:LEU:HB3	0.42	1.91	5	1
1:A:27:GLN:HB3	1:A:31:SER:OG	0.42	2.15	7	1
1:A:92:VAL:HG22	1:A:92:VAL:O	0.41	2.15	7	1
1:A:139:ASP:CG	1:A:247:ALA:HB1	0.41	2.39	8	1
1:A:37:VAL:CG1	1:A:41:GLU:HG2	0.41	2.45	6	1
1:A:127:ILE:HD11	1:A:235:ILE:HG12	0.41	1.92	7	1
1:A:92:VAL:HB	1:A:102:ASP:OD1	0.41	2.15	9	1
1:A:61:VAL:HG13	1:A:85:PHE:CD1	0.41	2.50	2	1
1:A:53:TYR:HB2	1:A:55:SER:OG	0.41	2.14	8	1
1:A:158:GLU:HA	1:A:186:ILE:CD1	0.41	2.45	10	1
1:A:148:PHE:CD1	1:A:148:PHE:C	0.41	2.98	2	1
1:A:77:ASP:H	1:A:80:TYR:HB2	0.41	1.76	7	1
1:A:187:LYS:HD2	1:A:194:THR:CG2	0.41	2.46	10	1
1:A:6:GLU:O	1:A:10:GLU:HG3	0.41	2.15	1	2
1:A:251:VAL:HG13	1:A:252:VAL:N	0.41	2.31	3	2
1:A:151:PHE:CD2	1:A:168:LEU:HD11	0.41	2.51	5	1
1:A:165:LEU:C	1:A:165:LEU:HD23	0.41	2.41	7	1
1:A:185:ARG:HG2	1:A:220:TRP:HA	0.41	1.92	5	1
1:A:5:HIS:O	1:A:9:VAL:HG22	0.41	2.16	10	1
1:A:148:PHE:HD1	1:A:148:PHE:O	0.41	1.97	10	1
1:A:15:VAL:HG23	1:A:19:TYR:CE1	0.41	2.50	6	1
1:A:85:PHE:CZ	1:A:103:PHE:HE1	0.41	2.34	6	1
1:A:23:LEU:HD13	1:A:24:SER:N	0.41	2.30	4	1
1:A:46:GLN:HE21	1:A:46:GLN:HA	0.41	1.76	9	1
1:A:92:VAL:CB	1:A:99:CYS:HA	0.41	2.46	10	1
1:A:140:PRO:HG2	1:A:243:ILE:HD11	0.41	1.91	2	1
1:A:29:ASP:CG	1:A:30:GLY:N	0.41	2.79	8	1
1:A:110:VAL:C	1:A:112:TYR:H	0.41	2.23	4	1
1:A:188:GLN:CG	1:A:193:ALA:HB3	0.41	2.46	4	1
1:A:148:PHE:C	1:A:148:PHE:HD1	0.41	2.23	10	1
1:A:105:THR:O	1:A:108:ASP:HB3	0.40	2.16	8	1
1:A:146:SER:HA	1:A:229:TRP:O	0.40	2.16	7	1
1:A:214:ILE:O	1:A:219:VAL:HG12	0.40	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:ASP:CB	1:A:204:THR:HA	0.40	2.46	5	1
1:A:167:LEU:O	1:A:171:ASP:HB2	0.40	2.16	7	1
1:A:92:VAL:CG1	1:A:102:ASP:HB3	0.40	2.47	10	1
1:A:140:PRO:HA	1:A:148:PHE:O	0.40	2.16	10	1
1:A:187:LYS:HB3	1:A:221:ASN:OD1	0.40	2.16	10	1
1:A:139:ASP:OD2	1:A:247:ALA:HB1	0.40	2.17	4	2
1:A:50:PRO:CD	1:A:59:PRO:HA	0.40	2.46	5	1
1:A:53:TYR:HB2	1:A:54:PRO:HD2	0.40	1.94	6	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	231/258 (90%)	193±3 (84±1%)	30±3 (13±1%)	8±2 (4±1%)	4	32
All	All	2310/2580 (90%)	1931 (84%)	296 (13%)	83 (4%)	4	32

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	99	CYS	10
1	A	138	SER	10
1	A	20	PRO	7
1	A	53	TYR	6
1	A	54	PRO	6
1	A	31	SER	5
1	A	201	ASP	5
1	A	41	GLU	4
1	A	42	TYR	3
1	A	92	VAL	3
1	A	40	HIS	3
1	A	254	ALA	2
1	A	68	THR	2
1	A	158	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	230	PHE	2
1	A	257	ASP	2
1	A	235	ILE	2
1	A	134	GLY	1
1	A	200	ASP	1
1	A	58	ALA	1
1	A	202	GLY	1
1	A	112	TYR	1
1	A	177	ALA	1
1	A	156	THR	1
1	A	256	PHE	1
1	A	51	THR	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	200/224 (89%)	182±2 (91±1%)	18±2 (9±1%)	11	57
All	All	2000/2240 (89%)	1819 (91%)	181 (9%)	11	57

All 66 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	84	LEU	10
1	A	98	VAL	10
1	A	211	LEU	9
1	A	213	LEU	9
1	A	45	LEU	8
1	A	19	TYR	7
1	A	79	LYS	7
1	A	81	LEU	7
1	A	229	TRP	7
1	A	174	MET	6
1	A	103	PHE	5
1	A	168	LEU	5
1	A	217	MET	5

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Mol	Chain	Res	Type	Models (Total)
1	A	53	TYR	4
1	A	107	LEU	4
1	A	92	VAL	4
1	A	239	ARG	3
1	A	173	LYS	3
1	A	234	HIS	3
1	A	105	THR	3
1	A	27	GLN	3
1	A	167	LEU	2
1	A	23	LEU	2
1	A	93	PHE	2
1	A	148	PHE	2
1	A	36	LYS	2
1	A	40	HIS	2
1	A	162	PHE	2
1	A	169	LYS	2
1	A	241	LYS	2
1	A	82	GLN	2
1	A	176	LYS	2
1	A	203	GLU	2
1	A	46	GLN	2
1	A	243	ILE	2
1	A	60	ASN	1
1	A	63	GLU	1
1	A	16	GLU	1
1	A	22	LEU	1
1	A	39	GLN	1
1	A	85	PHE	1
1	A	188	GLN	1
1	A	5	HIS	1
1	A	56	GLU	1
1	A	196	GLN	1
1	A	28	GLU	1
1	A	110	VAL	1
1	A	219	VAL	1
1	A	242	HIS	1
1	A	68	THR	1
1	A	90	ASP	1
1	A	133	GLU	1
1	A	165	LEU	1
1	A	181	MET	1
1	A	11	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	33	ILE	1
1	A	48	SER	1
1	A	129	THR	1
1	A	175	ARG	1
1	A	201	ASP	1
1	A	235	ILE	1
1	A	253	ARG	1
1	A	97	SER	1
1	A	228	ARG	1
1	A	9	VAL	1
1	A	139	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *yih.str.txt*

7.1.1 Bookkeeping [i](#)

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	2691
Number of shifts mapped to atoms	2691
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	249	2.58 ± 0.11	Should be applied
$^{13}\text{C}_\beta$	237	2.92 ± 0.15	Should be applied
$^{13}\text{C}'$	164	2.90 ± 0.13	Should be applied
^{15}N	238	0.16 ± 0.21	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 2466 atoms were assigned a chemical shift out of a possible 3107. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1042/1154 (90%)	449/467 (96%)	377/464 (81%)	216/223 (97%)
Sidechain	1330/1650 (81%)	897/1078 (83%)	429/526 (82%)	4/46 (9%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	94/303 (31%)	56/148 (38%)	36/133 (27%)	2/22 (9%)
Overall	2466/3107 (79%)	1402/1693 (83%)	842/1123 (75%)	222/291 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 2689 atoms were assigned a chemical shift out of a possible 3451. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1145/1281 (89%)	494/518 (95%)	413/516 (80%)	238/247 (96%)
Sidechain	1448/1859 (78%)	973/1210 (80%)	471/594 (79%)	4/55 (7%)
Aromatic	96/311 (31%)	57/152 (38%)	37/135 (27%)	2/24 (8%)
Overall	2689/3451 (78%)	1524/1880 (81%)	921/1245 (74%)	244/326 (75%)

7.1.4 Statistically unusual chemical shifts ⓘ

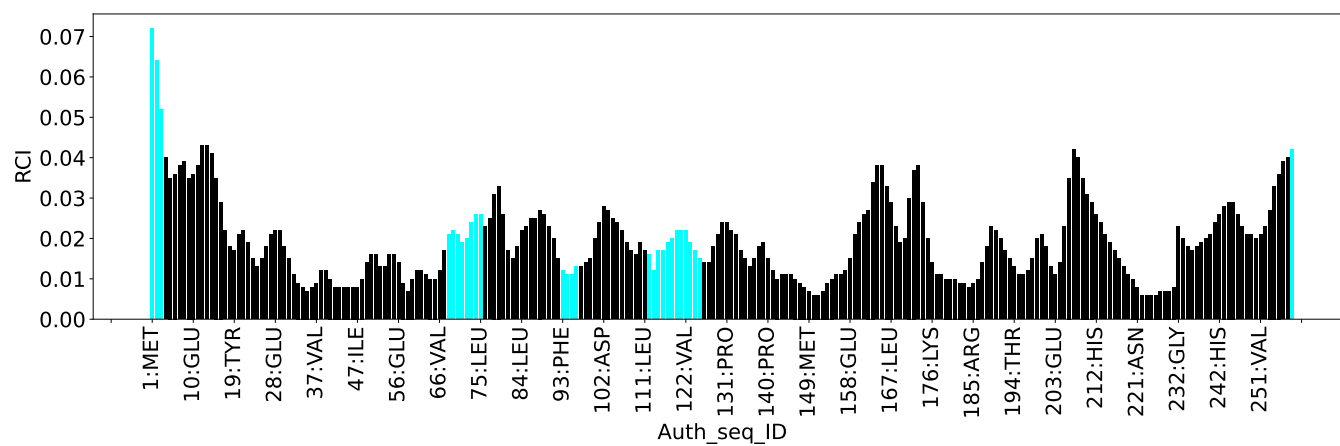
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	234	HIS	CE1	115.05	126.08 – 149.12	-9.8
1	A	168	LEU	HD11	-1.26	-0.61 – 2.12	-7.4
1	A	168	LEU	HD12	-1.26	-0.61 – 2.12	-7.4
1	A	168	LEU	HD13	-1.26	-0.61 – 2.12	-7.4
1	A	168	LEU	HD21	-0.91	-0.65 – 2.13	-5.9
1	A	168	LEU	HD22	-0.91	-0.65 – 2.13	-5.9
1	A	168	LEU	HD23	-0.91	-0.65 – 2.13	-5.9
1	A	54	PRO	CG	20.90	21.69 – 32.72	-5.7
1	A	145	GLY	N	129.71	91.59 – 127.52	5.6
1	A	109	GLY	N	129.54	91.59 – 127.52	5.6
1	A	253	ARG	CD	38.49	38.57 – 47.75	-5.1
1	A	202	GLY	N	127.77	91.59 – 127.52	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



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	2669
Intra-residue ($ i-j =0$)	563
Sequential ($ i-j =1$)	827
Medium range ($ i-j >1$ and $ i-j <5$)	535
Long range ($ i-j \geq 5$)	744
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	388
Number of unmapped restraints	0
Number of restraints per residue	11.8
Number of long range restraints per residue ¹	2.9

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)	119.9	0.2
0.2-0.5 (Medium)	89.1	0.5
>0.5 (Large)	8.8	1.35

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)	41.3	9.64
10.0-20.0 (Medium)	2.1	19.58
>20.0 (Large)	0.2	23.16

9 Distance violation analysis ⓘ

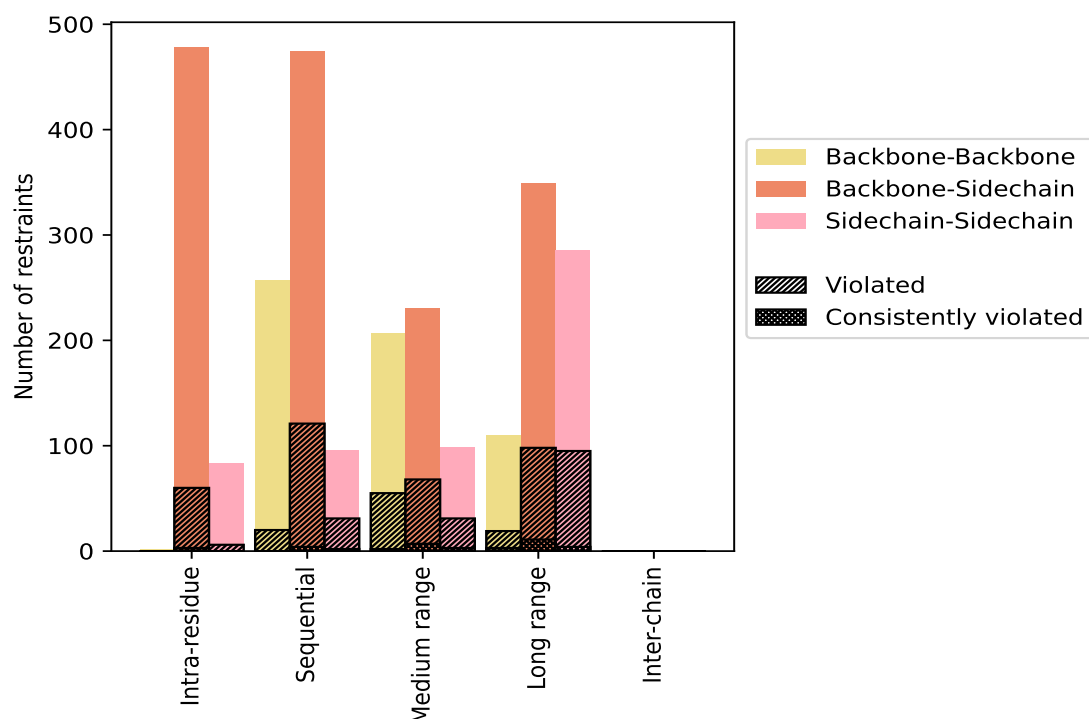
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	563	21.1	66	11.7	2.5	3	0.5	0.1
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	478	17.9	60	12.6	2.2	3	0.6	0.1
Sidechain-Sidechain	83	3.1	6	7.2	0.2	0	0.0	0.0
Sequential ($i-j =1$)	827	31.0	172	20.8	6.4	6	0.7	0.2
Backbone-Backbone	257	9.6	20	7.8	0.7	0	0.0	0.0
Backbone-Sidechain	474	17.8	121	25.5	4.5	4	0.8	0.1
Sidechain-Sidechain	96	3.6	31	32.3	1.2	2	2.1	0.1
Medium range ($i-j >1$ & $i-j <5$)	535	20.0	154	28.8	5.8	12	2.2	0.4
Backbone-Backbone	207	7.8	55	26.6	2.1	2	1.0	0.1
Backbone-Sidechain	230	8.6	68	29.6	2.5	7	3.0	0.3
Sidechain-Sidechain	98	3.7	31	31.6	1.2	3	3.1	0.1
Long range ($i-j \geq 5$)	744	27.9	212	28.5	7.9	18	2.4	0.7
Backbone-Backbone	110	4.1	19	17.3	0.7	3	2.7	0.1
Backbone-Sidechain	349	13.1	98	28.1	3.7	11	3.2	0.4
Sidechain-Sidechain	285	10.7	95	33.3	3.6	4	1.4	0.1
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2669	100.0	604	22.6	22.6	39	1.5	1.5
Backbone-Backbone	576	21.6	94	16.3	3.5	5	0.9	0.2
Backbone-Sidechain	1531	57.4	347	22.7	13.0	25	1.6	0.9
Sidechain-Sidechain	562	21.1	163	29.0	6.1	9	1.6	0.3

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

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



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

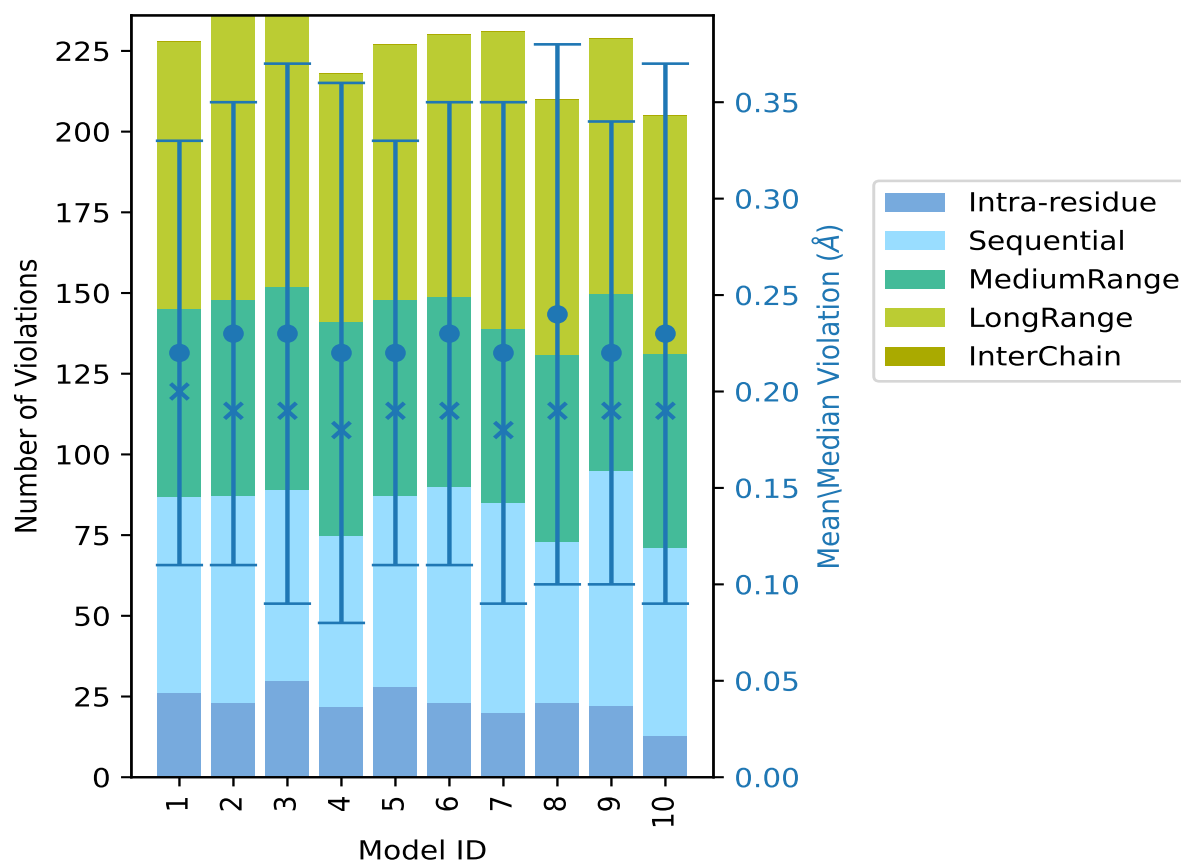
9.2 Distance violation statistics for each model [i](#)

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	26	61	58	83	0	228	0.22	0.77	0.11	0.2
2	23	64	61	88	0	236	0.23	0.81	0.12	0.19
3	30	59	63	84	0	236	0.23	1.3	0.14	0.19
4	22	53	66	77	0	218	0.22	1.35	0.14	0.18
5	28	59	61	79	0	227	0.22	0.84	0.11	0.19
6	23	67	59	81	0	230	0.23	0.76	0.12	0.19
7	20	65	54	92	0	231	0.22	0.95	0.13	0.18
8	23	50	58	79	0	210	0.24	0.81	0.14	0.19
9	22	73	55	79	0	229	0.22	0.84	0.12	0.19
10	13	58	60	74	0	205	0.23	1.04	0.14	0.19

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, 2065(IR:497, SQ:655, MR:381, LR:532, 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	%
25	56	47	62	0	190	1	10.0
10	28	32	32	0	102	2	20.0
7	20	11	29	0	67	3	30.0

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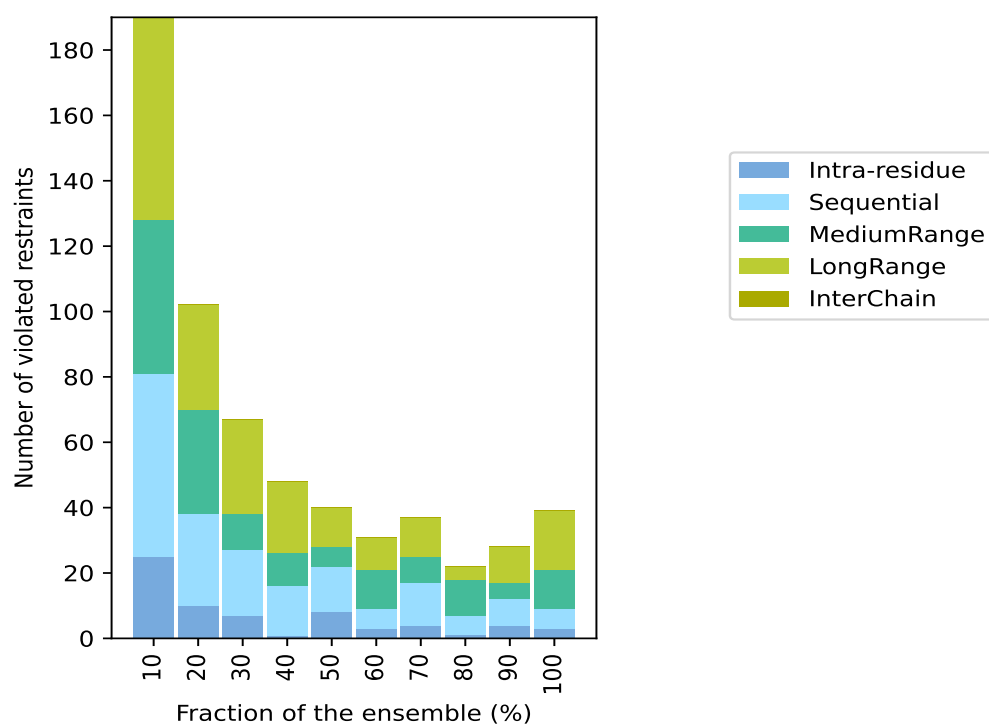
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	15	10	22	0	48	4	40.0
8	14	6	12	0	40	5	50.0
3	6	12	10	0	31	6	60.0
4	13	8	12	0	37	7	70.0
1	6	11	4	0	22	8	80.0
4	8	5	11	0	28	9	90.0
3	6	12	18	0	39	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 ⓘ

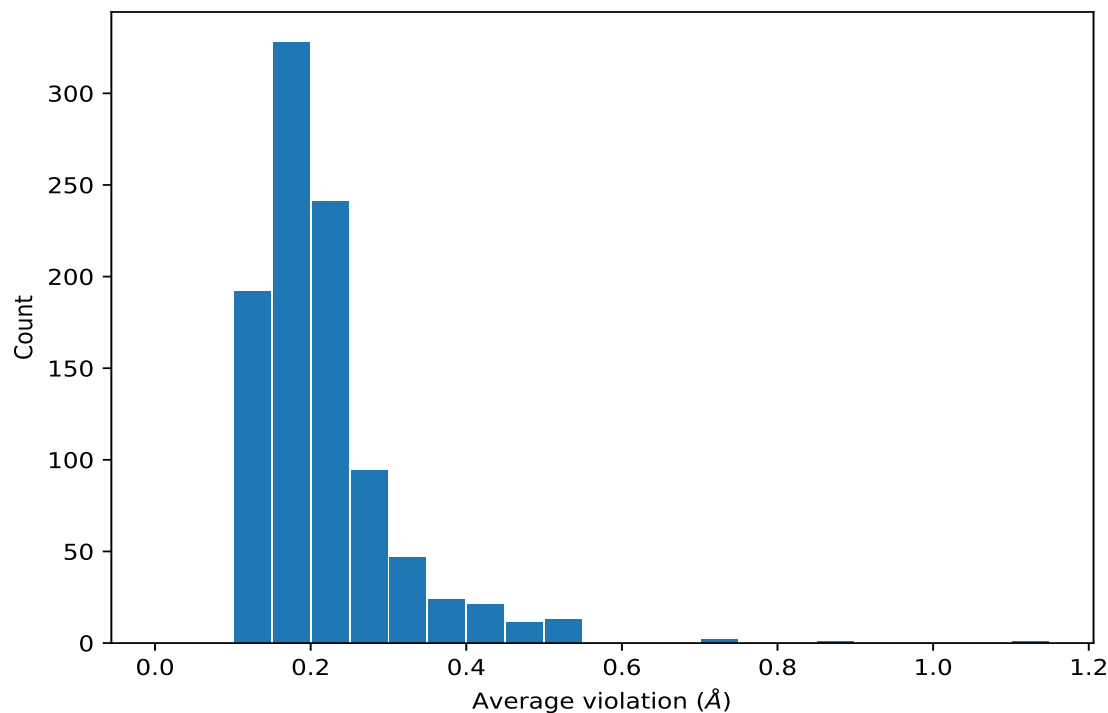


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



9.4.2 Table: Most violated distance restraints [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)
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	10	0.72	0.06	0.72
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	10	0.72	0.06	0.72
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	10	0.5	0.06	0.5
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	10	0.5	0.06	0.5
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	10	0.5	0.06	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	10	0.5	0.06	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	10	0.5	0.06	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	10	0.5	0.06	0.5
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	10	0.49	0.18	0.48
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	10	0.49	0.18	0.48
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	10	0.49	0.18	0.48
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	10	0.45	0.1	0.45
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	10	0.45	0.1	0.45
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	10	0.45	0.1	0.45
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	10	0.44	0.04	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	10	0.42	0.1	0.39
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	10	0.42	0.1	0.39
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	10	0.42	0.1	0.39
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	10	0.4	0.02	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	10	0.4	0.02	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	10	0.4	0.02	0.41
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	10	0.39	0.13	0.38
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	10	0.39	0.13	0.38
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	10	0.36	0.08	0.36
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	10	0.36	0.08	0.36
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	10	0.36	0.08	0.36
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	10	0.36	0.08	0.36
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	10	0.36	0.08	0.36
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	10	0.36	0.08	0.36
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	10	0.35	0.09	0.32
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	10	0.35	0.09	0.32
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	10	0.34	0.07	0.32
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	10	0.34	0.13	0.34
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	10	0.34	0.13	0.34
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	10	0.34	0.13	0.34
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	10	0.32	0.08	0.32
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	10	0.32	0.08	0.32
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	10	0.32	0.08	0.32
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	10	0.32	0.11	0.29
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	10	0.32	0.11	0.29
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	10	0.32	0.08	0.32
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	10	0.32	0.08	0.32
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	10	0.32	0.08	0.32
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	10	0.3	0.09	0.32
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	10	0.3	0.07	0.32
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	10	0.29	0.04	0.3
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	10	0.29	0.07	0.3
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	10	0.29	0.07	0.3
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	10	0.29	0.07	0.3
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	10	0.29	0.07	0.3
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	10	0.29	0.07	0.3
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	10	0.29	0.07	0.3
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	10	0.29	0.14	0.23
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	10	0.27	0.04	0.27
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	10	0.27	0.04	0.27
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	10	0.27	0.04	0.27
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	10	0.26	0.07	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	10	0.26	0.07	0.25
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	10	0.26	0.07	0.25
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	10	0.26	0.05	0.25
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	10	0.25	0.02	0.26
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	10	0.25	0.06	0.26
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	10	0.25	0.07	0.24
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	10	0.25	0.07	0.24
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	10	0.25	0.07	0.24
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	10	0.25	0.06	0.26
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	10	0.25	0.06	0.26
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	10	0.25	0.06	0.26
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	10	0.24	0.09	0.21
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	10	0.24	0.09	0.21
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	10	0.24	0.09	0.21
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	10	0.23	0.05	0.24
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	10	0.23	0.05	0.24
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	10	0.23	0.05	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	10	0.22	0.03	0.23
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	10	0.22	0.03	0.23
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	10	0.22	0.03	0.23
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	10	0.22	0.03	0.21
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	10	0.21	0.05	0.22
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	10	0.2	0.03	0.2
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	10	0.19	0.04	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	10	0.18	0.04	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	10	0.18	0.04	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	10	0.18	0.04	0.18
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	10	0.17	0.02	0.16
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	10	0.16	0.02	0.16
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	10	0.16	0.02	0.15
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	10	0.15	0.01	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	10	0.15	0.01	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	10	0.15	0.01	0.16
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	9	0.46	0.23	0.32
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	9	0.34	0.07	0.32
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	9	0.31	0.18	0.35
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	9	0.31	0.18	0.35
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	9	0.31	0.18	0.35
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	9	0.3	0.06	0.29
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	9	0.3	0.09	0.32
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	9	0.28	0.11	0.33
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	9	0.28	0.11	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	9	0.27	0.06	0.27
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	9	0.27	0.19	0.17
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	9	0.27	0.19	0.17
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	9	0.27	0.19	0.17
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	9	0.25	0.1	0.25
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	9	0.25	0.1	0.25
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	9	0.25	0.1	0.25
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	9	0.24	0.24	0.15
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	9	0.24	0.07	0.23
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	9	0.24	0.07	0.25
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	9	0.24	0.07	0.25
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	9	0.24	0.07	0.25
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	9	0.24	0.04	0.24
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	9	0.24	0.06	0.23
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	9	0.24	0.04	0.24
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	9	0.24	0.04	0.24
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	9	0.24	0.04	0.24
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	9	0.24	0.07	0.27
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	9	0.24	0.07	0.27
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	9	0.23	0.06	0.24
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	9	0.23	0.06	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	9	0.23	0.06	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	9	0.23	0.06	0.25
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	9	0.23	0.03	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	9	0.23	0.03	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	9	0.23	0.03	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	9	0.22	0.06	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	9	0.22	0.06	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	9	0.22	0.06	0.21
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	9	0.19	0.06	0.17
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	9	0.19	0.05	0.2
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	9	0.19	0.05	0.2
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	9	0.19	0.05	0.2
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	9	0.19	0.05	0.2
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	9	0.18	0.03	0.18
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	9	0.18	0.03	0.18
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	9	0.18	0.03	0.18
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	9	0.16	0.02	0.17
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	9	0.15	0.04	0.14
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	9	0.15	0.02	0.14
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	9	0.15	0.02	0.14
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	9	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	9	0.14	0.02	0.13
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	9	0.13	0.03	0.12
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	9	0.13	0.03	0.12
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	9	0.13	0.03	0.12
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	9	0.13	0.03	0.12
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	9	0.13	0.03	0.12
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	9	0.13	0.03	0.12
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	8	0.48	0.16	0.51
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	8	0.48	0.16	0.51
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	8	0.35	0.06	0.35
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	8	0.35	0.06	0.35
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	8	0.35	0.06	0.35
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	8	0.3	0.08	0.28
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	8	0.29	0.12	0.29
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	8	0.29	0.12	0.29
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	8	0.29	0.12	0.29
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	8	0.28	0.21	0.22
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	8	0.28	0.21	0.22
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	8	0.25	0.05	0.26
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	8	0.25	0.08	0.24
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	8	0.23	0.07	0.24
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	8	0.23	0.07	0.24
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	8	0.23	0.07	0.24
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	8	0.22	0.07	0.21
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	8	0.21	0.04	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	8	0.21	0.04	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	8	0.21	0.04	0.2
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	8	0.21	0.05	0.2
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	8	0.2	0.08	0.18
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	8	0.2	0.08	0.18
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	8	0.2	0.11	0.15
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	8	0.18	0.07	0.15
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	8	0.18	0.07	0.15
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	8	0.17	0.05	0.16
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	8	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	8	0.16	0.06	0.15
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	8	0.15	0.03	0.14
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	8	0.15	0.03	0.14
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	8	0.15	0.03	0.14
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	8	0.15	0.02	0.15
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	8	0.15	0.02	0.15
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	8	0.15	0.02	0.15
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	8	0.15	0.02	0.14
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	8	0.14	0.03	0.13
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	8	0.14	0.03	0.14
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	7	0.42	0.05	0.41
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	7	0.42	0.05	0.41
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	7	0.42	0.05	0.41
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	7	0.42	0.05	0.41
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	7	0.35	0.06	0.33
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	7	0.35	0.06	0.33
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	7	0.31	0.18	0.26
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	7	0.31	0.18	0.26
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	7	0.31	0.18	0.26
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	7	0.3	0.14	0.3
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	7	0.26	0.05	0.27
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	7	0.26	0.05	0.27
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	7	0.26	0.05	0.27
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	7	0.26	0.09	0.27
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	7	0.26	0.09	0.27
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	7	0.26	0.09	0.21
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	7	0.23	0.07	0.22
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	7	0.23	0.07	0.22
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	7	0.23	0.07	0.22
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	7	0.23	0.04	0.24
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	7	0.23	0.04	0.24
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	7	0.23	0.04	0.24
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	7	0.22	0.05	0.22
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	7	0.22	0.06	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	7	0.22	0.06	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	7	0.22	0.06	0.19
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	7	0.22	0.02	0.21
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	7	0.22	0.02	0.21
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	7	0.21	0.07	0.2
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	7	0.21	0.07	0.2
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	7	0.21	0.07	0.2
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	7	0.21	0.09	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	7	0.21	0.07	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	7	0.21	0.07	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	7	0.21	0.07	0.21
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	7	0.21	0.05	0.2
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	7	0.2	0.06	0.19
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	7	0.2	0.06	0.19
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	7	0.2	0.04	0.2
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	7	0.2	0.04	0.2
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	7	0.18	0.08	0.15
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	7	0.18	0.08	0.15
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	7	0.18	0.08	0.15
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	7	0.18	0.06	0.17
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	7	0.18	0.06	0.17
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	7	0.18	0.06	0.17
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	7	0.18	0.04	0.17
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	7	0.18	0.05	0.17
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	7	0.18	0.05	0.17
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	7	0.18	0.05	0.17
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	7	0.18	0.02	0.18
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	7	0.18	0.02	0.18
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	7	0.18	0.02	0.18
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	7	0.17	0.01	0.17
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	7	0.17	0.01	0.17
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	7	0.16	0.03	0.16
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	7	0.16	0.03	0.16
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	7	0.16	0.03	0.16
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	7	0.16	0.03	0.16
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	7	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	7	0.16	0.03	0.16
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	7	0.16	0.03	0.16
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	7	0.16	0.03	0.16
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	7	0.16	0.03	0.16
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	7	0.16	0.01	0.16
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	7	0.16	0.01	0.16
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	7	0.16	0.01	0.16
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	7	0.15	0.04	0.14
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	7	0.15	0.04	0.14
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	7	0.15	0.04	0.14
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	7	0.15	0.03	0.14
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	7	0.15	0.02	0.15
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	7	0.15	0.02	0.15
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	7	0.15	0.02	0.15
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	7	0.15	0.03	0.15
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	7	0.14	0.03	0.13
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	7	0.14	0.07	0.11
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	7	0.14	0.02	0.14
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	7	0.14	0.02	0.14
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	7	0.12	0.02	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	7	0.12	0.01	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	7	0.12	0.01	0.12
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	7	0.12	0.01	0.12
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	7	0.12	0.01	0.12
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	7	0.12	0.01	0.12
(1,1879)	1:187:A:LYS:HB2	1:221:A:ASN:HD22	6	0.89	0.27	0.94
(1,2312)	1:56:A:GLU:H	1:58:A:ALA:H	6	0.35	0.1	0.35
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD11	6	0.33	0.07	0.31
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD12	6	0.33	0.07	0.31
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD13	6	0.33	0.07	0.31
(1,2303)	1:19:A:TYR:HB2	1:21:A:ASP:H	6	0.32	0.09	0.3
(1,40)	1:255:A:GLY:HA3	1:257:A:ASP:H	6	0.29	0.12	0.28
(1,1043)	1:42:A:TYR:HA	1:67:A:CYS:HB2	6	0.27	0.07	0.26
(1,2093)	1:239:A:ARG:HB3	1:241:A:LYS:H	6	0.25	0.13	0.22
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG2	6	0.25	0.05	0.27
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG3	6	0.25	0.05	0.27
(1,411)	1:187:A:LYS:HB2	1:188:A:GLN:H	6	0.23	0.08	0.22
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG21	6	0.22	0.07	0.24
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG22	6	0.22	0.07	0.24
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG23	6	0.22	0.07	0.24
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG21	6	0.22	0.07	0.24
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG22	6	0.22	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG23	6	0.22	0.07	0.24
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG21	6	0.22	0.07	0.24
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG22	6	0.22	0.07	0.24
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG23	6	0.22	0.07	0.24
(1,129)	1:79:A:LYS:HE2	1:80:A:TYR:H	6	0.21	0.09	0.2
(1,129)	1:79:A:LYS:HE3	1:80:A:TYR:H	6	0.21	0.09	0.2
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD2	6	0.21	0.04	0.2
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD3	6	0.21	0.04	0.2
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD2	6	0.21	0.04	0.2
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD3	6	0.21	0.04	0.2
(1,621)	1:117:A:GLU:H	1:118:A:GLU:HB3	6	0.21	0.14	0.16
(1,572)	1:79:A:LYS:HB2	1:80:A:TYR:H	6	0.2	0.07	0.18
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD21	6	0.19	0.07	0.2
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD22	6	0.19	0.07	0.2
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD23	6	0.19	0.07	0.2
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD21	6	0.19	0.06	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD22	6	0.19	0.06	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD23	6	0.19	0.06	0.18
(1,2187)	1:107:A:LEU:HB2	1:111:A:LEU:H	6	0.18	0.04	0.16
(1,2610)	1:98:A:VAL:HG21	1:99:A:CYS:HB2	6	0.18	0.05	0.19
(1,2610)	1:98:A:VAL:HG22	1:99:A:CYS:HB2	6	0.18	0.05	0.19
(1,2610)	1:98:A:VAL:HG23	1:99:A:CYS:HB2	6	0.18	0.05	0.19
(1,1069)	1:242:A:HIS:HA	1:245:A:SER:H	6	0.17	0.04	0.18
(1,2318)	1:49:A:PHE:HD2	1:60:A:ASN:H	6	0.17	0.05	0.16
(1,2491)	1:168:A:LEU:HD21	1:174:A:MET:H	6	0.17	0.04	0.16
(1,2491)	1:168:A:LEU:HD22	1:174:A:MET:H	6	0.17	0.04	0.16
(1,2491)	1:168:A:LEU:HD23	1:174:A:MET:H	6	0.17	0.04	0.16
(1,1995)	1:51:A:THR:H	1:53:A:TYR:H	6	0.16	0.03	0.16
(1,1353)	1:181:A:MET:HE1	1:228:A:ARG:H	6	0.16	0.03	0.17
(1,1353)	1:181:A:MET:HE2	1:228:A:ARG:H	6	0.16	0.03	0.17
(1,1353)	1:181:A:MET:HE3	1:228:A:ARG:H	6	0.16	0.03	0.17
(1,2096)	1:251:A:VAL:HG21	1:253:A:ARG:H	6	0.16	0.04	0.14
(1,2096)	1:251:A:VAL:HG22	1:253:A:ARG:H	6	0.16	0.04	0.14
(1,2096)	1:251:A:VAL:HG23	1:253:A:ARG:H	6	0.16	0.04	0.14
(1,2129)	1:222:A:VAL:HG11	1:256:A:PHE:H	6	0.16	0.06	0.12
(1,2129)	1:222:A:VAL:HG12	1:256:A:PHE:H	6	0.16	0.06	0.12
(1,2129)	1:222:A:VAL:HG13	1:256:A:PHE:H	6	0.16	0.06	0.12
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD11	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD12	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD13	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD21	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD22	6	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD23	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD11	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD12	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD13	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD21	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD22	6	0.15	0.02	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD23	6	0.15	0.02	0.15
(1,2248)	1:64:A:VAL:HG21	1:83:A:HIS:H	6	0.15	0.04	0.13
(1,2248)	1:64:A:VAL:HG22	1:83:A:HIS:H	6	0.15	0.04	0.13
(1,2248)	1:64:A:VAL:HG23	1:83:A:HIS:H	6	0.15	0.04	0.13
(1,490)	1:48:A:SER:HB2	1:60:A:ASN:HB2	6	0.14	0.03	0.13
(1,1051)	1:137:A:ALA:HB1	1:151:A:PHE:HE1	6	0.13	0.02	0.13
(1,1051)	1:137:A:ALA:HB2	1:151:A:PHE:HE1	6	0.13	0.02	0.13
(1,1051)	1:137:A:ALA:HB3	1:151:A:PHE:HE1	6	0.13	0.02	0.13
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD11	6	0.12	0.01	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD12	6	0.12	0.01	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD13	6	0.12	0.01	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG21	6	0.12	0.01	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG22	6	0.12	0.01	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG23	6	0.12	0.01	0.12
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD2	5	0.51	0.01	0.51
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD3	5	0.51	0.01	0.51
(1,2323)	1:58:A:ALA:HB1	1:92:A:VAL:H	5	0.41	0.15	0.43
(1,2323)	1:58:A:ALA:HB2	1:92:A:VAL:H	5	0.41	0.15	0.43
(1,2323)	1:58:A:ALA:HB3	1:92:A:VAL:H	5	0.41	0.15	0.43
(1,794)	1:258:A:SER:HA	1:258:A:SER:HB2	5	0.38	0.01	0.38
(1,550)	1:258:A:SER:H	1:258:A:SER:HB3	5	0.37	0.16	0.27
(1,922)	1:176:A:LYS:HG3	1:177:A:ALA:H	5	0.34	0.14	0.31
(1,1621)	1:4:A:ASP:H	1:4:A:ASP:HB3	5	0.34	0.02	0.34
(1,989)	1:200:A:ASP:HA	1:207:A:GLY:H	5	0.26	0.13	0.21
(1,111)	1:175:A:ARG:HD2	1:176:A:LYS:H	5	0.26	0.07	0.3
(1,111)	1:175:A:ARG:HD3	1:176:A:LYS:H	5	0.26	0.07	0.3
(1,527)	1:61:A:VAL:HG21	1:82:A:GLN:HG2	5	0.26	0.14	0.17
(1,527)	1:61:A:VAL:HG22	1:82:A:GLN:HG2	5	0.26	0.14	0.17
(1,527)	1:61:A:VAL:HG23	1:82:A:GLN:HG2	5	0.26	0.14	0.17
(1,1942)	1:144:A:ARG:H	1:234:A:HIS:HA	5	0.26	0.05	0.26
(1,563)	1:257:A:ASP:HB2	1:258:A:SER:HB2	5	0.24	0.09	0.24
(1,563)	1:257:A:ASP:HB3	1:258:A:SER:HB2	5	0.24	0.09	0.24
(1,1959)	1:187:A:LYS:H	1:189:A:ASP:H	5	0.22	0.09	0.17
(1,1439)	1:58:A:ALA:HB1	1:94:A:HIS:H	5	0.22	0.07	0.2
(1,1439)	1:58:A:ALA:HB2	1:94:A:HIS:H	5	0.22	0.07	0.2
(1,1439)	1:58:A:ALA:HB3	1:94:A:HIS:H	5	0.22	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD11	5	0.21	0.06	0.21
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD12	5	0.21	0.06	0.21
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD13	5	0.21	0.06	0.21
(1,2078)	1:100:A:LEU:H	1:102:A:ASP:H	5	0.21	0.05	0.21
(1,2241)	1:31:A:SER:H	1:32:A:ILE:H	5	0.19	0.06	0.2
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG2	5	0.18	0.04	0.19
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG3	5	0.18	0.04	0.19
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB2	5	0.18	0.05	0.16
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB3	5	0.18	0.05	0.16
(1,1171)	1:51:A:THR:HG21	1:52:A:HIS:H	5	0.18	0.04	0.17
(1,1171)	1:51:A:THR:HG22	1:52:A:HIS:H	5	0.18	0.04	0.17
(1,1171)	1:51:A:THR:HG23	1:52:A:HIS:H	5	0.18	0.04	0.17
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE1	5	0.18	0.06	0.16
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE2	5	0.18	0.06	0.16
(1,2359)	1:40:A:HIS:HA	1:42:A:TYR:H	5	0.17	0.07	0.15
(1,440)	1:27:A:GLN:HG3	1:28:A:GLU:H	5	0.17	0.07	0.13
(1,1935)	1:141:A:ILE:HD11	1:148:A:PHE:H	5	0.17	0.05	0.16
(1,1935)	1:141:A:ILE:HD12	1:148:A:PHE:H	5	0.17	0.05	0.16
(1,1935)	1:141:A:ILE:HD13	1:148:A:PHE:H	5	0.17	0.05	0.16
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE21	5	0.17	0.04	0.15
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE22	5	0.17	0.04	0.15
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG21	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG22	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG23	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG21	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG22	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG23	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG21	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG22	5	0.17	0.04	0.14
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG23	5	0.17	0.04	0.14
(1,560)	1:240:A:PHE:H	1:241:A:LYS:HB2	5	0.16	0.04	0.15
(1,768)	1:248:A:ARG:HA	1:251:A:VAL:HB	5	0.16	0.02	0.16
(1,1035)	1:22:A:LEU:HD21	1:23:A:LEU:H	5	0.16	0.03	0.16
(1,1035)	1:22:A:LEU:HD22	1:23:A:LEU:H	5	0.16	0.03	0.16
(1,1035)	1:22:A:LEU:HD23	1:23:A:LEU:H	5	0.16	0.03	0.16
(1,2227)	1:17:A:ALA:H	1:19:A:TYR:H	5	0.15	0.01	0.15
(1,345)	1:6:A:GLU:HA	1:6:A:GLU:HG2	5	0.15	0.03	0.14
(1,777)	1:42:A:TYR:HD1	1:66:A:VAL:HA	5	0.15	0.03	0.15
(1,777)	1:42:A:TYR:HD2	1:66:A:VAL:HA	5	0.15	0.03	0.15
(1,2040)	1:210:A:MET:H	1:211:A:LEU:HB3	5	0.15	0.04	0.13
(1,324)	1:105:A:THR:HB	1:106:A:GLU:H	5	0.14	0.03	0.13
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD11	5	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD12	5	0.14	0.03	0.14
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD13	5	0.14	0.03	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD11	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD12	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD13	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD11	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD12	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD13	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD11	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD12	5	0.14	0.02	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD13	5	0.14	0.02	0.14
(1,1919)	1:35:A:VAL:H	1:45:A:LEU:H	5	0.13	0.02	0.14
(1,332)	1:9:A:VAL:HA	1:13:A:GLU:HG3	5	0.13	0.04	0.11
(1,1461)	1:43:A:MET:HE1	1:66:A:VAL:H	5	0.12	0.01	0.12
(1,1461)	1:43:A:MET:HE2	1:66:A:VAL:H	5	0.12	0.01	0.12
(1,1461)	1:43:A:MET:HE3	1:66:A:VAL:H	5	0.12	0.01	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG21	5	0.12	0.0	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG22	5	0.12	0.0	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG23	5	0.12	0.0	0.12
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD21	5	0.11	0.01	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD22	5	0.11	0.01	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD23	5	0.11	0.01	0.11
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG21	4	0.51	0.3	0.5
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG22	4	0.51	0.3	0.5
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG23	4	0.51	0.3	0.5
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD11	4	0.4	0.13	0.44
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD12	4	0.4	0.13	0.44
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD13	4	0.4	0.13	0.44
(1,930)	1:36:A:LYS:HG2	1:41:A:GLU:HA	4	0.32	0.16	0.29
(1,930)	1:36:A:LYS:HG3	1:41:A:GLU:HA	4	0.32	0.16	0.29
(1,215)	1:29:A:ASP:HB2	1:30:A:GLY:H	4	0.31	0.12	0.36
(1,991)	1:88:A:VAL:HG21	1:107:A:LEU:HA	4	0.31	0.06	0.33
(1,991)	1:88:A:VAL:HG22	1:107:A:LEU:HA	4	0.31	0.06	0.33
(1,991)	1:88:A:VAL:HG23	1:107:A:LEU:HA	4	0.31	0.06	0.33
(1,588)	1:31:A:SER:HB2	1:49:A:PHE:H	4	0.3	0.02	0.3
(1,1497)	1:127:A:ILE:HG21	1:128:A:PRO:HG3	4	0.29	0.08	0.28
(1,1497)	1:127:A:ILE:HG22	1:128:A:PRO:HG3	4	0.29	0.08	0.28
(1,1497)	1:127:A:ILE:HG23	1:128:A:PRO:HG3	4	0.29	0.08	0.28
(1,2631)	1:235:A:ILE:HD11	1:127:A:ILE:H	4	0.27	0.12	0.25
(1,2631)	1:235:A:ILE:HD12	1:127:A:ILE:H	4	0.27	0.12	0.25
(1,2631)	1:235:A:ILE:HD13	1:127:A:ILE:H	4	0.27	0.12	0.25
(1,1190)	1:1:A:MET:HA	1:2:A:ASP:H	4	0.26	0.21	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1291)	1:177:A:ALA:HA	1:229:A:TRP:HH2	4	0.26	0.21	0.15
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD11	4	0.24	0.1	0.24
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD12	4	0.24	0.1	0.24
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD13	4	0.24	0.1	0.24
(1,99)	1:171:A:ASP:HB2	1:174:A:MET:HB3	4	0.24	0.07	0.26
(1,738)	1:186:A:ILE:HA	1:220:A:TRP:HD1	4	0.24	0.03	0.22
(1,709)	1:79:A:LYS:HD2	1:80:A:TYR:H	4	0.24	0.07	0.22
(1,709)	1:79:A:LYS:HD3	1:80:A:TYR:H	4	0.24	0.07	0.22
(1,1666)	1:251:A:VAL:HG21	1:257:A:ASP:H	4	0.23	0.06	0.23
(1,1666)	1:251:A:VAL:HG22	1:257:A:ASP:H	4	0.23	0.06	0.23
(1,1666)	1:251:A:VAL:HG23	1:257:A:ASP:H	4	0.23	0.06	0.23
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD11	4	0.23	0.08	0.2
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD12	4	0.23	0.08	0.2
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD13	4	0.23	0.08	0.2
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD21	4	0.23	0.1	0.22
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD22	4	0.23	0.1	0.22
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD23	4	0.23	0.1	0.22
(1,2654)	1:103:A:PHE:HE1	1:85:A:PHE:HB3	4	0.22	0.07	0.21
(1,2654)	1:103:A:PHE:HE2	1:85:A:PHE:HB3	4	0.22	0.07	0.21
(1,2089)	1:257:A:ASP:H	1:258:A:SER:H	4	0.22	0.13	0.16
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG11	4	0.22	0.06	0.2
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG12	4	0.22	0.06	0.2
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG13	4	0.22	0.06	0.2
(1,1790)	1:4:A:ASP:HB2	1:5:A:HIS:H	4	0.22	0.06	0.22
(1,2196)	1:88:A:VAL:HG21	1:90:A:ASP:H	4	0.22	0.08	0.22
(1,2196)	1:88:A:VAL:HG22	1:90:A:ASP:H	4	0.22	0.08	0.22
(1,2196)	1:88:A:VAL:HG23	1:90:A:ASP:H	4	0.22	0.08	0.22
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD11	4	0.21	0.05	0.22
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD12	4	0.21	0.05	0.22
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD13	4	0.21	0.05	0.22
(1,1440)	1:58:A:ALA:HB1	1:99:A:CYS:HB2	4	0.2	0.06	0.2
(1,1440)	1:58:A:ALA:HB2	1:99:A:CYS:HB2	4	0.2	0.06	0.2
(1,1440)	1:58:A:ALA:HB3	1:99:A:CYS:HB2	4	0.2	0.06	0.2
(1,2361)	1:42:A:TYR:H	1:43:A:MET:H	4	0.2	0.03	0.2
(1,1701)	1:256:A:PHE:H	1:257:A:ASP:H	4	0.2	0.06	0.2
(1,2075)	1:173:A:LYS:H	1:176:A:LYS:HG2	4	0.19	0.05	0.18
(1,851)	1:171:A:ASP:HB3	1:173:A:LYS:HG3	4	0.19	0.06	0.16
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD1	4	0.19	0.04	0.16
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD2	4	0.19	0.04	0.16
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD1	4	0.19	0.04	0.16
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD2	4	0.19	0.04	0.16
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD1	4	0.19	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD2	4	0.19	0.04	0.16
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG11	4	0.17	0.06	0.16
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG12	4	0.17	0.06	0.16
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG13	4	0.17	0.06	0.16
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG11	4	0.17	0.06	0.16
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG12	4	0.17	0.06	0.16
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG13	4	0.17	0.06	0.16
(1,536)	1:24:A:SER:HB2	1:25:A:LYS:H	4	0.17	0.06	0.16
(1,536)	1:24:A:SER:HB3	1:25:A:LYS:H	4	0.17	0.06	0.16
(1,1027)	1:135:A:TRP:HA	1:154:A:HIS:HD2	4	0.17	0.04	0.18
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG11	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG12	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG13	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG11	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG12	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG13	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG11	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG12	4	0.17	0.03	0.18
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG13	4	0.17	0.03	0.18
(1,2207)	1:161:A:ALA:H	1:164:A:MET:H	4	0.17	0.03	0.17
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG21	4	0.16	0.02	0.17
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG22	4	0.16	0.02	0.17
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG23	4	0.16	0.02	0.17
(1,1585)	1:11:A:GLU:H	1:11:A:GLU:HG3	4	0.16	0.07	0.16
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG21	4	0.16	0.04	0.16
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG22	4	0.16	0.04	0.16
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG23	4	0.16	0.04	0.16
(1,1694)	1:211:A:LEU:HD11	1:213:A:LEU:H	4	0.15	0.06	0.12
(1,1694)	1:211:A:LEU:HD12	1:213:A:LEU:H	4	0.15	0.06	0.12
(1,1694)	1:211:A:LEU:HD13	1:213:A:LEU:H	4	0.15	0.06	0.12
(1,1817)	1:81:A:LEU:H	1:82:A:GLN:HB2	4	0.15	0.03	0.15
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG11	4	0.15	0.02	0.14
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG12	4	0.15	0.02	0.14
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG13	4	0.15	0.02	0.14
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG21	4	0.15	0.02	0.14
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG22	4	0.15	0.02	0.14
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG23	4	0.15	0.02	0.14
(1,60)	1:134:A:GLY:HA3	1:164:A:MET:HB2	4	0.14	0.06	0.12
(1,2306)	1:176:A:LYS:H	1:229:A:TRP:HE1	4	0.14	0.03	0.14
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD1	4	0.14	0.02	0.15
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD2	4	0.14	0.02	0.15
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD1	4	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD2	4	0.14	0.02	0.15
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD1	4	0.14	0.02	0.15
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD2	4	0.14	0.02	0.15
(1,1079)	1:152:A:ALA:HB1	1:224:A:VAL:HA	4	0.13	0.02	0.13
(1,1079)	1:152:A:ALA:HB2	1:224:A:VAL:HA	4	0.13	0.02	0.13
(1,1079)	1:152:A:ALA:HB3	1:224:A:VAL:HA	4	0.13	0.02	0.13
(1,1158)	1:53:A:TYR:HA	1:57:A:GLU:H	4	0.13	0.01	0.12
(1,2426)	1:125:A:SER:HA	1:126:A:ASP:HB3	4	0.12	0.02	0.12
(1,2496)	1:251:A:VAL:HG11	1:253:A:ARG:H	4	0.12	0.02	0.11
(1,2496)	1:251:A:VAL:HG12	1:253:A:ARG:H	4	0.12	0.02	0.11
(1,2496)	1:251:A:VAL:HG13	1:253:A:ARG:H	4	0.12	0.02	0.11
(1,493)	1:243:A:ILE:HA	1:245:A:SER:H	4	0.11	0.01	0.12
(1,742)	1:41:A:GLU:HA	1:43:A:MET:H	3	0.49	0.07	0.51
(1,1188)	1:257:A:ASP:HA	1:258:A:SER:H	3	0.46	0.1	0.52
(1,2390)	1:30:A:GLY:H	1:32:A:ILE:H	3	0.43	0.06	0.41
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD2	3	0.37	0.14	0.3
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD3	3	0.37	0.14	0.3
(1,891)	1:73:A:ARG:HA	1:73:A:ARG:HD2	3	0.36	0.02	0.36
(1,2346)	1:52:A:HIS:H	1:57:A:GLU:HG3	3	0.29	0.21	0.15
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB2	3	0.28	0.22	0.14
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB3	3	0.28	0.22	0.14
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB2	3	0.28	0.22	0.14
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB3	3	0.28	0.22	0.14
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB2	3	0.28	0.22	0.14
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB3	3	0.28	0.22	0.14
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG2	3	0.28	0.04	0.26
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG3	3	0.28	0.04	0.26
(1,526)	1:82:A:GLN:H	1:82:A:GLN:HG2	3	0.28	0.22	0.13
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD11	3	0.24	0.08	0.22
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD12	3	0.24	0.08	0.22
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD13	3	0.24	0.08	0.22
(1,1627)	1:1:A:MET:HB2	1:2:A:ASP:H	3	0.24	0.02	0.23
(1,1627)	1:1:A:MET:HB3	1:2:A:ASP:H	3	0.24	0.02	0.23
(1,488)	1:96:A:GLY:H	1:97:A:SER:HB3	3	0.23	0.17	0.12
(1,2558)	1:92:A:VAL:HG11	1:99:A:CYS:HB3	3	0.23	0.03	0.23
(1,2558)	1:92:A:VAL:HG12	1:99:A:CYS:HB3	3	0.23	0.03	0.23
(1,2558)	1:92:A:VAL:HG13	1:99:A:CYS:HB3	3	0.23	0.03	0.23
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE1	3	0.22	0.11	0.15
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE2	3	0.22	0.11	0.15
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE3	3	0.22	0.11	0.15
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG2	3	0.22	0.05	0.23
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG3	3	0.22	0.05	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2242)	1:29:A:ASP:H	1:32:A:ILE:H	3	0.22	0.07	0.23
(1,1377)	1:131:A:PRO:HD3	1:132:A:PHE:H	3	0.21	0.02	0.22
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG21	3	0.21	0.04	0.23
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG22	3	0.21	0.04	0.23
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG23	3	0.21	0.04	0.23
(1,1735)	1:217:A:MET:HB2	1:218:A:ASP:H	3	0.21	0.08	0.19
(1,781)	1:159:A:GLU:HA	1:162:A:PHE:HB3	3	0.2	0.04	0.2
(1,401)	1:46:A:GLN:HG3	1:63:A:GLU:H	3	0.2	0.03	0.19
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD21	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD22	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD23	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD21	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD22	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD23	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD21	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD22	3	0.2	0.07	0.2
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD23	3	0.2	0.07	0.2
(1,2285)	1:142:A:THR:HG21	1:239:A:ARG:H	3	0.2	0.07	0.19
(1,2285)	1:142:A:THR:HG22	1:239:A:ARG:H	3	0.2	0.07	0.19
(1,2285)	1:142:A:THR:HG23	1:239:A:ARG:H	3	0.2	0.07	0.19
(1,1554)	1:181:A:MET:HB3	1:226:A:VAL:H	3	0.19	0.01	0.2
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD11	3	0.19	0.03	0.2
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD12	3	0.19	0.03	0.2
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD13	3	0.19	0.03	0.2
(1,54)	1:189:A:ASP:HB2	1:190:A:GLY:HA2	3	0.19	0.04	0.21
(1,54)	1:189:A:ASP:HB3	1:190:A:GLY:HA2	3	0.19	0.04	0.21
(1,1994)	1:53:A:TYR:H	1:56:A:GLU:H	3	0.18	0.08	0.14
(1,2194)	1:75:A:LEU:H	1:76:A:TYR:HB3	3	0.18	0.07	0.16
(1,2271)	1:29:A:ASP:H	1:30:A:GLY:H	3	0.18	0.04	0.2
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE1	3	0.17	0.02	0.18
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE2	3	0.17	0.02	0.18
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE3	3	0.17	0.02	0.18
(1,193)	1:163:A:ALA:HA	1:166:A:ASP:HB3	3	0.17	0.03	0.19
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD21	3	0.17	0.05	0.19
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD22	3	0.17	0.05	0.19
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD23	3	0.17	0.05	0.19
(1,2025)	1:186:A:ILE:H	1:196:A:GLN:H	3	0.17	0.06	0.15
(1,1196)	1:105:A:THR:HG21	1:106:A:GLU:H	3	0.16	0.06	0.12
(1,1196)	1:105:A:THR:HG22	1:106:A:GLU:H	3	0.16	0.06	0.12
(1,1196)	1:105:A:THR:HG23	1:106:A:GLU:H	3	0.16	0.06	0.12
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG11	3	0.16	0.04	0.18
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG12	3	0.16	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG13	3	0.16	0.04	0.18
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG11	3	0.16	0.04	0.18
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG12	3	0.16	0.04	0.18
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG13	3	0.16	0.04	0.18
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG11	3	0.16	0.04	0.18
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG12	3	0.16	0.04	0.18
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG13	3	0.16	0.04	0.18
(1,1730)	1:146:A:SER:H	1:234:A:HIS:HA	3	0.16	0.04	0.13
(1,232)	1:186:A:ILE:HB	1:194:A:THR:HB	3	0.16	0.05	0.14
(1,689)	1:187:A:LYS:HD3	1:220:A:TRP:HB3	3	0.16	0.03	0.17
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB2	3	0.16	0.04	0.16
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB3	3	0.16	0.04	0.16
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB2	3	0.16	0.04	0.16
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB3	3	0.16	0.04	0.16
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB2	3	0.16	0.04	0.16
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB3	3	0.16	0.04	0.16
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD11	3	0.16	0.02	0.15
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD12	3	0.16	0.02	0.15
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD13	3	0.16	0.02	0.15
(1,1164)	1:126:A:ASP:HA	1:127:A:ILE:H	3	0.15	0.02	0.14
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD21	3	0.15	0.04	0.14
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD22	3	0.15	0.04	0.14
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD23	3	0.15	0.04	0.14
(1,2157)	1:208:A:SER:H	1:211:A:LEU:H	3	0.15	0.02	0.17
(1,289)	1:158:A:GLU:HG2	1:159:A:GLU:H	3	0.15	0.03	0.16
(1,1747)	1:11:A:GLU:HA	1:13:A:GLU:H	3	0.15	0.05	0.14
(1,1420)	1:58:A:ALA:HB1	1:93:A:PHE:HB2	3	0.15	0.04	0.14
(1,1420)	1:58:A:ALA:HB2	1:93:A:PHE:HB2	3	0.15	0.04	0.14
(1,1420)	1:58:A:ALA:HB3	1:93:A:PHE:HB2	3	0.15	0.04	0.14
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE1	3	0.15	0.02	0.15
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE2	3	0.15	0.02	0.15
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE1	3	0.15	0.02	0.15
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE2	3	0.15	0.02	0.15
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE1	3	0.15	0.02	0.15
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE2	3	0.15	0.02	0.15
(1,362)	1:133:A:GLU:HG2	1:134:A:GLY:HA3	3	0.14	0.02	0.14
(1,362)	1:133:A:GLU:HG3	1:134:A:GLY:HA3	3	0.14	0.02	0.14
(1,722)	1:43:A:MET:HG2	1:64:A:VAL:HA	3	0.14	0.03	0.13
(1,808)	1:141:A:ILE:HA	1:142:A:THR:HB	3	0.14	0.03	0.13
(1,984)	1:168:A:LEU:HD21	1:225:A:VAL:H	3	0.14	0.05	0.12
(1,984)	1:168:A:LEU:HD22	1:225:A:VAL:H	3	0.14	0.05	0.12
(1,984)	1:168:A:LEU:HD23	1:225:A:VAL:H	3	0.14	0.05	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2294)	1:76:A:TYR:HB3	1:81:A:LEU:H	3	0.14	0.05	0.11
(1,416)	1:9:A:VAL:HA	1:13:A:GLU:H	3	0.14	0.01	0.14
(1,1543)	1:188:A:GLN:H	1:194:A:THR:H	3	0.14	0.02	0.15
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD11	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD12	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD13	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD11	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD12	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD13	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD11	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD12	3	0.13	0.0	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD13	3	0.13	0.0	0.13
(1,2235)	1:82:A:GLN:H	1:84:A:LEU:H	3	0.13	0.02	0.14
(1,228)	1:186:A:ILE:H	1:194:A:THR:HB	3	0.13	0.02	0.12
(1,1537)	1:138:A:SER:H	1:150:A:ALA:H	3	0.13	0.02	0.11
(1,2252)	1:159:A:GLU:H	1:160:A:GLN:HB2	3	0.13	0.01	0.13
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE21	3	0.12	0.01	0.12
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE22	3	0.12	0.01	0.12
(1,211)	1:81:A:LEU:HB3	1:84:A:LEU:HG	3	0.12	0.01	0.11
(1,230)	1:194:A:THR:H	1:194:A:THR:HB	3	0.12	0.02	0.11
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG21	3	0.12	0.02	0.11
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG22	3	0.12	0.02	0.11
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG23	3	0.12	0.02	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD11	3	0.11	0.0	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD12	3	0.11	0.0	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD13	3	0.11	0.0	0.11
(1,1405)	1:33:A:ILE:HG21	1:49:A:PHE:HD2	3	0.11	0.01	0.1
(1,1405)	1:33:A:ILE:HG22	1:49:A:PHE:HD2	3	0.11	0.01	0.1
(1,1405)	1:33:A:ILE:HG23	1:49:A:PHE:HD2	3	0.11	0.01	0.1
(1,399)	1:220:A:TRP:HB2	1:220:A:TRP:HE1	3	0.1	0.0	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB1	3	0.1	0.0	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB2	3	0.1	0.0	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB3	3	0.1	0.0	0.1
(1,2659)	1:5:A:HIS:HD1	1:8:A:LEU:HD23	2	1.1	0.26	1.1
(1,175)	1:3:A:ASP:HB2	1:7:A:GLN:HE21	2	0.5	0.32	0.5
(1,175)	1:3:A:ASP:HB3	1:7:A:GLN:HE21	2	0.5	0.32	0.5
(1,1739)	1:167:A:LEU:H	1:167:A:LEU:HG	2	0.44	0.04	0.44
(1,1073)	1:176:A:LYS:HA	1:229:A:TRP:HE1	2	0.44	0.32	0.44
(1,667)	1:147:A:THR:HA	1:148:A:PHE:HD1	2	0.42	0.06	0.42
(1,456)	1:116:A:GLU:HG2	1:117:A:GLU:H	2	0.36	0.03	0.36
(1,456)	1:116:A:GLU:HG3	1:117:A:GLU:H	2	0.36	0.03	0.36
(1,1626)	1:102:A:ASP:H	1:102:A:ASP:HB3	2	0.36	0.05	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB1	2	0.34	0.02	0.34
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB2	2	0.34	0.02	0.34
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB3	2	0.34	0.02	0.34
(1,926)	1:176:A:LYS:HG2	1:177:A:ALA:H	2	0.33	0.02	0.33
(1,1765)	1:104:A:LEU:H	1:105:A:THR:HB	2	0.32	0.04	0.32
(1,2046)	1:61:A:VAL:HB	1:86:A:GLN:H	2	0.32	0.16	0.32
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD11	2	0.3	0.12	0.3
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD12	2	0.3	0.12	0.3
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD13	2	0.3	0.12	0.3
(1,2360)	1:41:A:GLU:H	1:42:A:TYR:H	2	0.28	0.03	0.28
(1,260)	1:119:A:THR:HB	1:120:A:GLU:H	2	0.27	0.17	0.27
(1,521)	1:122:A:VAL:H	1:122:A:VAL:HB	2	0.26	0.01	0.26
(1,1213)	1:42:A:TYR:H	1:43:A:MET:HA	2	0.26	0.14	0.26
(1,1222)	1:9:A:VAL:HG11	1:10:A:GLU:HG2	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG11	1:10:A:GLU:HG3	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG12	1:10:A:GLU:HG2	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG12	1:10:A:GLU:HG3	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG13	1:10:A:GLU:HG2	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG21	1:10:A:GLU:HG2	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG22	1:10:A:GLU:HG2	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG22	1:10:A:GLU:HG3	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG23	1:10:A:GLU:HG2	2	0.26	0.1	0.26
(1,1222)	1:9:A:VAL:HG23	1:10:A:GLU:HG3	2	0.26	0.1	0.26
(1,109)	1:95:A:ARG:HD2	1:96:A:GLY:H	2	0.26	0.02	0.26
(1,109)	1:95:A:ARG:HD3	1:96:A:GLY:H	2	0.26	0.02	0.26
(1,1794)	1:200:A:ASP:HB3	1:201:A:ASP:H	2	0.26	0.03	0.26
(1,1202)	1:61:A:VAL:HG21	1:62:A:ILE:H	2	0.24	0.01	0.24
(1,1202)	1:61:A:VAL:HG22	1:62:A:ILE:H	2	0.24	0.01	0.24
(1,1202)	1:61:A:VAL:HG23	1:62:A:ILE:H	2	0.24	0.01	0.24
(1,334)	1:10:A:GLU:H	1:10:A:GLU:HG2	2	0.24	0.02	0.24
(1,334)	1:10:A:GLU:H	1:10:A:GLU:HG3	2	0.24	0.02	0.24
(1,1074)	1:176:A:LYS:HA	1:176:A:LYS:HG2	2	0.24	0.04	0.24
(1,1714)	1:211:A:LEU:H	1:213:A:LEU:HB2	2	0.24	0.08	0.24
(1,330)	1:83:A:HIS:H	1:85:A:PHE:HB3	2	0.22	0.08	0.22
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD11	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD12	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD13	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD11	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD12	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD13	2	0.22	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD11	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD12	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD13	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD11	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD12	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD13	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD11	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD12	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD13	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD11	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD12	2	0.22	0.04	0.22
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD13	2	0.22	0.04	0.22
(1,1678)	1:159:A:GLU:HB3	1:160:A:GLN:H	2	0.21	0.06	0.21
(1,475)	1:219:A:VAL:HB	1:258:A:SER:H	2	0.21	0.0	0.21
(1,1372)	1:137:A:ALA:HA	1:151:A:PHE:HD1	2	0.2	0.04	0.2
(1,2385)	1:29:A:ASP:HA	1:31:A:SER:H	2	0.2	0.03	0.2
(1,2440)	1:84:A:LEU:H	1:87:A:GLU:HB2	2	0.2	0.1	0.2
(1,2440)	1:84:A:LEU:H	1:87:A:GLU:HB3	2	0.2	0.1	0.2
(1,45)	1:47:A:ILE:HD11	1:85:A:PHE:HD1	2	0.2	0.01	0.2
(1,45)	1:47:A:ILE:HD11	1:85:A:PHE:HD2	2	0.2	0.01	0.2
(1,45)	1:47:A:ILE:HD12	1:85:A:PHE:HD1	2	0.2	0.01	0.2
(1,45)	1:47:A:ILE:HD12	1:85:A:PHE:HD2	2	0.2	0.01	0.2
(1,45)	1:47:A:ILE:HD13	1:85:A:PHE:HD1	2	0.2	0.01	0.2
(1,45)	1:47:A:ILE:HD13	1:85:A:PHE:HD2	2	0.2	0.01	0.2
(1,1704)	1:136:A:THR:H	1:154:A:HIS:HD2	2	0.2	0.01	0.2
(1,2415)	1:141:A:ILE:HD11	1:240:A:PHE:HB3	2	0.2	0.02	0.2
(1,2415)	1:141:A:ILE:HD12	1:240:A:PHE:HB3	2	0.2	0.02	0.2
(1,2415)	1:141:A:ILE:HD13	1:240:A:PHE:HB3	2	0.2	0.02	0.2
(1,725)	1:117:A:GLU:H	1:117:A:GLU:HB2	2	0.2	0.05	0.2
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG21	2	0.2	0.04	0.2
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG22	2	0.2	0.04	0.2
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG23	2	0.2	0.04	0.2
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG21	2	0.2	0.04	0.2
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG22	2	0.2	0.04	0.2
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG23	2	0.2	0.04	0.2
(1,1111)	1:219:A:VAL:HG21	1:256:A:PHE:HB3	2	0.2	0.09	0.2
(1,1111)	1:219:A:VAL:HG22	1:256:A:PHE:HB3	2	0.2	0.09	0.2
(1,1111)	1:219:A:VAL:HG23	1:256:A:PHE:HB3	2	0.2	0.09	0.2
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG21	2	0.2	0.02	0.2
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG22	2	0.2	0.02	0.2
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG23	2	0.2	0.02	0.2
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG21	2	0.2	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG22	2	0.2	0.02	0.2
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG23	2	0.2	0.02	0.2
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG21	2	0.2	0.02	0.2
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG22	2	0.2	0.02	0.2
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG23	2	0.2	0.02	0.2
(1,1230)	1:199:A:ASP:HA	1:201:A:ASP:H	2	0.2	0.09	0.2
(1,406)	1:187:A:LYS:HB3	1:220:A:TRP:HD1	2	0.19	0.08	0.19
(1,1608)	1:132:A:PHE:H	1:135:A:TRP:HB3	2	0.19	0.04	0.19
(1,1900)	1:37:A:VAL:H	1:43:A:MET:H	2	0.19	0.01	0.19
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD11	2	0.19	0.08	0.19
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD12	2	0.19	0.08	0.19
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD13	2	0.19	0.08	0.19
(1,284)	1:158:A:GLU:HG3	1:195:A:TYR:HB3	2	0.18	0.04	0.18
(1,423)	1:185:A:ARG:HB2	1:220:A:TRP:HD1	2	0.18	0.02	0.18
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG11	2	0.18	0.04	0.18
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG12	2	0.18	0.04	0.18
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG13	2	0.18	0.04	0.18
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG11	2	0.18	0.04	0.18
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG12	2	0.18	0.04	0.18
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG13	2	0.18	0.04	0.18
(1,618)	1:172:A:SER:HB2	1:175:A:ARG:HB2	2	0.18	0.02	0.18
(1,618)	1:172:A:SER:HB2	1:175:A:ARG:HB3	2	0.18	0.02	0.18
(1,618)	1:172:A:SER:HB3	1:175:A:ARG:HB2	2	0.18	0.02	0.18
(1,618)	1:172:A:SER:HB3	1:175:A:ARG:HB3	2	0.18	0.02	0.18
(1,866)	1:251:A:VAL:HG21	1:256:A:PHE:HA	2	0.18	0.01	0.18
(1,866)	1:251:A:VAL:HG22	1:256:A:PHE:HA	2	0.18	0.01	0.18
(1,866)	1:251:A:VAL:HG23	1:256:A:PHE:HA	2	0.18	0.01	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG21	2	0.18	0.0	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG22	2	0.18	0.0	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG23	2	0.18	0.0	0.18
(1,2038)	1:155:A:VAL:HA	1:161:A:ALA:H	2	0.18	0.05	0.18
(1,717)	1:187:A:LYS:HD3	1:188:A:GLN:H	2	0.18	0.02	0.18
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE1	2	0.18	0.04	0.18
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE2	2	0.18	0.04	0.18
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE3	2	0.18	0.04	0.18
(1,1589)	1:70:A:LEU:H	1:70:A:LEU:HG	2	0.17	0.03	0.17
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG11	2	0.17	0.01	0.17
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG12	2	0.17	0.01	0.17
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG13	2	0.17	0.01	0.17
(1,2063)	1:40:A:HIS:H	1:41:A:GLU:H	2	0.17	0.05	0.17
(1,528)	1:82:A:GLN:H	1:82:A:GLN:HG3	2	0.16	0.06	0.16
(1,2438)	1:186:A:ILE:HG21	1:188:A:GLN:HB2	2	0.16	0.06	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2438)	1:186:A:ILE:HG22	1:188:A:GLN:HB2	2	0.16	0.06	0.16
(1,2438)	1:186:A:ILE:HG23	1:188:A:GLN:HB2	2	0.16	0.06	0.16
(1,2162)	1:135:A:TRP:H	1:136:A:THR:HA	2	0.16	0.02	0.16
(1,160)	1:100:A:LEU:HB3	1:103:A:PHE:HD1	2	0.16	0.03	0.16
(1,160)	1:100:A:LEU:HB3	1:103:A:PHE:HD2	2	0.16	0.03	0.16
(1,218)	1:74:A:ASP:HB2	1:75:A:LEU:H	2	0.16	0.01	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG11	2	0.16	0.0	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG12	2	0.16	0.0	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG13	2	0.16	0.0	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG11	2	0.16	0.0	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG12	2	0.16	0.0	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG13	2	0.16	0.0	0.16
(1,573)	1:20:A:PRO:HB2	1:21:A:ASP:H	2	0.16	0.02	0.16
(1,590)	1:8:A:LEU:HD21	1:31:A:SER:HB2	2	0.16	0.03	0.16
(1,590)	1:8:A:LEU:HD22	1:31:A:SER:HB2	2	0.16	0.03	0.16
(1,590)	1:8:A:LEU:HD23	1:31:A:SER:HB2	2	0.16	0.03	0.16
(1,1983)	1:162:A:PHE:HD1	1:165:A:LEU:H	2	0.16	0.04	0.16
(1,1983)	1:162:A:PHE:HD2	1:165:A:LEU:H	2	0.16	0.04	0.16
(1,2183)	1:165:A:LEU:HD21	1:167:A:LEU:H	2	0.16	0.02	0.16
(1,2183)	1:165:A:LEU:HD22	1:167:A:LEU:H	2	0.16	0.02	0.16
(1,2183)	1:165:A:LEU:HD23	1:167:A:LEU:H	2	0.16	0.02	0.16
(1,115)	1:186:A:ILE:HB	1:195:A:TYR:HB3	2	0.16	0.05	0.16
(1,2220)	1:101:A:PHE:H	1:103:A:PHE:H	2	0.16	0.01	0.16
(1,2245)	1:83:A:HIS:H	1:86:A:GLN:H	2	0.16	0.01	0.16
(1,341)	1:159:A:GLU:HG2	1:162:A:PHE:HD1	2	0.15	0.01	0.15
(1,341)	1:159:A:GLU:HG2	1:162:A:PHE:HD2	2	0.15	0.01	0.15
(1,341)	1:159:A:GLU:HG3	1:162:A:PHE:HD1	2	0.15	0.01	0.15
(1,341)	1:159:A:GLU:HG3	1:162:A:PHE:HD2	2	0.15	0.01	0.15
(1,2338)	1:134:A:GLY:H	1:135:A:TRP:HD1	2	0.15	0.01	0.15
(1,471)	1:146:A:SER:HB2	1:148:A:PHE:H	2	0.15	0.02	0.15
(1,471)	1:146:A:SER:HB3	1:148:A:PHE:H	2	0.15	0.02	0.15
(1,1986)	1:160:A:GLN:H	1:163:A:ALA:H	2	0.15	0.04	0.15
(1,2518)	1:194:A:THR:HG21	1:196:A:GLN:HG2	2	0.15	0.03	0.15
(1,2518)	1:194:A:THR:HG21	1:196:A:GLN:HG3	2	0.15	0.03	0.15
(1,2518)	1:194:A:THR:HG22	1:196:A:GLN:HG2	2	0.15	0.03	0.15
(1,2518)	1:194:A:THR:HG22	1:196:A:GLN:HG3	2	0.15	0.03	0.15
(1,2518)	1:194:A:THR:HG23	1:196:A:GLN:HG2	2	0.15	0.03	0.15
(1,2518)	1:194:A:THR:HG23	1:196:A:GLN:HG3	2	0.15	0.03	0.15
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG21	2	0.14	0.03	0.14
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG22	2	0.14	0.03	0.14
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG23	2	0.14	0.03	0.14
(1,631)	1:208:A:SER:HB3	1:209:A:ARG:H	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,641)	1:116:A:GLU:H	1:116:A:GLU:HB3	2	0.14	0.02	0.14
(1,2064)	1:36:A:LYS:HG2	1:40:A:HIS:H	2	0.14	0.02	0.14
(1,2064)	1:36:A:LYS:HG3	1:40:A:HIS:H	2	0.14	0.02	0.14
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD11	2	0.14	0.01	0.14
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD12	2	0.14	0.01	0.14
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD13	2	0.14	0.01	0.14
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG21	2	0.14	0.01	0.14
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG22	2	0.14	0.01	0.14
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG23	2	0.14	0.01	0.14
(1,2204)	1:39:A:GLN:H	1:41:A:GLU:H	2	0.14	0.02	0.14
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG21	2	0.13	0.02	0.13
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG22	2	0.13	0.02	0.13
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG23	2	0.13	0.02	0.13
(1,1241)	1:8:A:LEU:HD11	1:53:A:TYR:HE1	2	0.13	0.02	0.13
(1,1241)	1:8:A:LEU:HD11	1:53:A:TYR:HE2	2	0.13	0.02	0.13
(1,1241)	1:8:A:LEU:HD12	1:53:A:TYR:HE1	2	0.13	0.02	0.13
(1,1241)	1:8:A:LEU:HD12	1:53:A:TYR:HE2	2	0.13	0.02	0.13
(1,1241)	1:8:A:LEU:HD13	1:53:A:TYR:HE1	2	0.13	0.02	0.13
(1,1241)	1:8:A:LEU:HD13	1:53:A:TYR:HE2	2	0.13	0.02	0.13
(1,1865)	1:193:A:ALA:HB1	1:194:A:THR:H	2	0.13	0.02	0.13
(1,1865)	1:193:A:ALA:HB2	1:194:A:THR:H	2	0.13	0.02	0.13
(1,1865)	1:193:A:ALA:HB3	1:194:A:THR:H	2	0.13	0.02	0.13
(1,2021)	1:8:A:LEU:H	1:10:A:GLU:H	2	0.13	0.03	0.13
(1,2029)	1:1:A:MET:HG2	1:3:A:ASP:H	2	0.13	0.01	0.13
(1,2029)	1:1:A:MET:HG3	1:3:A:ASP:H	2	0.13	0.01	0.13
(1,2418)	1:145:A:GLY:HA3	1:234:A:HIS:HA	2	0.13	0.0	0.13
(1,265)	1:100:A:LEU:HD21	1:101:A:PHE:HB2	2	0.12	0.02	0.12
(1,265)	1:100:A:LEU:HD22	1:101:A:PHE:HB2	2	0.12	0.02	0.12
(1,265)	1:100:A:LEU:HD23	1:101:A:PHE:HB2	2	0.12	0.02	0.12
(1,596)	1:101:A:PHE:HA	1:104:A:LEU:HB2	2	0.12	0.01	0.12
(1,596)	1:101:A:PHE:HA	1:104:A:LEU:HB3	2	0.12	0.01	0.12
(1,695)	1:8:A:LEU:HD21	1:31:A:SER:HA	2	0.12	0.02	0.12
(1,695)	1:8:A:LEU:HD22	1:31:A:SER:HA	2	0.12	0.02	0.12
(1,695)	1:8:A:LEU:HD23	1:31:A:SER:HA	2	0.12	0.02	0.12
(1,1915)	1:181:A:MET:H	1:228:A:ARG:H	2	0.12	0.02	0.12
(1,2209)	1:98:A:VAL:H	1:101:A:PHE:H	2	0.12	0.02	0.12
(1,2281)	1:62:A:ILE:HD11	1:63:A:GLU:H	2	0.12	0.02	0.12
(1,2281)	1:62:A:ILE:HD12	1:63:A:GLU:H	2	0.12	0.02	0.12
(1,2281)	1:62:A:ILE:HD13	1:63:A:GLU:H	2	0.12	0.02	0.12
(1,2587)	1:92:A:VAL:HG21	1:103:A:PHE:H	2	0.12	0.02	0.12
(1,2587)	1:92:A:VAL:HG22	1:103:A:PHE:H	2	0.12	0.02	0.12
(1,2587)	1:92:A:VAL:HG23	1:103:A:PHE:H	2	0.12	0.02	0.12

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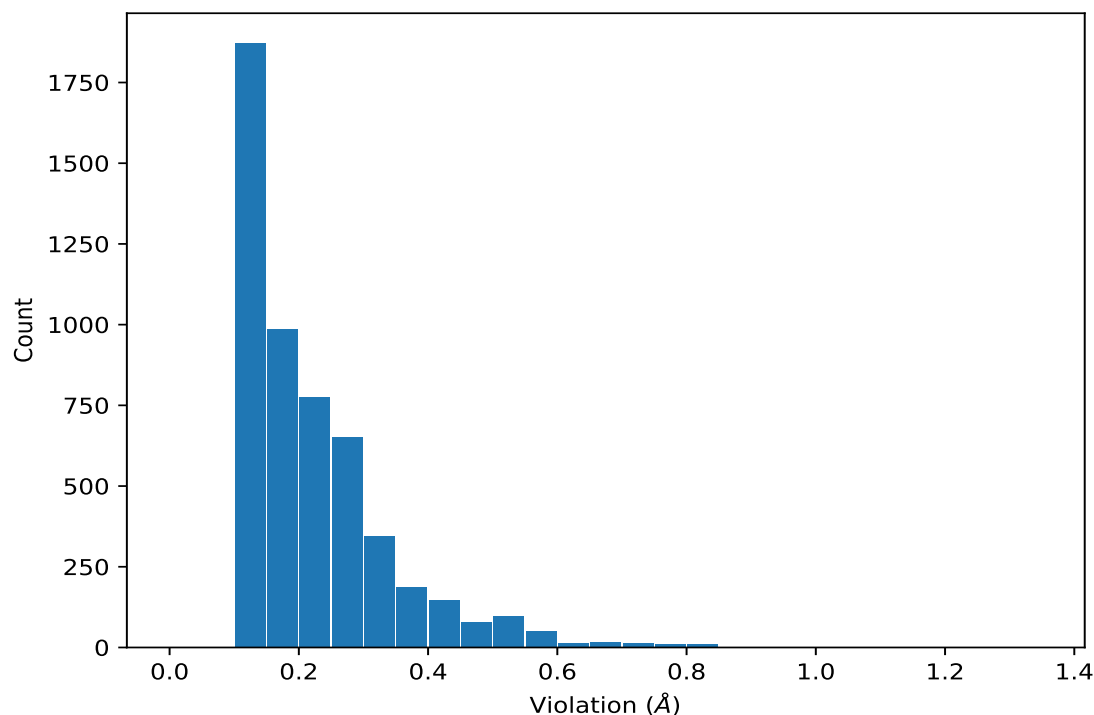
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,640)	1:9:A:VAL:HG11	1:10:A:GLU:HB2	2	0.12	0.02	0.12
(1,640)	1:9:A:VAL:HG12	1:10:A:GLU:HB2	2	0.12	0.02	0.12
(1,640)	1:9:A:VAL:HG13	1:10:A:GLU:HB2	2	0.12	0.02	0.12
(1,640)	1:9:A:VAL:HG21	1:10:A:GLU:HB2	2	0.12	0.02	0.12
(1,640)	1:9:A:VAL:HG22	1:10:A:GLU:HB2	2	0.12	0.02	0.12
(1,640)	1:9:A:VAL:HG23	1:10:A:GLU:HB2	2	0.12	0.02	0.12
(1,273)	1:135:A:TRP:HA	1:136:A:THR:HB	2	0.12	0.01	0.12
(1,1201)	1:61:A:VAL:HG21	1:85:A:PHE:HB2	2	0.12	0.01	0.12
(1,1201)	1:61:A:VAL:HG22	1:85:A:PHE:HB2	2	0.12	0.01	0.12
(1,1201)	1:61:A:VAL:HG23	1:85:A:PHE:HB2	2	0.12	0.01	0.12
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG21	2	0.12	0.01	0.12
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG22	2	0.12	0.01	0.12
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG23	2	0.12	0.01	0.12
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD11	2	0.12	0.01	0.12
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD12	2	0.12	0.01	0.12
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD13	2	0.12	0.01	0.12
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE1	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE2	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE3	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE1	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE2	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE3	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE1	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE2	2	0.12	0.02	0.12
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE3	2	0.12	0.02	0.12
(1,2356)	1:217:A:MET:H	1:219:A:VAL:H	2	0.12	0.02	0.12
(1,1273)	1:143:A:ASP:HA	1:144:A:ARG:HA	2	0.12	0.0	0.12
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG21	2	0.11	0.0	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG22	2	0.11	0.0	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG23	2	0.11	0.0	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG21	2	0.11	0.0	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG22	2	0.11	0.0	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG23	2	0.11	0.0	0.11
(1,1072)	1:186:A:ILE:HG21	1:188:A:GLN:HA	2	0.11	0.0	0.11
(1,1072)	1:186:A:ILE:HG22	1:188:A:GLN:HA	2	0.11	0.0	0.11
(1,1072)	1:186:A:ILE:HG23	1:188:A:GLN:HA	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)
(1,2659)	1:5:A:HIS:HD1	1:8:A:LEU:HD23	4	1.35
(1,1879)	1:187:A:LYS:HB2	1:221:A:ASN:HD22	3	1.3
(1,1879)	1:187:A:LYS:HB2	1:221:A:ASN:HD22	10	1.04
(1,1879)	1:187:A:LYS:HB2	1:221:A:ASN:HD22	7	0.95
(1,1879)	1:187:A:LYS:HB2	1:221:A:ASN:HD22	4	0.94
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	10	0.89
(1,2659)	1:5:A:HIS:HD1	1:8:A:LEU:HD23	5	0.84
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG21	9	0.84
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG22	9	0.84
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG23	9	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	3	0.82
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	3	0.82
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	4	0.82
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	4	0.82
(1,175)	1:3:A:ASP:HB2	1:7:A:GLN:HE21	8	0.81
(1,175)	1:3:A:ASP:HB3	1:7:A:GLN:HE21	8	0.81
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	2	0.81
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	9	0.8
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	5	0.78
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	5	0.78
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG21	1	0.77
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG22	1	0.77
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG23	1	0.77
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	6	0.76
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	6	0.76
(1,1073)	1:176:A:LYS:HA	1:229:A:TRP:HE1	8	0.75
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	8	0.75
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	8	0.75
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	8	0.75
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	3	0.74
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	3	0.74
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	8	0.73
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	8	0.73
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	8	0.73
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	2	0.72
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	2	0.72
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	7	0.71
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	7	0.71
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	7	0.71
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	8	0.71
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	8	0.71
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	9	0.71
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	9	0.71
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	4	0.7
(1,2588)	1:92:A:VAL:H	1:92:A:VAL:HG21	7	0.68
(1,2588)	1:92:A:VAL:H	1:92:A:VAL:HG22	7	0.68
(1,2588)	1:92:A:VAL:H	1:92:A:VAL:HG23	7	0.68
(1,2378)	1:3:A:ASP:HA	1:7:A:GLN:HE22	10	0.68
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	6	0.68
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	6	0.68
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	6	0.68
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	7	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	7	0.68
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	10	0.68
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	10	0.68
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	9	0.67
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	9	0.67
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	10	0.65
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	6	0.65
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	6	0.65
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	10	0.63
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	10	0.63
(1,1190)	1:1:A:MET:HA	1:2:A:ASP:H	2	0.63
(1,1030)	1:220:A:TRP:HA	1:220:A:TRP:HD1	3	0.63
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	1	0.62
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	1	0.62
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	1	0.62
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	10	0.62
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	10	0.62
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	10	0.62
(1,1291)	1:177:A:ALA:HA	1:229:A:TRP:HH2	8	0.62
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	7	0.61
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	7	0.61
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	7	0.61
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	4	0.6
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	4	0.6
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	4	0.6
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB2	3	0.6
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB3	3	0.6
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB2	3	0.6
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB3	3	0.6
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB2	3	0.6
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB3	3	0.6
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB2	1	0.6
(1,200)	1:166:A:ASP:HB2	1:167:A:LEU:HB3	1	0.6
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	9	0.59
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	9	0.59
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	9	0.59
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	9	0.59
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	9	0.59
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	9	0.59
(1,2346)	1:52:A:HIS:H	1:57:A:GLU:HG3	2	0.59
(1,2323)	1:58:A:ALA:HB1	1:92:A:VAL:H	7	0.59
(1,2323)	1:58:A:ALA:HB2	1:92:A:VAL:H	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2323)	1:58:A:ALA:HB3	1:92:A:VAL:H	7	0.59
(1,526)	1:82:A:GLN:H	1:82:A:GLN:HG2	8	0.59
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	8	0.58
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	8	0.58
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	8	0.58
(1,1879)	1:187:A:LYS:HB2	1:221:A:ASN:HD22	8	0.58
(1,930)	1:36:A:LYS:HG2	1:41:A:GLU:HA	7	0.58
(1,930)	1:36:A:LYS:HG3	1:41:A:GLU:HA	7	0.58
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	6	0.58
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	6	0.58
(1,742)	1:41:A:GLU:HA	1:43:A:MET:H	6	0.57
(1,550)	1:258:A:SER:H	1:258:A:SER:HB3	7	0.57
(1,2625)	1:235:A:ILE:HG21	1:239:A:ARG:H	8	0.56
(1,2625)	1:235:A:ILE:HG22	1:239:A:ARG:H	8	0.56
(1,2625)	1:235:A:ILE:HG23	1:239:A:ARG:H	8	0.56
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	6	0.56
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	6	0.56
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	6	0.56
(1,922)	1:176:A:LYS:HG3	1:177:A:ALA:H	2	0.56
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	2	0.56
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	2	0.56
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	4	0.56
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	4	0.56
(1,550)	1:258:A:SER:H	1:258:A:SER:HB3	5	0.56
(1,335)	1:3:A:ASP:HA	1:6:A:GLU:HG2	8	0.56
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD2	9	0.56
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD3	9	0.56
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	9	0.55
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	9	0.55
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	9	0.55
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	1	0.54
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	1	0.54
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	1	0.54
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	1	0.54
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	1	0.54
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	1	0.54
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	8	0.54
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	8	0.54
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	8	0.54
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	8	0.54
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	8	0.54
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2323)	1:58:A:ALA:HB1	1:92:A:VAL:H	1	0.54
(1,2323)	1:58:A:ALA:HB2	1:92:A:VAL:H	1	0.54
(1,2323)	1:58:A:ALA:HB3	1:92:A:VAL:H	1	0.54
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD11	1	0.54
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD12	1	0.54
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD13	1	0.54
(1,1188)	1:257:A:ASP:HA	1:258:A:SER:H	3	0.54
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	4	0.54
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	4	0.54
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	2	0.53
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	2	0.53
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	2	0.53
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	3	0.53
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	3	0.53
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	3	0.53
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	3	0.53
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	9	0.53
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	9	0.53
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD2	3	0.53
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD3	3	0.53
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	3	0.52
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	3	0.52
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	3	0.52
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	3	0.52
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	3	0.52
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	3	0.52
(1,1188)	1:257:A:ASP:HA	1:258:A:SER:H	7	0.52
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	6	0.52
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	6	0.52
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	6	0.52
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	6	0.52
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	6	0.52
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	6	0.52
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD2	8	0.52
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD3	8	0.52
(1,40)	1:255:A:GLY:HA3	1:257:A:ASP:H	8	0.52
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	10	0.51
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	10	0.51
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	10	0.51
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	10	0.51
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	10	0.51
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	6	0.51
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	6	0.51
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	6	0.51
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	7	0.51
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	7	0.51
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	7	0.51
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	1	0.51
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	1	0.51
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	1	0.51
(1,2390)	1:30:A:GLY:H	1:32:A:ILE:H	3	0.51
(1,989)	1:200:A:ASP:HA	1:207:A:GLY:H	8	0.51
(1,742)	1:41:A:GLU:HA	1:43:A:MET:H	1	0.51
(1,621)	1:117:A:GLU:H	1:118:A:GLU:HB3	9	0.51
(1,527)	1:61:A:VAL:HG21	1:82:A:GLN:HG2	2	0.51
(1,527)	1:61:A:VAL:HG22	1:82:A:GLN:HG2	2	0.51
(1,527)	1:61:A:VAL:HG23	1:82:A:GLN:HG2	2	0.51
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD2	1	0.51
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD3	1	0.51
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD2	10	0.51
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD3	10	0.51
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	2	0.5
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	2	0.5
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	2	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	2	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	2	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	2	0.5
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	6	0.5
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	6	0.5
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	6	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	6	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	6	0.5
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	6	0.5
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	6	0.5
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	6	0.5
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	6	0.5
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	5	0.5
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	5	0.5
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	5	0.5
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	10	0.5
(1,1879)	1:187:A:LYS:HB2	1:221:A:ASN:HD22	2	0.5
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD2	6	0.5
(1,107)	1:95:A:ARG:HB2	1:95:A:ARG:HD3	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	5	0.5
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	4	0.49
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	4	0.49
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	4	0.49
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	3	0.49
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	3	0.49
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	3	0.49
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	6	0.49
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	6	0.49
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	6	0.49
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	10	0.49
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	10	0.49
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	10	0.49
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	10	0.49
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	10	0.49
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	1	0.49
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	1	0.49
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	1	0.49
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	4	0.48
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	4	0.48
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	4	0.48
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	4	0.48
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	4	0.48
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	4	0.48
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	10	0.48
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	10	0.48
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	10	0.48
(1,2046)	1:61:A:VAL:HB	1:86:A:GLN:H	2	0.48
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	7	0.48
(1,1739)	1:167:A:LEU:H	1:167:A:LEU:HG	1	0.48
(1,667)	1:147:A:THR:HA	1:148:A:PHE:HD1	2	0.48
(1,566)	1:249:A:GLU:HA	1:252:A:VAL:HB	8	0.48
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	7	0.48
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	7	0.48
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	4	0.48
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	10	0.48
(1,2312)	1:56:A:GLU:H	1:58:A:ALA:H	6	0.47
(1,2303)	1:19:A:TYR:HB2	1:21:A:ASP:H	7	0.47
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	2	0.47
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	2	0.47
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	2	0.47
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	10	0.47
(1,488)	1:96:A:GLY:H	1:97:A:SER:HB3	5	0.47
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	1	0.47
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	1	0.47
(1,419)	1:188:A:GLN:H	1:188:A:GLN:HG2	2	0.47
(1,419)	1:188:A:GLN:H	1:188:A:GLN:HG3	2	0.47
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	5	0.47
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	2	0.46
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	2	0.46
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	2	0.46
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD11	2	0.46
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD12	2	0.46
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD13	2	0.46
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	10	0.46
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	10	0.46
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	10	0.46
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	2	0.46
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	2	0.46
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	2	0.46
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	2	0.46
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	2	0.46
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	2	0.46
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	1	0.46
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	1	0.46
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	3	0.46
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	6	0.46
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	3	0.45
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	3	0.45
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	3	0.45
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	1	0.45
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	1	0.45
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	1	0.45
(1,2089)	1:257:A:ASP:H	1:258:A:SER:H	2	0.45
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	4	0.45
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	4	0.45
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	5	0.45
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	5	0.45
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	5	0.45
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	5	0.45
(1,2631)	1:235:A:ILE:HD11	1:127:A:ILE:H	8	0.44
(1,2631)	1:235:A:ILE:HD12	1:127:A:ILE:H	8	0.44
(1,2631)	1:235:A:ILE:HD13	1:127:A:ILE:H	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	4	0.44
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	4	0.44
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	4	0.44
(1,2312)	1:56:A:GLU:H	1:58:A:ALA:H	1	0.44
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	9	0.44
(1,922)	1:176:A:LYS:HG3	1:177:A:ALA:H	3	0.44
(1,260)	1:119:A:THR:HB	1:120:A:GLU:H	5	0.44
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	7	0.44
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD11	2	0.43
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD12	2	0.43
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD13	2	0.43
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	10	0.43
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	10	0.43
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	10	0.43
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	10	0.43
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	10	0.43
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	10	0.43
(1,2323)	1:58:A:ALA:HB1	1:92:A:VAL:H	6	0.43
(1,2323)	1:58:A:ALA:HB2	1:92:A:VAL:H	6	0.43
(1,2323)	1:58:A:ALA:HB3	1:92:A:VAL:H	6	0.43
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	5	0.43
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	2	0.43
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	2	0.43
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	2	0.43
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	6	0.43
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	6	0.43
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	6	0.43
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	1	0.43
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	1	0.43
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	8	0.43
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD11	4	0.42
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD12	4	0.42
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD13	4	0.42
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	3	0.42
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	3	0.42
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	3	0.42
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	7	0.42
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	7	0.42
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	7	0.42
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	2	0.42
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	10	0.42
(1,2093)	1:239:A:ARG:HB3	1:241:A:LYS:H	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	3	0.42
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD11	6	0.42
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD12	6	0.42
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD13	6	0.42
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	7	0.42
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	8	0.42
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	7	0.42
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	7	0.42
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	5	0.42
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	5	0.42
(1,215)	1:29:A:ASP:HB2	1:30:A:GLY:H	7	0.42
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	1	0.42
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	8	0.42
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	5	0.41
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	5	0.41
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	5	0.41
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	9	0.41
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	9	0.41
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	9	0.41
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	5	0.41
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	5	0.41
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	5	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	1	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	1	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	1	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	4	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	4	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	4	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	5	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	5	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	5	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	6	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	6	0.41
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	6	0.41
(1,2390)	1:30:A:GLY:H	1:32:A:ILE:H	9	0.41
(1,2093)	1:239:A:ARG:HB3	1:241:A:LYS:H	3	0.41
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	6	0.41
(1,1626)	1:102:A:ASP:H	1:102:A:ASP:HB3	2	0.41
(1,1213)	1:42:A:TYR:H	1:43:A:MET:HA	7	0.41
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	5	0.41
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	5	0.41
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	7	0.41
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	6	0.41
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	6	0.41
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	1	0.41
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	1	0.41
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	1	0.41
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	1	0.41
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	8	0.41
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	8	0.41
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	8	0.41
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	8	0.41
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	4	0.41
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	4	0.41
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	4	0.41
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	4	0.41
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	4	0.41
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	4	0.41
(1,215)	1:29:A:ASP:HB2	1:30:A:GLY:H	3	0.41
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	6	0.41
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD11	4	0.41
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD12	4	0.41
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD13	4	0.41
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	7	0.4
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	7	0.4
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	7	0.4
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	7	0.4
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	7	0.4
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	7	0.4
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	3	0.4
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	3	0.4
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	3	0.4
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	10	0.4
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	10	0.4
(1,2303)	1:19:A:TYR:HB2	1:21:A:ASP:H	9	0.4
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	2	0.4
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	2	0.4
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	2	0.4
(1,1739)	1:167:A:LEU:H	1:167:A:LEU:HG	6	0.4
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	4	0.4
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	4	0.4
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	4	0.4
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	4	0.4
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	4	0.4
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	1	0.4
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	1	0.4
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	7	0.4
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	7	0.4
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	7	0.4
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	7	0.4
(1,563)	1:257:A:ASP:HB2	1:258:A:SER:HB2	2	0.4
(1,563)	1:257:A:ASP:HB3	1:258:A:SER:HB2	2	0.4
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	2	0.4
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	2	0.4
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	9	0.4
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	9	0.4
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	8	0.4
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	8	0.4
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	8	0.4
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	2	0.39
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	8	0.39
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	8	0.39
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	8	0.39
(1,1959)	1:187:A:LYS:H	1:189:A:ASP:H	5	0.39
(1,1497)	1:127:A:ILE:HG21	1:128:A:PRO:HG3	8	0.39
(1,1497)	1:127:A:ILE:HG22	1:128:A:PRO:HG3	8	0.39
(1,1497)	1:127:A:ILE:HG23	1:128:A:PRO:HG3	8	0.39
(1,794)	1:258:A:SER:HA	1:258:A:SER:HB2	3	0.39
(1,742)	1:41:A:GLU:HA	1:43:A:MET:H	5	0.39
(1,622)	1:95:A:ARG:HB2	1:96:A:GLY:H	5	0.39
(1,456)	1:116:A:GLU:HG2	1:117:A:GLU:H	3	0.39
(1,456)	1:116:A:GLU:HG3	1:117:A:GLU:H	3	0.39
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	5	0.38
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	5	0.38
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	5	0.38
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	6	0.38
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	6	0.38
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	6	0.38
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	2	0.38
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	2	0.38
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	2	0.38
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	9	0.38
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	9	0.38
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	3	0.38
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	6	0.38
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	2	0.38
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	8	0.38
(1,1565)	1:188:A:GLN:HB3	1:189:A:ASP:H	2	0.38
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	10	0.38
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE1	5	0.38
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE2	5	0.38
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE3	5	0.38
(1,1388)	1:163:A:ALA:HB1	1:164:A:MET:HB3	10	0.38
(1,1388)	1:163:A:ALA:HB2	1:164:A:MET:HB3	10	0.38
(1,1388)	1:163:A:ALA:HB3	1:164:A:MET:HB3	10	0.38
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	1	0.38
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	1	0.38
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	1	0.38
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	1	0.38
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	1	0.38
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	1	0.38
(1,891)	1:73:A:ARG:HA	1:73:A:ARG:HD2	8	0.38
(1,794)	1:258:A:SER:HA	1:258:A:SER:HB2	6	0.38
(1,794)	1:258:A:SER:HA	1:258:A:SER:HB2	7	0.38
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	2	0.38
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	6	0.38
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	6	0.38
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	6	0.38
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	6	0.38
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	9	0.38
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	3	0.38
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	3	0.38
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	3	0.38
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG21	5	0.37
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG22	5	0.37
(1,2660)	1:101:A:PHE:HD1	1:92:A:VAL:HG23	5	0.37
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG21	5	0.37
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG22	5	0.37
(1,2660)	1:101:A:PHE:HD2	1:92:A:VAL:HG23	5	0.37
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	2	0.37
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	2	0.37
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	2	0.37
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	6	0.37
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	6	0.37
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	10	0.37
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	10	0.37
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	10	0.37
(1,2617)	1:217:A:MET:HE1	1:252:A:VAL:HG21	8	0.37
(1,2617)	1:217:A:MET:HE1	1:252:A:VAL:HG22	8	0.37
(1,2617)	1:217:A:MET:HE1	1:252:A:VAL:HG23	8	0.37
(1,2617)	1:217:A:MET:HE2	1:252:A:VAL:HG21	8	0.37
(1,2617)	1:217:A:MET:HE2	1:252:A:VAL:HG22	8	0.37
(1,2617)	1:217:A:MET:HE2	1:252:A:VAL:HG23	8	0.37
(1,2617)	1:217:A:MET:HE3	1:252:A:VAL:HG21	8	0.37
(1,2617)	1:217:A:MET:HE3	1:252:A:VAL:HG22	8	0.37
(1,2617)	1:217:A:MET:HE3	1:252:A:VAL:HG23	8	0.37
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG11	8	0.37
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG12	8	0.37
(1,2488)	1:154:A:HIS:HB3	1:155:A:VAL:HG13	8	0.37
(1,2407)	1:33:A:ILE:HD11	1:47:A:ILE:HD11	2	0.37
(1,2407)	1:33:A:ILE:HD11	1:47:A:ILE:HD12	2	0.37
(1,2407)	1:33:A:ILE:HD11	1:47:A:ILE:HD13	2	0.37
(1,2407)	1:33:A:ILE:HD12	1:47:A:ILE:HD11	2	0.37
(1,2407)	1:33:A:ILE:HD12	1:47:A:ILE:HD12	2	0.37
(1,2407)	1:33:A:ILE:HD12	1:47:A:ILE:HD13	2	0.37
(1,2407)	1:33:A:ILE:HD13	1:47:A:ILE:HD11	2	0.37
(1,2407)	1:33:A:ILE:HD13	1:47:A:ILE:HD12	2	0.37
(1,2407)	1:33:A:ILE:HD13	1:47:A:ILE:HD13	2	0.37
(1,2390)	1:30:A:GLY:H	1:32:A:ILE:H	6	0.37
(1,2367)	1:96:A:GLY:H	1:97:A:SER:H	5	0.37
(1,1902)	1:202:A:GLY:H	1:204:A:THR:HA	9	0.37
(1,1732)	1:57:A:GLU:H	1:57:A:GLU:HG3	2	0.37
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	4	0.37
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	4	0.37
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB1	5	0.37
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB2	5	0.37
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB3	5	0.37
(1,1222)	1:9:A:VAL:HG11	1:10:A:GLU:HG2	10	0.37
(1,1222)	1:9:A:VAL:HG11	1:10:A:GLU:HG3	10	0.37
(1,1222)	1:9:A:VAL:HG12	1:10:A:GLU:HG2	10	0.37
(1,1222)	1:9:A:VAL:HG12	1:10:A:GLU:HG3	10	0.37
(1,1222)	1:9:A:VAL:HG13	1:10:A:GLU:HG2	10	0.37
(1,1222)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	10	0.37
(1,1222)	1:9:A:VAL:HG21	1:10:A:GLU:HG2	10	0.37
(1,1222)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	10	0.37
(1,1222)	1:9:A:VAL:HG22	1:10:A:GLU:HG2	10	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:9:A:VAL:HG22	1:10:A:GLU:HG3	10	0.37
(1,1222)	1:9:A:VAL:HG23	1:10:A:GLU:HG2	10	0.37
(1,1222)	1:9:A:VAL:HG23	1:10:A:GLU:HG3	10	0.37
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	10	0.37
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	10	0.37
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	10	0.37
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	10	0.37
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	10	0.37
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	10	0.37
(1,991)	1:88:A:VAL:HG21	1:107:A:LEU:HA	6	0.37
(1,991)	1:88:A:VAL:HG22	1:107:A:LEU:HA	6	0.37
(1,991)	1:88:A:VAL:HG23	1:107:A:LEU:HA	6	0.37
(1,794)	1:258:A:SER:HA	1:258:A:SER:HB2	5	0.37
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	1	0.37
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD2	10	0.37
(1,616)	1:172:A:SER:HB2	1:175:A:ARG:HD3	10	0.37
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD2	10	0.37
(1,616)	1:172:A:SER:HB3	1:175:A:ARG:HD3	10	0.37
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	4	0.37
(1,83)	1:138:A:SER:H	1:151:A:PHE:HB3	2	0.37
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	6	0.37
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	6	0.37
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	6	0.37
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	7	0.36
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	7	0.36
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	7	0.36
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	7	0.36
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	7	0.36
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	7	0.36
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	4	0.36
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	4	0.36
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	4	0.36
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	8	0.36
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	8	0.36
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	8	0.36
(1,2312)	1:56:A:GLU:H	1:58:A:ALA:H	10	0.36
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	1	0.36
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	1	0.36
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	1	0.36
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	1	0.36
(1,1765)	1:104:A:LEU:H	1:105:A:THR:HB	8	0.36
(1,1621)	1:4:A:ASP:H	1:4:A:ASP:HB3	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	9	0.36
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	9	0.36
(1,1321)	1:89:A:MET:HA	1:92:A:VAL:HG21	7	0.36
(1,1321)	1:89:A:MET:HA	1:92:A:VAL:HG22	7	0.36
(1,1321)	1:89:A:MET:HA	1:92:A:VAL:HG23	7	0.36
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD21	3	0.36
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD22	3	0.36
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD23	3	0.36
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	9	0.36
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	9	0.36
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	9	0.36
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	9	0.36
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	9	0.36
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	9	0.36
(1,891)	1:73:A:ARG:HA	1:73:A:ARG:HD2	3	0.36
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	8	0.36
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	8	0.36
(1,794)	1:258:A:SER:HA	1:258:A:SER:HB2	2	0.36
(1,667)	1:147:A:THR:HA	1:148:A:PHE:HD1	10	0.36
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	5	0.36
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	5	0.36
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	8	0.36
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	8	0.36
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	1	0.36
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	1	0.36
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	5	0.36
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	5	0.36
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD11	6	0.36
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD12	6	0.36
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD13	6	0.36
(1,129)	1:79:A:LYS:HE2	1:80:A:TYR:H	7	0.36
(1,129)	1:79:A:LYS:HE3	1:80:A:TYR:H	7	0.36
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	5	0.36
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	5	0.36
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	5	0.36
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	5	0.35
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	5	0.35
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	5	0.35
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	9	0.35
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	9	0.35
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	9	0.35
(1,2564)	1:142:A:THR:HG21	1:234:A:HIS:HB3	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2564)	1:142:A:THR:HG22	1:234:A:HIS:HB3	7	0.35
(1,2564)	1:142:A:THR:HG23	1:234:A:HIS:HB3	7	0.35
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	4	0.35
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	6	0.35
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	6	0.35
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	6	0.35
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	3	0.35
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	3	0.35
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	3	0.35
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	8	0.35
(1,1621)	1:4:A:ASP:H	1:4:A:ASP:HB3	3	0.35
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	1	0.35
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	3	0.35
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	5	0.35
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	5	0.35
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	5	0.35
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	4	0.35
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	4	0.35
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	4	0.35
(1,926)	1:176:A:LYS:HG2	1:177:A:ALA:H	1	0.35
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	10	0.35
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	3	0.35
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	3	0.35
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	3	0.35
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	3	0.35
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	3	0.35
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	3	0.35
(1,411)	1:187:A:LYS:HB2	1:188:A:GLN:H	2	0.35
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD11	10	0.35
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD12	10	0.35
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD13	10	0.35
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD11	10	0.35
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD12	10	0.35
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD13	10	0.35
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	1	0.35
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	1	0.35
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	1	0.35
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	8	0.34
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	8	0.34
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	8	0.34
(1,2654)	1:103:A:PHE:HE1	1:85:A:PHE:HB3	3	0.34
(1,2654)	1:103:A:PHE:HE2	1:85:A:PHE:HB3	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	3	0.34
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	3	0.34
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	3	0.34
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	7	0.34
(1,2312)	1:56:A:GLU:H	1:58:A:ALA:H	2	0.34
(1,2312)	1:56:A:GLU:H	1:58:A:ALA:H	5	0.34
(1,2221)	1:41:A:GLU:H	1:42:A:TYR:HD1	5	0.34
(1,2221)	1:41:A:GLU:H	1:42:A:TYR:HD2	5	0.34
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	4	0.34
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	1	0.34
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	4	0.34
(1,1942)	1:144:A:ARG:H	1:234:A:HIS:HA	3	0.34
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	2	0.34
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	6	0.34
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	6	0.34
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	6	0.34
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	8	0.34
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	8	0.34
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	8	0.34
(1,1621)	1:4:A:ASP:H	1:4:A:ASP:HB3	1	0.34
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	4	0.34
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	4	0.34
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	4	0.34
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	4	0.34
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	10	0.34
(1,1043)	1:42:A:TYR:HA	1:67:A:CYS:HB2	1	0.34
(1,1043)	1:42:A:TYR:HA	1:67:A:CYS:HB2	6	0.34
(1,991)	1:88:A:VAL:HG21	1:107:A:LEU:HA	2	0.34
(1,991)	1:88:A:VAL:HG22	1:107:A:LEU:HA	2	0.34
(1,991)	1:88:A:VAL:HG23	1:107:A:LEU:HA	2	0.34
(1,891)	1:73:A:ARG:HA	1:73:A:ARG:HD2	5	0.34
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	4	0.34
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	4	0.34
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	4	0.34
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	3	0.34
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	3	0.34
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	3	0.34
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	8	0.34
(1,709)	1:79:A:LYS:HD2	1:80:A:TYR:H	8	0.34
(1,709)	1:79:A:LYS:HD3	1:80:A:TYR:H	8	0.34
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	7	0.34
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	7	0.34
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	7	0.34
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	5	0.34
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	5	0.34
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	5	0.34
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	3	0.34
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	10	0.34
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	10	0.34
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	10	0.34
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD11	9	0.33
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD12	9	0.33
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD13	9	0.33
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	2	0.33
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	2	0.33
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	2	0.33
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	1	0.33
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	1	0.33
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	1	0.33
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	7	0.33
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	7	0.33
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	7	0.33
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	3	0.33
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	3	0.33
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	3	0.33
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	2	0.33
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	2	0.33
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	2	0.33
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	2	0.33
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	2	0.33
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	2	0.33
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	2	0.33
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	2	0.33
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	2	0.33
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	10	0.33
(1,2303)	1:19:A:TYR:HB2	1:21:A:ASP:H	3	0.33
(1,2196)	1:88:A:VAL:HG21	1:90:A:ASP:H	5	0.33
(1,2196)	1:88:A:VAL:HG22	1:90:A:ASP:H	5	0.33
(1,2196)	1:88:A:VAL:HG23	1:90:A:ASP:H	5	0.33
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	3	0.33
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	3	0.33
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	3	0.33
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	1	0.33
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	1	0.33
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	1	0.33
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	2	0.33
(1,1497)	1:127:A:ILE:HG21	1:128:A:PRO:HG3	3	0.33
(1,1497)	1:127:A:ILE:HG22	1:128:A:PRO:HG3	3	0.33
(1,1497)	1:127:A:ILE:HG23	1:128:A:PRO:HG3	3	0.33
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG2	3	0.33
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG3	3	0.33
(1,1019)	1:213:A:LEU:HD21	1:214:A:ILE:HG21	5	0.33
(1,1019)	1:213:A:LEU:HD21	1:214:A:ILE:HG22	5	0.33
(1,1019)	1:213:A:LEU:HD21	1:214:A:ILE:HG23	5	0.33
(1,1019)	1:213:A:LEU:HD22	1:214:A:ILE:HG21	5	0.33
(1,1019)	1:213:A:LEU:HD22	1:214:A:ILE:HG22	5	0.33
(1,1019)	1:213:A:LEU:HD22	1:214:A:ILE:HG23	5	0.33
(1,1019)	1:213:A:LEU:HD23	1:214:A:ILE:HG21	5	0.33
(1,1019)	1:213:A:LEU:HD23	1:214:A:ILE:HG22	5	0.33
(1,1019)	1:213:A:LEU:HD23	1:214:A:ILE:HG23	5	0.33
(1,930)	1:36:A:LYS:HG2	1:41:A:GLU:HA	5	0.33
(1,930)	1:36:A:LYS:HG3	1:41:A:GLU:HA	5	0.33
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	6	0.33
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	6	0.33
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	2	0.33
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	9	0.33
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	4	0.33
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	4	0.33
(1,588)	1:31:A:SER:HB2	1:49:A:PHE:H	1	0.33
(1,572)	1:79:A:LYS:HB2	1:80:A:TYR:H	4	0.33
(1,456)	1:116:A:GLU:HG2	1:117:A:GLU:H	9	0.33
(1,456)	1:116:A:GLU:HG3	1:117:A:GLU:H	9	0.33
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	9	0.33
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	9	0.33
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	8	0.33
(1,40)	1:255:A:GLY:HA3	1:257:A:ASP:H	3	0.33
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	4	0.32
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	4	0.32
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	4	0.32
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	4	0.32
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	4	0.32
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	2	0.32
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	4	0.32
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	3	0.32
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	9	0.32
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	9	0.32
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	9	0.32
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	3	0.32
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	3	0.32
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	3	0.32
(1,1858)	1:91:A:SER:H	1:92:A:VAL:HG21	7	0.32
(1,1858)	1:91:A:SER:H	1:92:A:VAL:HG22	7	0.32
(1,1858)	1:91:A:SER:H	1:92:A:VAL:HG23	7	0.32
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	4	0.32
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	4	0.32
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	4	0.32
(1,1735)	1:217:A:MET:HB2	1:218:A:ASP:H	5	0.32
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	9	0.32
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	9	0.32
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	9	0.32
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	5	0.32
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	7	0.32
(1,1621)	1:4:A:ASP:H	1:4:A:ASP:HB3	2	0.32
(1,1621)	1:4:A:ASP:H	1:4:A:ASP:HB3	9	0.32
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	7	0.32
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG11	8	0.32
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG12	8	0.32
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG13	8	0.32
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB1	4	0.32
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB2	4	0.32
(1,1480)	1:176:A:LYS:HB2	1:177:A:ALA:HB3	4	0.32
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	1	0.32
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	1	0.32
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	1	0.32
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	3	0.32
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	3	0.32
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	3	0.32
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	10	0.32
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	10	0.32
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	10	0.32
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	1	0.32
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	10	0.32
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	5	0.32
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	5	0.32
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	5	0.32
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	5	0.32
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	5	0.32
(1,991)	1:88:A:VAL:HG21	1:107:A:LEU:HA	3	0.32
(1,991)	1:88:A:VAL:HG22	1:107:A:LEU:HA	3	0.32
(1,991)	1:88:A:VAL:HG23	1:107:A:LEU:HA	3	0.32
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	1	0.32
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	1	0.32
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	1	0.32
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	5	0.32
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	6	0.32
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	6	0.32
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	6	0.32
(1,716)	1:187:A:LYS:HB2	1:187:A:LYS:HD3	9	0.32
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	9	0.32
(1,588)	1:31:A:SER:HB2	1:49:A:PHE:H	6	0.32
(1,527)	1:61:A:VAL:HG21	1:82:A:GLN:HG2	10	0.32
(1,527)	1:61:A:VAL:HG22	1:82:A:GLN:HG2	10	0.32
(1,527)	1:61:A:VAL:HG23	1:82:A:GLN:HG2	10	0.32
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	6	0.32
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	6	0.32
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	6	0.32
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	3	0.32
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	3	0.32
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	10	0.32
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	10	0.32
(1,111)	1:175:A:ARG:HD2	1:176:A:LYS:H	2	0.32
(1,111)	1:175:A:ARG:HD3	1:176:A:LYS:H	2	0.32
(1,111)	1:175:A:ARG:HD2	1:176:A:LYS:H	9	0.32
(1,111)	1:175:A:ARG:HD3	1:176:A:LYS:H	9	0.32
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	6	0.32
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	6	0.32
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	3	0.32
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	7	0.32
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	7	0.32
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	7	0.32
(1,40)	1:255:A:GLY:HA3	1:257:A:ASP:H	10	0.32
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	10	0.31
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	10	0.31
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	10	0.31
(1,2631)	1:235:A:ILE:HD11	1:127:A:ILE:H	4	0.31
(1,2631)	1:235:A:ILE:HD12	1:127:A:ILE:H	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2631)	1:235:A:ILE:HD13	1:127:A:ILE:H	4	0.31
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	1	0.31
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	1	0.31
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	1	0.31
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	5	0.31
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	5	0.31
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	5	0.31
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	9	0.31
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	9	0.31
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	9	0.31
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG21	1	0.31
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG22	1	0.31
(1,2623)	1:242:A:HIS:H	1:141:A:ILE:HG23	1	0.31
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	4	0.31
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	4	0.31
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	4	0.31
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	9	0.31
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	9	0.31
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	9	0.31
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	10	0.31
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	10	0.31
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	10	0.31
(1,2440)	1:84:A:LEU:H	1:87:A:GLU:HB2	3	0.31
(1,2440)	1:84:A:LEU:H	1:87:A:GLU:HB3	3	0.31
(1,2360)	1:41:A:GLU:H	1:42:A:TYR:H	5	0.31
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	2	0.31
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	6	0.31
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	6	0.31
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	6	0.31
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG2	7	0.31
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG3	7	0.31
(1,1807)	1:125:A:SER:H	1:125:A:SER:HB3	9	0.31
(1,1714)	1:211:A:LEU:H	1:213:A:LEU:HB2	5	0.31
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	6	0.31
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	6	0.31
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	6	0.31
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	3	0.31
(1,1666)	1:251:A:VAL:HG21	1:257:A:ASP:H	5	0.31
(1,1666)	1:251:A:VAL:HG22	1:257:A:ASP:H	5	0.31
(1,1666)	1:251:A:VAL:HG23	1:257:A:ASP:H	5	0.31
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	3	0.31
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	6	0.31
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	6	0.31
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	6	0.31
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	3	0.31
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	3	0.31
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	3	0.31
(1,1188)	1:257:A:ASP:HA	1:258:A:SER:H	6	0.31
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	2	0.31
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	1	0.31
(1,1043)	1:42:A:TYR:HA	1:67:A:CYS:HB2	7	0.31
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	3	0.31
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	4	0.31
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	8	0.31
(1,926)	1:176:A:LYS:HG2	1:177:A:ALA:H	9	0.31
(1,922)	1:176:A:LYS:HG3	1:177:A:ALA:H	8	0.31
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	4	0.31
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	8	0.31
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	5	0.31
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	5	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	2	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	2	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	2	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	2	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	2	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	2	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	5	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	5	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	5	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	5	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	5	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	5	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	10	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	10	0.31
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	10	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	10	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	10	0.31
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	10	0.31
(1,411)	1:187:A:LYS:HB2	1:188:A:GLN:H	6	0.31
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	6	0.31
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD11	8	0.31
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD12	8	0.31
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD13	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:29:A:ASP:HB2	1:30:A:GLY:H	6	0.31
(1,99)	1:171:A:ASP:HB2	1:174:A:MET:HB3	5	0.31
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	4	0.3
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	4	0.3
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	4	0.3
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	5	0.3
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	5	0.3
(1,2242)	1:29:A:ASP:H	1:32:A:ILE:H	6	0.3
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	8	0.3
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	8	0.3
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	8	0.3
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	2	0.3
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	2	0.3
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	2	0.3
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	6	0.3
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	1	0.3
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	4	0.3
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	5	0.3
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	10	0.3
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	10	0.3
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	10	0.3
(1,1790)	1:4:A:ASP:HB2	1:5:A:HIS:H	4	0.3
(1,1759)	1:89:A:MET:HE1	1:90:A:ASP:H	6	0.3
(1,1759)	1:89:A:MET:HE2	1:90:A:ASP:H	6	0.3
(1,1759)	1:89:A:MET:HE3	1:90:A:ASP:H	6	0.3
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	10	0.3
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	10	0.3
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	2	0.3
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	2	0.3
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	2	0.3
(1,1626)	1:102:A:ASP:H	1:102:A:ASP:HB3	4	0.3
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	9	0.3
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	9	0.3
(1,1439)	1:58:A:ALA:HB1	1:94:A:HIS:H	4	0.3
(1,1439)	1:58:A:ALA:HB2	1:94:A:HIS:H	4	0.3
(1,1439)	1:58:A:ALA:HB3	1:94:A:HIS:H	4	0.3
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	7	0.3
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	7	0.3
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	7	0.3
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	7	0.3
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	7	0.3
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	7	0.3
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	7	0.3
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	7	0.3
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG21	9	0.3
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG22	9	0.3
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG23	9	0.3
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG21	9	0.3
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG22	9	0.3
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG23	9	0.3
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG21	9	0.3
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG22	9	0.3
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG23	9	0.3
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	10	0.3
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	10	0.3
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	10	0.3
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	3	0.3
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	3	0.3
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	3	0.3
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	3	0.3
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	5	0.3
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	5	0.3
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	5	0.3
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	9	0.3
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	3	0.3
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	3	0.3
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	10	0.3
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	1	0.3
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	1	0.3
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	1	0.3
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	7	0.3
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	7	0.3
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	7	0.3
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	7	0.3
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	7	0.3
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	7	0.3
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	4	0.3
(1,330)	1:83:A:HIS:H	1:85:A:PHE:HB3	2	0.3
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	1	0.3
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD2	2	0.3
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD3	2	0.3
(1,111)	1:175:A:ARG:HD2	1:176:A:LYS:H	1	0.3
(1,111)	1:175:A:ARG:HD3	1:176:A:LYS:H	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	4	0.3
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	4	0.3
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	1	0.3
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD11	8	0.29
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD12	8	0.29
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD13	8	0.29
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG21	2	0.29
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG22	2	0.29
(1,2622)	1:239:A:ARG:H	1:127:A:ILE:HG23	2	0.29
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD21	2	0.29
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD22	2	0.29
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD23	2	0.29
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD21	2	0.29
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD22	2	0.29
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD23	2	0.29
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD21	2	0.29
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD22	2	0.29
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD23	2	0.29
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	8	0.29
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	8	0.29
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	8	0.29
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	3	0.29
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	10	0.29
(1,2285)	1:142:A:THR:HG21	1:239:A:ARG:H	1	0.29
(1,2285)	1:142:A:THR:HG22	1:239:A:ARG:H	1	0.29
(1,2285)	1:142:A:THR:HG23	1:239:A:ARG:H	1	0.29
(1,2241)	1:31:A:SER:H	1:32:A:ILE:H	6	0.29
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD21	1	0.29
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD22	1	0.29
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD23	1	0.29
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	4	0.29
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	4	0.29
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	4	0.29
(1,2093)	1:239:A:ARG:HB3	1:241:A:LYS:H	5	0.29
(1,1994)	1:53:A:TYR:H	1:56:A:GLU:H	8	0.29
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG2	8	0.29
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG3	8	0.29
(1,1794)	1:200:A:ASP:HB3	1:201:A:ASP:H	1	0.29
(1,1765)	1:104:A:LEU:H	1:105:A:THR:HB	7	0.29
(1,1701)	1:256:A:PHE:H	1:257:A:ASP:H	7	0.29
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	6	0.29
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	6	0.29
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	3	0.29
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	3	0.29
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	3	0.29
(1,1439)	1:58:A:ALA:HB1	1:94:A:HIS:H	3	0.29
(1,1439)	1:58:A:ALA:HB2	1:94:A:HIS:H	3	0.29
(1,1439)	1:58:A:ALA:HB3	1:94:A:HIS:H	3	0.29
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	2	0.29
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	2	0.29
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	2	0.29
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	6	0.29
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	6	0.29
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	6	0.29
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	1	0.29
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	1	0.29
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	1	0.29
(1,989)	1:200:A:ASP:HA	1:207:A:GLY:H	2	0.29
(1,851)	1:171:A:ASP:HB3	1:173:A:LYS:HG3	2	0.29
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	1	0.29
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	1	0.29
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	1	0.29
(1,738)	1:186:A:ILE:HA	1:220:A:TRP:HD1	6	0.29
(1,588)	1:31:A:SER:HB2	1:49:A:PHE:H	3	0.29
(1,422)	1:22:A:LEU:HD11	1:36:A:LYS:HB2	9	0.29
(1,422)	1:22:A:LEU:HD11	1:36:A:LYS:HB3	9	0.29
(1,422)	1:22:A:LEU:HD12	1:36:A:LYS:HB2	9	0.29
(1,422)	1:22:A:LEU:HD12	1:36:A:LYS:HB3	9	0.29
(1,422)	1:22:A:LEU:HD13	1:36:A:LYS:HB2	9	0.29
(1,422)	1:22:A:LEU:HD13	1:36:A:LYS:HB3	9	0.29
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	3	0.29
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	7	0.29
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	7	0.29
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	7	0.29
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	10	0.29
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	10	0.29
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	5	0.29
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD11	7	0.29
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD12	7	0.29
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD13	7	0.29
(1,21)	1:135:A:TRP:HZ2	1:164:A:MET:HB2	10	0.29
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD11	5	0.28
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD12	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD13	5	0.28
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	6	0.28
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	6	0.28
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	6	0.28
(1,2359)	1:40:A:HIS:HA	1:42:A:TYR:H	3	0.28
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	9	0.28
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	6	0.28
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG2	3	0.28
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG3	3	0.28
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	5	0.28
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	8	0.28
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	5	0.28
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	5	0.28
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	6	0.28
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	8	0.28
(1,1440)	1:58:A:ALA:HB1	1:99:A:CYS:HB2	7	0.28
(1,1440)	1:58:A:ALA:HB2	1:99:A:CYS:HB2	7	0.28
(1,1440)	1:58:A:ALA:HB3	1:99:A:CYS:HB2	7	0.28
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	9	0.28
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	9	0.28
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	9	0.28
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	9	0.28
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	9	0.28
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	9	0.28
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	9	0.28
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	9	0.28
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	9	0.28
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	9	0.28
(1,1237)	1:252:A:VAL:HG11	1:253:A:ARG:H	8	0.28
(1,1237)	1:252:A:VAL:HG12	1:253:A:ARG:H	8	0.28
(1,1237)	1:252:A:VAL:HG13	1:253:A:ARG:H	8	0.28
(1,1230)	1:199:A:ASP:HA	1:201:A:ASP:H	2	0.28
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	4	0.28
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	4	0.28
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	4	0.28
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	7	0.28
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	7	0.28
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	7	0.28
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG21	6	0.28
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG22	6	0.28
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG23	6	0.28
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG21	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG22	6	0.28
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG23	6	0.28
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG21	6	0.28
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG22	6	0.28
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG23	6	0.28
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	5	0.28
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	6	0.28
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	8	0.28
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	8	0.28
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	8	0.28
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	8	0.28
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	8	0.28
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	8	0.28
(1,1111)	1:219:A:VAL:HG21	1:256:A:PHE:HB3	7	0.28
(1,1111)	1:219:A:VAL:HG22	1:256:A:PHE:HB3	7	0.28
(1,1111)	1:219:A:VAL:HG23	1:256:A:PHE:HB3	7	0.28
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	2	0.28
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	5	0.28
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD21	3	0.28
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD22	3	0.28
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD23	3	0.28
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	9	0.28
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	9	0.28
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	9	0.28
(1,718)	1:187:A:LYS:HD3	1:220:A:TRP:HD1	9	0.28
(1,706)	1:87:A:GLU:HB2	1:88:A:VAL:H	9	0.28
(1,706)	1:87:A:GLU:HB3	1:88:A:VAL:H	9	0.28
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	1	0.28
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	3	0.28
(1,563)	1:257:A:ASP:HB2	1:258:A:SER:HB2	1	0.28
(1,563)	1:257:A:ASP:HB3	1:258:A:SER:HB2	1	0.28
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	1	0.28
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	8	0.28
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	10	0.28
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	2	0.28
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	2	0.28
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	9	0.28
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	1	0.28
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	1	0.28
(1,109)	1:95:A:ARG:HD2	1:96:A:GLY:H	5	0.28
(1,109)	1:95:A:ARG:HD3	1:96:A:GLY:H	5	0.28
(1,99)	1:171:A:ASP:HB2	1:174:A:MET:HB3	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	9	0.27
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	9	0.27
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	9	0.27
(1,2632)	1:240:A:PHE:H	1:235:A:ILE:HG21	8	0.27
(1,2632)	1:240:A:PHE:H	1:235:A:ILE:HG22	8	0.27
(1,2632)	1:240:A:PHE:H	1:235:A:ILE:HG23	8	0.27
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	7	0.27
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	7	0.27
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	7	0.27
(1,2558)	1:92:A:VAL:HG11	1:99:A:CYS:HB3	3	0.27
(1,2558)	1:92:A:VAL:HG12	1:99:A:CYS:HB3	3	0.27
(1,2558)	1:92:A:VAL:HG13	1:99:A:CYS:HB3	3	0.27
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	3	0.27
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	3	0.27
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE1	1	0.27
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE2	1	0.27
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD11	9	0.27
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD12	9	0.27
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD13	9	0.27
(1,2318)	1:49:A:PHE:HD2	1:60:A:ASN:H	4	0.27
(1,2194)	1:75:A:LEU:H	1:76:A:TYR:HB3	8	0.27
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	2	0.27
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	9	0.27
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	3	0.27
(1,2129)	1:222:A:VAL:HG11	1:256:A:PHE:H	3	0.27
(1,2129)	1:222:A:VAL:HG12	1:256:A:PHE:H	3	0.27
(1,2129)	1:222:A:VAL:HG13	1:256:A:PHE:H	3	0.27
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	6	0.27
(1,2075)	1:173:A:LYS:H	1:176:A:LYS:HG2	10	0.27
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	5	0.27
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	5	0.27
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	5	0.27
(1,2043)	1:85:A:PHE:HD1	1:86:A:GLN:H	2	0.27
(1,2043)	1:85:A:PHE:HD2	1:86:A:GLN:H	2	0.27
(1,1942)	1:144:A:ARG:H	1:234:A:HIS:HA	7	0.27
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	3	0.27
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	3	0.27
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	3	0.27
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	9	0.27
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	9	0.27
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	9	0.27
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1775)	1:6:A:GLU:H	1:6:A:GLU:HG3	4	0.27
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	1	0.27
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	1	0.27
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	1	0.27
(1,1678)	1:159:A:GLU:HB3	1:160:A:GLN:H	4	0.27
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	2	0.27
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	9	0.27
(1,1666)	1:251:A:VAL:HG21	1:257:A:ASP:H	8	0.27
(1,1666)	1:251:A:VAL:HG22	1:257:A:ASP:H	8	0.27
(1,1666)	1:251:A:VAL:HG23	1:257:A:ASP:H	8	0.27
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	2	0.27
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	2	0.27
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	8	0.27
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	8	0.27
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG2	3	0.27
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG3	3	0.27
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD2	1	0.27
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD3	1	0.27
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD2	1	0.27
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD3	1	0.27
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	6	0.27
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	6	0.27
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	6	0.27
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	5	0.27
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	5	0.27
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	5	0.27
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD21	5	0.27
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD22	5	0.27
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD23	5	0.27
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	3	0.27
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	3	0.27
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	3	0.27
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	3	0.27
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	3	0.27
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	3	0.27
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD1	7	0.27
(1,1122)	1:15:A:VAL:HG11	1:19:A:TYR:HD2	7	0.27
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD1	7	0.27
(1,1122)	1:15:A:VAL:HG12	1:19:A:TYR:HD2	7	0.27
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD1	7	0.27
(1,1122)	1:15:A:VAL:HG13	1:19:A:TYR:HD2	7	0.27
(1,1074)	1:176:A:LYS:HA	1:176:A:LYS:HG2	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	2	0.27
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	2	0.27
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	2	0.27
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD21	5	0.27
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD22	5	0.27
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD23	5	0.27
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	6	0.27
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	8	0.27
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	1	0.27
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	3	0.27
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	6	0.27
(1,588)	1:31:A:SER:HB2	1:49:A:PHE:H	4	0.27
(1,550)	1:258:A:SER:H	1:258:A:SER:HB3	3	0.27
(1,536)	1:24:A:SER:HB2	1:25:A:LYS:H	10	0.27
(1,536)	1:24:A:SER:HB3	1:25:A:LYS:H	10	0.27
(1,521)	1:122:A:VAL:H	1:122:A:VAL:HB	8	0.27
(1,440)	1:27:A:GLN:HG3	1:28:A:GLU:H	5	0.27
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	9	0.27
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	9	0.27
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	9	0.27
(1,406)	1:187:A:LYS:HB3	1:220:A:TRP:HD1	1	0.27
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	1	0.27
(1,129)	1:79:A:LYS:HE2	1:80:A:TYR:H	8	0.27
(1,129)	1:79:A:LYS:HE3	1:80:A:TYR:H	8	0.27
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	9	0.27
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	9	0.27
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	6	0.27
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	1	0.27
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	1	0.27
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	1	0.27
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD11	1	0.27
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD12	1	0.27
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD13	1	0.27
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	2	0.26
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	2	0.26
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	2	0.26
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	2	0.26
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	2	0.26
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	2	0.26
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	4	0.26
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	4	0.26
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	1	0.26
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	1	0.26
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	1	0.26
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	2	0.26
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	2	0.26
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	2	0.26
(1,2499)	1:213:A:LEU:HD21	1:216:A:ILE:HD11	10	0.26
(1,2499)	1:213:A:LEU:HD21	1:216:A:ILE:HD12	10	0.26
(1,2499)	1:213:A:LEU:HD21	1:216:A:ILE:HD13	10	0.26
(1,2499)	1:213:A:LEU:HD22	1:216:A:ILE:HD11	10	0.26
(1,2499)	1:213:A:LEU:HD22	1:216:A:ILE:HD12	10	0.26
(1,2499)	1:213:A:LEU:HD22	1:216:A:ILE:HD13	10	0.26
(1,2499)	1:213:A:LEU:HD23	1:216:A:ILE:HD11	10	0.26
(1,2499)	1:213:A:LEU:HD23	1:216:A:ILE:HD12	10	0.26
(1,2499)	1:213:A:LEU:HD23	1:216:A:ILE:HD13	10	0.26
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	7	0.26
(1,2377)	1:5:A:HIS:H	1:7:A:GLN:HE22	10	0.26
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	6	0.26
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	7	0.26
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	7	0.26
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	7	0.26
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	7	0.26
(1,2323)	1:58:A:ALA:HB1	1:92:A:VAL:H	10	0.26
(1,2323)	1:58:A:ALA:HB2	1:92:A:VAL:H	10	0.26
(1,2323)	1:58:A:ALA:HB3	1:92:A:VAL:H	10	0.26
(1,2303)	1:19:A:TYR:HB2	1:21:A:ASP:H	1	0.26
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	7	0.26
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	7	0.26
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	7	0.26
(1,2035)	1:3:A:ASP:H	1:4:A:ASP:H	8	0.26
(1,2025)	1:186:A:ILE:H	1:196:A:GLN:H	5	0.26
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG2	1	0.26
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG3	1	0.26
(1,1942)	1:144:A:ARG:H	1:234:A:HIS:HA	8	0.26
(1,1935)	1:141:A:ILE:HD11	1:148:A:PHE:H	9	0.26
(1,1935)	1:141:A:ILE:HD12	1:148:A:PHE:H	9	0.26
(1,1935)	1:141:A:ILE:HD13	1:148:A:PHE:H	9	0.26
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	4	0.26
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	4	0.26
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	4	0.26
(1,1694)	1:211:A:LEU:HD11	1:213:A:LEU:H	4	0.26
(1,1694)	1:211:A:LEU:HD12	1:213:A:LEU:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:211:A:LEU:HD13	1:213:A:LEU:H	4	0.26
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	4	0.26
(1,1627)	1:1:A:MET:HB2	1:2:A:ASP:H	1	0.26
(1,1627)	1:1:A:MET:HB3	1:2:A:ASP:H	1	0.26
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	1	0.26
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	1	0.26
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	1	0.26
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	9	0.26
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	9	0.26
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	9	0.26
(1,1299)	1:183:A:ALA:HA	1:184:A:TRP:HB3	2	0.26
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	9	0.26
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	9	0.26
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	9	0.26
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD11	6	0.26
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD12	6	0.26
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD13	6	0.26
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD11	6	0.26
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD12	6	0.26
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD13	6	0.26
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD11	6	0.26
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD12	6	0.26
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD13	6	0.26
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD11	6	0.26
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD12	6	0.26
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD13	6	0.26
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD11	6	0.26
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD12	6	0.26
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD13	6	0.26
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD11	6	0.26
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD12	6	0.26
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD13	6	0.26
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	6	0.26
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	6	0.26
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	6	0.26
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG2	6	0.26
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG3	6	0.26
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	6	0.26
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	9	0.26
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	9	0.26
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	9	0.26
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	9	0.26
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	9	0.26
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	9	0.26
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	9	0.26
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	9	0.26
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	9	0.26
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	1	0.26
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	6	0.26
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	2	0.26
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	6	0.26
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	8	0.26
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	8	0.26
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	8	0.26
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	4	0.26
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	3	0.26
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB2	2	0.26
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB3	2	0.26
(1,521)	1:122:A:VAL:H	1:122:A:VAL:HB	9	0.26
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	2	0.26
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	6	0.26
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	8	0.26
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	9	0.26
(1,334)	1:10:A:GLU:H	1:10:A:GLU:HG2	8	0.26
(1,334)	1:10:A:GLU:H	1:10:A:GLU:HG3	8	0.26
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	3	0.26
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG11	9	0.26
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG12	9	0.26
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG13	9	0.26
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG11	9	0.26
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG12	9	0.26
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG13	9	0.26
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	5	0.26
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	5	0.26
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	5	0.26
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	9	0.25
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	9	0.25
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	9	0.25
(1,2610)	1:98:A:VAL:HG21	1:99:A:CYS:HB2	2	0.25
(1,2610)	1:98:A:VAL:HG22	1:99:A:CYS:HB2	2	0.25
(1,2610)	1:98:A:VAL:HG23	1:99:A:CYS:HB2	2	0.25
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	1	0.25
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	1	0.25
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	3	0.25
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	3	0.25
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	3	0.25
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	5	0.25
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	5	0.25
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	5	0.25
(1,2491)	1:168:A:LEU:HD21	1:174:A:MET:H	5	0.25
(1,2491)	1:168:A:LEU:HD22	1:174:A:MET:H	5	0.25
(1,2491)	1:168:A:LEU:HD23	1:174:A:MET:H	5	0.25
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	2	0.25
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	2	0.25
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	2	0.25
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	5	0.25
(1,2361)	1:42:A:TYR:H	1:43:A:MET:H	1	0.25
(1,2360)	1:41:A:GLU:H	1:42:A:TYR:H	10	0.25
(1,2303)	1:19:A:TYR:HB2	1:21:A:ASP:H	6	0.25
(1,2196)	1:88:A:VAL:HG21	1:90:A:ASP:H	6	0.25
(1,2196)	1:88:A:VAL:HG22	1:90:A:ASP:H	6	0.25
(1,2196)	1:88:A:VAL:HG23	1:90:A:ASP:H	6	0.25
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	1	0.25
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	1	0.25
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	7	0.25
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	7	0.25
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	7	0.25
(1,2078)	1:100:A:LEU:H	1:102:A:ASP:H	1	0.25
(1,2078)	1:100:A:LEU:H	1:102:A:ASP:H	2	0.25
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	7	0.25
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	2	0.25
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	2	0.25
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	4	0.25
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	4	0.25
(1,1625)	1:2:A:ASP:H	1:2:A:ASP:HB3	4	0.25
(1,1585)	1:11:A:GLU:H	1:11:A:GLU:HG3	7	0.25
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	4	0.25
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	1	0.25
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	1	0.25
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	1	0.25
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	5	0.25
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	5	0.25
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	5	0.25
(1,1440)	1:58:A:ALA:HB1	1:99:A:CYS:HB2	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1440)	1:58:A:ALA:HB2	1:99:A:CYS:HB2	2	0.25
(1,1440)	1:58:A:ALA:HB3	1:99:A:CYS:HB2	2	0.25
(1,1421)	1:58:A:ALA:HB1	1:89:A:MET:HG2	1	0.25
(1,1421)	1:58:A:ALA:HB1	1:89:A:MET:HG3	1	0.25
(1,1421)	1:58:A:ALA:HB2	1:89:A:MET:HG2	1	0.25
(1,1421)	1:58:A:ALA:HB2	1:89:A:MET:HG3	1	0.25
(1,1421)	1:58:A:ALA:HB3	1:89:A:MET:HG2	1	0.25
(1,1421)	1:58:A:ALA:HB3	1:89:A:MET:HG3	1	0.25
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD2	6	0.25
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD3	6	0.25
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD2	6	0.25
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD3	6	0.25
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	2	0.25
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	2	0.25
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	2	0.25
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	2	0.25
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	10	0.25
(1,1372)	1:137:A:ALA:HA	1:151:A:PHE:HD1	4	0.25
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	2	0.25
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	2	0.25
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	2	0.25
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD1	3	0.25
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD2	3	0.25
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD1	3	0.25
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD2	3	0.25
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD1	3	0.25
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD2	3	0.25
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	2	0.25
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	2	0.25
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	2	0.25
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	4	0.25
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	4	0.25
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	4	0.25
(1,1202)	1:61:A:VAL:HG21	1:62:A:ILE:H	1	0.25
(1,1202)	1:61:A:VAL:HG22	1:62:A:ILE:H	1	0.25
(1,1202)	1:61:A:VAL:HG23	1:62:A:ILE:H	1	0.25
(1,1194)	1:68:A:THR:H	1:68:A:THR:HG21	3	0.25
(1,1194)	1:68:A:THR:H	1:68:A:THR:HG22	3	0.25
(1,1194)	1:68:A:THR:H	1:68:A:THR:HG23	3	0.25
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG21	5	0.25
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG22	5	0.25
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG23	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG21	5	0.25
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG22	5	0.25
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG23	5	0.25
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG21	5	0.25
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG22	5	0.25
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG23	5	0.25
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG2	1	0.25
(1,1144)	1:116:A:GLU:HA	1:116:A:GLU:HG3	1	0.25
(1,1140)	1:220:A:TRP:HB2	1:221:A:ASN:HA	4	0.25
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	3	0.25
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	2	0.25
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	2	0.25
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	2	0.25
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	6	0.25
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	6	0.25
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	6	0.25
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	9	0.25
(1,930)	1:36:A:LYS:HG2	1:41:A:GLU:HA	6	0.25
(1,930)	1:36:A:LYS:HG3	1:41:A:GLU:HA	6	0.25
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	2	0.25
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	6	0.25
(1,781)	1:159:A:GLU:HA	1:162:A:PHE:HB3	5	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	2	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	2	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	2	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	6	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	6	0.25
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	6	0.25
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	6	0.25
(1,725)	1:117:A:GLU:H	1:117:A:GLU:HB2	3	0.25
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	1	0.25
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	1	0.25
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	1	0.25
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	1	0.25
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	6	0.25
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	6	0.25
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	6	0.25
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	6	0.25
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	3	0.25
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	3	0.25
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	8	0.25
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	3	0.25
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	3	0.25
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	3	0.25
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	9	0.25
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	9	0.25
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	9	0.25
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	9	0.25
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	9	0.25
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	9	0.25
(1,401)	1:46:A:GLN:HG3	1:63:A:GLU:H	10	0.25
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	5	0.25
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	9	0.25
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	6	0.25
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	6	0.25
(1,361)	1:133:A:GLU:HG2	1:134:A:GLY:H	8	0.25
(1,361)	1:133:A:GLU:HG3	1:134:A:GLY:H	8	0.25
(1,129)	1:79:A:LYS:HE2	1:80:A:TYR:H	2	0.25
(1,129)	1:79:A:LYS:HE3	1:80:A:TYR:H	2	0.25
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD2	4	0.25
(1,113)	1:175:A:ARG:HA	1:175:A:ARG:HD3	4	0.25
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	4	0.25
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	4	0.25
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	4	0.25
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD11	3	0.24
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD12	3	0.24
(1,2666)	1:98:A:VAL:HA	1:8:A:LEU:HD13	3	0.24
(1,2628)	1:235:A:ILE:HD11	1:239:A:ARG:H	3	0.24
(1,2628)	1:235:A:ILE:HD12	1:239:A:ARG:H	3	0.24
(1,2628)	1:235:A:ILE:HD13	1:239:A:ARG:H	3	0.24
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	3	0.24
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	3	0.24
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	3	0.24
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	3	0.24
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	3	0.24
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	3	0.24
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	3	0.24
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	3	0.24
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	3	0.24
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	5	0.24
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	9	0.24
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	4	0.24
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	1	0.24
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD21	10	0.24
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD22	10	0.24
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD23	10	0.24
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	5	0.24
(1,2187)	1:107:A:LEU:HB2	1:111:A:LEU:H	9	0.24
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	1	0.24
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	8	0.24
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	9	0.24
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	4	0.24
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	5	0.24
(1,2104)	1:40:A:HIS:H	1:42:A:TYR:H	1	0.24
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	4	0.24
(1,1959)	1:187:A:LYS:H	1:189:A:ASP:H	9	0.24
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	7	0.24
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	7	0.24
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	7	0.24
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	10	0.24
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	10	0.24
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	10	0.24
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG11	7	0.24
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG12	7	0.24
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG13	7	0.24
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	6	0.24
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	6	0.24
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	6	0.24
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	5	0.24
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	5	0.24
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	5	0.24
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	5	0.24
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	5	0.24
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	5	0.24
(1,1283)	1:66:A:VAL:HG11	1:76:A:TYR:HE1	8	0.24
(1,1283)	1:66:A:VAL:HG11	1:76:A:TYR:HE2	8	0.24
(1,1283)	1:66:A:VAL:HG12	1:76:A:TYR:HE1	8	0.24
(1,1283)	1:66:A:VAL:HG12	1:76:A:TYR:HE2	8	0.24
(1,1283)	1:66:A:VAL:HG13	1:76:A:TYR:HE1	8	0.24
(1,1283)	1:66:A:VAL:HG13	1:76:A:TYR:HE2	8	0.24
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	8	0.24
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	8	0.24
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	8	0.24
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	10	0.24
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	10	0.24
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	1	0.24
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	1	0.24
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	1	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	2	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	2	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	2	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	6	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	6	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	6	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	10	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	10	0.24
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	10	0.24
(1,1202)	1:61:A:VAL:HG21	1:62:A:ILE:H	6	0.24
(1,1202)	1:61:A:VAL:HG22	1:62:A:ILE:H	6	0.24
(1,1202)	1:61:A:VAL:HG23	1:62:A:ILE:H	6	0.24
(1,1196)	1:105:A:THR:HG21	1:106:A:GLU:H	6	0.24
(1,1196)	1:105:A:THR:HG22	1:106:A:GLU:H	6	0.24
(1,1196)	1:105:A:THR:HG23	1:106:A:GLU:H	6	0.24
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG21	6	0.24
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG22	6	0.24
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG23	6	0.24
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	8	0.24
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	8	0.24
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	8	0.24
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	8	0.24
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	8	0.24
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	8	0.24
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	8	0.24
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	8	0.24
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	8	0.24
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	1	0.24
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	1	0.24
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	1	0.24
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	9	0.24
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	9	0.24
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	9	0.24
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	9	0.24
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	9	0.24
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	9	0.24
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	8	0.24
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	8	0.24
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	8	0.24
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	9	0.24
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG21	9	0.24
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG22	9	0.24
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG23	9	0.24
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	5	0.24
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	8	0.24
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	8	0.24
(1,572)	1:79:A:LYS:HB2	1:80:A:TYR:H	10	0.24
(1,563)	1:257:A:ASP:HB2	1:258:A:SER:HB2	9	0.24
(1,563)	1:257:A:ASP:HB3	1:258:A:SER:HB2	9	0.24
(1,550)	1:258:A:SER:H	1:258:A:SER:HB3	6	0.24
(1,411)	1:187:A:LYS:HB2	1:188:A:GLN:H	9	0.24
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	10	0.24
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	3	0.24
(1,109)	1:95:A:ARG:HD2	1:96:A:GLY:H	7	0.24
(1,109)	1:95:A:ARG:HD3	1:96:A:GLY:H	7	0.24
(1,82)	1:95:A:ARG:HB2	1:96:A:GLY:HA3	10	0.24
(1,60)	1:134:A:GLY:HA3	1:164:A:MET:HB2	10	0.24
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	4	0.24
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	4	0.24
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	4	0.24
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD11	10	0.24
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD12	10	0.24
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD13	10	0.24
(1,2654)	1:103:A:PHE:HE1	1:85:A:PHE:HB3	1	0.23
(1,2654)	1:103:A:PHE:HE2	1:85:A:PHE:HB3	1	0.23
(1,2558)	1:92:A:VAL:HG11	1:99:A:CYS:HB3	5	0.23
(1,2558)	1:92:A:VAL:HG12	1:99:A:CYS:HB3	5	0.23
(1,2558)	1:92:A:VAL:HG13	1:99:A:CYS:HB3	5	0.23
(1,2504)	1:74:A:ASP:HB3	1:75:A:LEU:HD11	10	0.23
(1,2504)	1:74:A:ASP:HB3	1:75:A:LEU:HD12	10	0.23
(1,2504)	1:74:A:ASP:HB3	1:75:A:LEU:HD13	10	0.23
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG21	1	0.23
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG22	1	0.23
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG23	1	0.23
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG21	1	0.23
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG22	1	0.23
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG23	1	0.23
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG21	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG22	1	0.23
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG23	1	0.23
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	9	0.23
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	9	0.23
(1,2385)	1:29:A:ASP:HA	1:31:A:SER:H	1	0.23
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	3	0.23
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	1	0.23
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	5	0.23
(1,2242)	1:29:A:ASP:H	1:32:A:ILE:H	3	0.23
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	3	0.23
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	8	0.23
(1,2187)	1:107:A:LEU:HB2	1:111:A:LEU:H	4	0.23
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	3	0.23
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	7	0.23
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	2	0.23
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	10	0.23
(1,2096)	1:251:A:VAL:HG21	1:253:A:ARG:H	3	0.23
(1,2096)	1:251:A:VAL:HG22	1:253:A:ARG:H	3	0.23
(1,2096)	1:251:A:VAL:HG23	1:253:A:ARG:H	3	0.23
(1,2040)	1:210:A:MET:H	1:211:A:LEU:HB3	10	0.23
(1,2038)	1:155:A:VAL:HA	1:161:A:ALA:H	3	0.23
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	9	0.23
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	9	0.23
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	9	0.23
(1,1794)	1:200:A:ASP:HB3	1:201:A:ASP:H	4	0.23
(1,1790)	1:4:A:ASP:HB2	1:5:A:HIS:H	8	0.23
(1,1627)	1:1:A:MET:HB2	1:2:A:ASP:H	9	0.23
(1,1627)	1:1:A:MET:HB3	1:2:A:ASP:H	9	0.23
(1,1608)	1:132:A:PHE:H	1:135:A:TRP:HB3	5	0.23
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	7	0.23
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE21	1	0.23
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE22	1	0.23
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG2	5	0.23
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG3	5	0.23
(1,1377)	1:131:A:PRO:HD3	1:132:A:PHE:H	7	0.23
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	1	0.23
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	1	0.23
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	1	0.23
(1,1171)	1:51:A:THR:HG21	1:52:A:HIS:H	9	0.23
(1,1171)	1:51:A:THR:HG22	1:52:A:HIS:H	9	0.23
(1,1171)	1:51:A:THR:HG23	1:52:A:HIS:H	9	0.23
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG21	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG22	2	0.23
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG23	2	0.23
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG21	2	0.23
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG22	2	0.23
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG23	2	0.23
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG21	2	0.23
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG22	2	0.23
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG23	2	0.23
(1,1027)	1:135:A:TRP:HA	1:154:A:HIS:HD2	6	0.23
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	8	0.23
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	1	0.23
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG21	5	0.23
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG22	5	0.23
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG23	5	0.23
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG21	5	0.23
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG22	5	0.23
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG23	5	0.23
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG2	1	0.23
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG3	1	0.23
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG21	8	0.23
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG22	8	0.23
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG23	8	0.23
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	10	0.23
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	10	0.23
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	10	0.23
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	10	0.23
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	2	0.23
(1,550)	1:258:A:SER:H	1:258:A:SER:HB3	2	0.23
(1,476)	1:219:A:VAL:HB	1:256:A:PHE:HB3	3	0.23
(1,440)	1:27:A:GLN:HG3	1:28:A:GLU:H	1	0.23
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	2	0.23
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	2	0.23
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	2	0.23
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	8	0.23
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	8	0.23
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	8	0.23
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	8	0.23
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	8	0.23
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	8	0.23
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	4	0.23
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	4	0.23
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	1	0.23
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	8	0.23
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	8	0.23
(1,284)	1:158:A:GLU:HG3	1:195:A:TYR:HB3	7	0.23
(1,232)	1:186:A:ILE:HB	1:194:A:THR:HB	3	0.23
(1,174)	1:3:A:ASP:H	1:3:A:ASP:HB2	7	0.23
(1,174)	1:3:A:ASP:H	1:3:A:ASP:HB3	7	0.23
(1,99)	1:171:A:ASP:HB2	1:174:A:MET:HB3	2	0.23
(1,40)	1:255:A:GLY:HA3	1:257:A:ASP:H	5	0.23
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD11	2	0.23
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD12	2	0.23
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD13	2	0.23
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	5	0.23
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	5	0.23
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	5	0.23
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	6	0.22
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	6	0.22
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	6	0.22
(1,2610)	1:98:A:VAL:HG21	1:99:A:CYS:HB2	9	0.22
(1,2610)	1:98:A:VAL:HG22	1:99:A:CYS:HB2	9	0.22
(1,2610)	1:98:A:VAL:HG23	1:99:A:CYS:HB2	9	0.22
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG11	1	0.22
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG12	1	0.22
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG13	1	0.22
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG11	1	0.22
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG12	1	0.22
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG13	1	0.22
(1,2553)	1:142:A:THR:HG21	1:235:A:ILE:HG12	7	0.22
(1,2553)	1:142:A:THR:HG22	1:235:A:ILE:HG12	7	0.22
(1,2553)	1:142:A:THR:HG23	1:235:A:ILE:HG12	7	0.22
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	10	0.22
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	10	0.22
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	10	0.22
(1,2438)	1:186:A:ILE:HG21	1:188:A:GLN:HB2	3	0.22
(1,2438)	1:186:A:ILE:HG22	1:188:A:GLN:HB2	3	0.22
(1,2438)	1:186:A:ILE:HG23	1:188:A:GLN:HB2	3	0.22
(1,2415)	1:141:A:ILE:HD11	1:240:A:PHE:HB3	8	0.22
(1,2415)	1:141:A:ILE:HD12	1:240:A:PHE:HB3	8	0.22
(1,2415)	1:141:A:ILE:HD13	1:240:A:PHE:HB3	8	0.22
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	1	0.22
(1,2359)	1:40:A:HIS:HA	1:42:A:TYR:H	8	0.22
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE1	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE2	6	0.22
(1,2303)	1:19:A:TYR:HB2	1:21:A:ASP:H	10	0.22
(1,2248)	1:64:A:VAL:HG21	1:83:A:HIS:H	10	0.22
(1,2248)	1:64:A:VAL:HG22	1:83:A:HIS:H	10	0.22
(1,2248)	1:64:A:VAL:HG23	1:83:A:HIS:H	10	0.22
(1,2241)	1:31:A:SER:H	1:32:A:ILE:H	1	0.22
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	4	0.22
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	5	0.22
(1,2063)	1:40:A:HIS:H	1:41:A:GLU:H	4	0.22
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	1	0.22
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	1	0.22
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	1	0.22
(1,1942)	1:144:A:ARG:H	1:234:A:HIS:HA	2	0.22
(1,1931)	1:64:A:VAL:H	1:82:A:GLN:H	10	0.22
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	7	0.22
(1,1790)	1:4:A:ASP:HB2	1:5:A:HIS:H	7	0.22
(1,1747)	1:11:A:GLU:HA	1:13:A:GLU:H	9	0.22
(1,1730)	1:146:A:SER:H	1:234:A:HIS:HA	9	0.22
(1,1627)	1:1:A:MET:HB2	1:2:A:ASP:H	6	0.22
(1,1627)	1:1:A:MET:HB3	1:2:A:ASP:H	6	0.22
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	1	0.22
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	1	0.22
(1,1497)	1:127:A:ILE:HG21	1:128:A:PRO:HG3	4	0.22
(1,1497)	1:127:A:ILE:HG22	1:128:A:PRO:HG3	4	0.22
(1,1497)	1:127:A:ILE:HG23	1:128:A:PRO:HG3	4	0.22
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE1	6	0.22
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE2	6	0.22
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE3	6	0.22
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD2	3	0.22
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD3	3	0.22
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD2	3	0.22
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD3	3	0.22
(1,1377)	1:131:A:PRO:HD3	1:132:A:PHE:H	9	0.22
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	7	0.22
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	1	0.22
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	1	0.22
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	1	0.22
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	7	0.22
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	7	0.22
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	7	0.22
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG21	1	0.22
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG22	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG23	1	0.22
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG21	1	0.22
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG22	1	0.22
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG23	1	0.22
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG21	1	0.22
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG22	1	0.22
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG23	1	0.22
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	4	0.22
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	10	0.22
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	10	0.22
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	10	0.22
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	10	0.22
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	10	0.22
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	10	0.22
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	10	0.22
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	10	0.22
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	10	0.22
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	2	0.22
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	2	0.22
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	2	0.22
(1,1069)	1:242:A:HIS:HA	1:245:A:SER:H	2	0.22
(1,1069)	1:242:A:HIS:HA	1:245:A:SER:H	4	0.22
(1,1043)	1:42:A:TYR:HA	1:67:A:CYS:HB2	5	0.22
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	8	0.22
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	8	0.22
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	8	0.22
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	6	0.22
(1,922)	1:176:A:LYS:HG3	1:177:A:ALA:H	6	0.22
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	4	0.22
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	2	0.22
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	2	0.22
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	2	0.22
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	7	0.22
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	7	0.22
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	7	0.22
(1,738)	1:186:A:ILE:HA	1:220:A:TRP:HD1	1	0.22
(1,738)	1:186:A:ILE:HA	1:220:A:TRP:HD1	8	0.22
(1,738)	1:186:A:ILE:HA	1:220:A:TRP:HD1	9	0.22
(1,709)	1:79:A:LYS:HD2	1:80:A:TYR:H	3	0.22
(1,709)	1:79:A:LYS:HD3	1:80:A:TYR:H	3	0.22
(1,709)	1:79:A:LYS:HD2	1:80:A:TYR:H	7	0.22
(1,709)	1:79:A:LYS:HD3	1:80:A:TYR:H	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	6	0.22
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD21	4	0.22
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD22	4	0.22
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD23	4	0.22
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	7	0.22
(1,621)	1:117:A:GLU:H	1:118:A:GLU:HB3	10	0.22
(1,528)	1:82:A:GLN:H	1:82:A:GLN:HG3	5	0.22
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	3	0.22
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD11	8	0.22
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD12	8	0.22
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD13	8	0.22
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	1	0.22
(1,371)	1:65:A:GLY:HA3	1:66:A:VAL:HB	7	0.22
(1,334)	1:10:A:GLU:H	1:10:A:GLU:HG2	10	0.22
(1,334)	1:10:A:GLU:H	1:10:A:GLU:HG3	10	0.22
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	6	0.22
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD11	1	0.22
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD12	1	0.22
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD13	1	0.22
(1,54)	1:189:A:ASP:HB2	1:190:A:GLY:HA2	5	0.22
(1,54)	1:189:A:ASP:HB3	1:190:A:GLY:HA2	5	0.22
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD11	10	0.22
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD12	10	0.22
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD13	10	0.22
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	2	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	2	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	2	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	10	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	10	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	10	0.21
(1,2610)	1:98:A:VAL:HG21	1:99:A:CYS:HB2	7	0.21
(1,2610)	1:98:A:VAL:HG22	1:99:A:CYS:HB2	7	0.21
(1,2610)	1:98:A:VAL:HG23	1:99:A:CYS:HB2	7	0.21
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	7	0.21
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	7	0.21
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	7	0.21
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG21	2	0.21
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG22	2	0.21
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG23	2	0.21
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG21	2	0.21
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG22	2	0.21
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG23	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG21	2	0.21
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG22	2	0.21
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG23	2	0.21
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	3	0.21
(1,2424)	1:107:A:LEU:HB3	1:108:A:ASP:HB3	2	0.21
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	8	0.21
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	8	0.21
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	8	0.21
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	8	0.21
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	8	0.21
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	8	0.21
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	8	0.21
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	8	0.21
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	8	0.21
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG11	5	0.21
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG12	5	0.21
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG13	5	0.21
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG11	5	0.21
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG12	5	0.21
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG13	5	0.21
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG11	5	0.21
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG12	5	0.21
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG13	5	0.21
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	2	0.21
(1,2323)	1:58:A:ALA:HB1	1:92:A:VAL:H	5	0.21
(1,2323)	1:58:A:ALA:HB2	1:92:A:VAL:H	5	0.21
(1,2323)	1:58:A:ALA:HB3	1:92:A:VAL:H	5	0.21
(1,2294)	1:76:A:TYR:HB3	1:81:A:LEU:H	4	0.21
(1,2271)	1:29:A:ASP:H	1:30:A:GLY:H	1	0.21
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	4	0.21
(1,2129)	1:222:A:VAL:HG11	1:256:A:PHE:H	8	0.21
(1,2129)	1:222:A:VAL:HG12	1:256:A:PHE:H	8	0.21
(1,2129)	1:222:A:VAL:HG13	1:256:A:PHE:H	8	0.21
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	4	0.21
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	9	0.21
(1,2096)	1:251:A:VAL:HG21	1:253:A:ARG:H	6	0.21
(1,2096)	1:251:A:VAL:HG22	1:253:A:ARG:H	6	0.21
(1,2096)	1:251:A:VAL:HG23	1:253:A:ARG:H	6	0.21
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG21	4	0.21
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG22	4	0.21
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG23	4	0.21
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2078)	1:100:A:LEU:H	1:102:A:ASP:H	6	0.21
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	4	0.21
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	4	0.21
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	4	0.21
(1,1972)	1:202:A:GLY:H	1:203:A:GLU:H	3	0.21
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG2	6	0.21
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG3	6	0.21
(1,1964)	1:12:A:LEU:HB3	1:14:A:ALA:H	4	0.21
(1,1927)	1:77:A:ASP:H	1:80:A:TYR:HA	8	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	5	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	5	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	5	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	8	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	8	0.21
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	8	0.21
(1,1704)	1:136:A:THR:H	1:154:A:HIS:HD2	3	0.21
(1,1607)	1:36:A:LYS:HB2	1:45:A:LEU:H	7	0.21
(1,1607)	1:36:A:LYS:HB3	1:45:A:LEU:H	7	0.21
(1,1585)	1:11:A:GLU:H	1:11:A:GLU:HG3	4	0.21
(1,1497)	1:127:A:ILE:HG21	1:128:A:PRO:HG3	5	0.21
(1,1497)	1:127:A:ILE:HG22	1:128:A:PRO:HG3	5	0.21
(1,1497)	1:127:A:ILE:HG23	1:128:A:PRO:HG3	5	0.21
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	2	0.21
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	2	0.21
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	2	0.21
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	4	0.21
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	4	0.21
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	4	0.21
(1,1353)	1:181:A:MET:HE1	1:228:A:ARG:H	1	0.21
(1,1353)	1:181:A:MET:HE2	1:228:A:ARG:H	1	0.21
(1,1353)	1:181:A:MET:HE3	1:228:A:ARG:H	1	0.21
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	3	0.21
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	3	0.21
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	3	0.21
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	5	0.21
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	5	0.21
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	5	0.21
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD21	4	0.21
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD22	4	0.21
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD23	4	0.21
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	9	0.21
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	9	0.21
(1,1171)	1:51:A:THR:HG21	1:52:A:HIS:H	5	0.21
(1,1171)	1:51:A:THR:HG22	1:52:A:HIS:H	5	0.21
(1,1171)	1:51:A:THR:HG23	1:52:A:HIS:H	5	0.21
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	7	0.21
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	7	0.21
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	7	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	8	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	8	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	8	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	10	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	10	0.21
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	10	0.21
(1,1043)	1:42:A:TYR:HA	1:67:A:CYS:HB2	4	0.21
(1,989)	1:200:A:ASP:HA	1:207:A:GLY:H	7	0.21
(1,984)	1:168:A:LEU:HD21	1:225:A:VAL:H	9	0.21
(1,984)	1:168:A:LEU:HD22	1:225:A:VAL:H	9	0.21
(1,984)	1:168:A:LEU:HD23	1:225:A:VAL:H	9	0.21
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD21	9	0.21
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD22	9	0.21
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD23	9	0.21
(1,952)	1:72:A:LYS:HG2	1:73:A:ARG:H	2	0.21
(1,952)	1:72:A:LYS:HG3	1:73:A:ARG:H	2	0.21
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	3	0.21
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	7	0.21
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	5	0.21
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	7	0.21
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	7	0.21
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	7	0.21
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	7	0.21
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	9	0.21
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	9	0.21
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	9	0.21
(1,621)	1:117:A:GLU:H	1:118:A:GLU:HB3	5	0.21
(1,579)	1:20:A:PRO:HB3	1:21:A:ASP:H	4	0.21
(1,560)	1:240:A:PHE:H	1:241:A:LYS:HB2	9	0.21
(1,475)	1:219:A:VAL:HB	1:258:A:SER:H	4	0.21
(1,475)	1:219:A:VAL:HB	1:258:A:SER:H	7	0.21
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	8	0.21
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	8	0.21
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	8	0.21
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	4	0.21
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	4	0.21
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	6	0.21
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	6	0.21
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	7	0.21
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	7	0.21
(1,423)	1:185:A:ARG:HB2	1:220:A:TRP:HD1	3	0.21
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	6	0.21
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	6	0.21
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	6	0.21
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	6	0.21
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	6	0.21
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	6	0.21
(1,411)	1:187:A:LYS:HB2	1:188:A:GLN:H	1	0.21
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	10	0.21
(1,304)	1:16:A:GLU:H	1:16:A:GLU:HG2	7	0.21
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	9	0.21
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	9	0.21
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	9	0.21
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	9	0.21
(1,158)	1:141:A:ILE:HB	1:142:A:THR:H	10	0.21
(1,142)	1:19:A:TYR:HB2	1:22:A:LEU:HB2	5	0.21
(1,142)	1:19:A:TYR:HB2	1:22:A:LEU:HB3	5	0.21
(1,111)	1:175:A:ARG:HD2	1:176:A:LYS:H	10	0.21
(1,111)	1:175:A:ARG:HD3	1:176:A:LYS:H	10	0.21
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	5	0.21
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	5	0.21
(1,54)	1:189:A:ASP:HB2	1:190:A:GLY:HA2	9	0.21
(1,54)	1:189:A:ASP:HB3	1:190:A:GLY:HA2	9	0.21
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	2	0.21
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	2	0.21
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	2	0.21
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	3	0.21
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	3	0.21
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	3	0.21
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	6	0.21
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	6	0.21
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	6	0.21
(1,45)	1:47:A:ILE:HD11	1:85:A:PHE:HD1	2	0.21
(1,45)	1:47:A:ILE:HD11	1:85:A:PHE:HD2	2	0.21
(1,45)	1:47:A:ILE:HD12	1:85:A:PHE:HD1	2	0.21
(1,45)	1:47:A:ILE:HD12	1:85:A:PHE:HD2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:47:A:ILE:HD13	1:85:A:PHE:HD1	2	0.21
(1,45)	1:47:A:ILE:HD13	1:85:A:PHE:HD2	2	0.21
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD11	9	0.21
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD12	9	0.21
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD13	9	0.21
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	4	0.2
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	4	0.2
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	4	0.2
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	5	0.2
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	5	0.2
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	5	0.2
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	8	0.2
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	8	0.2
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	8	0.2
(1,2629)	1:234:A:HIS:HD2	1:239:A:ARG:H	7	0.2
(1,2626)	1:234:A:HIS:HD2	1:239:A:ARG:H	7	0.2
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	2	0.2
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	2	0.2
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	2	0.2
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD21	9	0.2
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD22	9	0.2
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD23	9	0.2
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD21	9	0.2
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD22	9	0.2
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD23	9	0.2
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD21	9	0.2
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD22	9	0.2
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD23	9	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	9	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	9	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	9	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	10	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	10	0.2
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	10	0.2
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	10	0.2
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	10	0.2
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	10	0.2
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	1	0.2
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	1	0.2
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	1	0.2
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	3	0.2
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	3	0.2
(1,2361)	1:42:A:TYR:H	1:43:A:MET:H	6	0.2
(1,2328)	1:162:A:PHE:H	1:164:A:MET:H	8	0.2
(1,2271)	1:29:A:ASP:H	1:30:A:GLY:H	7	0.2
(1,2241)	1:31:A:SER:H	1:32:A:ILE:H	3	0.2
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	5	0.2
(1,2207)	1:161:A:ALA:H	1:164:A:MET:H	6	0.2
(1,2097)	1:222:A:VAL:HG21	1:257:A:ASP:H	5	0.2
(1,2097)	1:222:A:VAL:HG22	1:257:A:ASP:H	5	0.2
(1,2097)	1:222:A:VAL:HG23	1:257:A:ASP:H	5	0.2
(1,2078)	1:100:A:LEU:H	1:102:A:ASP:H	9	0.2
(1,2075)	1:173:A:LYS:H	1:176:A:LYS:HG2	1	0.2
(1,1995)	1:51:A:THR:H	1:53:A:TYR:H	7	0.2
(1,1995)	1:51:A:THR:H	1:53:A:TYR:H	10	0.2
(1,1983)	1:162:A:PHE:HD1	1:165:A:LEU:H	2	0.2
(1,1983)	1:162:A:PHE:HD2	1:165:A:LEU:H	2	0.2
(1,1942)	1:144:A:ARG:H	1:234:A:HIS:HA	9	0.2
(1,1900)	1:37:A:VAL:H	1:43:A:MET:H	9	0.2
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	10	0.2
(1,1701)	1:256:A:PHE:H	1:257:A:ASP:H	1	0.2
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	8	0.2
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	8	0.2
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	8	0.2
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	2	0.2
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	5	0.2
(1,1589)	1:70:A:LEU:H	1:70:A:LEU:HG	4	0.2
(1,1578)	1:175:A:ARG:HA	1:177:A:ALA:H	4	0.2
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	2	0.2
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	3	0.2
(1,1554)	1:181:A:MET:HB3	1:226:A:VAL:H	2	0.2
(1,1554)	1:181:A:MET:HB3	1:226:A:VAL:H	3	0.2
(1,1503)	1:179:A:HIS:H	1:227:A:ALA:HA	4	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	5	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	5	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	5	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	6	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	6	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	6	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	10	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	10	0.2
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	10	0.2
(1,1439)	1:58:A:ALA:HB1	1:94:A:HIS:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1439)	1:58:A:ALA:HB2	1:94:A:HIS:H	8	0.2
(1,1439)	1:58:A:ALA:HB3	1:94:A:HIS:H	8	0.2
(1,1420)	1:58:A:ALA:HB1	1:93:A:PHE:HB2	7	0.2
(1,1420)	1:58:A:ALA:HB2	1:93:A:PHE:HB2	7	0.2
(1,1420)	1:58:A:ALA:HB3	1:93:A:PHE:HB2	7	0.2
(1,1396)	1:216:A:ILE:HG21	1:217:A:MET:H	5	0.2
(1,1396)	1:216:A:ILE:HG22	1:217:A:MET:H	5	0.2
(1,1396)	1:216:A:ILE:HG23	1:217:A:MET:H	5	0.2
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	5	0.2
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	5	0.2
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	5	0.2
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	5	0.2
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	5	0.2
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	5	0.2
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	5	0.2
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	5	0.2
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	5	0.2
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	8	0.2
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	8	0.2
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	8	0.2
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	8	0.2
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	8	0.2
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	8	0.2
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	10	0.2
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	10	0.2
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	10	0.2
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG11	7	0.2
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG12	7	0.2
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG13	7	0.2
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG11	7	0.2
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG12	7	0.2
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG13	7	0.2
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG11	7	0.2
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG12	7	0.2
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG13	7	0.2
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	9	0.2
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	9	0.2
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	9	0.2
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	7	0.2
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	7	0.2
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	7	0.2
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	7	0.2
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	7	0.2
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	7	0.2
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	7	0.2
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	7	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	3	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	3	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	3	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	5	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	5	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	5	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG21	7	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG22	7	0.2
(1,1084)	1:246:A:THR:H	1:246:A:THR:HG23	7	0.2
(1,1074)	1:176:A:LYS:HA	1:176:A:LYS:HG2	4	0.2
(1,1069)	1:242:A:HIS:HA	1:245:A:SER:H	6	0.2
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB2	1	0.2
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB3	1	0.2
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB2	1	0.2
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB3	1	0.2
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB2	1	0.2
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB3	1	0.2
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	7	0.2
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	7	0.2
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	7	0.2
(1,991)	1:88:A:VAL:HG21	1:107:A:LEU:HA	5	0.2
(1,991)	1:88:A:VAL:HG22	1:107:A:LEU:HA	5	0.2
(1,991)	1:88:A:VAL:HG23	1:107:A:LEU:HA	5	0.2
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	6	0.2
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	7	0.2
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	9	0.2
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	9	0.2
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	9	0.2
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	9	0.2
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	7	0.2
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	7	0.2
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG2	10	0.2
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG3	10	0.2
(1,781)	1:159:A:GLU:HA	1:162:A:PHE:HB3	10	0.2
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	4	0.2
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	8	0.2
(1,682)	1:3:A:ASP:HA	1:6:A:GLU:HB2	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,682)	1:3:A:ASP:HA	1:6:A:GLU:HB3	8	0.2
(1,618)	1:172:A:SER:HB2	1:175:A:ARG:HB2	2	0.2
(1,618)	1:172:A:SER:HB2	1:175:A:ARG:HB3	2	0.2
(1,618)	1:172:A:SER:HB3	1:175:A:ARG:HB2	2	0.2
(1,618)	1:172:A:SER:HB3	1:175:A:ARG:HB3	2	0.2
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	10	0.2
(1,560)	1:240:A:PHE:H	1:241:A:LYS:HB2	2	0.2
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB2	9	0.2
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB3	9	0.2
(1,490)	1:48:A:SER:HB2	1:60:A:ASN:HB2	7	0.2
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	8	0.2
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	5	0.2
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	5	0.2
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	5	0.2
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	5	0.2
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	7	0.2
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	7	0.2
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	7	0.2
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	7	0.2
(1,458)	1:63:A:GLU:HB2	1:64:A:VAL:H	9	0.2
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD11	7	0.2
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD12	7	0.2
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD13	7	0.2
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	10	0.2
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	10	0.2
(1,345)	1:6:A:GLU:HA	1:6:A:GLU:HG2	1	0.2
(1,332)	1:9:A:VAL:HA	1:13:A:GLU:HG3	1	0.2
(1,324)	1:105:A:THR:HB	1:106:A:GLU:H	5	0.2
(1,193)	1:163:A:ALA:HA	1:166:A:ASP:HB3	4	0.2
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	4	0.2
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	5	0.2
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG11	3	0.2
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG12	3	0.2
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG13	3	0.2
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG11	3	0.2
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG12	3	0.2
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG13	3	0.2
(1,115)	1:186:A:ILE:HB	1:195:A:TYR:HB3	6	0.2
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD11	2	0.2
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD12	2	0.2
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD13	2	0.2
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	3	0.2
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	3	0.2
(1,2654)	1:103:A:PHE:HE1	1:85:A:PHE:HB3	7	0.19
(1,2654)	1:103:A:PHE:HE2	1:85:A:PHE:HB3	7	0.19
(1,2631)	1:235:A:ILE:HD11	1:127:A:ILE:H	3	0.19
(1,2631)	1:235:A:ILE:HD12	1:127:A:ILE:H	3	0.19
(1,2631)	1:235:A:ILE:HD13	1:127:A:ILE:H	3	0.19
(1,2558)	1:92:A:VAL:HG11	1:99:A:CYS:HB3	8	0.19
(1,2558)	1:92:A:VAL:HG12	1:99:A:CYS:HB3	8	0.19
(1,2558)	1:92:A:VAL:HG13	1:99:A:CYS:HB3	8	0.19
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD21	4	0.19
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD22	4	0.19
(1,2540)	1:10:A:GLU:H	1:12:A:LEU:HD23	4	0.19
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	5	0.19
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	5	0.19
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	5	0.19
(1,2537)	1:76:A:TYR:HB2	1:81:A:LEU:HD21	8	0.19
(1,2537)	1:76:A:TYR:HB2	1:81:A:LEU:HD22	8	0.19
(1,2537)	1:76:A:TYR:HB2	1:81:A:LEU:HD23	8	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	1	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	1	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	1	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	7	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	7	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	7	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	9	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	9	0.19
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	9	0.19
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	8	0.19
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	9	0.19
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	4	0.19
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	4	0.19
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	4	0.19
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	4	0.19
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	4	0.19
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	4	0.19
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	4	0.19
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	4	0.19
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	4	0.19
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD11	8	0.19
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD12	8	0.19
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD13	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	4	0.19
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	7	0.19
(1,2361)	1:42:A:TYR:H	1:43:A:MET:H	5	0.19
(1,2285)	1:142:A:THR:HG21	1:239:A:ARG:H	3	0.19
(1,2285)	1:142:A:THR:HG22	1:239:A:ARG:H	3	0.19
(1,2285)	1:142:A:THR:HG23	1:239:A:ARG:H	3	0.19
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	6	0.19
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	10	0.19
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	8	0.19
(1,1986)	1:160:A:GLN:H	1:163:A:ALA:H	8	0.19
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	10	0.19
(1,1817)	1:81:A:LEU:H	1:82:A:GLN:HB2	2	0.19
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	2	0.19
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	3	0.19
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	6	0.19
(1,1735)	1:217:A:MET:HB2	1:218:A:ASP:H	4	0.19
(1,1704)	1:136:A:THR:H	1:154:A:HIS:HD2	8	0.19
(1,1701)	1:256:A:PHE:H	1:257:A:ASP:H	9	0.19
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	9	0.19
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	5	0.19
(1,1669)	1:37:A:VAL:H	1:44:A:THR:HB	10	0.19
(1,1666)	1:251:A:VAL:HG21	1:257:A:ASP:H	7	0.19
(1,1666)	1:251:A:VAL:HG22	1:257:A:ASP:H	7	0.19
(1,1666)	1:251:A:VAL:HG23	1:257:A:ASP:H	7	0.19
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD11	9	0.19
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD12	9	0.19
(1,1651)	1:141:A:ILE:H	1:243:A:ILE:HD13	9	0.19
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD11	2	0.19
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD12	2	0.19
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD13	2	0.19
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE21	9	0.19
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE22	9	0.19
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	3	0.19
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	3	0.19
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	3	0.19
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD2	7	0.19
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD3	7	0.19
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD2	7	0.19
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD3	7	0.19
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	6	0.19
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	6	0.19
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:131:A:PRO:HD3	1:132:A:PHE:H	6	0.19
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	8	0.19
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	8	0.19
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	8	0.19
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD11	1	0.19
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD12	1	0.19
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD13	1	0.19
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD21	1	0.19
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD22	1	0.19
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD23	1	0.19
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD11	1	0.19
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD12	1	0.19
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD13	1	0.19
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD21	1	0.19
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD22	1	0.19
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD23	1	0.19
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	7	0.19
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	7	0.19
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	7	0.19
(1,1216)	1:142:A:THR:HG21	1:234:A:HIS:HA	10	0.19
(1,1216)	1:142:A:THR:HG22	1:234:A:HIS:HA	10	0.19
(1,1216)	1:142:A:THR:HG23	1:234:A:HIS:HA	10	0.19
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG21	7	0.19
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG22	7	0.19
(1,1166)	1:104:A:LEU:H	1:105:A:THR:HG23	7	0.19
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	1	0.19
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	1	0.19
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	1	0.19
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	4	0.19
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	4	0.19
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	4	0.19
(1,1035)	1:22:A:LEU:HD21	1:23:A:LEU:H	7	0.19
(1,1035)	1:22:A:LEU:HD22	1:23:A:LEU:H	7	0.19
(1,1035)	1:22:A:LEU:HD23	1:23:A:LEU:H	7	0.19
(1,1027)	1:135:A:TRP:HA	1:154:A:HIS:HD2	7	0.19
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	3	0.19
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	3	0.19
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	3	0.19
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	10	0.19
(1,866)	1:251:A:VAL:HG21	1:256:A:PHE:HA	2	0.19
(1,866)	1:251:A:VAL:HG22	1:256:A:PHE:HA	2	0.19
(1,866)	1:251:A:VAL:HG23	1:256:A:PHE:HA	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:171:A:ASP:HB3	1:173:A:LYS:HG3	5	0.19
(1,831)	1:127:A:ILE:HD11	1:140:A:PRO:HG2	9	0.19
(1,831)	1:127:A:ILE:HD11	1:140:A:PRO:HG3	9	0.19
(1,831)	1:127:A:ILE:HD12	1:140:A:PRO:HG2	9	0.19
(1,831)	1:127:A:ILE:HD12	1:140:A:PRO:HG3	9	0.19
(1,831)	1:127:A:ILE:HD13	1:140:A:PRO:HG2	9	0.19
(1,831)	1:127:A:ILE:HD13	1:140:A:PRO:HG3	9	0.19
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	6	0.19
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	6	0.19
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	6	0.19
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	7	0.19
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	7	0.19
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	7	0.19
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	5	0.19
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	5	0.19
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG2	4	0.19
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG3	4	0.19
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG2	5	0.19
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG3	5	0.19
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	1	0.19
(1,777)	1:42:A:TYR:HD1	1:66:A:VAL:HA	7	0.19
(1,777)	1:42:A:TYR:HD2	1:66:A:VAL:HA	7	0.19
(1,768)	1:248:A:ARG:HA	1:251:A:VAL:HB	2	0.19
(1,717)	1:187:A:LYS:HD3	1:188:A:GLN:H	3	0.19
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD21	9	0.19
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD22	9	0.19
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD23	9	0.19
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	2	0.19
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	8	0.19
(1,590)	1:8:A:LEU:HD21	1:31:A:SER:HB2	10	0.19
(1,590)	1:8:A:LEU:HD22	1:31:A:SER:HB2	10	0.19
(1,590)	1:8:A:LEU:HD23	1:31:A:SER:HB2	10	0.19
(1,572)	1:79:A:LYS:HB2	1:80:A:TYR:H	9	0.19
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	2	0.19
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	3	0.19
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	3	0.19
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	10	0.19
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	10	0.19
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	10	0.19
(1,401)	1:46:A:GLN:HG3	1:63:A:GLU:H	4	0.19
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	3	0.19
(1,338)	1:9:A:VAL:HG11	1:13:A:GLU:HG2	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:9:A:VAL:HG12	1:13:A:GLU:HG2	10	0.19
(1,338)	1:9:A:VAL:HG13	1:13:A:GLU:HG2	10	0.19
(1,338)	1:9:A:VAL:HG21	1:13:A:GLU:HG2	10	0.19
(1,338)	1:9:A:VAL:HG22	1:13:A:GLU:HG2	10	0.19
(1,338)	1:9:A:VAL:HG23	1:13:A:GLU:HG2	10	0.19
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	3	0.19
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	3	0.19
(1,289)	1:158:A:GLU:HG2	1:159:A:GLU:H	2	0.19
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	4	0.19
(1,193)	1:163:A:ALA:HA	1:166:A:ASP:HB3	7	0.19
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	8	0.19
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	8	0.19
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	8	0.19
(1,160)	1:100:A:LEU:HB3	1:103:A:PHE:HD1	8	0.19
(1,160)	1:100:A:LEU:HB3	1:103:A:PHE:HD2	8	0.19
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	7	0.19
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	7	0.19
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	7	0.19
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	7	0.19
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	7	0.19
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	7	0.19
(1,53)	1:32:A:ILE:HD11	1:48:A:SER:HB3	9	0.19
(1,53)	1:32:A:ILE:HD12	1:48:A:SER:HB3	9	0.19
(1,53)	1:32:A:ILE:HD13	1:48:A:SER:HB3	9	0.19
(1,45)	1:47:A:ILE:HD11	1:85:A:PHE:HD1	1	0.19
(1,45)	1:47:A:ILE:HD11	1:85:A:PHE:HD2	1	0.19
(1,45)	1:47:A:ILE:HD12	1:85:A:PHE:HD1	1	0.19
(1,45)	1:47:A:ILE:HD12	1:85:A:PHE:HD2	1	0.19
(1,45)	1:47:A:ILE:HD13	1:85:A:PHE:HD1	1	0.19
(1,45)	1:47:A:ILE:HD13	1:85:A:PHE:HD2	1	0.19
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD11	7	0.19
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD12	7	0.19
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD13	7	0.19
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE1	1	0.19
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE2	1	0.19
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE3	1	0.19
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG11	5	0.18
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG12	5	0.18
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG13	5	0.18
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG21	5	0.18
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG22	5	0.18
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG23	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	6	0.18
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	6	0.18
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	6	0.18
(1,2491)	1:168:A:LEU:HD21	1:174:A:MET:H	9	0.18
(1,2491)	1:168:A:LEU:HD22	1:174:A:MET:H	9	0.18
(1,2491)	1:168:A:LEU:HD23	1:174:A:MET:H	9	0.18
(1,2415)	1:141:A:ILE:HD11	1:240:A:PHE:HB3	3	0.18
(1,2415)	1:141:A:ILE:HD12	1:240:A:PHE:HB3	3	0.18
(1,2415)	1:141:A:ILE:HD13	1:240:A:PHE:HB3	3	0.18
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG11	4	0.18
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG12	4	0.18
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG13	4	0.18
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG11	4	0.18
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG12	4	0.18
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG13	4	0.18
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG11	4	0.18
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG12	4	0.18
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG13	4	0.18
(1,2385)	1:29:A:ASP:HA	1:31:A:SER:H	6	0.18
(1,2306)	1:176:A:LYS:H	1:229:A:TRP:HE1	7	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD21	6	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD22	6	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD23	6	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD21	8	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD22	8	0.18
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD23	8	0.18
(1,2207)	1:161:A:ALA:H	1:164:A:MET:H	4	0.18
(1,2205)	1:37:A:VAL:H	1:41:A:GLU:H	10	0.18
(1,2196)	1:88:A:VAL:HG21	1:90:A:ASP:H	1	0.18
(1,2196)	1:88:A:VAL:HG22	1:90:A:ASP:H	1	0.18
(1,2196)	1:88:A:VAL:HG23	1:90:A:ASP:H	1	0.18
(1,2183)	1:165:A:LEU:HD21	1:167:A:LEU:H	5	0.18
(1,2183)	1:165:A:LEU:HD22	1:167:A:LEU:H	5	0.18
(1,2183)	1:165:A:LEU:HD23	1:167:A:LEU:H	5	0.18
(1,2162)	1:135:A:TRP:H	1:136:A:THR:HA	5	0.18
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	6	0.18
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG21	7	0.18
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG22	7	0.18
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG23	7	0.18
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	9	0.18
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	9	0.18
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG21	5	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG22	5	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG23	5	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG21	6	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG22	6	0.18
(1,2037)	1:86:A:GLN:H	1:88:A:VAL:HG23	6	0.18
(1,1935)	1:141:A:ILE:HD11	1:148:A:PHE:H	8	0.18
(1,1935)	1:141:A:ILE:HD12	1:148:A:PHE:H	8	0.18
(1,1935)	1:141:A:ILE:HD13	1:148:A:PHE:H	8	0.18
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	1	0.18
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	1	0.18
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	1	0.18
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	7	0.18
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	7	0.18
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	7	0.18
(1,1900)	1:37:A:VAL:H	1:43:A:MET:H	10	0.18
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	5	0.18
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	1	0.18
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	1	0.18
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	5	0.18
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	5	0.18
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	5	0.18
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	5	0.18
(1,1615)	1:121:A:PRO:HG2	1:122:A:VAL:H	9	0.18
(1,1615)	1:121:A:PRO:HG3	1:122:A:VAL:H	9	0.18
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	2	0.18
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	6	0.18
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	1	0.18
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	1	0.18
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	1	0.18
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	1	0.18
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	1	0.18
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	1	0.18
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD2	2	0.18
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD3	2	0.18
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD2	2	0.18
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD3	2	0.18
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	3	0.18
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	4	0.18
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	8	0.18
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	8	0.18
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	8	0.18
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	10	0.18
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	10	0.18
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	10	0.18
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD11	3	0.18
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD12	3	0.18
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD13	3	0.18
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD11	3	0.18
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD12	3	0.18
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD13	3	0.18
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD11	3	0.18
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD12	3	0.18
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD13	3	0.18
(1,1353)	1:181:A:MET:HE1	1:228:A:ARG:H	6	0.18
(1,1353)	1:181:A:MET:HE2	1:228:A:ARG:H	6	0.18
(1,1353)	1:181:A:MET:HE3	1:228:A:ARG:H	6	0.18
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	7	0.18
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	7	0.18
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	7	0.18
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	4	0.18
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	4	0.18
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	4	0.18
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG11	3	0.18
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG12	3	0.18
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG13	3	0.18
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG11	3	0.18
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG12	3	0.18
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG13	3	0.18
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG11	3	0.18
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG12	3	0.18
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG13	3	0.18
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	3	0.18
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	3	0.18
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	3	0.18
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG11	8	0.18
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG12	8	0.18
(1,1206)	1:151:A:PHE:HD1	1:225:A:VAL:HG13	8	0.18
(1,1164)	1:126:A:ASP:HA	1:127:A:ILE:H	6	0.18
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	2	0.18
(1,1137)	1:93:A:PHE:HA	1:94:A:HIS:HD2	8	0.18
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	1	0.18
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	1	0.18
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	1	0.18
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	1	0.18
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	1	0.18
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	1	0.18
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	1	0.18
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	1	0.18
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	3	0.18
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	3	0.18
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	3	0.18
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	8	0.18
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	8	0.18
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	8	0.18
(1,1043)	1:42:A:TYR:HA	1:67:A:CYS:HB2	8	0.18
(1,1035)	1:22:A:LEU:HD21	1:23:A:LEU:H	6	0.18
(1,1035)	1:22:A:LEU:HD22	1:23:A:LEU:H	6	0.18
(1,1035)	1:22:A:LEU:HD23	1:23:A:LEU:H	6	0.18
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG21	4	0.18
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG22	4	0.18
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG23	4	0.18
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG21	6	0.18
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG22	6	0.18
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG23	6	0.18
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG11	4	0.18
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG12	4	0.18
(1,995)	1:154:A:HIS:HD2	1:155:A:VAL:HG13	4	0.18
(1,989)	1:200:A:ASP:HA	1:207:A:GLY:H	4	0.18
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD21	7	0.18
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD22	7	0.18
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD23	7	0.18
(1,922)	1:176:A:LYS:HG3	1:177:A:ALA:H	7	0.18
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG11	10	0.18
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG12	10	0.18
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG13	10	0.18
(1,808)	1:141:A:ILE:HA	1:142:A:THR:HB	9	0.18
(1,777)	1:42:A:TYR:HD1	1:66:A:VAL:HA	9	0.18
(1,777)	1:42:A:TYR:HD2	1:66:A:VAL:HA	9	0.18
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	1	0.18
(1,758)	1:128:A:PRO:HG3	1:151:A:PHE:HD1	4	0.18
(1,722)	1:43:A:MET:HG2	1:64:A:VAL:HA	1	0.18
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	1	0.18
(1,689)	1:187:A:LYS:HD3	1:220:A:TRP:HB3	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:244:A:ASN:HB2	1:245:A:SER:HA	9	0.18
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	6	0.18
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	9	0.18
(1,573)	1:20:A:PRO:HB2	1:21:A:ASP:H	9	0.18
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	1	0.18
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	9	0.18
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	9	0.18
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	9	0.18
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	9	0.18
(1,434)	1:188:A:GLN:HG2	1:189:A:ASP:H	9	0.18
(1,434)	1:188:A:GLN:HG3	1:189:A:ASP:H	9	0.18
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB1	1	0.18
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB2	1	0.18
(1,420)	1:188:A:GLN:HG2	1:192:A:ALA:HB3	1	0.18
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB1	1	0.18
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB2	1	0.18
(1,420)	1:188:A:GLN:HG3	1:192:A:ALA:HB3	1	0.18
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	1	0.18
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	5	0.18
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	6	0.18
(1,326)	1:51:A:THR:HB	1:52:A:HIS:H	9	0.18
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	7	0.18
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	7	0.18
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	7	0.18
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	7	0.18
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	8	0.18
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	8	0.18
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	3	0.18
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	3	0.18
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	3	0.18
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	6	0.18
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	7	0.18
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	2	0.18
(1,175)	1:3:A:ASP:HB2	1:7:A:GLN:HE21	4	0.18
(1,175)	1:3:A:ASP:HB3	1:7:A:GLN:HE21	4	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	2	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	2	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	2	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	3	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	3	0.18
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	3	0.18
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	2	0.18
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	2	0.18
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	2	0.18
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	2	0.18
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	2	0.18
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	6	0.18
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	6	0.18
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	6	0.18
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	6	0.18
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	6	0.18
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	6	0.18
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD11	7	0.18
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD12	7	0.18
(1,41)	1:146:A:SER:H	1:235:A:ILE:HD13	7	0.18
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD11	7	0.18
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD12	7	0.18
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD13	7	0.18
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	2	0.18
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	2	0.18
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	2	0.18
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE1	6	0.18
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE2	6	0.18
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE3	6	0.18
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	1	0.17
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	1	0.17
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	1	0.17
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	5	0.17
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	5	0.17
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	5	0.17
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	10	0.17
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	10	0.17
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	10	0.17
(1,2610)	1:98:A:VAL:HG21	1:99:A:CYS:HB2	5	0.17
(1,2610)	1:98:A:VAL:HG22	1:99:A:CYS:HB2	5	0.17
(1,2610)	1:98:A:VAL:HG23	1:99:A:CYS:HB2	5	0.17
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	2	0.17
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	2	0.17
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	2	0.17
(1,2518)	1:194:A:THR:HG21	1:196:A:GLN:HG2	3	0.17
(1,2518)	1:194:A:THR:HG21	1:196:A:GLN:HG3	3	0.17
(1,2518)	1:194:A:THR:HG22	1:196:A:GLN:HG2	3	0.17
(1,2518)	1:194:A:THR:HG22	1:196:A:GLN:HG3	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2518)	1:194:A:THR:HG23	1:196:A:GLN:HG2	3	0.17
(1,2518)	1:194:A:THR:HG23	1:196:A:GLN:HG3	3	0.17
(1,2513)	1:251:A:VAL:HB	1:252:A:VAL:HG21	8	0.17
(1,2513)	1:251:A:VAL:HB	1:252:A:VAL:HG22	8	0.17
(1,2513)	1:251:A:VAL:HB	1:252:A:VAL:HG23	8	0.17
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	1	0.17
(1,2443)	1:14:A:ALA:H	1:16:A:GLU:HB3	6	0.17
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	5	0.17
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	5	0.17
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	5	0.17
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	5	0.17
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	5	0.17
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	5	0.17
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	5	0.17
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	5	0.17
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	5	0.17
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG11	10	0.17
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG12	10	0.17
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG13	10	0.17
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG11	10	0.17
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG12	10	0.17
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG13	10	0.17
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG11	10	0.17
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG12	10	0.17
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG13	10	0.17
(1,2405)	1:26:A:LYS:H	1:33:A:ILE:HD11	9	0.17
(1,2405)	1:26:A:LYS:H	1:33:A:ILE:HD12	9	0.17
(1,2405)	1:26:A:LYS:H	1:33:A:ILE:HD13	9	0.17
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	6	0.17
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	9	0.17
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	9	0.17
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	9	0.17
(1,2357)	1:42:A:TYR:H	1:44:A:THR:H	9	0.17
(1,2318)	1:49:A:PHE:HD2	1:60:A:ASN:H	6	0.17
(1,2255)	1:155:A:VAL:H	1:161:A:ALA:HB1	5	0.17
(1,2255)	1:155:A:VAL:H	1:161:A:ALA:HB2	5	0.17
(1,2255)	1:155:A:VAL:H	1:161:A:ALA:HB3	5	0.17
(1,2248)	1:64:A:VAL:HG21	1:83:A:HIS:H	1	0.17
(1,2248)	1:64:A:VAL:HG22	1:83:A:HIS:H	1	0.17
(1,2248)	1:64:A:VAL:HG23	1:83:A:HIS:H	1	0.17
(1,2227)	1:17:A:ALA:H	1:19:A:TYR:H	1	0.17
(1,2227)	1:17:A:ALA:H	1:19:A:TYR:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2187)	1:107:A:LEU:HB2	1:111:A:LEU:H	2	0.17
(1,2176)	1:143:A:ASP:H	1:146:A:SER:H	9	0.17
(1,2157)	1:208:A:SER:H	1:211:A:LEU:H	2	0.17
(1,2157)	1:208:A:SER:H	1:211:A:LEU:H	10	0.17
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	2	0.17
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	5	0.17
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	7	0.17
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	9	0.17
(1,2105)	1:178:A:ASN:H	1:229:A:TRP:HE1	7	0.17
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	7	0.17
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	10	0.17
(1,2089)	1:257:A:ASP:H	1:258:A:SER:H	9	0.17
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	10	0.17
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	10	0.17
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	10	0.17
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	1	0.17
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	1	0.17
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	1	0.17
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	6	0.17
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	6	0.17
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	6	0.17
(1,1995)	1:51:A:THR:H	1:53:A:TYR:H	2	0.17
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	4	0.17
(1,1959)	1:187:A:LYS:H	1:189:A:ASP:H	1	0.17
(1,1817)	1:81:A:LEU:H	1:82:A:GLN:HB2	6	0.17
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	3	0.17
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	8	0.17
(1,1767)	1:160:A:GLN:HG2	1:164:A:MET:H	5	0.17
(1,1767)	1:160:A:GLN:HG3	1:164:A:MET:H	5	0.17
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	9	0.17
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	9	0.17
(1,1679)	1:155:A:VAL:HG21	1:160:A:GLN:H	7	0.17
(1,1679)	1:155:A:VAL:HG22	1:160:A:GLN:H	7	0.17
(1,1679)	1:155:A:VAL:HG23	1:160:A:GLN:H	7	0.17
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	4	0.17
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	6	0.17
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	6	0.17
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	6	0.17
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	10	0.17
(1,1554)	1:181:A:MET:HB3	1:226:A:VAL:H	10	0.17
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG11	2	0.17
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG12	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG13	2	0.17
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	8	0.17
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	8	0.17
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	8	0.17
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	3	0.17
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	3	0.17
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	3	0.17
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE1	7	0.17
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE2	7	0.17
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE1	7	0.17
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE2	7	0.17
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE1	7	0.17
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE2	7	0.17
(1,1353)	1:181:A:MET:HE1	1:228:A:ARG:H	8	0.17
(1,1353)	1:181:A:MET:HE2	1:228:A:ARG:H	8	0.17
(1,1353)	1:181:A:MET:HE3	1:228:A:ARG:H	8	0.17
(1,1353)	1:181:A:MET:HE1	1:228:A:ARG:H	9	0.17
(1,1353)	1:181:A:MET:HE2	1:228:A:ARG:H	9	0.17
(1,1353)	1:181:A:MET:HE3	1:228:A:ARG:H	9	0.17
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD1	2	0.17
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD2	2	0.17
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD1	2	0.17
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD2	2	0.17
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD1	2	0.17
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD2	2	0.17
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD11	7	0.17
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD12	7	0.17
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD13	7	0.17
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD21	7	0.17
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD22	7	0.17
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD23	7	0.17
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD11	7	0.17
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD12	7	0.17
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD13	7	0.17
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD21	7	0.17
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD22	7	0.17
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD23	7	0.17
(1,1265)	1:61:A:VAL:HG11	1:85:A:PHE:HB3	2	0.17
(1,1265)	1:61:A:VAL:HG12	1:85:A:PHE:HB3	2	0.17
(1,1265)	1:61:A:VAL:HG13	1:85:A:PHE:HB3	2	0.17
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD11	1	0.17
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD12	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	1:167:A:LEU:HD11	1:168:A:LEU:HD13	1	0.17
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD11	1	0.17
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD12	1	0.17
(1,1251)	1:167:A:LEU:HD12	1:168:A:LEU:HD13	1	0.17
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD11	1	0.17
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD12	1	0.17
(1,1251)	1:167:A:LEU:HD13	1:168:A:LEU:HD13	1	0.17
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD11	1	0.17
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD12	1	0.17
(1,1251)	1:167:A:LEU:HD21	1:168:A:LEU:HD13	1	0.17
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD11	1	0.17
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD12	1	0.17
(1,1251)	1:167:A:LEU:HD22	1:168:A:LEU:HD13	1	0.17
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD11	1	0.17
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD12	1	0.17
(1,1251)	1:167:A:LEU:HD23	1:168:A:LEU:HD13	1	0.17
(1,1203)	1:92:A:VAL:HG11	1:103:A:PHE:HD1	5	0.17
(1,1203)	1:92:A:VAL:HG11	1:103:A:PHE:HD2	5	0.17
(1,1203)	1:92:A:VAL:HG12	1:103:A:PHE:HD1	5	0.17
(1,1203)	1:92:A:VAL:HG12	1:103:A:PHE:HD2	5	0.17
(1,1203)	1:92:A:VAL:HG13	1:103:A:PHE:HD1	5	0.17
(1,1203)	1:92:A:VAL:HG13	1:103:A:PHE:HD2	5	0.17
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD21	6	0.17
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD22	6	0.17
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD23	6	0.17
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG21	6	0.17
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG22	6	0.17
(1,1174)	1:47:A:ILE:HG21	1:61:A:VAL:HG23	6	0.17
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG21	6	0.17
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG22	6	0.17
(1,1174)	1:47:A:ILE:HG22	1:61:A:VAL:HG23	6	0.17
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG21	6	0.17
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG22	6	0.17
(1,1174)	1:47:A:ILE:HG23	1:61:A:VAL:HG23	6	0.17
(1,1171)	1:51:A:THR:HG21	1:52:A:HIS:H	6	0.17
(1,1171)	1:51:A:THR:HG22	1:52:A:HIS:H	6	0.17
(1,1171)	1:51:A:THR:HG23	1:52:A:HIS:H	6	0.17
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG21	4	0.17
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG22	4	0.17
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG23	4	0.17
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG21	4	0.17
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG22	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG23	4	0.17
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG21	4	0.17
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG22	4	0.17
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG23	4	0.17
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	5	0.17
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	5	0.17
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	5	0.17
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	8	0.17
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	8	0.17
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	8	0.17
(1,921)	1:176:A:LYS:HG3	1:229:A:TRP:HE1	8	0.17
(1,866)	1:251:A:VAL:HG21	1:256:A:PHE:HA	1	0.17
(1,866)	1:251:A:VAL:HG22	1:256:A:PHE:HA	1	0.17
(1,866)	1:251:A:VAL:HG23	1:256:A:PHE:HA	1	0.17
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	3	0.17
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	2	0.17
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	7	0.17
(1,689)	1:187:A:LYS:HD3	1:220:A:TRP:HB3	3	0.17
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	5	0.17
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	7	0.17
(1,572)	1:79:A:LYS:HB2	1:80:A:TYR:H	8	0.17
(1,527)	1:61:A:VAL:HG21	1:82:A:GLN:HG2	4	0.17
(1,527)	1:61:A:VAL:HG22	1:82:A:GLN:HG2	4	0.17
(1,527)	1:61:A:VAL:HG23	1:82:A:GLN:HG2	4	0.17
(1,527)	1:61:A:VAL:HG21	1:82:A:GLN:HG2	9	0.17
(1,527)	1:61:A:VAL:HG22	1:82:A:GLN:HG2	9	0.17
(1,527)	1:61:A:VAL:HG23	1:82:A:GLN:HG2	9	0.17
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	7	0.17
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG2	4	0.17
(1,474)	1:158:A:GLU:HA	1:160:A:GLN:HG3	4	0.17
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	9	0.17
(1,401)	1:46:A:GLN:HG3	1:63:A:GLU:H	6	0.17
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	8	0.17
(1,362)	1:133:A:GLU:HG2	1:134:A:GLY:HA3	5	0.17
(1,362)	1:133:A:GLU:HG3	1:134:A:GLY:HA3	5	0.17
(1,345)	1:6:A:GLU:HA	1:6:A:GLU:HG2	6	0.17
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	6	0.17
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	6	0.17
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	2	0.17
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	2	0.17
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	9	0.17
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	10	0.17
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	10	0.17
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	9	0.17
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	9	0.17
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	9	0.17
(1,282)	1:158:A:GLU:HG3	1:159:A:GLU:H	3	0.17
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	3	0.17
(1,218)	1:74:A:ASP:HB2	1:75:A:LEU:H	8	0.17
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	10	0.17
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	10	0.17
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	10	0.17
(1,40)	1:255:A:GLY:HA3	1:257:A:ASP:H	7	0.17
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG21	3	0.17
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG22	3	0.17
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG23	3	0.17
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	2	0.17
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	2	0.17
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	2	0.17
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	9	0.16
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	9	0.16
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	9	0.16
(1,2552)	1:104:A:LEU:H	1:104:A:LEU:HD11	9	0.16
(1,2552)	1:104:A:LEU:H	1:104:A:LEU:HD12	9	0.16
(1,2552)	1:104:A:LEU:H	1:104:A:LEU:HD13	9	0.16
(1,2491)	1:168:A:LEU:HD21	1:174:A:MET:H	3	0.16
(1,2491)	1:168:A:LEU:HD22	1:174:A:MET:H	3	0.16
(1,2491)	1:168:A:LEU:HD23	1:174:A:MET:H	3	0.16
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	4	0.16
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	4	0.16
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	8	0.16
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	8	0.16
(1,2391)	1:30:A:GLY:H	1:31:A:SER:HB3	7	0.16
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	10	0.16
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	8	0.16
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	8	0.16
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	8	0.16
(1,2361)	1:42:A:TYR:H	1:43:A:MET:H	10	0.16
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE1	2	0.16
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE2	2	0.16
(1,2338)	1:134:A:GLY:H	1:135:A:TRP:HD1	5	0.16
(1,2318)	1:49:A:PHE:HD2	1:60:A:ASN:H	3	0.16
(1,2318)	1:49:A:PHE:HD2	1:60:A:ASN:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2245)	1:83:A:HIS:H	1:86:A:GLN:H	4	0.16
(1,2220)	1:101:A:PHE:H	1:103:A:PHE:H	4	0.16
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	8	0.16
(1,2207)	1:161:A:ALA:H	1:164:A:MET:H	3	0.16
(1,2204)	1:39:A:GLN:H	1:41:A:GLU:H	10	0.16
(1,2194)	1:75:A:LEU:H	1:76:A:TYR:HB3	9	0.16
(1,2187)	1:107:A:LEU:HB2	1:111:A:LEU:H	8	0.16
(1,2169)	1:13:A:GLU:H	1:16:A:GLU:HG3	7	0.16
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	3	0.16
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	5	0.16
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	1	0.16
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	8	0.16
(1,2093)	1:239:A:ARG:HB3	1:241:A:LYS:H	8	0.16
(1,2075)	1:173:A:LYS:H	1:176:A:LYS:HG2	9	0.16
(1,2064)	1:36:A:LYS:HG2	1:40:A:HIS:H	9	0.16
(1,2064)	1:36:A:LYS:HG3	1:40:A:HIS:H	9	0.16
(1,2050)	1:64:A:VAL:HG21	1:80:A:TYR:H	6	0.16
(1,2050)	1:64:A:VAL:HG22	1:80:A:TYR:H	6	0.16
(1,2050)	1:64:A:VAL:HG23	1:80:A:TYR:H	6	0.16
(1,2040)	1:210:A:MET:H	1:211:A:LEU:HB3	2	0.16
(1,2021)	1:8:A:LEU:H	1:10:A:GLU:H	4	0.16
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	3	0.16
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	3	0.16
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	3	0.16
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG2	10	0.16
(1,1966)	1:171:A:ASP:H	1:175:A:ARG:HG3	10	0.16
(1,1959)	1:187:A:LYS:H	1:189:A:ASP:H	2	0.16
(1,1935)	1:141:A:ILE:HD11	1:148:A:PHE:H	2	0.16
(1,1935)	1:141:A:ILE:HD12	1:148:A:PHE:H	2	0.16
(1,1935)	1:141:A:ILE:HD13	1:148:A:PHE:H	2	0.16
(1,1827)	1:152:A:ALA:HB1	1:251:A:VAL:H	5	0.16
(1,1827)	1:152:A:ALA:HB2	1:251:A:VAL:H	5	0.16
(1,1827)	1:152:A:ALA:HB3	1:251:A:VAL:H	5	0.16
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	4	0.16
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	7	0.16
(1,1714)	1:211:A:LEU:H	1:213:A:LEU:HB2	10	0.16
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	1	0.16
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	2	0.16
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	8	0.16
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	9	0.16
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	9	0.16
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD11	9	0.16
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD12	9	0.16
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD13	9	0.16
(1,1582)	1:152:A:ALA:H	1:251:A:VAL:HA	3	0.16
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	4	0.16
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	4	0.16
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	4	0.16
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	6	0.16
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	6	0.16
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	6	0.16
(1,1537)	1:138:A:SER:H	1:150:A:ALA:H	5	0.16
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG11	9	0.16
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG12	9	0.16
(1,1512)	1:54:A:PRO:HD3	1:98:A:VAL:HG13	9	0.16
(1,1511)	1:127:A:ILE:HG21	1:140:A:PRO:HA	2	0.16
(1,1511)	1:127:A:ILE:HG22	1:140:A:PRO:HA	2	0.16
(1,1511)	1:127:A:ILE:HG23	1:140:A:PRO:HA	2	0.16
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	5	0.16
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	5	0.16
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	5	0.16
(1,1493)	1:141:A:ILE:HG21	1:148:A:PHE:HB3	7	0.16
(1,1493)	1:141:A:ILE:HG22	1:148:A:PHE:HB3	7	0.16
(1,1493)	1:141:A:ILE:HG23	1:148:A:PHE:HB3	7	0.16
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	3	0.16
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	3	0.16
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	3	0.16
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	8	0.16
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	8	0.16
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	8	0.16
(1,1439)	1:58:A:ALA:HB1	1:94:A:HIS:H	5	0.16
(1,1439)	1:58:A:ALA:HB2	1:94:A:HIS:H	5	0.16
(1,1439)	1:58:A:ALA:HB3	1:94:A:HIS:H	5	0.16
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	4	0.16
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	4	0.16
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	4	0.16
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	6	0.16
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	6	0.16
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	6	0.16
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	7	0.16
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	7	0.16
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	7	0.16
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	1	0.16
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	1	0.16
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	1	0.16
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	1	0.16
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	1	0.16
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	1	0.16
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	1	0.16
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	1	0.16
(1,1372)	1:137:A:ALA:HA	1:151:A:PHE:HD1	5	0.16
(1,1349)	1:181:A:MET:HE1	1:203:A:GLU:H	9	0.16
(1,1349)	1:181:A:MET:HE2	1:203:A:GLU:H	9	0.16
(1,1349)	1:181:A:MET:HE3	1:203:A:GLU:H	9	0.16
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	1	0.16
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	1	0.16
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	1	0.16
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	1	0.16
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	1	0.16
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	1	0.16
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD1	4	0.16
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD2	4	0.16
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD1	4	0.16
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD2	4	0.16
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD1	4	0.16
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD2	4	0.16
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD1	9	0.16
(1,1319)	1:92:A:VAL:HG21	1:103:A:PHE:HD2	9	0.16
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD1	9	0.16
(1,1319)	1:92:A:VAL:HG22	1:103:A:PHE:HD2	9	0.16
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD1	9	0.16
(1,1319)	1:92:A:VAL:HG23	1:103:A:PHE:HD2	9	0.16
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	2	0.16
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	2	0.16
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	2	0.16
(1,1286)	1:35:A:VAL:HG11	1:36:A:LYS:H	9	0.16
(1,1286)	1:35:A:VAL:HG12	1:36:A:LYS:H	9	0.16
(1,1286)	1:35:A:VAL:HG13	1:36:A:LYS:H	9	0.16
(1,1222)	1:9:A:VAL:HG11	1:10:A:GLU:HG2	8	0.16
(1,1222)	1:9:A:VAL:HG11	1:10:A:GLU:HG3	8	0.16
(1,1222)	1:9:A:VAL:HG12	1:10:A:GLU:HG2	8	0.16
(1,1222)	1:9:A:VAL:HG12	1:10:A:GLU:HG3	8	0.16
(1,1222)	1:9:A:VAL:HG13	1:10:A:GLU:HG2	8	0.16
(1,1222)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:9:A:VAL:HG21	1:10:A:GLU:HG2	8	0.16
(1,1222)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	8	0.16
(1,1222)	1:9:A:VAL:HG22	1:10:A:GLU:HG2	8	0.16
(1,1222)	1:9:A:VAL:HG22	1:10:A:GLU:HG3	8	0.16
(1,1222)	1:9:A:VAL:HG23	1:10:A:GLU:HG2	8	0.16
(1,1222)	1:9:A:VAL:HG23	1:10:A:GLU:HG3	8	0.16
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	8	0.16
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	8	0.16
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	8	0.16
(1,1209)	1:84:A:LEU:HD21	1:85:A:PHE:H	2	0.16
(1,1209)	1:84:A:LEU:HD22	1:85:A:PHE:H	2	0.16
(1,1209)	1:84:A:LEU:HD23	1:85:A:PHE:H	2	0.16
(1,1190)	1:1:A:MET:HA	1:2:A:ASP:H	7	0.16
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	6	0.16
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	6	0.16
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	6	0.16
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	6	0.16
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	6	0.16
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	6	0.16
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	6	0.16
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	6	0.16
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	6	0.16
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB2	5	0.16
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB3	5	0.16
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB2	5	0.16
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB3	5	0.16
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB2	5	0.16
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB3	5	0.16
(1,1051)	1:137:A:ALA:HB1	1:151:A:PHE:HE1	2	0.16
(1,1051)	1:137:A:ALA:HB2	1:151:A:PHE:HE1	2	0.16
(1,1051)	1:137:A:ALA:HB3	1:151:A:PHE:HE1	2	0.16
(1,1035)	1:22:A:LEU:HD21	1:23:A:LEU:H	1	0.16
(1,1035)	1:22:A:LEU:HD22	1:23:A:LEU:H	1	0.16
(1,1035)	1:22:A:LEU:HD23	1:23:A:LEU:H	1	0.16
(1,1027)	1:135:A:TRP:HA	1:154:A:HIS:HD2	5	0.16
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG21	1	0.16
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG22	1	0.16
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG23	1	0.16
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	2	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	2	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	2	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	7	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	7	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	7	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	9	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	9	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	9	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	10	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	10	0.16
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	10	0.16
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG11	7	0.16
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG12	7	0.16
(1,902)	1:89:A:MET:HA	1:92:A:VAL:HG13	7	0.16
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	7	0.16
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	9	0.16
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG21	7	0.16
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG22	7	0.16
(1,830)	1:140:A:PRO:HG2	1:147:A:THR:HG23	7	0.16
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG21	7	0.16
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG22	7	0.16
(1,830)	1:140:A:PRO:HG3	1:147:A:THR:HG23	7	0.16
(1,781)	1:159:A:GLU:HA	1:162:A:PHE:HB3	7	0.16
(1,778)	1:80:A:TYR:HA	1:82:A:GLN:H	10	0.16
(1,768)	1:248:A:ARG:HA	1:251:A:VAL:HB	6	0.16
(1,768)	1:248:A:ARG:HA	1:251:A:VAL:HB	10	0.16
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG21	3	0.16
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG22	3	0.16
(1,766)	1:156:A:THR:HA	1:186:A:ILE:HG23	3	0.16
(1,717)	1:187:A:LYS:HD3	1:188:A:GLN:H	2	0.16
(1,709)	1:79:A:LYS:HD2	1:80:A:TYR:H	5	0.16
(1,709)	1:79:A:LYS:HD3	1:80:A:TYR:H	5	0.16
(1,641)	1:116:A:GLU:H	1:116:A:GLU:HB3	6	0.16
(1,631)	1:208:A:SER:HB3	1:209:A:ARG:H	10	0.16
(1,629)	1:170:A:THR:HA	1:175:A:ARG:HD2	2	0.16
(1,629)	1:170:A:THR:HA	1:175:A:ARG:HD3	2	0.16
(1,618)	1:172:A:SER:HB2	1:175:A:ARG:HB2	4	0.16
(1,618)	1:172:A:SER:HB2	1:175:A:ARG:HB3	4	0.16
(1,618)	1:172:A:SER:HB3	1:175:A:ARG:HB2	4	0.16
(1,618)	1:172:A:SER:HB3	1:175:A:ARG:HB3	4	0.16
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	3	0.16
(1,567)	1:252:A:VAL:H	1:252:A:VAL:HB	8	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG11	7	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG12	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG13	7	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG11	7	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG12	7	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG13	7	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG11	10	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG12	10	0.16
(1,539)	1:24:A:SER:HB2	1:34:A:VAL:HG13	10	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG11	10	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG12	10	0.16
(1,539)	1:24:A:SER:HB3	1:34:A:VAL:HG13	10	0.16
(1,536)	1:24:A:SER:HB2	1:25:A:LYS:H	2	0.16
(1,536)	1:24:A:SER:HB3	1:25:A:LYS:H	2	0.16
(1,536)	1:24:A:SER:HB2	1:25:A:LYS:H	6	0.16
(1,536)	1:24:A:SER:HB3	1:25:A:LYS:H	6	0.16
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB2	6	0.16
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB3	6	0.16
(1,532)	1:258:A:SER:H	1:258:A:SER:HB2	5	0.16
(1,471)	1:146:A:SER:HB2	1:148:A:PHE:H	4	0.16
(1,471)	1:146:A:SER:HB3	1:148:A:PHE:H	4	0.16
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	6	0.16
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	10	0.16
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD1	6	0.16
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD2	6	0.16
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD1	6	0.16
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD2	6	0.16
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD1	6	0.16
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD2	6	0.16
(1,423)	1:185:A:ARG:HB2	1:220:A:TRP:HD1	5	0.16
(1,341)	1:159:A:GLU:HG2	1:162:A:PHE:HD1	5	0.16
(1,341)	1:159:A:GLU:HG2	1:162:A:PHE:HD2	5	0.16
(1,341)	1:159:A:GLU:HG3	1:162:A:PHE:HD1	5	0.16
(1,341)	1:159:A:GLU:HG3	1:162:A:PHE:HD2	5	0.16
(1,316)	1:16:A:GLU:HG2	1:20:A:PRO:HA	4	0.16
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	3	0.16
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	3	0.16
(1,298)	1:41:A:GLU:HG2	1:42:A:TYR:H	4	0.16
(1,298)	1:41:A:GLU:HG3	1:42:A:TYR:H	4	0.16
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	10	0.16
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	10	0.16
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	10	0.16
(1,289)	1:158:A:GLU:HG2	1:159:A:GLU:H	9	0.16
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD11	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD12	1	0.16
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD13	1	0.16
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	10	0.16
(1,196)	1:126:A:ASP:HB2	1:127:A:ILE:HD11	7	0.16
(1,196)	1:126:A:ASP:HB2	1:127:A:ILE:HD12	7	0.16
(1,196)	1:126:A:ASP:HB2	1:127:A:ILE:HD13	7	0.16
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD11	7	0.16
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD12	7	0.16
(1,176)	1:126:A:ASP:HB3	1:127:A:ILE:HD13	7	0.16
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	6	0.16
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	6	0.16
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	6	0.16
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	3	0.16
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	3	0.16
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	1	0.16
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	1	0.16
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	1	0.16
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	1	0.16
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	1	0.16
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	1	0.16
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	10	0.16
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	10	0.16
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	10	0.16
(1,2650)	1:103:A:PHE:HE1	1:85:A:PHE:HB2	4	0.15
(1,2650)	1:103:A:PHE:HE2	1:85:A:PHE:HB2	4	0.15
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	6	0.15
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	6	0.15
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	6	0.15
(1,2587)	1:92:A:VAL:HG21	1:103:A:PHE:H	9	0.15
(1,2587)	1:92:A:VAL:HG22	1:103:A:PHE:H	9	0.15
(1,2587)	1:92:A:VAL:HG23	1:103:A:PHE:H	9	0.15
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG11	6	0.15
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG12	6	0.15
(1,2568)	1:89:A:MET:HG2	1:92:A:VAL:HG13	6	0.15
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG11	6	0.15
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG12	6	0.15
(1,2568)	1:89:A:MET:HG3	1:92:A:VAL:HG13	6	0.15
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG11	3	0.15
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG12	3	0.15
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG13	3	0.15
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG21	3	0.15
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG22	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG23	3	0.15
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	3	0.15
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	3	0.15
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	3	0.15
(1,2496)	1:251:A:VAL:HG11	1:253:A:ARG:H	6	0.15
(1,2496)	1:251:A:VAL:HG12	1:253:A:ARG:H	6	0.15
(1,2496)	1:251:A:VAL:HG13	1:253:A:ARG:H	6	0.15
(1,2491)	1:168:A:LEU:HD21	1:174:A:MET:H	1	0.15
(1,2491)	1:168:A:LEU:HD22	1:174:A:MET:H	1	0.15
(1,2491)	1:168:A:LEU:HD23	1:174:A:MET:H	1	0.15
(1,2481)	1:107:A:LEU:HD21	1:111:A:LEU:H	5	0.15
(1,2481)	1:107:A:LEU:HD22	1:111:A:LEU:H	5	0.15
(1,2481)	1:107:A:LEU:HD23	1:111:A:LEU:H	5	0.15
(1,2471)	1:25:A:LYS:HG2	1:33:A:ILE:HD11	2	0.15
(1,2471)	1:25:A:LYS:HG2	1:33:A:ILE:HD12	2	0.15
(1,2471)	1:25:A:LYS:HG2	1:33:A:ILE:HD13	2	0.15
(1,2460)	1:12:A:LEU:HD11	1:29:A:ASP:HB2	9	0.15
(1,2460)	1:12:A:LEU:HD12	1:29:A:ASP:HB2	9	0.15
(1,2460)	1:12:A:LEU:HD13	1:29:A:ASP:HB2	9	0.15
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	6	0.15
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	6	0.15
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	10	0.15
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	10	0.15
(1,2426)	1:125:A:SER:HA	1:126:A:ASP:HB3	6	0.15
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	9	0.15
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	9	0.15
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	9	0.15
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	9	0.15
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	9	0.15
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	9	0.15
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	9	0.15
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	9	0.15
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	9	0.15
(1,2419)	1:216:A:ILE:HD11	1:217:A:MET:H	4	0.15
(1,2419)	1:216:A:ILE:HD12	1:217:A:MET:H	4	0.15
(1,2419)	1:216:A:ILE:HD13	1:217:A:MET:H	4	0.15
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD11	10	0.15
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD12	10	0.15
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD13	10	0.15
(1,2379)	1:211:A:LEU:HB2	1:214:A:ILE:H	8	0.15
(1,2371)	1:129:A:THR:H	1:130:A:ASP:H	4	0.15
(1,2359)	1:40:A:HIS:HA	1:42:A:TYR:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2346)	1:52:A:HIS:H	1:57:A:GLU:HG3	9	0.15
(1,2312)	1:56:A:GLU:H	1:58:A:ALA:H	7	0.15
(1,2245)	1:83:A:HIS:H	1:86:A:GLN:H	2	0.15
(1,2240)	1:26:A:LYS:H	1:32:A:ILE:H	5	0.15
(1,2235)	1:82:A:GLN:H	1:84:A:LEU:H	8	0.15
(1,2227)	1:17:A:ALA:H	1:19:A:TYR:H	3	0.15
(1,2220)	1:101:A:PHE:H	1:103:A:PHE:H	5	0.15
(1,2209)	1:98:A:VAL:H	1:101:A:PHE:H	7	0.15
(1,2191)	1:5:A:HIS:HA	1:10:A:GLU:H	7	0.15
(1,2187)	1:107:A:LEU:HB2	1:111:A:LEU:H	3	0.15
(1,2187)	1:107:A:LEU:HB2	1:111:A:LEU:H	5	0.15
(1,2162)	1:135:A:TRP:H	1:136:A:THR:HA	1	0.15
(1,2052)	1:209:A:ARG:H	1:211:A:LEU:H	10	0.15
(1,2046)	1:61:A:VAL:HB	1:86:A:GLN:H	9	0.15
(1,2025)	1:186:A:ILE:H	1:196:A:GLN:H	2	0.15
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	2	0.15
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	2	0.15
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	2	0.15
(1,1995)	1:51:A:THR:H	1:53:A:TYR:H	3	0.15
(1,1919)	1:35:A:VAL:H	1:45:A:LEU:H	1	0.15
(1,1919)	1:35:A:VAL:H	1:45:A:LEU:H	2	0.15
(1,1915)	1:181:A:MET:H	1:228:A:ARG:H	9	0.15
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	1	0.15
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	8	0.15
(1,1865)	1:193:A:ALA:HB1	1:194:A:THR:H	9	0.15
(1,1865)	1:193:A:ALA:HB2	1:194:A:THR:H	9	0.15
(1,1865)	1:193:A:ALA:HB3	1:194:A:THR:H	9	0.15
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	1	0.15
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	9	0.15
(1,1727)	1:57:A:GLU:H	1:58:A:ALA:HB1	7	0.15
(1,1727)	1:57:A:GLU:H	1:58:A:ALA:HB2	7	0.15
(1,1727)	1:57:A:GLU:H	1:58:A:ALA:HB3	7	0.15
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	4	0.15
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	6	0.15
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	7	0.15
(1,1678)	1:159:A:GLU:HB3	1:160:A:GLN:H	3	0.15
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	1	0.15
(1,1666)	1:251:A:VAL:HG21	1:257:A:ASP:H	10	0.15
(1,1666)	1:251:A:VAL:HG22	1:257:A:ASP:H	10	0.15
(1,1666)	1:251:A:VAL:HG23	1:257:A:ASP:H	10	0.15
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	3	0.15
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	3	0.15
(1,1608)	1:132:A:PHE:H	1:135:A:TRP:HB3	1	0.15
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	7	0.15
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	8	0.15
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	6	0.15
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE21	5	0.15
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE22	5	0.15
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	8	0.15
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG2	10	0.15
(1,1564)	1:61:A:VAL:H	1:89:A:MET:HG3	10	0.15
(1,1543)	1:188:A:GLN:H	1:194:A:THR:H	5	0.15
(1,1543)	1:188:A:GLN:H	1:194:A:THR:H	10	0.15
(1,1472)	1:158:A:GLU:H	1:186:A:ILE:HG21	2	0.15
(1,1472)	1:158:A:GLU:H	1:186:A:ILE:HG22	2	0.15
(1,1472)	1:158:A:GLU:H	1:186:A:ILE:HG23	2	0.15
(1,1440)	1:58:A:ALA:HB1	1:99:A:CYS:HB2	6	0.15
(1,1440)	1:58:A:ALA:HB2	1:99:A:CYS:HB2	6	0.15
(1,1440)	1:58:A:ALA:HB3	1:99:A:CYS:HB2	6	0.15
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	1	0.15
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	1	0.15
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	1	0.15
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	2	0.15
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	2	0.15
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	2	0.15
(1,1433)	1:43:A:MET:HE1	1:44:A:THR:H	8	0.15
(1,1433)	1:43:A:MET:HE2	1:44:A:THR:H	8	0.15
(1,1433)	1:43:A:MET:HE3	1:44:A:THR:H	8	0.15
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE1	9	0.15
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE2	9	0.15
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE3	9	0.15
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD2	10	0.15
(1,1418)	1:19:A:TYR:HD1	1:20:A:PRO:HD3	10	0.15
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD2	10	0.15
(1,1418)	1:19:A:TYR:HD2	1:20:A:PRO:HD3	10	0.15
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	3	0.15
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	3	0.15
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	3	0.15
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE1	2	0.15
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE2	2	0.15
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE1	2	0.15
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE2	2	0.15
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE1	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE2	2	0.15
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD11	8	0.15
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD12	8	0.15
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD13	8	0.15
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD11	8	0.15
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD12	8	0.15
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD13	8	0.15
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD11	8	0.15
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD12	8	0.15
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD13	8	0.15
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	4	0.15
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	4	0.15
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	4	0.15
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	4	0.15
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	4	0.15
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	4	0.15
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	1	0.15
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	1	0.15
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	1	0.15
(1,1291)	1:177:A:ALA:HA	1:229:A:TRP:HH2	3	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD11	4	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD12	4	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD13	4	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD21	4	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD22	4	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD23	4	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD11	4	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD12	4	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD13	4	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD21	4	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD22	4	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD23	4	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD11	6	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD12	6	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD13	6	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD21	6	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD22	6	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD23	6	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD11	6	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD12	6	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD13	6	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD21	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD22	6	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD23	6	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD11	8	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD12	8	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD13	8	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD21	8	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD22	8	0.15
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD23	8	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD11	8	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD12	8	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD13	8	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD21	8	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD22	8	0.15
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD23	8	0.15
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG21	6	0.15
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG22	6	0.15
(1,1271)	1:45:A:LEU:HA	1:64:A:VAL:HG23	6	0.15
(1,1247)	1:132:A:PHE:HD1	1:168:A:LEU:HD11	3	0.15
(1,1247)	1:132:A:PHE:HD1	1:168:A:LEU:HD12	3	0.15
(1,1247)	1:132:A:PHE:HD1	1:168:A:LEU:HD13	3	0.15
(1,1247)	1:132:A:PHE:HD2	1:168:A:LEU:HD11	3	0.15
(1,1247)	1:132:A:PHE:HD2	1:168:A:LEU:HD12	3	0.15
(1,1247)	1:132:A:PHE:HD2	1:168:A:LEU:HD13	3	0.15
(1,1241)	1:8:A:LEU:HD11	1:53:A:TYR:HE1	6	0.15
(1,1241)	1:8:A:LEU:HD11	1:53:A:TYR:HE2	6	0.15
(1,1241)	1:8:A:LEU:HD12	1:53:A:TYR:HE1	6	0.15
(1,1241)	1:8:A:LEU:HD12	1:53:A:TYR:HE2	6	0.15
(1,1241)	1:8:A:LEU:HD13	1:53:A:TYR:HE1	6	0.15
(1,1241)	1:8:A:LEU:HD13	1:53:A:TYR:HE2	6	0.15
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG11	5	0.15
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG12	5	0.15
(1,1217)	1:249:A:GLU:HA	1:252:A:VAL:HG13	5	0.15
(1,1171)	1:51:A:THR:HG21	1:52:A:HIS:H	4	0.15
(1,1171)	1:51:A:THR:HG22	1:52:A:HIS:H	4	0.15
(1,1171)	1:51:A:THR:HG23	1:52:A:HIS:H	4	0.15
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	2	0.15
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	2	0.15
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	2	0.15
(1,1079)	1:152:A:ALA:HB1	1:224:A:VAL:HA	9	0.15
(1,1079)	1:152:A:ALA:HB2	1:224:A:VAL:HA	9	0.15
(1,1079)	1:152:A:ALA:HB3	1:224:A:VAL:HA	9	0.15
(1,1069)	1:242:A:HIS:HA	1:245:A:SER:H	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1035)	1:22:A:LEU:HD21	1:23:A:LEU:H	5	0.15
(1,1035)	1:22:A:LEU:HD22	1:23:A:LEU:H	5	0.15
(1,1035)	1:22:A:LEU:HD23	1:23:A:LEU:H	5	0.15
(1,992)	1:100:A:LEU:H	1:100:A:LEU:HD21	10	0.15
(1,992)	1:100:A:LEU:H	1:100:A:LEU:HD22	10	0.15
(1,992)	1:100:A:LEU:H	1:100:A:LEU:HD23	10	0.15
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	7	0.15
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	1	0.15
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	1	0.15
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	1	0.15
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	5	0.15
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	3	0.15
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	3	0.15
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	3	0.15
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	7	0.15
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	9	0.15
(1,777)	1:42:A:TYR:HD1	1:66:A:VAL:HA	5	0.15
(1,777)	1:42:A:TYR:HD2	1:66:A:VAL:HA	5	0.15
(1,768)	1:248:A:ARG:HA	1:251:A:VAL:HB	3	0.15
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	8	0.15
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	8	0.15
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	8	0.15
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	9	0.15
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	5	0.15
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	7	0.15
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG21	2	0.15
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG22	2	0.15
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG23	2	0.15
(1,563)	1:257:A:ASP:HB2	1:258:A:SER:HB2	6	0.15
(1,563)	1:257:A:ASP:HB3	1:258:A:SER:HB2	6	0.15
(1,563)	1:257:A:ASP:HB2	1:258:A:SER:HB2	10	0.15
(1,563)	1:257:A:ASP:HB3	1:258:A:SER:HB2	10	0.15
(1,560)	1:240:A:PHE:H	1:241:A:LYS:HB2	8	0.15
(1,490)	1:48:A:SER:HB2	1:60:A:ASN:HB2	3	0.15
(1,490)	1:48:A:SER:HB2	1:60:A:ASN:HB2	5	0.15
(1,489)	1:97:A:SER:HB3	1:98:A:VAL:H	1	0.15
(1,479)	1:128:A:PRO:HB2	1:151:A:PHE:HE1	5	0.15
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	2	0.15
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	9	0.15
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	5	0.15
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD1	10	0.15
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD1	10	0.15
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD2	10	0.15
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD1	10	0.15
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD2	10	0.15
(1,416)	1:9:A:VAL:HA	1:13:A:GLU:H	3	0.15
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	4	0.15
(1,324)	1:105:A:THR:HB	1:106:A:GLU:H	2	0.15
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	2	0.15
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	2	0.15
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	2	0.15
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	1	0.15
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	5	0.15
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	8	0.15
(1,233)	1:19:A:TYR:HB3	1:22:A:LEU:HG	2	0.15
(1,230)	1:194:A:THR:H	1:194:A:THR:HB	7	0.15
(1,228)	1:186:A:ILE:H	1:194:A:THR:HB	2	0.15
(1,218)	1:74:A:ASP:HB2	1:75:A:LEU:H	6	0.15
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	1	0.15
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	1	0.15
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	1	0.15
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	4	0.15
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	4	0.15
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	4	0.15
(1,129)	1:79:A:LYS:HE2	1:80:A:TYR:H	3	0.15
(1,129)	1:79:A:LYS:HE3	1:80:A:TYR:H	3	0.15
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	2	0.15
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	2	0.15
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD2	8	0.15
(1,110)	1:95:A:ARG:H	1:95:A:ARG:HD3	8	0.15
(1,40)	1:255:A:GLY:HA3	1:257:A:ASP:H	4	0.15
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD11	9	0.15
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD12	9	0.15
(1,33)	1:142:A:THR:HB	1:235:A:ILE:HD13	9	0.15
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	9	0.15
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	9	0.15
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	9	0.15
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE1	7	0.15
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE2	7	0.15
(1,16)	1:61:A:VAL:HA	1:89:A:MET:HE3	7	0.15
(1,2654)	1:103:A:PHE:HE1	1:85:A:PHE:HB3	10	0.14
(1,2654)	1:103:A:PHE:HE2	1:85:A:PHE:HB3	10	0.14
(1,2610)	1:98:A:VAL:HG21	1:99:A:CYS:HB2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2610)	1:98:A:VAL:HG22	1:99:A:CYS:HB2	8	0.14
(1,2610)	1:98:A:VAL:HG23	1:99:A:CYS:HB2	8	0.14
(1,2491)	1:168:A:LEU:HD21	1:174:A:MET:H	4	0.14
(1,2491)	1:168:A:LEU:HD22	1:174:A:MET:H	4	0.14
(1,2491)	1:168:A:LEU:HD23	1:174:A:MET:H	4	0.14
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG21	5	0.14
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG22	5	0.14
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG23	5	0.14
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG21	5	0.14
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG22	5	0.14
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG23	5	0.14
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG21	5	0.14
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG22	5	0.14
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG23	5	0.14
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG21	6	0.14
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG22	6	0.14
(1,2444)	1:185:A:ARG:HG3	1:186:A:ILE:HG23	6	0.14
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	7	0.14
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	7	0.14
(1,2372)	1:128:A:PRO:HG2	1:129:A:THR:H	4	0.14
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	6	0.14
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	6	0.14
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	6	0.14
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	7	0.14
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	7	0.14
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	7	0.14
(1,2338)	1:134:A:GLY:H	1:135:A:TRP:HD1	1	0.14
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG21	4	0.14
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG22	4	0.14
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG23	4	0.14
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	2	0.14
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	2	0.14
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	2	0.14
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	4	0.14
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	4	0.14
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	4	0.14
(1,2306)	1:176:A:LYS:H	1:229:A:TRP:HE1	2	0.14
(1,2281)	1:62:A:ILE:HD11	1:63:A:GLU:H	2	0.14
(1,2281)	1:62:A:ILE:HD12	1:63:A:GLU:H	2	0.14
(1,2281)	1:62:A:ILE:HD13	1:63:A:GLU:H	2	0.14
(1,2252)	1:159:A:GLU:H	1:160:A:GLN:HB2	9	0.14
(1,2235)	1:82:A:GLN:H	1:84:A:LEU:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2227)	1:17:A:ALA:H	1:19:A:TYR:H	6	0.14
(1,2227)	1:17:A:ALA:H	1:19:A:TYR:H	7	0.14
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD21	9	0.14
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD22	9	0.14
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD23	9	0.14
(1,2183)	1:165:A:LEU:HD21	1:167:A:LEU:H	2	0.14
(1,2183)	1:165:A:LEU:HD22	1:167:A:LEU:H	2	0.14
(1,2183)	1:165:A:LEU:HD23	1:167:A:LEU:H	2	0.14
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	10	0.14
(1,2103)	1:251:A:VAL:H	1:253:A:ARG:H	8	0.14
(1,2096)	1:251:A:VAL:HG21	1:253:A:ARG:H	2	0.14
(1,2096)	1:251:A:VAL:HG22	1:253:A:ARG:H	2	0.14
(1,2096)	1:251:A:VAL:HG23	1:253:A:ARG:H	2	0.14
(1,2089)	1:257:A:ASP:H	1:258:A:SER:H	1	0.14
(1,2045)	1:209:A:ARG:H	1:212:A:HIS:H	5	0.14
(1,2029)	1:1:A:MET:HG2	1:3:A:ASP:H	6	0.14
(1,2029)	1:1:A:MET:HG3	1:3:A:ASP:H	6	0.14
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	4	0.14
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	4	0.14
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	4	0.14
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	10	0.14
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	10	0.14
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	10	0.14
(1,1995)	1:51:A:THR:H	1:53:A:TYR:H	8	0.14
(1,1994)	1:53:A:TYR:H	1:56:A:GLU:H	4	0.14
(1,1963)	1:77:A:ASP:H	1:79:A:LYS:H	8	0.14
(1,1919)	1:35:A:VAL:H	1:45:A:LEU:H	6	0.14
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	2	0.14
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	5	0.14
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	9	0.14
(1,1793)	1:200:A:ASP:HA	1:201:A:ASP:H	9	0.14
(1,1790)	1:4:A:ASP:HB2	1:5:A:HIS:H	10	0.14
(1,1747)	1:11:A:GLU:HA	1:13:A:GLU:H	7	0.14
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	6	0.14
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	6	0.14
(1,1731)	1:54:A:PRO:HA	1:57:A:GLU:H	3	0.14
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	10	0.14
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	2	0.14
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	7	0.14
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	7	0.14
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	7	0.14
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1589)	1:70:A:LEU:H	1:70:A:LEU:HG	3	0.14
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD11	4	0.14
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD12	4	0.14
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD13	4	0.14
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE21	6	0.14
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE22	6	0.14
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	10	0.14
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	10	0.14
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	10	0.14
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB2	5	0.14
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB3	5	0.14
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB2	5	0.14
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB3	5	0.14
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB2	5	0.14
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB3	5	0.14
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE1	9	0.14
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE2	9	0.14
(1,1456)	1:217:A:MET:HA	1:217:A:MET:HE3	9	0.14
(1,1420)	1:58:A:ALA:HB1	1:93:A:PHE:HB2	10	0.14
(1,1420)	1:58:A:ALA:HB2	1:93:A:PHE:HB2	10	0.14
(1,1420)	1:58:A:ALA:HB3	1:93:A:PHE:HB2	10	0.14
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD11	2	0.14
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD12	2	0.14
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD13	2	0.14
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD11	2	0.14
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD12	2	0.14
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD13	2	0.14
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD11	2	0.14
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD12	2	0.14
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD13	2	0.14
(1,1389)	1:33:A:ILE:HG21	1:34:A:VAL:H	7	0.14
(1,1389)	1:33:A:ILE:HG22	1:34:A:VAL:H	7	0.14
(1,1389)	1:33:A:ILE:HG23	1:34:A:VAL:H	7	0.14
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	4	0.14
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	4	0.14
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	4	0.14
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	4	0.14
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	4	0.14
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	4	0.14
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	4	0.14
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	4	0.14
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD11	5	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD12	5	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD13	5	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD11	5	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD12	5	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD13	5	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD11	5	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD12	5	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD13	5	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD11	9	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD12	9	0.14
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD13	9	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD11	9	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD12	9	0.14
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD13	9	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD11	9	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD12	9	0.14
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD13	9	0.14
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	9	0.14
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	9	0.14
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	9	0.14
(1,1291)	1:177:A:ALA:HA	1:229:A:TRP:HH2	6	0.14
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD21	8	0.14
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD22	8	0.14
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD23	8	0.14
(1,1190)	1:1:A:MET:HA	1:2:A:ASP:H	6	0.14
(1,1164)	1:126:A:ASP:HA	1:127:A:ILE:H	2	0.14
(1,1164)	1:126:A:ASP:HA	1:127:A:ILE:H	9	0.14
(1,1158)	1:53:A:TYR:HA	1:57:A:GLU:H	9	0.14
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG21	2	0.14
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG22	2	0.14
(1,1098)	1:168:A:LEU:HD21	1:180:A:VAL:HG23	2	0.14
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG21	2	0.14
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG22	2	0.14
(1,1098)	1:168:A:LEU:HD22	1:180:A:VAL:HG23	2	0.14
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG21	2	0.14
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG22	2	0.14
(1,1098)	1:168:A:LEU:HD23	1:180:A:VAL:HG23	2	0.14
(1,1091)	1:252:A:VAL:HA	1:252:A:VAL:HG21	8	0.14
(1,1091)	1:252:A:VAL:HA	1:252:A:VAL:HG22	8	0.14
(1,1091)	1:252:A:VAL:HA	1:252:A:VAL:HG23	8	0.14
(1,1079)	1:152:A:ALA:HB1	1:224:A:VAL:HA	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:152:A:ALA:HB2	1:224:A:VAL:HA	2	0.14
(1,1079)	1:152:A:ALA:HB3	1:224:A:VAL:HA	2	0.14
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	6	0.14
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	6	0.14
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	6	0.14
(1,1069)	1:242:A:HIS:HA	1:245:A:SER:H	5	0.14
(1,1051)	1:137:A:ALA:HB1	1:151:A:PHE:HE1	4	0.14
(1,1051)	1:137:A:ALA:HB2	1:151:A:PHE:HE1	4	0.14
(1,1051)	1:137:A:ALA:HB3	1:151:A:PHE:HE1	4	0.14
(1,1051)	1:137:A:ALA:HB1	1:151:A:PHE:HE1	9	0.14
(1,1051)	1:137:A:ALA:HB2	1:151:A:PHE:HE1	9	0.14
(1,1051)	1:137:A:ALA:HB3	1:151:A:PHE:HE1	9	0.14
(1,1021)	1:213:A:LEU:HD21	1:214:A:ILE:HA	10	0.14
(1,1021)	1:213:A:LEU:HD22	1:214:A:ILE:HA	10	0.14
(1,1021)	1:213:A:LEU:HD23	1:214:A:ILE:HA	10	0.14
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG21	9	0.14
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG22	9	0.14
(1,1020)	1:182:A:SER:HB2	1:225:A:VAL:HG23	9	0.14
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE21	8	0.14
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE22	8	0.14
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	8	0.14
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	10	0.14
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG21	2	0.14
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG22	2	0.14
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG23	2	0.14
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	4	0.14
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	4	0.14
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	4	0.14
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	6	0.14
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	6	0.14
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	6	0.14
(1,930)	1:36:A:LYS:HG2	1:41:A:GLU:HA	1	0.14
(1,930)	1:36:A:LYS:HG3	1:41:A:GLU:HA	1	0.14
(1,924)	1:176:A:LYS:H	1:176:A:LYS:HG2	4	0.14
(1,878)	1:45:A:LEU:HD21	1:107:A:LEU:HD21	5	0.14
(1,878)	1:45:A:LEU:HD21	1:107:A:LEU:HD22	5	0.14
(1,878)	1:45:A:LEU:HD21	1:107:A:LEU:HD23	5	0.14
(1,878)	1:45:A:LEU:HD22	1:107:A:LEU:HD21	5	0.14
(1,878)	1:45:A:LEU:HD22	1:107:A:LEU:HD22	5	0.14
(1,878)	1:45:A:LEU:HD22	1:107:A:LEU:HD23	5	0.14
(1,878)	1:45:A:LEU:HD23	1:107:A:LEU:HD21	5	0.14
(1,878)	1:45:A:LEU:HD23	1:107:A:LEU:HD22	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:45:A:LEU:HD23	1:107:A:LEU:HD23	5	0.14
(1,851)	1:171:A:ASP:HB3	1:173:A:LYS:HG3	3	0.14
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	9	0.14
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	9	0.14
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	4	0.14
(1,768)	1:248:A:ARG:HA	1:251:A:VAL:HB	1	0.14
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	1	0.14
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	1	0.14
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	1	0.14
(1,725)	1:117:A:GLU:H	1:117:A:GLU:HB2	8	0.14
(1,695)	1:8:A:LEU:HD21	1:31:A:SER:HA	1	0.14
(1,695)	1:8:A:LEU:HD22	1:31:A:SER:HA	1	0.14
(1,695)	1:8:A:LEU:HD23	1:31:A:SER:HA	1	0.14
(1,683)	1:6:A:GLU:HB2	1:7:A:GLN:HE21	3	0.14
(1,683)	1:6:A:GLU:HB3	1:7:A:GLN:HE21	3	0.14
(1,649)	1:50:A:PRO:HA	1:53:A:TYR:H	6	0.14
(1,640)	1:9:A:VAL:HG11	1:10:A:GLU:HB2	9	0.14
(1,640)	1:9:A:VAL:HG12	1:10:A:GLU:HB2	9	0.14
(1,640)	1:9:A:VAL:HG13	1:10:A:GLU:HB2	9	0.14
(1,640)	1:9:A:VAL:HG21	1:10:A:GLU:HB2	9	0.14
(1,640)	1:9:A:VAL:HG22	1:10:A:GLU:HB2	9	0.14
(1,640)	1:9:A:VAL:HG23	1:10:A:GLU:HB2	9	0.14
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	1	0.14
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	4	0.14
(1,573)	1:20:A:PRO:HB2	1:21:A:ASP:H	7	0.14
(1,572)	1:79:A:LYS:HB2	1:80:A:TYR:H	6	0.14
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB2	1	0.14
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB3	1	0.14
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	4	0.14
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	6	0.14
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD1	8	0.14
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD2	8	0.14
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD1	8	0.14
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD2	8	0.14
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD1	8	0.14
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD2	8	0.14
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	10	0.14
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	10	0.14
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	10	0.14
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	10	0.14
(1,451)	1:146:A:SER:HB2	1:148:A:PHE:HA	4	0.14
(1,451)	1:146:A:SER:HB3	1:148:A:PHE:HA	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD11	10	0.14
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD12	10	0.14
(1,441)	1:27:A:GLN:HG3	1:32:A:ILE:HD13	10	0.14
(1,416)	1:9:A:VAL:HA	1:13:A:GLU:H	4	0.14
(1,411)	1:187:A:LYS:HB2	1:188:A:GLN:H	10	0.14
(1,407)	1:187:A:LYS:HB3	1:188:A:GLN:H	8	0.14
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	5	0.14
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	3	0.14
(1,385)	1:88:A:VAL:HG21	1:106:A:GLU:HG2	4	0.14
(1,385)	1:88:A:VAL:HG21	1:106:A:GLU:HG3	4	0.14
(1,385)	1:88:A:VAL:HG22	1:106:A:GLU:HG2	4	0.14
(1,385)	1:88:A:VAL:HG22	1:106:A:GLU:HG3	4	0.14
(1,385)	1:88:A:VAL:HG23	1:106:A:GLU:HG2	4	0.14
(1,385)	1:88:A:VAL:HG23	1:106:A:GLU:HG3	4	0.14
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	2	0.14
(1,362)	1:133:A:GLU:HG2	1:134:A:GLY:HA3	4	0.14
(1,362)	1:133:A:GLU:HG3	1:134:A:GLY:HA3	4	0.14
(1,345)	1:6:A:GLU:HA	1:6:A:GLU:HG2	7	0.14
(1,341)	1:159:A:GLU:HG2	1:162:A:PHE:HD1	8	0.14
(1,341)	1:159:A:GLU:HG2	1:162:A:PHE:HD2	8	0.14
(1,341)	1:159:A:GLU:HG3	1:162:A:PHE:HD1	8	0.14
(1,341)	1:159:A:GLU:HG3	1:162:A:PHE:HD2	8	0.14
(1,332)	1:9:A:VAL:HA	1:13:A:GLU:HG3	4	0.14
(1,330)	1:83:A:HIS:H	1:85:A:PHE:HB3	4	0.14
(1,299)	1:40:A:HIS:H	1:41:A:GLU:HG2	7	0.14
(1,299)	1:40:A:HIS:H	1:41:A:GLU:HG3	7	0.14
(1,284)	1:158:A:GLU:HG3	1:195:A:TYR:HB3	6	0.14
(1,268)	1:101:A:PHE:HB3	1:102:A:ASP:H	5	0.14
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	2	0.14
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	4	0.14
(1,265)	1:100:A:LEU:HD21	1:101:A:PHE:HB2	2	0.14
(1,265)	1:100:A:LEU:HD22	1:101:A:PHE:HB2	2	0.14
(1,265)	1:100:A:LEU:HD23	1:101:A:PHE:HB2	2	0.14
(1,232)	1:186:A:ILE:HB	1:194:A:THR:HB	10	0.14
(1,227)	1:188:A:GLN:H	1:194:A:THR:HB	7	0.14
(1,211)	1:81:A:LEU:HB3	1:84:A:LEU:HG	3	0.14
(1,111)	1:175:A:ARG:HD2	1:176:A:LYS:H	7	0.14
(1,111)	1:175:A:ARG:HD3	1:176:A:LYS:H	7	0.14
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	10	0.14
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	10	0.14
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	10	0.14
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	10	0.14
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	10	0.14
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD11	5	0.14
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD12	5	0.14
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD13	5	0.14
(1,52)	1:32:A:ILE:HD11	1:48:A:SER:HB2	7	0.14
(1,52)	1:32:A:ILE:HD12	1:48:A:SER:HB2	7	0.14
(1,52)	1:32:A:ILE:HD13	1:48:A:SER:HB2	7	0.14
(1,25)	1:214:A:ILE:HD11	1:215:A:THR:HA	5	0.14
(1,25)	1:214:A:ILE:HD12	1:215:A:THR:HA	5	0.14
(1,25)	1:214:A:ILE:HD13	1:215:A:THR:HA	5	0.14
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	8	0.14
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	8	0.14
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	8	0.14
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	7	0.13
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	7	0.13
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	7	0.13
(1,2631)	1:235:A:ILE:HD11	1:127:A:ILE:H	5	0.13
(1,2631)	1:235:A:ILE:HD12	1:127:A:ILE:H	5	0.13
(1,2631)	1:235:A:ILE:HD13	1:127:A:ILE:H	5	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG11	4	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG12	4	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG13	4	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG21	4	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG22	4	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG23	4	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG11	10	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG12	10	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG13	10	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG21	10	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG22	10	0.13
(1,2565)	1:121:A:PRO:HB2	1:122:A:VAL:HG23	10	0.13
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG21	6	0.13
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG22	6	0.13
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG23	6	0.13
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG21	6	0.13
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG22	6	0.13
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG23	6	0.13
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG21	6	0.13
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG22	6	0.13
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG23	6	0.13
(1,2447)	1:140:A:PRO:HG2	1:141:A:ILE:HD11	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2447)	1:140:A:PRO:HG2	1:141:A:ILE:HD12	2	0.13
(1,2447)	1:140:A:PRO:HG2	1:141:A:ILE:HD13	2	0.13
(1,2447)	1:140:A:PRO:HG3	1:141:A:ILE:HD11	2	0.13
(1,2447)	1:140:A:PRO:HG3	1:141:A:ILE:HD12	2	0.13
(1,2447)	1:140:A:PRO:HG3	1:141:A:ILE:HD13	2	0.13
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	2	0.13
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	2	0.13
(1,2426)	1:125:A:SER:HA	1:126:A:ASP:HB3	9	0.13
(1,2422)	1:79:A:LYS:HE2	1:82:A:GLN:HB2	7	0.13
(1,2422)	1:79:A:LYS:HE3	1:82:A:GLN:HB2	7	0.13
(1,2418)	1:145:A:GLY:HA3	1:234:A:HIS:HA	3	0.13
(1,2418)	1:145:A:GLY:HA3	1:234:A:HIS:HA	4	0.13
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD11	6	0.13
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD12	6	0.13
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD13	6	0.13
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG11	9	0.13
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG12	9	0.13
(1,2411)	1:214:A:ILE:HD11	1:224:A:VAL:HG13	9	0.13
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG11	9	0.13
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG12	9	0.13
(1,2411)	1:214:A:ILE:HD12	1:224:A:VAL:HG13	9	0.13
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG11	9	0.13
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG12	9	0.13
(1,2411)	1:214:A:ILE:HD13	1:224:A:VAL:HG13	9	0.13
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD11	3	0.13
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD12	3	0.13
(1,2399)	1:151:A:PHE:HB3	1:223:A:ILE:HD13	3	0.13
(1,2376)	1:156:A:THR:HB	1:157:A:SER:H	3	0.13
(1,2356)	1:217:A:MET:H	1:219:A:VAL:H	7	0.13
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE1	5	0.13
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE2	5	0.13
(1,2318)	1:49:A:PHE:HD2	1:60:A:ASN:H	1	0.13
(1,2306)	1:176:A:LYS:H	1:229:A:TRP:HE1	10	0.13
(1,2271)	1:29:A:ASP:H	1:30:A:GLY:H	10	0.13
(1,2252)	1:159:A:GLU:H	1:160:A:GLN:HB2	2	0.13
(1,2248)	1:64:A:VAL:HG21	1:83:A:HIS:H	5	0.13
(1,2248)	1:64:A:VAL:HG22	1:83:A:HIS:H	5	0.13
(1,2248)	1:64:A:VAL:HG23	1:83:A:HIS:H	5	0.13
(1,2248)	1:64:A:VAL:HG21	1:83:A:HIS:H	6	0.13
(1,2248)	1:64:A:VAL:HG22	1:83:A:HIS:H	6	0.13
(1,2248)	1:64:A:VAL:HG23	1:83:A:HIS:H	6	0.13
(1,2248)	1:64:A:VAL:HG21	1:83:A:HIS:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2248)	1:64:A:VAL:HG22	1:83:A:HIS:H	7	0.13
(1,2248)	1:64:A:VAL:HG23	1:83:A:HIS:H	7	0.13
(1,2241)	1:31:A:SER:H	1:32:A:ILE:H	7	0.13
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	1	0.13
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	7	0.13
(1,2207)	1:161:A:ALA:H	1:164:A:MET:H	2	0.13
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	9	0.13
(1,2129)	1:222:A:VAL:HG11	1:256:A:PHE:H	2	0.13
(1,2129)	1:222:A:VAL:HG12	1:256:A:PHE:H	2	0.13
(1,2129)	1:222:A:VAL:HG13	1:256:A:PHE:H	2	0.13
(1,2126)	1:252:A:VAL:H	1:254:A:ALA:H	5	0.13
(1,2118)	1:174:A:MET:H	1:180:A:VAL:HG11	9	0.13
(1,2118)	1:174:A:MET:H	1:180:A:VAL:HG12	9	0.13
(1,2118)	1:174:A:MET:H	1:180:A:VAL:HG13	9	0.13
(1,2111)	1:157:A:SER:H	1:160:A:GLN:H	2	0.13
(1,2096)	1:251:A:VAL:HG21	1:253:A:ARG:H	1	0.13
(1,2096)	1:251:A:VAL:HG22	1:253:A:ARG:H	1	0.13
(1,2096)	1:251:A:VAL:HG23	1:253:A:ARG:H	1	0.13
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG21	3	0.13
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG22	3	0.13
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG23	3	0.13
(1,2093)	1:239:A:ARG:HB3	1:241:A:LYS:H	10	0.13
(1,2089)	1:257:A:ASP:H	1:258:A:SER:H	10	0.13
(1,2075)	1:173:A:LYS:H	1:176:A:LYS:HG2	4	0.13
(1,2073)	1:103:A:PHE:H	1:106:A:GLU:H	3	0.13
(1,2040)	1:210:A:MET:H	1:211:A:LEU:HB3	4	0.13
(1,2038)	1:155:A:VAL:HA	1:161:A:ALA:H	7	0.13
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	8	0.13
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	8	0.13
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	8	0.13
(1,1959)	1:187:A:LYS:H	1:189:A:ASP:H	6	0.13
(1,1935)	1:141:A:ILE:HD11	1:148:A:PHE:H	1	0.13
(1,1935)	1:141:A:ILE:HD12	1:148:A:PHE:H	1	0.13
(1,1935)	1:141:A:ILE:HD13	1:148:A:PHE:H	1	0.13
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	6	0.13
(1,1860)	1:42:A:TYR:H	1:42:A:TYR:HB3	7	0.13
(1,1817)	1:81:A:LEU:H	1:82:A:GLN:HB2	1	0.13
(1,1785)	1:82:A:GLN:H	1:84:A:LEU:HG	10	0.13
(1,1730)	1:146:A:SER:H	1:234:A:HIS:HA	1	0.13
(1,1730)	1:146:A:SER:H	1:234:A:HIS:HA	4	0.13
(1,1719)	1:127:A:ILE:H	1:127:A:ILE:HG12	2	0.13
(1,1719)	1:127:A:ILE:H	1:127:A:ILE:HG13	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:211:A:LEU:HD11	1:213:A:LEU:H	2	0.13
(1,1694)	1:211:A:LEU:HD12	1:213:A:LEU:H	2	0.13
(1,1694)	1:211:A:LEU:HD13	1:213:A:LEU:H	2	0.13
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	6	0.13
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	10	0.13
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	2	0.13
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	2	0.13
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	2	0.13
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	3	0.13
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE21	2	0.13
(1,1569)	1:26:A:LYS:H	1:27:A:GLN:HE22	2	0.13
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	10	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	2	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	2	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	2	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	7	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	7	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	7	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	9	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	9	0.13
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	9	0.13
(1,1486)	1:210:A:MET:HE1	1:225:A:VAL:HA	2	0.13
(1,1486)	1:210:A:MET:HE2	1:225:A:VAL:HA	2	0.13
(1,1486)	1:210:A:MET:HE3	1:225:A:VAL:HA	2	0.13
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD11	7	0.13
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD12	7	0.13
(1,1468)	1:152:A:ALA:HA	1:223:A:ILE:HD13	7	0.13
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE1	1	0.13
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE2	1	0.13
(1,1465)	1:43:A:MET:HB2	1:43:A:MET:HE3	1	0.13
(1,1461)	1:43:A:MET:HE1	1:66:A:VAL:H	1	0.13
(1,1461)	1:43:A:MET:HE2	1:66:A:VAL:H	1	0.13
(1,1461)	1:43:A:MET:HE3	1:66:A:VAL:H	1	0.13
(1,1461)	1:43:A:MET:HE1	1:66:A:VAL:H	7	0.13
(1,1461)	1:43:A:MET:HE2	1:66:A:VAL:H	7	0.13
(1,1461)	1:43:A:MET:HE3	1:66:A:VAL:H	7	0.13
(1,1440)	1:58:A:ALA:HB1	1:99:A:CYS:HB2	3	0.13
(1,1440)	1:58:A:ALA:HB2	1:99:A:CYS:HB2	3	0.13
(1,1440)	1:58:A:ALA:HB3	1:99:A:CYS:HB2	3	0.13
(1,1439)	1:58:A:ALA:HB1	1:94:A:HIS:H	9	0.13
(1,1439)	1:58:A:ALA:HB2	1:94:A:HIS:H	9	0.13
(1,1439)	1:58:A:ALA:HB3	1:94:A:HIS:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE1	7	0.13
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE2	7	0.13
(1,1419)	1:140:A:PRO:HA	1:149:A:MET:HE3	7	0.13
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	4	0.13
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	4	0.13
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	4	0.13
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG21	3	0.13
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG22	3	0.13
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG23	3	0.13
(1,1405)	1:33:A:ILE:HG21	1:49:A:PHE:HD2	8	0.13
(1,1405)	1:33:A:ILE:HG22	1:49:A:PHE:HD2	8	0.13
(1,1405)	1:33:A:ILE:HG23	1:49:A:PHE:HD2	8	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD11	1	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD12	1	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD13	1	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD11	1	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD12	1	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD13	1	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD11	1	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD12	1	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD13	1	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD11	6	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD12	6	0.13
(1,1393)	1:33:A:ILE:HG21	1:33:A:ILE:HD13	6	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD11	6	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD12	6	0.13
(1,1393)	1:33:A:ILE:HG22	1:33:A:ILE:HD13	6	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD11	6	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD12	6	0.13
(1,1393)	1:33:A:ILE:HG23	1:33:A:ILE:HD13	6	0.13
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	2	0.13
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	2	0.13
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	2	0.13
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	2	0.13
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	2	0.13
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	2	0.13
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	2	0.13
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	2	0.13
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	2	0.13
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	6	0.13
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	6	0.13
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	6	0.13
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	6	0.13
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	6	0.13
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	6	0.13
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	6	0.13
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	6	0.13
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB1	3	0.13
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB2	3	0.13
(1,1365)	1:137:A:ALA:HA	1:250:A:ALA:HB3	3	0.13
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	5	0.13
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	5	0.13
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	5	0.13
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	5	0.13
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	5	0.13
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	5	0.13
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG11	6	0.13
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG12	6	0.13
(1,1292)	1:152:A:ALA:HA	1:224:A:VAL:HG13	6	0.13
(1,1201)	1:61:A:VAL:HG21	1:85:A:PHE:HB2	1	0.13
(1,1201)	1:61:A:VAL:HG22	1:85:A:PHE:HB2	1	0.13
(1,1201)	1:61:A:VAL:HG23	1:85:A:PHE:HB2	1	0.13
(1,1171)	1:51:A:THR:HG21	1:52:A:HIS:H	1	0.13
(1,1171)	1:51:A:THR:HG22	1:52:A:HIS:H	1	0.13
(1,1171)	1:51:A:THR:HG23	1:52:A:HIS:H	1	0.13
(1,1158)	1:53:A:TYR:HA	1:57:A:GLU:H	10	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	6	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	6	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	6	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	8	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	8	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	8	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	10	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	10	0.13
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	10	0.13
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	7	0.13
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	7	0.13
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	7	0.13
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	7	0.13
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	7	0.13
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	7	0.13
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG21	8	0.13
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG22	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG23	8	0.13
(1,989)	1:200:A:ASP:HA	1:207:A:GLY:H	5	0.13
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG21	7	0.13
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG22	7	0.13
(1,988)	1:118:A:GLU:HA	1:119:A:THR:HG23	7	0.13
(1,964)	1:24:A:SER:HA	1:35:A:VAL:HA	10	0.13
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD21	6	0.13
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD22	6	0.13
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD23	6	0.13
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD11	3	0.13
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD12	3	0.13
(1,938)	1:104:A:LEU:HA	1:104:A:LEU:HD13	3	0.13
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD21	5	0.13
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD22	5	0.13
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD23	5	0.13
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD11	4	0.13
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD12	4	0.13
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD13	4	0.13
(1,881)	1:165:A:LEU:HA	1:168:A:LEU:HG	3	0.13
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	3	0.13
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	3	0.13
(1,862)	1:47:A:ILE:HA	1:60:A:ASN:HA	10	0.13
(1,851)	1:171:A:ASP:HB3	1:173:A:LYS:HG3	10	0.13
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD11	10	0.13
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD12	10	0.13
(1,820)	1:213:A:LEU:H	1:213:A:LEU:HD13	10	0.13
(1,808)	1:141:A:ILE:HA	1:142:A:THR:HB	10	0.13
(1,802)	1:140:A:PRO:HG2	1:141:A:ILE:H	10	0.13
(1,802)	1:140:A:PRO:HG3	1:141:A:ILE:H	10	0.13
(1,786)	1:131:A:PRO:HG3	1:132:A:PHE:H	7	0.13
(1,779)	1:5:A:HIS:HA	1:8:A:LEU:HD11	2	0.13
(1,779)	1:5:A:HIS:HA	1:8:A:LEU:HD12	2	0.13
(1,779)	1:5:A:HIS:HA	1:8:A:LEU:HD13	2	0.13
(1,722)	1:43:A:MET:HG2	1:64:A:VAL:HA	6	0.13
(1,713)	1:187:A:LYS:HD2	1:188:A:GLN:H	3	0.13
(1,676)	1:245:A:SER:HA	1:247:A:ALA:HB1	5	0.13
(1,676)	1:245:A:SER:HA	1:247:A:ALA:HB2	5	0.13
(1,676)	1:245:A:SER:HA	1:247:A:ALA:HB3	5	0.13
(1,613)	1:188:A:GLN:H	1:188:A:GLN:HB3	8	0.13
(1,596)	1:101:A:PHE:HA	1:104:A:LEU:HB2	9	0.13
(1,596)	1:101:A:PHE:HA	1:104:A:LEU:HB3	9	0.13
(1,590)	1:8:A:LEU:HD21	1:31:A:SER:HB2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:8:A:LEU:HD22	1:31:A:SER:HB2	7	0.13
(1,590)	1:8:A:LEU:HD23	1:31:A:SER:HB2	7	0.13
(1,560)	1:240:A:PHE:H	1:241:A:LYS:HB2	3	0.13
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB2	4	0.13
(1,534)	1:23:A:LEU:HA	1:24:A:SER:HB3	4	0.13
(1,526)	1:82:A:GLN:H	1:82:A:GLN:HG2	1	0.13
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	7	0.13
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	8	0.13
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	10	0.13
(1,471)	1:146:A:SER:HB2	1:148:A:PHE:H	1	0.13
(1,471)	1:146:A:SER:HB3	1:148:A:PHE:H	1	0.13
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	4	0.13
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	4	0.13
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	4	0.13
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	4	0.13
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	4	0.13
(1,440)	1:27:A:GLN:HG3	1:28:A:GLU:H	9	0.13
(1,428)	1:15:A:VAL:HA	1:18:A:ILE:H	4	0.13
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	4	0.13
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	4	0.13
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	4	0.13
(1,411)	1:187:A:LYS:HB2	1:188:A:GLN:H	5	0.13
(1,405)	1:43:A:MET:HA	1:64:A:VAL:HB	7	0.13
(1,370)	1:66:A:VAL:HB	1:67:A:CYS:H	7	0.13
(1,324)	1:105:A:THR:HB	1:106:A:GLU:H	3	0.13
(1,324)	1:105:A:THR:HB	1:106:A:GLU:H	10	0.13
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD11	10	0.13
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD12	10	0.13
(1,287)	1:158:A:GLU:HG3	1:186:A:ILE:HD13	10	0.13
(1,273)	1:135:A:TRP:HA	1:136:A:THR:HB	7	0.13
(1,266)	1:101:A:PHE:H	1:101:A:PHE:HB3	9	0.13
(1,262)	1:127:A:ILE:HD11	1:147:A:THR:HB	7	0.13
(1,262)	1:127:A:ILE:HD12	1:147:A:THR:HB	7	0.13
(1,262)	1:127:A:ILE:HD13	1:147:A:THR:HB	7	0.13
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	9	0.13
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	10	0.13
(1,193)	1:163:A:ALA:HA	1:166:A:ASP:HB3	10	0.13
(1,169)	1:27:A:GLN:HB3	1:32:A:ILE:HB	2	0.13
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG21	5	0.13
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG22	5	0.13
(1,163)	1:60:A:ASN:HB3	1:62:A:ILE:HG23	5	0.13
(1,160)	1:100:A:LEU:HB3	1:103:A:PHE:HD1	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:100:A:LEU:HB3	1:103:A:PHE:HD2	9	0.13
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG11	5	0.13
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG12	5	0.13
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG13	5	0.13
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG11	5	0.13
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG12	5	0.13
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG13	5	0.13
(1,129)	1:79:A:LYS:HE2	1:80:A:TYR:H	1	0.13
(1,129)	1:79:A:LYS:HE3	1:80:A:TYR:H	1	0.13
(1,99)	1:171:A:ASP:HB2	1:174:A:MET:HB3	4	0.13
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	4	0.13
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	4	0.13
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	4	0.13
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	4	0.13
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	4	0.13
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	4	0.13
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD11	4	0.13
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD12	4	0.13
(1,63)	1:213:A:LEU:HB2	1:216:A:ILE:HD13	4	0.13
(1,54)	1:189:A:ASP:HB2	1:190:A:GLY:HA2	2	0.13
(1,54)	1:189:A:ASP:HB3	1:190:A:GLY:HA2	2	0.13
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD11	4	0.13
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD12	4	0.13
(1,32)	1:234:A:HIS:HA	1:235:A:ILE:HD13	4	0.13
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD11	3	0.13
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD12	3	0.13
(1,27)	1:185:A:ARG:H	1:186:A:ILE:HD13	3	0.13
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE1	8	0.13
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE2	8	0.13
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE3	8	0.13
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE1	8	0.13
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE2	8	0.13
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE3	8	0.13
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE1	8	0.13
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE2	8	0.13
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE3	8	0.13
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	9	0.13
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	9	0.13
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	9	0.13
(1,1)	1:135:A:TRP:HE1	1:164:A:MET:HE1	10	0.13
(1,1)	1:135:A:TRP:HE1	1:164:A:MET:HE2	10	0.13
(1,1)	1:135:A:TRP:HE1	1:164:A:MET:HE3	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2635)	1:235:A:ILE:HD11	1:229:A:TRP:HA	9	0.12
(1,2635)	1:235:A:ILE:HD12	1:229:A:TRP:HA	9	0.12
(1,2635)	1:235:A:ILE:HD13	1:229:A:TRP:HA	9	0.12
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG21	10	0.12
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG22	10	0.12
(1,2633)	1:234:A:HIS:HD2	1:141:A:ILE:HG23	10	0.12
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG21	1	0.12
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG22	1	0.12
(1,2621)	1:240:A:PHE:H	1:127:A:ILE:HG23	1	0.12
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD21	4	0.12
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD22	4	0.12
(1,2570)	1:37:A:VAL:HG11	1:107:A:LEU:HD23	4	0.12
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD21	4	0.12
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD22	4	0.12
(1,2570)	1:37:A:VAL:HG12	1:107:A:LEU:HD23	4	0.12
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD21	4	0.12
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD22	4	0.12
(1,2570)	1:37:A:VAL:HG13	1:107:A:LEU:HD23	4	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG21	3	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG22	3	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG23	3	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG21	5	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG22	5	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG23	5	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG21	9	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG22	9	0.12
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG23	9	0.12
(1,2549)	1:142:A:THR:HG21	1:240:A:PHE:HB3	3	0.12
(1,2549)	1:142:A:THR:HG22	1:240:A:PHE:HB3	3	0.12
(1,2549)	1:142:A:THR:HG23	1:240:A:PHE:HB3	3	0.12
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG21	8	0.12
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG22	8	0.12
(1,2543)	1:148:A:PHE:HA	1:226:A:VAL:HG23	8	0.12
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	6	0.12
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	6	0.12
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	6	0.12
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD21	8	0.12
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD22	8	0.12
(1,2539)	1:11:A:GLU:H	1:12:A:LEU:HD23	8	0.12
(1,2518)	1:194:A:THR:HG21	1:196:A:GLN:HG2	4	0.12
(1,2518)	1:194:A:THR:HG21	1:196:A:GLN:HG3	4	0.12
(1,2518)	1:194:A:THR:HG22	1:196:A:GLN:HG2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2518)	1:194:A:THR:HG22	1:196:A:GLN:HG3	4	0.12
(1,2518)	1:194:A:THR:HG23	1:196:A:GLN:HG2	4	0.12
(1,2518)	1:194:A:THR:HG23	1:196:A:GLN:HG3	4	0.12
(1,2491)	1:168:A:LEU:HD21	1:174:A:MET:H	6	0.12
(1,2491)	1:168:A:LEU:HD22	1:174:A:MET:H	6	0.12
(1,2491)	1:168:A:LEU:HD23	1:174:A:MET:H	6	0.12
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG21	3	0.12
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG22	3	0.12
(1,2454)	1:45:A:LEU:HD11	1:64:A:VAL:HG23	3	0.12
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG21	3	0.12
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG22	3	0.12
(1,2454)	1:45:A:LEU:HD12	1:64:A:VAL:HG23	3	0.12
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG21	3	0.12
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG22	3	0.12
(1,2454)	1:45:A:LEU:HD13	1:64:A:VAL:HG23	3	0.12
(1,2449)	1:23:A:LEU:HD11	1:33:A:ILE:HD11	7	0.12
(1,2449)	1:23:A:LEU:HD11	1:33:A:ILE:HD12	7	0.12
(1,2449)	1:23:A:LEU:HD11	1:33:A:ILE:HD13	7	0.12
(1,2449)	1:23:A:LEU:HD12	1:33:A:ILE:HD11	7	0.12
(1,2449)	1:23:A:LEU:HD12	1:33:A:ILE:HD12	7	0.12
(1,2449)	1:23:A:LEU:HD12	1:33:A:ILE:HD13	7	0.12
(1,2449)	1:23:A:LEU:HD13	1:33:A:ILE:HD11	7	0.12
(1,2449)	1:23:A:LEU:HD13	1:33:A:ILE:HD12	7	0.12
(1,2449)	1:23:A:LEU:HD13	1:33:A:ILE:HD13	7	0.12
(1,2449)	1:23:A:LEU:HD21	1:33:A:ILE:HD11	7	0.12
(1,2449)	1:23:A:LEU:HD21	1:33:A:ILE:HD12	7	0.12
(1,2449)	1:23:A:LEU:HD21	1:33:A:ILE:HD13	7	0.12
(1,2449)	1:23:A:LEU:HD22	1:33:A:ILE:HD11	7	0.12
(1,2449)	1:23:A:LEU:HD22	1:33:A:ILE:HD12	7	0.12
(1,2449)	1:23:A:LEU:HD22	1:33:A:ILE:HD13	7	0.12
(1,2449)	1:23:A:LEU:HD23	1:33:A:ILE:HD11	7	0.12
(1,2449)	1:23:A:LEU:HD23	1:33:A:ILE:HD12	7	0.12
(1,2449)	1:23:A:LEU:HD23	1:33:A:ILE:HD13	7	0.12
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD11	9	0.12
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD12	9	0.12
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD13	9	0.12
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	8	0.12
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	8	0.12
(1,2426)	1:125:A:SER:HA	1:126:A:ASP:HB3	1	0.12
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD11	1	0.12
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD12	1	0.12
(1,2421)	1:18:A:ILE:HD11	1:100:A:LEU:HD13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD11	1	0.12
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD12	1	0.12
(1,2421)	1:18:A:ILE:HD12	1:100:A:LEU:HD13	1	0.12
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD11	1	0.12
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD12	1	0.12
(1,2421)	1:18:A:ILE:HD13	1:100:A:LEU:HD13	1	0.12
(1,2359)	1:40:A:HIS:HA	1:42:A:TYR:H	9	0.12
(1,2346)	1:52:A:HIS:H	1:57:A:GLU:HG3	4	0.12
(1,2285)	1:142:A:THR:HG21	1:239:A:ARG:H	4	0.12
(1,2285)	1:142:A:THR:HG22	1:239:A:ARG:H	4	0.12
(1,2285)	1:142:A:THR:HG23	1:239:A:ARG:H	4	0.12
(1,2242)	1:29:A:ASP:H	1:32:A:ILE:H	8	0.12
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD21	2	0.12
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD22	2	0.12
(1,2210)	1:98:A:VAL:H	1:100:A:LEU:HD23	2	0.12
(1,2161)	1:125:A:SER:HB3	1:127:A:ILE:H	4	0.12
(1,2157)	1:208:A:SER:H	1:211:A:LEU:H	9	0.12
(1,2156)	1:15:A:VAL:H	1:18:A:ILE:HB	7	0.12
(1,2129)	1:222:A:VAL:HG11	1:256:A:PHE:H	6	0.12
(1,2129)	1:222:A:VAL:HG12	1:256:A:PHE:H	6	0.12
(1,2129)	1:222:A:VAL:HG13	1:256:A:PHE:H	6	0.12
(1,2129)	1:222:A:VAL:HG11	1:256:A:PHE:H	10	0.12
(1,2129)	1:222:A:VAL:HG12	1:256:A:PHE:H	10	0.12
(1,2129)	1:222:A:VAL:HG13	1:256:A:PHE:H	10	0.12
(1,2096)	1:251:A:VAL:HG21	1:253:A:ARG:H	4	0.12
(1,2096)	1:251:A:VAL:HG22	1:253:A:ARG:H	4	0.12
(1,2096)	1:251:A:VAL:HG23	1:253:A:ARG:H	4	0.12
(1,2096)	1:251:A:VAL:HG21	1:253:A:ARG:H	9	0.12
(1,2096)	1:251:A:VAL:HG22	1:253:A:ARG:H	9	0.12
(1,2096)	1:251:A:VAL:HG23	1:253:A:ARG:H	9	0.12
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	7	0.12
(1,2078)	1:100:A:LEU:H	1:102:A:ASP:H	3	0.12
(1,2064)	1:36:A:LYS:HG2	1:40:A:HIS:H	4	0.12
(1,2064)	1:36:A:LYS:HG3	1:40:A:HIS:H	4	0.12
(1,2063)	1:40:A:HIS:H	1:41:A:GLU:H	6	0.12
(1,2029)	1:1:A:MET:HG2	1:3:A:ASP:H	3	0.12
(1,2029)	1:1:A:MET:HG3	1:3:A:ASP:H	3	0.12
(1,1995)	1:51:A:THR:H	1:53:A:TYR:H	9	0.12
(1,1994)	1:53:A:TYR:H	1:56:A:GLU:H	7	0.12
(1,1992)	1:93:A:PHE:H	1:94:A:HIS:HB2	5	0.12
(1,1992)	1:93:A:PHE:H	1:94:A:HIS:HB3	5	0.12
(1,1983)	1:162:A:PHE:HD1	1:165:A:LEU:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1983)	1:162:A:PHE:HD2	1:165:A:LEU:H	1	0.12
(1,1944)	1:61:A:VAL:H	1:86:A:GLN:HG3	9	0.12
(1,1935)	1:141:A:ILE:HD11	1:148:A:PHE:H	3	0.12
(1,1935)	1:141:A:ILE:HD12	1:148:A:PHE:H	3	0.12
(1,1935)	1:141:A:ILE:HD13	1:148:A:PHE:H	3	0.12
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG21	10	0.12
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG22	10	0.12
(1,1923)	1:35:A:VAL:H	1:47:A:ILE:HG23	10	0.12
(1,1919)	1:35:A:VAL:H	1:45:A:LEU:H	7	0.12
(1,1887)	1:143:A:ASP:H	1:145:A:GLY:H	7	0.12
(1,1882)	1:12:A:LEU:HD21	1:31:A:SER:H	4	0.12
(1,1882)	1:12:A:LEU:HD22	1:31:A:SER:H	4	0.12
(1,1882)	1:12:A:LEU:HD23	1:31:A:SER:H	4	0.12
(1,1869)	1:27:A:GLN:HB3	1:27:A:GLN:HE21	5	0.12
(1,1869)	1:27:A:GLN:HB3	1:27:A:GLN:HE22	5	0.12
(1,1817)	1:81:A:LEU:H	1:82:A:GLN:HB2	4	0.12
(1,1735)	1:217:A:MET:HB2	1:218:A:ASP:H	6	0.12
(1,1692)	1:211:A:LEU:HA	1:213:A:LEU:H	4	0.12
(1,1688)	1:251:A:VAL:HB	1:252:A:VAL:H	3	0.12
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	7	0.12
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	8	0.12
(1,1599)	1:93:A:PHE:H	1:94:A:HIS:H	6	0.12
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	1	0.12
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	3	0.12
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	10	0.12
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD11	5	0.12
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD12	5	0.12
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD13	5	0.12
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	1	0.12
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG21	5	0.12
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG22	5	0.12
(1,1541)	1:77:A:ASP:H	1:78:A:THR:HG23	5	0.12
(1,1534)	1:143:A:ASP:H	1:144:A:ARG:HA	6	0.12
(1,1513)	1:54:A:PRO:HD2	1:98:A:VAL:HG11	5	0.12
(1,1513)	1:54:A:PRO:HD2	1:98:A:VAL:HG12	5	0.12
(1,1513)	1:54:A:PRO:HD2	1:98:A:VAL:HG13	5	0.12
(1,1461)	1:43:A:MET:HE1	1:66:A:VAL:H	2	0.12
(1,1461)	1:43:A:MET:HE2	1:66:A:VAL:H	2	0.12
(1,1461)	1:43:A:MET:HE3	1:66:A:VAL:H	2	0.12
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	9	0.12
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	9	0.12
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB1	8	0.12
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB2	8	0.12
(1,1381)	1:14:A:ALA:HB1	1:17:A:ALA:HB3	8	0.12
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB1	8	0.12
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB2	8	0.12
(1,1381)	1:14:A:ALA:HB2	1:17:A:ALA:HB3	8	0.12
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB1	8	0.12
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB2	8	0.12
(1,1381)	1:14:A:ALA:HB3	1:17:A:ALA:HB3	8	0.12
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE1	10	0.12
(1,1380)	1:14:A:ALA:HB1	1:101:A:PHE:HE2	10	0.12
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE1	10	0.12
(1,1380)	1:14:A:ALA:HB2	1:101:A:PHE:HE2	10	0.12
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE1	10	0.12
(1,1380)	1:14:A:ALA:HB3	1:101:A:PHE:HE2	10	0.12
(1,1375)	1:120:A:GLU:H	1:121:A:PRO:HD2	5	0.12
(1,1374)	1:130:A:ASP:H	1:131:A:PRO:HD2	9	0.12
(1,1353)	1:181:A:MET:HE1	1:228:A:ARG:H	2	0.12
(1,1353)	1:181:A:MET:HE2	1:228:A:ARG:H	2	0.12
(1,1353)	1:181:A:MET:HE3	1:228:A:ARG:H	2	0.12
(1,1353)	1:181:A:MET:HE1	1:228:A:ARG:H	4	0.12
(1,1353)	1:181:A:MET:HE2	1:228:A:ARG:H	4	0.12
(1,1353)	1:181:A:MET:HE3	1:228:A:ARG:H	4	0.12
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	2	0.12
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	2	0.12
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	2	0.12
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	2	0.12
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	2	0.12
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	2	0.12
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	10	0.12
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	10	0.12
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	10	0.12
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	10	0.12
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	10	0.12
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	10	0.12
(1,1324)	1:89:A:MET:HE1	1:92:A:VAL:HG21	3	0.12
(1,1324)	1:89:A:MET:HE1	1:92:A:VAL:HG22	3	0.12
(1,1324)	1:89:A:MET:HE1	1:92:A:VAL:HG23	3	0.12
(1,1324)	1:89:A:MET:HE2	1:92:A:VAL:HG21	3	0.12
(1,1324)	1:89:A:MET:HE2	1:92:A:VAL:HG22	3	0.12
(1,1324)	1:89:A:MET:HE2	1:92:A:VAL:HG23	3	0.12
(1,1324)	1:89:A:MET:HE3	1:92:A:VAL:HG21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	1:89:A:MET:HE3	1:92:A:VAL:HG22	3	0.12
(1,1324)	1:89:A:MET:HE3	1:92:A:VAL:HG23	3	0.12
(1,1273)	1:143:A:ASP:HA	1:144:A:ARG:HA	3	0.12
(1,1213)	1:42:A:TYR:H	1:43:A:MET:HA	3	0.12
(1,1196)	1:105:A:THR:HG21	1:106:A:GLU:H	7	0.12
(1,1196)	1:105:A:THR:HG22	1:106:A:GLU:H	7	0.12
(1,1196)	1:105:A:THR:HG23	1:106:A:GLU:H	7	0.12
(1,1196)	1:105:A:THR:HG21	1:106:A:GLU:H	8	0.12
(1,1196)	1:105:A:THR:HG22	1:106:A:GLU:H	8	0.12
(1,1196)	1:105:A:THR:HG23	1:106:A:GLU:H	8	0.12
(1,1158)	1:53:A:TYR:HA	1:57:A:GLU:H	2	0.12
(1,1158)	1:53:A:TYR:HA	1:57:A:GLU:H	7	0.12
(1,1079)	1:152:A:ALA:HB1	1:224:A:VAL:HA	4	0.12
(1,1079)	1:152:A:ALA:HB2	1:224:A:VAL:HA	4	0.12
(1,1079)	1:152:A:ALA:HB3	1:224:A:VAL:HA	4	0.12
(1,1073)	1:176:A:LYS:HA	1:229:A:TRP:HE1	4	0.12
(1,1051)	1:137:A:ALA:HB1	1:151:A:PHE:HE1	6	0.12
(1,1051)	1:137:A:ALA:HB2	1:151:A:PHE:HE1	6	0.12
(1,1051)	1:137:A:ALA:HB3	1:151:A:PHE:HE1	6	0.12
(1,1051)	1:137:A:ALA:HB1	1:151:A:PHE:HE1	8	0.12
(1,1051)	1:137:A:ALA:HB2	1:151:A:PHE:HE1	8	0.12
(1,1051)	1:137:A:ALA:HB3	1:151:A:PHE:HE1	8	0.12
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	1	0.12
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	1	0.12
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	1	0.12
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	3	0.12
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	3	0.12
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	3	0.12
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	9	0.12
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	9	0.12
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	9	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG21	1	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG22	1	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG23	1	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG21	2	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG22	2	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG23	2	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG21	3	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG22	3	0.12
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG23	3	0.12
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE21	7	0.12
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE22	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	3	0.12
(1,984)	1:168:A:LEU:HD21	1:225:A:VAL:H	3	0.12
(1,984)	1:168:A:LEU:HD22	1:225:A:VAL:H	3	0.12
(1,984)	1:168:A:LEU:HD23	1:225:A:VAL:H	3	0.12
(1,925)	1:176:A:LYS:HG2	1:229:A:TRP:HE1	8	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD11	1	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD12	1	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD13	1	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD11	3	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD12	3	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD13	3	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD11	8	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD12	8	0.12
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD13	8	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	1	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	1	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	2	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	2	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	6	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	6	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	9	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	9	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	10	0.12
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	10	0.12
(1,808)	1:141:A:ILE:HA	1:142:A:THR:HB	8	0.12
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	9	0.12
(1,777)	1:42:A:TYR:HD1	1:66:A:VAL:HA	10	0.12
(1,777)	1:42:A:TYR:HD2	1:66:A:VAL:HA	10	0.12
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE1	5	0.12
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE2	5	0.12
(1,760)	1:128:A:PRO:HG2	1:174:A:MET:HE3	5	0.12
(1,722)	1:43:A:MET:HG2	1:64:A:VAL:HA	7	0.12
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	2	0.12
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	3	0.12
(1,689)	1:187:A:LYS:HD3	1:220:A:TRP:HB3	1	0.12
(1,641)	1:116:A:GLU:H	1:116:A:GLU:HB3	1	0.12
(1,631)	1:208:A:SER:HB3	1:209:A:ARG:H	9	0.12
(1,596)	1:101:A:PHE:HA	1:104:A:LEU:HB2	2	0.12
(1,596)	1:101:A:PHE:HA	1:104:A:LEU:HB3	2	0.12
(1,560)	1:240:A:PHE:H	1:241:A:LYS:HB2	10	0.12
(1,531)	1:20:A:PRO:HA	1:22:A:LEU:H	4	0.12
(1,527)	1:61:A:VAL:HG21	1:82:A:GLN:HG2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:61:A:VAL:HG22	1:82:A:GLN:HG2	3	0.12
(1,527)	1:61:A:VAL:HG23	1:82:A:GLN:HG2	3	0.12
(1,526)	1:82:A:GLN:H	1:82:A:GLN:HG2	5	0.12
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	9	0.12
(1,493)	1:243:A:ILE:HA	1:245:A:SER:H	7	0.12
(1,493)	1:243:A:ILE:HA	1:245:A:SER:H	8	0.12
(1,488)	1:96:A:GLY:H	1:97:A:SER:HB3	9	0.12
(1,487)	1:97:A:SER:HB2	1:98:A:VAL:H	8	0.12
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	1	0.12
(1,472)	1:155:A:VAL:HG21	1:160:A:GLN:HG2	3	0.12
(1,472)	1:155:A:VAL:HG21	1:160:A:GLN:HG3	3	0.12
(1,472)	1:155:A:VAL:HG22	1:160:A:GLN:HG2	3	0.12
(1,472)	1:155:A:VAL:HG22	1:160:A:GLN:HG3	3	0.12
(1,472)	1:155:A:VAL:HG23	1:160:A:GLN:HG2	3	0.12
(1,472)	1:155:A:VAL:HG23	1:160:A:GLN:HG3	3	0.12
(1,440)	1:27:A:GLN:HG3	1:28:A:GLU:H	6	0.12
(1,426)	1:217:A:MET:HE1	1:252:A:VAL:HA	7	0.12
(1,426)	1:217:A:MET:HE2	1:252:A:VAL:HA	7	0.12
(1,426)	1:217:A:MET:HE3	1:252:A:VAL:HA	7	0.12
(1,416)	1:9:A:VAL:HA	1:13:A:GLU:H	1	0.12
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	2	0.12
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	6	0.12
(1,391)	1:4:A:ASP:HB2	1:7:A:GLN:HG2	3	0.12
(1,362)	1:133:A:GLU:HG2	1:134:A:GLY:HA3	1	0.12
(1,362)	1:133:A:GLU:HG3	1:134:A:GLY:HA3	1	0.12
(1,345)	1:6:A:GLU:HA	1:6:A:GLU:HG2	9	0.12
(1,301)	1:8:A:LEU:HA	1:11:A:GLU:HG3	7	0.12
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	4	0.12
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	4	0.12
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	7	0.12
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	7	0.12
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	7	0.12
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG21	8	0.12
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG22	8	0.12
(1,296)	1:156:A:THR:HB	1:186:A:ILE:HG23	8	0.12
(1,228)	1:186:A:ILE:H	1:194:A:THR:HB	1	0.12
(1,201)	1:163:A:ALA:HB1	1:166:A:ASP:HB2	8	0.12
(1,201)	1:163:A:ALA:HB2	1:166:A:ASP:HB2	8	0.12
(1,201)	1:163:A:ALA:HB3	1:166:A:ASP:HB2	8	0.12
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	3	0.12
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	7	0.12
(1,136)	1:75:A:LEU:HB3	1:76:A:TYR:HE1	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:75:A:LEU:HB3	1:76:A:TYR:HE2	3	0.12
(1,129)	1:79:A:LYS:HE2	1:80:A:TYR:H	5	0.12
(1,129)	1:79:A:LYS:HE3	1:80:A:TYR:H	5	0.12
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD1	3	0.12
(1,87)	1:18:A:ILE:HD11	1:19:A:TYR:HD2	3	0.12
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD1	3	0.12
(1,87)	1:18:A:ILE:HD12	1:19:A:TYR:HD2	3	0.12
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD1	3	0.12
(1,87)	1:18:A:ILE:HD13	1:19:A:TYR:HD2	3	0.12
(1,66)	1:22:A:LEU:H	1:23:A:LEU:HB2	10	0.12
(1,60)	1:134:A:GLY:HA3	1:164:A:MET:HB2	4	0.12
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD11	3	0.11
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD12	3	0.11
(1,2661)	1:49:A:PHE:H	1:8:A:LEU:HD13	3	0.11
(1,2630)	1:235:A:ILE:HD11	1:148:A:PHE:HA	3	0.11
(1,2630)	1:235:A:ILE:HD12	1:148:A:PHE:HA	3	0.11
(1,2630)	1:235:A:ILE:HD13	1:148:A:PHE:HA	3	0.11
(1,2620)	1:246:A:THR:H	1:141:A:ILE:HD11	1	0.11
(1,2620)	1:246:A:THR:H	1:141:A:ILE:HD12	1	0.11
(1,2620)	1:246:A:THR:H	1:141:A:ILE:HD13	1	0.11
(1,2610)	1:98:A:VAL:HG21	1:99:A:CYS:HB2	3	0.11
(1,2610)	1:98:A:VAL:HG22	1:99:A:CYS:HB2	3	0.11
(1,2610)	1:98:A:VAL:HG23	1:99:A:CYS:HB2	3	0.11
(1,2569)	1:66:A:VAL:HG11	1:67:A:CYS:H	9	0.11
(1,2569)	1:66:A:VAL:HG12	1:67:A:CYS:H	9	0.11
(1,2569)	1:66:A:VAL:HG13	1:67:A:CYS:H	9	0.11
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG21	1	0.11
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG22	1	0.11
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG23	1	0.11
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG21	7	0.11
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG22	7	0.11
(1,2554)	1:35:A:VAL:H	1:35:A:VAL:HG23	7	0.11
(1,2496)	1:251:A:VAL:HG11	1:253:A:ARG:H	3	0.11
(1,2496)	1:251:A:VAL:HG12	1:253:A:ARG:H	3	0.11
(1,2496)	1:251:A:VAL:HG13	1:253:A:ARG:H	3	0.11
(1,2496)	1:251:A:VAL:HG11	1:253:A:ARG:H	9	0.11
(1,2496)	1:251:A:VAL:HG12	1:253:A:ARG:H	9	0.11
(1,2496)	1:251:A:VAL:HG13	1:253:A:ARG:H	9	0.11
(1,2438)	1:186:A:ILE:HG21	1:188:A:GLN:HB2	10	0.11
(1,2438)	1:186:A:ILE:HG22	1:188:A:GLN:HB2	10	0.11
(1,2438)	1:186:A:ILE:HG23	1:188:A:GLN:HB2	10	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD11	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD12	4	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD13	4	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD11	10	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD12	10	0.11
(1,2437)	1:61:A:VAL:HB	1:62:A:ILE:HD13	10	0.11
(1,2432)	1:133:A:GLU:HG2	1:135:A:TRP:HB3	3	0.11
(1,2432)	1:133:A:GLU:HG3	1:135:A:TRP:HB3	3	0.11
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD11	1	0.11
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD12	1	0.11
(1,2412)	1:185:A:ARG:H	1:214:A:ILE:HD13	1	0.11
(1,2365)	1:186:A:ILE:HG21	1:194:A:THR:H	5	0.11
(1,2365)	1:186:A:ILE:HG22	1:194:A:THR:H	5	0.11
(1,2365)	1:186:A:ILE:HG23	1:194:A:THR:H	5	0.11
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE1	4	0.11
(1,2345)	1:52:A:HIS:H	1:53:A:TYR:HE2	4	0.11
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD11	2	0.11
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD12	2	0.11
(1,2339)	1:105:A:THR:H	1:107:A:LEU:HD13	2	0.11
(1,2336)	1:65:A:GLY:H	1:78:A:THR:HA	1	0.11
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG21	9	0.11
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG22	9	0.11
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG23	9	0.11
(1,2324)	1:88:A:VAL:HG21	1:92:A:VAL:H	10	0.11
(1,2324)	1:88:A:VAL:HG22	1:92:A:VAL:H	10	0.11
(1,2324)	1:88:A:VAL:HG23	1:92:A:VAL:H	10	0.11
(1,2318)	1:49:A:PHE:HD2	1:60:A:ASN:H	7	0.11
(1,2306)	1:176:A:LYS:H	1:229:A:TRP:HE1	5	0.11
(1,2294)	1:76:A:TYR:HB3	1:81:A:LEU:H	10	0.11
(1,2281)	1:62:A:ILE:HD11	1:63:A:GLU:H	6	0.11
(1,2281)	1:62:A:ILE:HD12	1:63:A:GLU:H	6	0.11
(1,2281)	1:62:A:ILE:HD13	1:63:A:GLU:H	6	0.11
(1,2252)	1:159:A:GLU:H	1:160:A:GLN:HB2	7	0.11
(1,2241)	1:31:A:SER:H	1:32:A:ILE:H	9	0.11
(1,2235)	1:82:A:GLN:H	1:84:A:LEU:H	3	0.11
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	3	0.11
(1,2204)	1:39:A:GLN:H	1:41:A:GLU:H	6	0.11
(1,2194)	1:75:A:LEU:H	1:76:A:TYR:HB3	7	0.11
(1,2150)	1:132:A:PHE:HB3	1:136:A:THR:H	1	0.11
(1,2123)	1:26:A:LYS:HB3	1:33:A:ILE:H	8	0.11
(1,2110)	1:155:A:VAL:HB	1:160:A:GLN:H	2	0.11
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG21	5	0.11
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG22	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:241:A:LYS:H	1:243:A:ILE:HG23	5	0.11
(1,2093)	1:239:A:ARG:HB3	1:241:A:LYS:H	9	0.11
(1,2090)	1:239:A:ARG:H	1:241:A:LYS:H	4	0.11
(1,2040)	1:210:A:MET:H	1:211:A:LEU:HB3	5	0.11
(1,2040)	1:210:A:MET:H	1:211:A:LEU:HB3	9	0.11
(1,2025)	1:186:A:ILE:H	1:196:A:GLN:H	9	0.11
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD21	9	0.11
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD22	9	0.11
(1,2004)	1:163:A:ALA:H	1:165:A:LEU:HD23	9	0.11
(1,1991)	1:90:A:ASP:H	1:93:A:PHE:H	2	0.11
(1,1975)	1:179:A:HIS:HB3	1:203:A:GLU:H	5	0.11
(1,1919)	1:35:A:VAL:H	1:45:A:LEU:H	3	0.11
(1,1897)	1:98:A:VAL:HA	1:100:A:LEU:H	1	0.11
(1,1865)	1:193:A:ALA:HB1	1:194:A:THR:H	1	0.11
(1,1865)	1:193:A:ALA:HB2	1:194:A:THR:H	1	0.11
(1,1865)	1:193:A:ALA:HB3	1:194:A:THR:H	1	0.11
(1,1829)	1:72:A:LYS:H	1:72:A:LYS:HG2	2	0.11
(1,1829)	1:72:A:LYS:H	1:72:A:LYS:HG3	2	0.11
(1,1773)	1:9:A:VAL:H	1:9:A:VAL:HB	10	0.11
(1,1701)	1:256:A:PHE:H	1:257:A:ASP:H	6	0.11
(1,1694)	1:211:A:LEU:HD11	1:213:A:LEU:H	3	0.11
(1,1694)	1:211:A:LEU:HD12	1:213:A:LEU:H	3	0.11
(1,1694)	1:211:A:LEU:HD13	1:213:A:LEU:H	3	0.11
(1,1694)	1:211:A:LEU:HD11	1:213:A:LEU:H	5	0.11
(1,1694)	1:211:A:LEU:HD12	1:213:A:LEU:H	5	0.11
(1,1694)	1:211:A:LEU:HD13	1:213:A:LEU:H	5	0.11
(1,1671)	1:138:A:SER:HB3	1:250:A:ALA:H	3	0.11
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD11	8	0.11
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD12	8	0.11
(1,1664)	1:212:A:HIS:H	1:213:A:LEU:HD13	8	0.11
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	1	0.11
(1,1593)	1:130:A:ASP:H	1:130:A:ASP:HB2	9	0.11
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD11	1	0.11
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD12	1	0.11
(1,1587)	1:14:A:ALA:H	1:100:A:LEU:HD13	1	0.11
(1,1567)	1:26:A:LYS:H	1:32:A:ILE:HB	7	0.11
(1,1543)	1:188:A:GLN:H	1:194:A:THR:H	8	0.11
(1,1537)	1:138:A:SER:H	1:150:A:ALA:H	2	0.11
(1,1537)	1:138:A:SER:H	1:150:A:ALA:H	7	0.11
(1,1461)	1:43:A:MET:HE1	1:66:A:VAL:H	6	0.11
(1,1461)	1:43:A:MET:HE2	1:66:A:VAL:H	6	0.11
(1,1461)	1:43:A:MET:HE3	1:66:A:VAL:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB2	6	0.11
(1,1457)	1:217:A:MET:HE1	1:257:A:ASP:HB3	6	0.11
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB2	6	0.11
(1,1457)	1:217:A:MET:HE2	1:257:A:ASP:HB3	6	0.11
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB2	6	0.11
(1,1457)	1:217:A:MET:HE3	1:257:A:ASP:HB3	6	0.11
(1,1452)	1:58:A:ALA:HA	1:99:A:CYS:HB2	5	0.11
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG21	6	0.11
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG22	6	0.11
(1,1411)	1:11:A:GLU:HA	1:98:A:VAL:HG23	6	0.11
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD11	6	0.11
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD12	6	0.11
(1,1362)	1:17:A:ALA:HB1	1:18:A:ILE:HD13	6	0.11
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD11	6	0.11
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD12	6	0.11
(1,1362)	1:17:A:ALA:HB2	1:18:A:ILE:HD13	6	0.11
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD11	6	0.11
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD12	6	0.11
(1,1362)	1:17:A:ALA:HB3	1:18:A:ILE:HD13	6	0.11
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	3	0.11
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	3	0.11
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	3	0.11
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	3	0.11
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	3	0.11
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	3	0.11
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	6	0.11
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	6	0.11
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	6	0.11
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	6	0.11
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	6	0.11
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	6	0.11
(1,1327)	1:128:A:PRO:HD2	1:151:A:PHE:HE1	3	0.11
(1,1291)	1:177:A:ALA:HA	1:229:A:TRP:HH2	2	0.11
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD11	9	0.11
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD12	9	0.11
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD13	9	0.11
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD21	9	0.11
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD22	9	0.11
(1,1281)	1:19:A:TYR:HE1	1:23:A:LEU:HD23	9	0.11
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD11	9	0.11
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD12	9	0.11
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD21	9	0.11
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD22	9	0.11
(1,1281)	1:19:A:TYR:HE2	1:23:A:LEU:HD23	9	0.11
(1,1273)	1:143:A:ASP:HA	1:144:A:ARG:HA	8	0.11
(1,1254)	1:119:A:THR:HA	1:119:A:THR:HG21	5	0.11
(1,1254)	1:119:A:THR:HA	1:119:A:THR:HG22	5	0.11
(1,1254)	1:119:A:THR:HA	1:119:A:THR:HG23	5	0.11
(1,1241)	1:8:A:LEU:HD11	1:53:A:TYR:HE1	1	0.11
(1,1241)	1:8:A:LEU:HD11	1:53:A:TYR:HE2	1	0.11
(1,1241)	1:8:A:LEU:HD12	1:53:A:TYR:HE1	1	0.11
(1,1241)	1:8:A:LEU:HD12	1:53:A:TYR:HE2	1	0.11
(1,1241)	1:8:A:LEU:HD13	1:53:A:TYR:HE1	1	0.11
(1,1241)	1:8:A:LEU:HD13	1:53:A:TYR:HE2	1	0.11
(1,1230)	1:199:A:ASP:HA	1:201:A:ASP:H	7	0.11
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD21	2	0.11
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD22	2	0.11
(1,1208)	1:83:A:HIS:HB2	1:84:A:LEU:HD23	2	0.11
(1,1201)	1:61:A:VAL:HG21	1:85:A:PHE:HB2	6	0.11
(1,1201)	1:61:A:VAL:HG22	1:85:A:PHE:HB2	6	0.11
(1,1201)	1:61:A:VAL:HG23	1:85:A:PHE:HB2	6	0.11
(1,1190)	1:1:A:MET:HA	1:2:A:ASP:H	9	0.11
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD21	4	0.11
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD22	4	0.11
(1,1177)	1:83:A:HIS:H	1:84:A:LEU:HD23	4	0.11
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG21	10	0.11
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG22	10	0.11
(1,1170)	1:127:A:ILE:HD11	1:129:A:THR:HG23	10	0.11
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG21	10	0.11
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG22	10	0.11
(1,1170)	1:127:A:ILE:HD12	1:129:A:THR:HG23	10	0.11
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG21	10	0.11
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG22	10	0.11
(1,1170)	1:127:A:ILE:HD13	1:129:A:THR:HG23	10	0.11
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB1	5	0.11
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB2	5	0.11
(1,1142)	1:57:A:GLU:HA	1:58:A:ALA:HB3	5	0.11
(1,1128)	1:251:A:VAL:HG21	1:256:A:PHE:HE1	10	0.11
(1,1128)	1:251:A:VAL:HG21	1:256:A:PHE:HE2	10	0.11
(1,1128)	1:251:A:VAL:HG22	1:256:A:PHE:HE1	10	0.11
(1,1128)	1:251:A:VAL:HG22	1:256:A:PHE:HE2	10	0.11
(1,1128)	1:251:A:VAL:HG23	1:256:A:PHE:HE1	10	0.11
(1,1128)	1:251:A:VAL:HG23	1:256:A:PHE:HE2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:51:A:THR:HG21	1:52:A:HIS:HD2	2	0.11
(1,1115)	1:51:A:THR:HG22	1:52:A:HIS:HD2	2	0.11
(1,1115)	1:51:A:THR:HG23	1:52:A:HIS:HD2	2	0.11
(1,1111)	1:219:A:VAL:HG21	1:256:A:PHE:HB3	8	0.11
(1,1111)	1:219:A:VAL:HG22	1:256:A:PHE:HB3	8	0.11
(1,1111)	1:219:A:VAL:HG23	1:256:A:PHE:HB3	8	0.11
(1,1088)	1:183:A:ALA:HB1	1:211:A:LEU:HD11	5	0.11
(1,1088)	1:183:A:ALA:HB1	1:211:A:LEU:HD12	5	0.11
(1,1088)	1:183:A:ALA:HB1	1:211:A:LEU:HD13	5	0.11
(1,1088)	1:183:A:ALA:HB2	1:211:A:LEU:HD11	5	0.11
(1,1088)	1:183:A:ALA:HB2	1:211:A:LEU:HD12	5	0.11
(1,1088)	1:183:A:ALA:HB2	1:211:A:LEU:HD13	5	0.11
(1,1088)	1:183:A:ALA:HB3	1:211:A:LEU:HD11	5	0.11
(1,1088)	1:183:A:ALA:HB3	1:211:A:LEU:HD12	5	0.11
(1,1088)	1:183:A:ALA:HB3	1:211:A:LEU:HD13	5	0.11
(1,1079)	1:152:A:ALA:HB1	1:224:A:VAL:HA	6	0.11
(1,1079)	1:152:A:ALA:HB2	1:224:A:VAL:HA	6	0.11
(1,1079)	1:152:A:ALA:HB3	1:224:A:VAL:HA	6	0.11
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	1	0.11
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	1	0.11
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	1	0.11
(1,1075)	1:137:A:ALA:HB1	1:150:A:ALA:H	5	0.11
(1,1075)	1:137:A:ALA:HB2	1:150:A:ALA:H	5	0.11
(1,1075)	1:137:A:ALA:HB3	1:150:A:ALA:H	5	0.11
(1,1072)	1:186:A:ILE:HG21	1:188:A:GLN:HA	3	0.11
(1,1072)	1:186:A:ILE:HG22	1:188:A:GLN:HA	3	0.11
(1,1072)	1:186:A:ILE:HG23	1:188:A:GLN:HA	3	0.11
(1,1072)	1:186:A:ILE:HG21	1:188:A:GLN:HA	6	0.11
(1,1072)	1:186:A:ILE:HG22	1:188:A:GLN:HA	6	0.11
(1,1072)	1:186:A:ILE:HG23	1:188:A:GLN:HA	6	0.11
(1,1069)	1:242:A:HIS:HA	1:245:A:SER:H	9	0.11
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB2	4	0.11
(1,1056)	1:136:A:THR:HG21	1:253:A:ARG:HB3	4	0.11
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB2	4	0.11
(1,1056)	1:136:A:THR:HG22	1:253:A:ARG:HB3	4	0.11
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB2	4	0.11
(1,1056)	1:136:A:THR:HG23	1:253:A:ARG:HB3	4	0.11
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	5	0.11
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	5	0.11
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	5	0.11
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	10	0.11
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	10	0.11
(1,1035)	1:22:A:LEU:HD21	1:23:A:LEU:H	10	0.11
(1,1035)	1:22:A:LEU:HD22	1:23:A:LEU:H	10	0.11
(1,1035)	1:22:A:LEU:HD23	1:23:A:LEU:H	10	0.11
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG21	4	0.11
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG22	4	0.11
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG23	4	0.11
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG21	9	0.11
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG22	9	0.11
(1,1033)	1:136:A:THR:H	1:136:A:THR:HG23	9	0.11
(1,1027)	1:135:A:TRP:HA	1:154:A:HIS:HD2	10	0.11
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE21	10	0.11
(1,1010)	1:26:A:LYS:HA	1:27:A:GLN:HE22	10	0.11
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	1	0.11
(1,990)	1:107:A:LEU:HA	1:110:A:VAL:HB	9	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD21	1	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD22	1	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD23	1	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD21	3	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD22	3	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD23	3	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD21	8	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD22	8	0.11
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD23	8	0.11
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD11	2	0.11
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD12	2	0.11
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD13	2	0.11
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD11	9	0.11
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD12	9	0.11
(1,904)	1:213:A:LEU:HA	1:213:A:LEU:HD13	9	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG21	2	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG22	2	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG23	2	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG21	2	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG22	2	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG23	2	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG21	4	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG22	4	0.11
(1,875)	1:127:A:ILE:HG12	1:147:A:THR:HG23	4	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG21	4	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG22	4	0.11
(1,875)	1:127:A:ILE:HG13	1:147:A:THR:HG23	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG2	7	0.11
(1,870)	1:133:A:GLU:HA	1:133:A:GLU:HG3	7	0.11
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	5	0.11
(1,741)	1:37:A:VAL:HG11	1:41:A:GLU:HA	2	0.11
(1,741)	1:37:A:VAL:HG12	1:41:A:GLU:HA	2	0.11
(1,741)	1:37:A:VAL:HG13	1:41:A:GLU:HA	2	0.11
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	6	0.11
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	7	0.11
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	8	0.11
(1,714)	1:187:A:LYS:HD2	1:220:A:TRP:HD1	10	0.11
(1,703)	1:116:A:GLU:HA	1:117:A:GLU:HB2	4	0.11
(1,695)	1:8:A:LEU:HD21	1:31:A:SER:HA	4	0.11
(1,695)	1:8:A:LEU:HD22	1:31:A:SER:HA	4	0.11
(1,695)	1:8:A:LEU:HD23	1:31:A:SER:HA	4	0.11
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD21	2	0.11
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD22	2	0.11
(1,686)	1:106:A:GLU:HB2	1:107:A:LEU:HD23	2	0.11
(1,621)	1:117:A:GLU:H	1:118:A:GLU:HB3	6	0.11
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB1	1	0.11
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB2	1	0.11
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB3	1	0.11
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG21	4	0.11
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG22	4	0.11
(1,577)	1:43:A:MET:HG2	1:64:A:VAL:HG23	4	0.11
(1,528)	1:82:A:GLN:H	1:82:A:GLN:HG3	7	0.11
(1,505)	1:26:A:LYS:HB2	1:27:A:GLN:HA	10	0.11
(1,493)	1:243:A:ILE:HA	1:245:A:SER:H	3	0.11
(1,490)	1:48:A:SER:HB2	1:60:A:ASN:HB2	1	0.11
(1,490)	1:48:A:SER:HB2	1:60:A:ASN:HB2	2	0.11
(1,488)	1:96:A:GLY:H	1:97:A:SER:HB3	7	0.11
(1,477)	1:219:A:VAL:HB	1:220:A:TRP:H	6	0.11
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	1	0.11
(1,470)	1:48:A:SER:HB2	1:60:A:ASN:HB3	2	0.11
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD1	3	0.11
(1,461)	1:19:A:TYR:HE1	1:101:A:PHE:HD2	3	0.11
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD1	3	0.11
(1,461)	1:19:A:TYR:HE2	1:101:A:PHE:HD2	3	0.11
(1,406)	1:187:A:LYS:HB3	1:220:A:TRP:HD1	6	0.11
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	1	0.11
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	5	0.11
(1,399)	1:220:A:TRP:HB2	1:220:A:TRP:HE1	5	0.11
(1,387)	1:66:A:VAL:HB	1:78:A:THR:HG21	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:66:A:VAL:HB	1:78:A:THR:HG22	8	0.11
(1,387)	1:66:A:VAL:HB	1:78:A:THR:HG23	8	0.11
(1,347)	1:3:A:ASP:HB2	1:6:A:GLU:HG2	8	0.11
(1,347)	1:3:A:ASP:HB3	1:6:A:GLU:HG2	8	0.11
(1,345)	1:6:A:GLU:HA	1:6:A:GLU:HG2	5	0.11
(1,342)	1:57:A:GLU:HA	1:57:A:GLU:HG2	2	0.11
(1,332)	1:9:A:VAL:HA	1:13:A:GLU:HG3	3	0.11
(1,332)	1:9:A:VAL:HA	1:13:A:GLU:HG3	6	0.11
(1,324)	1:105:A:THR:HB	1:106:A:GLU:H	4	0.11
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG2	5	0.11
(1,300)	1:37:A:VAL:H	1:41:A:GLU:HG3	5	0.11
(1,289)	1:158:A:GLU:HG2	1:159:A:GLU:H	5	0.11
(1,273)	1:135:A:TRP:HA	1:136:A:THR:HB	6	0.11
(1,265)	1:100:A:LEU:HD21	1:101:A:PHE:HB2	4	0.11
(1,265)	1:100:A:LEU:HD22	1:101:A:PHE:HB2	4	0.11
(1,265)	1:100:A:LEU:HD23	1:101:A:PHE:HB2	4	0.11
(1,230)	1:194:A:THR:H	1:194:A:THR:HB	8	0.11
(1,228)	1:186:A:ILE:H	1:194:A:THR:HB	6	0.11
(1,215)	1:29:A:ASP:HB2	1:30:A:GLY:H	1	0.11
(1,211)	1:81:A:LEU:HB3	1:84:A:LEU:HG	6	0.11
(1,211)	1:81:A:LEU:HB3	1:84:A:LEU:HG	10	0.11
(1,198)	1:166:A:ASP:HB2	1:167:A:LEU:H	6	0.11
(1,194)	1:2:A:ASP:HB2	1:3:A:ASP:H	5	0.11
(1,145)	1:108:A:ASP:HB2	1:109:A:GLY:H	3	0.11
(1,115)	1:186:A:ILE:HB	1:195:A:TYR:HB3	1	0.11
(1,60)	1:134:A:GLY:HA3	1:164:A:MET:HB2	7	0.11
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD11	5	0.11
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD12	5	0.11
(1,22)	1:24:A:SER:H	1:33:A:ILE:HD13	5	0.11
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG21	1	0.11
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG22	1	0.11
(1,9)	1:183:A:ALA:H	1:223:A:ILE:HG23	1	0.11
(1,7)	1:168:A:LEU:HD21	1:174:A:MET:HE1	7	0.11
(1,7)	1:168:A:LEU:HD21	1:174:A:MET:HE2	7	0.11
(1,7)	1:168:A:LEU:HD21	1:174:A:MET:HE3	7	0.11
(1,7)	1:168:A:LEU:HD22	1:174:A:MET:HE1	7	0.11
(1,7)	1:168:A:LEU:HD22	1:174:A:MET:HE2	7	0.11
(1,7)	1:168:A:LEU:HD22	1:174:A:MET:HE3	7	0.11
(1,7)	1:168:A:LEU:HD23	1:174:A:MET:HE1	7	0.11
(1,7)	1:168:A:LEU:HD23	1:174:A:MET:HE2	7	0.11
(1,7)	1:168:A:LEU:HD23	1:174:A:MET:HE3	7	0.11
(1,5)	1:174:A:MET:H	1:174:A:MET:HE1	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:174:A:MET:H	1:174:A:MET:HE2	6	0.11
(1,5)	1:174:A:MET:H	1:174:A:MET:HE3	6	0.11
(1,2587)	1:92:A:VAL:HG21	1:103:A:PHE:H	4	0.1
(1,2587)	1:92:A:VAL:HG22	1:103:A:PHE:H	4	0.1
(1,2587)	1:92:A:VAL:HG23	1:103:A:PHE:H	4	0.1
(1,2496)	1:251:A:VAL:HG11	1:253:A:ARG:H	1	0.1
(1,2496)	1:251:A:VAL:HG12	1:253:A:ARG:H	1	0.1
(1,2496)	1:251:A:VAL:HG13	1:253:A:ARG:H	1	0.1
(1,2440)	1:84:A:LEU:H	1:87:A:GLU:HB2	5	0.1
(1,2440)	1:84:A:LEU:H	1:87:A:GLU:HB3	5	0.1
(1,2426)	1:125:A:SER:HA	1:126:A:ASP:HB3	3	0.1
(1,2359)	1:40:A:HIS:HA	1:42:A:TYR:H	4	0.1
(1,2356)	1:217:A:MET:H	1:219:A:VAL:H	5	0.1
(1,2333)	1:51:A:THR:H	1:53:A:TYR:HE1	5	0.1
(1,2333)	1:51:A:THR:H	1:53:A:TYR:HE2	5	0.1
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG21	8	0.1
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG22	8	0.1
(1,2329)	1:162:A:PHE:H	1:223:A:ILE:HG23	8	0.1
(1,2294)	1:76:A:TYR:HB3	1:81:A:LEU:H	7	0.1
(1,2248)	1:64:A:VAL:HG21	1:83:A:HIS:H	3	0.1
(1,2248)	1:64:A:VAL:HG22	1:83:A:HIS:H	3	0.1
(1,2248)	1:64:A:VAL:HG23	1:83:A:HIS:H	3	0.1
(1,2211)	1:5:A:HIS:H	1:7:A:GLN:H	2	0.1
(1,2209)	1:98:A:VAL:H	1:101:A:PHE:H	9	0.1
(1,2196)	1:88:A:VAL:HG21	1:90:A:ASP:H	7	0.1
(1,2196)	1:88:A:VAL:HG22	1:90:A:ASP:H	7	0.1
(1,2196)	1:88:A:VAL:HG23	1:90:A:ASP:H	7	0.1
(1,2129)	1:222:A:VAL:HG11	1:256:A:PHE:H	9	0.1
(1,2129)	1:222:A:VAL:HG12	1:256:A:PHE:H	9	0.1
(1,2129)	1:222:A:VAL:HG13	1:256:A:PHE:H	9	0.1
(1,2055)	1:127:A:ILE:HD11	1:141:A:ILE:H	1	0.1
(1,2055)	1:127:A:ILE:HD12	1:141:A:ILE:H	1	0.1
(1,2055)	1:127:A:ILE:HD13	1:141:A:ILE:H	1	0.1
(1,2021)	1:8:A:LEU:H	1:10:A:GLU:H	5	0.1
(1,1998)	1:203:A:GLU:H	1:205:A:ALA:H	5	0.1
(1,1986)	1:160:A:GLN:H	1:163:A:ALA:H	1	0.1
(1,1915)	1:181:A:MET:H	1:228:A:ARG:H	4	0.1
(1,1883)	1:27:A:GLN:HB3	1:30:A:GLY:H	1	0.1
(1,1747)	1:11:A:GLU:HA	1:13:A:GLU:H	10	0.1
(1,1737)	1:72:A:LYS:HD2	1:73:A:ARG:H	8	0.1
(1,1737)	1:72:A:LYS:HD3	1:73:A:ARG:H	8	0.1
(1,1606)	1:50:A:PRO:HG3	1:53:A:TYR:H	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1585)	1:11:A:GLU:H	1:11:A:GLU:HG3	3	0.1
(1,1585)	1:11:A:GLU:H	1:11:A:GLU:HG3	5	0.1
(1,1547)	1:133:A:GLU:H	1:135:A:TRP:HB3	5	0.1
(1,1461)	1:43:A:MET:HE1	1:66:A:VAL:H	10	0.1
(1,1461)	1:43:A:MET:HE2	1:66:A:VAL:H	10	0.1
(1,1461)	1:43:A:MET:HE3	1:66:A:VAL:H	10	0.1
(1,1420)	1:58:A:ALA:HB1	1:93:A:PHE:HB2	6	0.1
(1,1420)	1:58:A:ALA:HB2	1:93:A:PHE:HB2	6	0.1
(1,1420)	1:58:A:ALA:HB3	1:93:A:PHE:HB2	6	0.1
(1,1414)	1:32:A:ILE:HG21	1:49:A:PHE:HD2	1	0.1
(1,1414)	1:32:A:ILE:HG22	1:49:A:PHE:HD2	1	0.1
(1,1414)	1:32:A:ILE:HG23	1:49:A:PHE:HD2	1	0.1
(1,1405)	1:33:A:ILE:HG21	1:49:A:PHE:HD2	2	0.1
(1,1405)	1:33:A:ILE:HG22	1:49:A:PHE:HD2	2	0.1
(1,1405)	1:33:A:ILE:HG23	1:49:A:PHE:HD2	2	0.1
(1,1405)	1:33:A:ILE:HG21	1:49:A:PHE:HD2	7	0.1
(1,1405)	1:33:A:ILE:HG22	1:49:A:PHE:HD2	7	0.1
(1,1405)	1:33:A:ILE:HG23	1:49:A:PHE:HD2	7	0.1
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE1	9	0.1
(1,1335)	1:254:A:ALA:HB1	1:256:A:PHE:HE2	9	0.1
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE1	9	0.1
(1,1335)	1:254:A:ALA:HB2	1:256:A:PHE:HE2	9	0.1
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE1	9	0.1
(1,1335)	1:254:A:ALA:HB3	1:256:A:PHE:HE2	9	0.1
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG11	8	0.1
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG12	8	0.1
(1,1267)	1:47:A:ILE:HG21	1:61:A:VAL:HG13	8	0.1
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG11	8	0.1
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG12	8	0.1
(1,1267)	1:47:A:ILE:HG22	1:61:A:VAL:HG13	8	0.1
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG11	8	0.1
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG12	8	0.1
(1,1267)	1:47:A:ILE:HG23	1:61:A:VAL:HG13	8	0.1
(1,1239)	1:8:A:LEU:HD11	1:9:A:VAL:H	9	0.1
(1,1239)	1:8:A:LEU:HD12	1:9:A:VAL:H	9	0.1
(1,1239)	1:8:A:LEU:HD13	1:9:A:VAL:H	9	0.1
(1,1155)	1:98:A:VAL:H	1:98:A:VAL:HG11	3	0.1
(1,1155)	1:98:A:VAL:H	1:98:A:VAL:HG12	3	0.1
(1,1155)	1:98:A:VAL:H	1:98:A:VAL:HG13	3	0.1
(1,1152)	1:127:A:ILE:HG21	1:147:A:THR:HG21	4	0.1
(1,1152)	1:127:A:ILE:HG21	1:147:A:THR:HG22	4	0.1
(1,1152)	1:127:A:ILE:HG21	1:147:A:THR:HG23	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1152)	1:127:A:ILE:HG22	1:147:A:THR:HG21	4	0.1
(1,1152)	1:127:A:ILE:HG22	1:147:A:THR:HG22	4	0.1
(1,1152)	1:127:A:ILE:HG22	1:147:A:THR:HG23	4	0.1
(1,1152)	1:127:A:ILE:HG23	1:147:A:THR:HG21	4	0.1
(1,1152)	1:127:A:ILE:HG23	1:147:A:THR:HG22	4	0.1
(1,1152)	1:127:A:ILE:HG23	1:147:A:THR:HG23	4	0.1
(1,1051)	1:137:A:ALA:HB1	1:151:A:PHE:HE1	10	0.1
(1,1051)	1:137:A:ALA:HB2	1:151:A:PHE:HE1	10	0.1
(1,1051)	1:137:A:ALA:HB3	1:151:A:PHE:HE1	10	0.1
(1,1048)	1:246:A:THR:HG21	1:247:A:ALA:HA	8	0.1
(1,1048)	1:246:A:THR:HG22	1:247:A:ALA:HA	8	0.1
(1,1048)	1:246:A:THR:HG23	1:247:A:ALA:HA	8	0.1
(1,1017)	1:150:A:ALA:HB1	1:226:A:VAL:HB	5	0.1
(1,1017)	1:150:A:ALA:HB2	1:226:A:VAL:HB	5	0.1
(1,1017)	1:150:A:ALA:HB3	1:226:A:VAL:HB	5	0.1
(1,984)	1:168:A:LEU:HD21	1:225:A:VAL:H	7	0.1
(1,984)	1:168:A:LEU:HD22	1:225:A:VAL:H	7	0.1
(1,984)	1:168:A:LEU:HD23	1:225:A:VAL:H	7	0.1
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD21	4	0.1
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD22	4	0.1
(1,958)	1:84:A:LEU:HA	1:84:A:LEU:HD23	4	0.1
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD21	4	0.1
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD22	4	0.1
(1,920)	1:165:A:LEU:HA	1:165:A:LEU:HD23	4	0.1
(1,798)	1:5:A:HIS:HA	1:9:A:VAL:HB	8	0.1
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG2	7	0.1
(1,790)	1:175:A:ARG:H	1:175:A:ARG:HG3	7	0.1
(1,777)	1:42:A:TYR:HD1	1:66:A:VAL:HA	2	0.1
(1,777)	1:42:A:TYR:HD2	1:66:A:VAL:HA	2	0.1
(1,763)	1:18:A:ILE:HG13	1:19:A:TYR:HE1	8	0.1
(1,763)	1:18:A:ILE:HG13	1:19:A:TYR:HE2	8	0.1
(1,640)	1:9:A:VAL:HG11	1:10:A:GLU:HB2	5	0.1
(1,640)	1:9:A:VAL:HG12	1:10:A:GLU:HB2	5	0.1
(1,640)	1:9:A:VAL:HG13	1:10:A:GLU:HB2	5	0.1
(1,640)	1:9:A:VAL:HG21	1:10:A:GLU:HB2	5	0.1
(1,640)	1:9:A:VAL:HG22	1:10:A:GLU:HB2	5	0.1
(1,640)	1:9:A:VAL:HG23	1:10:A:GLU:HB2	5	0.1
(1,621)	1:117:A:GLU:H	1:118:A:GLU:HB3	1	0.1
(1,621)	1:117:A:GLU:H	1:118:A:GLU:HB3	7	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB1	5	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB2	5	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB3	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB1	9	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB2	9	0.1
(1,606)	1:136:A:THR:HA	1:137:A:ALA:HB3	9	0.1
(1,572)	1:79:A:LYS:HB2	1:80:A:TYR:H	3	0.1
(1,570)	1:149:A:MET:HG2	1:150:A:ALA:H	3	0.1
(1,570)	1:149:A:MET:HG3	1:150:A:ALA:H	3	0.1
(1,536)	1:24:A:SER:HB2	1:25:A:LYS:H	1	0.1
(1,536)	1:24:A:SER:HB3	1:25:A:LYS:H	1	0.1
(1,493)	1:243:A:ILE:HA	1:245:A:SER:H	4	0.1
(1,490)	1:48:A:SER:HB2	1:60:A:ASN:HB2	4	0.1
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD1	7	0.1
(1,464)	1:18:A:ILE:HG21	1:101:A:PHE:HD2	7	0.1
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD1	7	0.1
(1,464)	1:18:A:ILE:HG22	1:101:A:PHE:HD2	7	0.1
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD1	7	0.1
(1,464)	1:18:A:ILE:HG23	1:101:A:PHE:HD2	7	0.1
(1,440)	1:27:A:GLN:HG3	1:28:A:GLU:H	3	0.1
(1,404)	1:64:A:VAL:H	1:64:A:VAL:HB	8	0.1
(1,399)	1:220:A:TRP:HB2	1:220:A:TRP:HE1	1	0.1
(1,399)	1:220:A:TRP:HB2	1:220:A:TRP:HE1	8	0.1
(1,383)	1:7:A:GLN:H	1:7:A:GLN:HG3	5	0.1
(1,332)	1:9:A:VAL:HA	1:13:A:GLU:HG3	8	0.1
(1,293)	1:39:A:GLN:H	1:41:A:GLU:HG2	2	0.1
(1,293)	1:39:A:GLN:H	1:41:A:GLU:HG3	2	0.1
(1,283)	1:158:A:GLU:HG3	1:162:A:PHE:HD1	2	0.1
(1,283)	1:158:A:GLU:HG3	1:162:A:PHE:HD2	2	0.1
(1,260)	1:119:A:THR:HB	1:120:A:GLU:H	7	0.1
(1,253)	1:16:A:GLU:H	1:18:A:ILE:HB	2	0.1
(1,232)	1:186:A:ILE:HB	1:194:A:THR:HB	7	0.1
(1,230)	1:194:A:THR:H	1:194:A:THR:HB	3	0.1
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG11	8	0.1
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG12	8	0.1
(1,148)	1:26:A:LYS:HE2	1:34:A:VAL:HG13	8	0.1
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG11	8	0.1
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG12	8	0.1
(1,148)	1:26:A:LYS:HE3	1:34:A:VAL:HG13	8	0.1
(1,60)	1:134:A:GLY:HA3	1:164:A:MET:HB2	2	0.1
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE1	2	0.1
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE2	2	0.1
(1,19)	1:47:A:ILE:HG21	1:89:A:MET:HE3	2	0.1
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE1	2	0.1
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE2	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:47:A:ILE:HG22	1:89:A:MET:HE3	2	0.1
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE1	2	0.1
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE2	2	0.1
(1,19)	1:47:A:ILE:HG23	1:89:A:MET:HE3	2	0.1

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

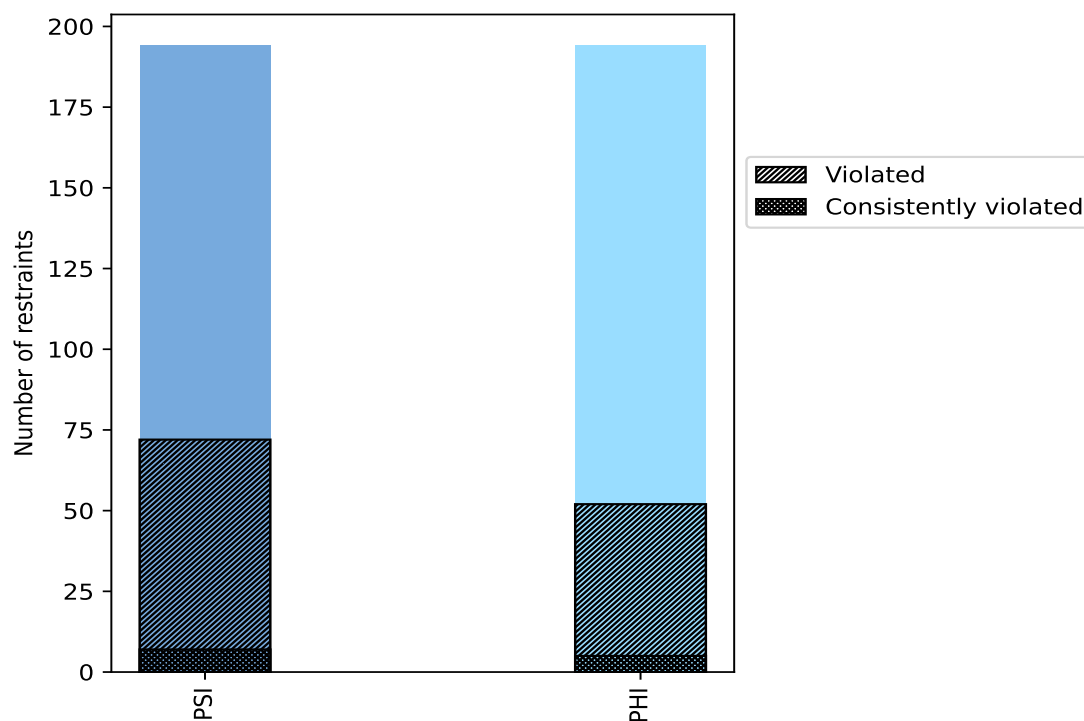
10.1 Summary of dihedral-angle violations [i](#)

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	194	50.0	72	37.1	18.6	7	3.6	1.8
PHI	194	50.0	52	26.8	13.4	5	2.6	1.3
Total	388	100.0	124	32.0	32.0	12	3.1	3.1

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](#)



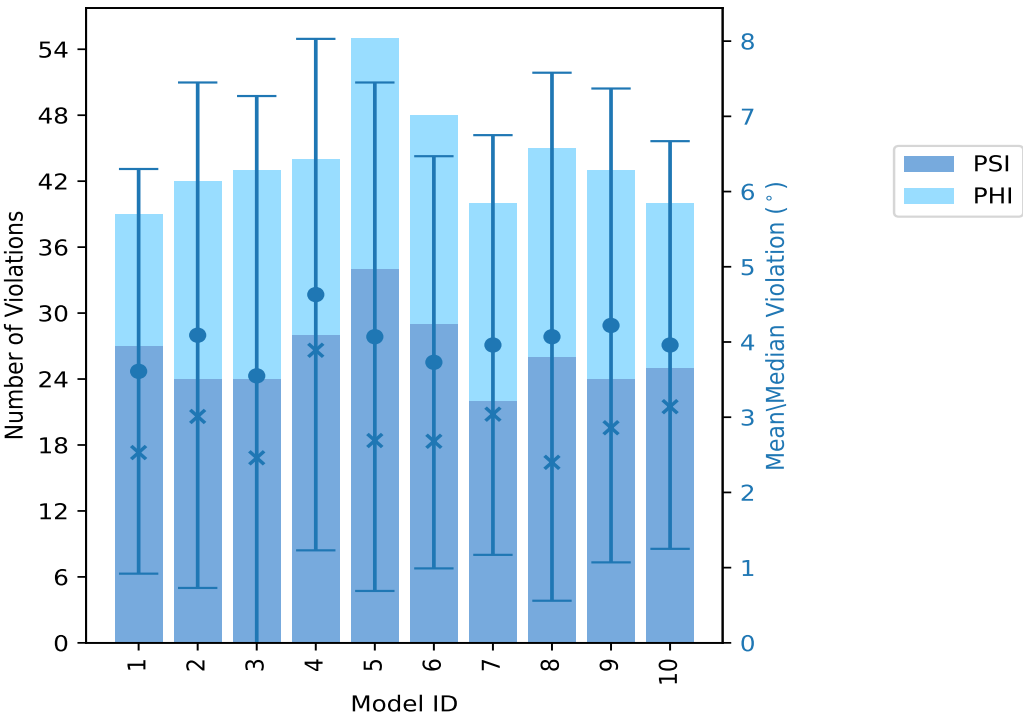
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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	27	12	39	3.61	12.24	2.69	2.53
2	24	18	42	4.09	14.94	3.36	3.01
3	24	19	43	3.55	23.16	3.72	2.46
4	28	16	44	4.63	20.73	3.4	3.89
5	34	21	55	4.07	19.58	3.38	2.69
6	29	19	48	3.73	13.92	2.74	2.68
7	22	18	40	3.96	13.06	2.79	3.04
8	26	19	45	4.07	17.91	3.51	2.4
9	24	19	43	4.22	14.06	3.15	2.86
10	25	15	40	3.96	13.17	2.71	3.14

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

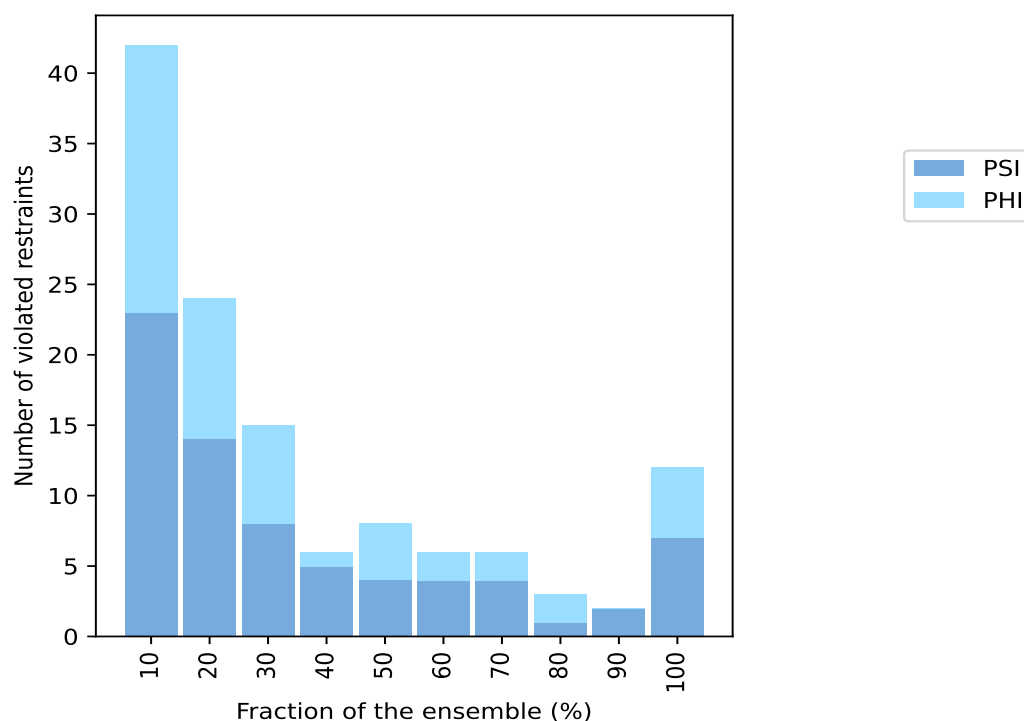
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
23	19	42	1	10.0
14	10	24	2	20.0
8	7	15	3	30.0
5	1	6	4	40.0
4	4	8	5	50.0
4	2	6	6	60.0
4	2	6	7	70.0
1	2	3	8	80.0
2	0	2	9	90.0
7	5	12	10	100.0

¹ Number of models with violations

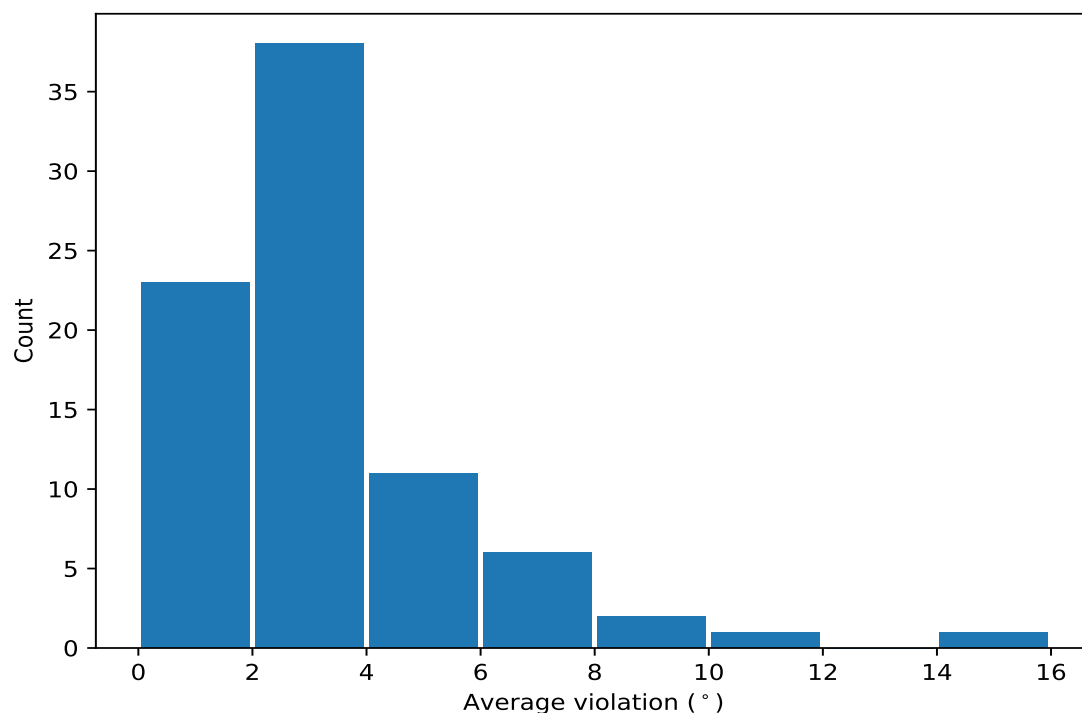
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	10	11.64	3.31	13.12
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	10	9.46	1.64	9.8
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	10	7.89	0.74	8.12
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	10	7.18	2.4	7.52
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	10	6.99	1.34	7.07
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	10	5.79	1.18	5.51
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	10	4.86	1.7	4.68
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	10	4.84	1.99	4.12
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	10	4.53	0.88	4.8
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	10	3.75	0.98	3.72
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	10	3.43	2.21	2.54
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	10	3.04	1.59	2.52
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	9	3.63	1.58	2.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	9	3.15	1.35	3.77
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	8	4.08	3.15	2.42
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	8	3.9	1.76	4.06
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	8	2.77	0.77	2.8
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	7	7.44	5.13	5.62
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	7	3.47	1.91	3.25
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	7	3.43	1.42	3.21
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	7	3.26	1.0	3.19
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	7	2.62	0.71	2.61
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	7	2.05	0.35	2.12
(1,132)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:GLY:N	6	14.8	7.26	16.42
(1,90)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:THR:N	6	3.51	2.0	3.4
(1,346)	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	1:230:A:PHE:N	6	3.2	1.06	2.76
(1,231)	1:159:A:GLU:C	1:160:A:GLN:N	1:160:A:GLN:CA	1:160:A:GLN:C	6	1.7	0.65	1.33
(1,35)	1:21:A:ASP:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	6	1.61	0.23	1.54
(1,48)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:VAL:N	6	1.39	0.25	1.38
(1,131)	1:94:A:HIS:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	5	8.2	2.11	7.17
(1,294)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:200:A:ASP:N	5	3.74	1.9	3.02
(1,66)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:PHE:N	5	3.4	1.64	2.6
(1,27)	1:16:A:GLU:C	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	5	2.78	1.38	2.65
(1,89)	1:66:A:VAL:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	5	1.81	0.6	1.75
(1,222)	1:155:A:VAL:N	1:155:A:VAL:CA	1:155:A:VAL:C	1:156:A:THR:N	5	1.71	0.8	1.33
(1,353)	1:237:A:PRO:C	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	5	1.48	0.46	1.32
(1,350)	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	1:235:A:ILE:N	5	1.45	0.42	1.26
(1,76)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLU:N	4	6.11	3.08	7.35
(1,128)	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	1:93:A:PHE:N	4	4.52	1.57	5.04
(1,92)	1:71:A:ALA:N	1:71:A:ALA:CA	1:71:A:ALA:C	1:72:A:LYS:N	4	2.46	1.4	2.37
(1,277)	1:186:A:ILE:C	1:187:A:LYS:N	1:187:A:LYS:CA	1:187:A:LYS:C	4	1.76	0.62	1.72
(1,186)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:ALA:N	4	1.55	0.3	1.61
(1,378)	1:250:A:ALA:N	1:250:A:ALA:CA	1:250:A:ALA:C	1:251:A:VAL:N	4	1.28	0.23	1.27
(1,356)	1:239:A:ARG:N	1:239:A:ARG:CA	1:239:A:ARG:C	1:240:A:PHE:N	3	4.25	0.29	4.11
(1,33)	1:20:A:PRO:C	1:21:A:ASP:N	1:21:A:ASP:CA	1:21:A:ASP:C	3	4.18	1.21	4.35
(1,142)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	1:104:A:LEU:N	3	2.99	0.49	2.83
(1,347)	1:232:A:GLY:C	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	3	2.94	1.47	3.1
(1,301)	1:205:A:ALA:C	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	3	2.92	1.04	3.37
(1,95)	1:72:A:LYS:C	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	3	2.87	0.86	2.76
(1,302)	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	1:207:A:GLY:N	3	2.83	0.33	2.97
(1,208)	1:148:A:PHE:N	1:148:A:PHE:CA	1:148:A:PHE:C	1:149:A:MET:N	3	2.63	0.49	2.63
(1,202)	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	1:146:A:SER:N	3	2.28	0.58	2.22
(1,134)	1:97:A:SER:N	1:97:A:SER:CA	1:97:A:SER:C	1:98:A:VAL:N	3	2.24	1.06	1.83
(1,153)	1:108:A:ASP:C	1:109:A:GLY:N	1:109:A:GLY:CA	1:109:A:GLY:C	3	2.09	0.47	2.17
(1,357)	1:239:A:ARG:C	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	3	1.69	0.22	1.66
(1,204)	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	1:147:A:THR:N	3	1.6	0.07	1.56
(1,238)	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	1:164:A:MET:N	3	1.54	0.15	1.62
(1,181)	1:133:A:GLU:C	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	3	1.47	0.07	1.52
(1,290)	1:197:A:ASP:N	1:197:A:ASP:CA	1:197:A:ASP:C	1:198:A:SER:N	2	6.43	1.02	6.43
(1,4)	1:5:A:HIS:N	1:5:A:HIS:CA	1:5:A:HIS:C	1:6:A:GLU:N	2	5.48	1.98	5.48
(1,227)	1:157:A:SER:C	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	2	5.36	0.19	5.36
(1,170)	1:128:A:PRO:N	1:128:A:PRO:CA	1:128:A:PRO:C	1:129:A:THR:N	2	4.33	2.56	4.33
(1,252)	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	1:171:A:ASP:N	2	3.62	1.14	3.62
(1,116)	1:85:A:PHE:N	1:85:A:PHE:CA	1:85:A:PHE:C	1:86:A:GLN:N	2	3.46	0.9	3.46

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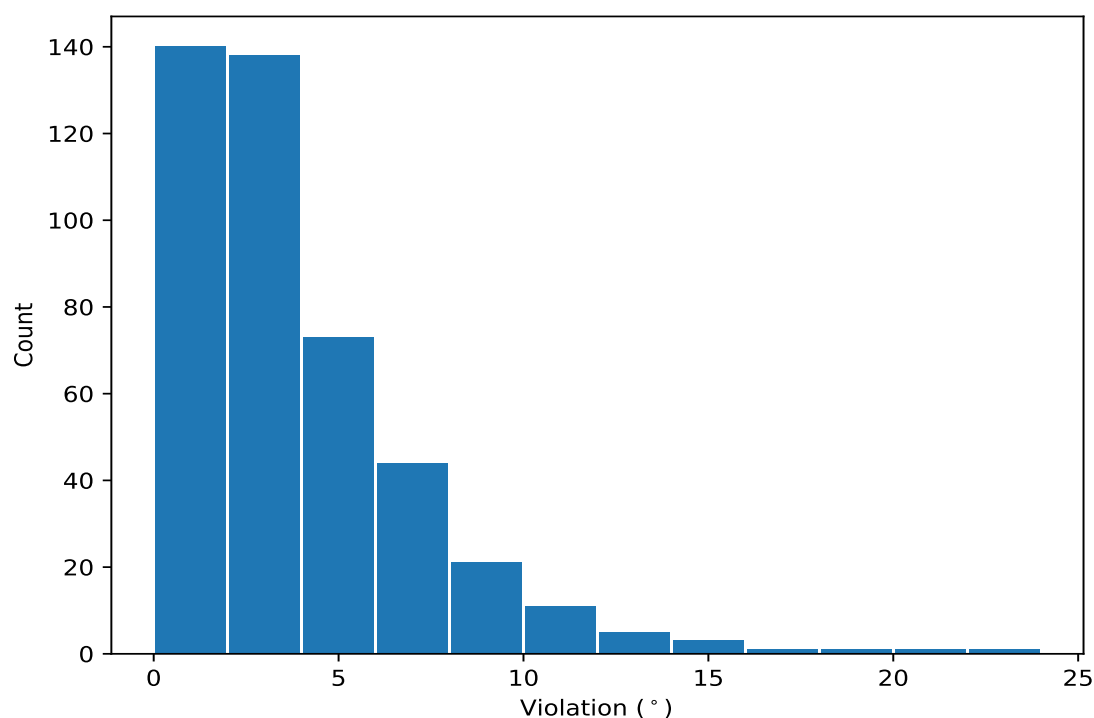
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,93)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	2	3.34	0.7	3.34
(1,341)	1:226:A:VAL:C	1:227:A:ALA:N	1:227:A:ALA:CA	1:227:A:ALA:C	2	2.84	0.71	2.84
(1,244)	1:166:A:ASP:N	1:166:A:ASP:CA	1:166:A:ASP:C	1:167:A:LEU:N	2	2.73	0.8	2.73
(1,288)	1:196:A:GLN:N	1:196:A:GLN:CA	1:196:A:GLN:C	1:197:A:ASP:N	2	2.7	0.88	2.7
(1,29)	1:17:A:ALA:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	2	2.54	1.3	2.54
(1,340)	1:226:A:VAL:N	1:226:A:VAL:CA	1:226:A:VAL:C	1:227:A:ALA:N	2	2.4	1.12	2.4
(1,129)	1:93:A:PHE:C	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	2	2.33	0.35	2.33
(1,69)	1:49:A:PHE:C	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	2	2.3	0.27	2.3
(1,81)	1:62:A:ILE:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	2	2.03	0.95	2.03
(1,354)	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	1:239:A:ARG:N	2	1.94	0.5	1.94
(1,82)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:VAL:N	2	1.83	0.41	1.83
(1,264)	1:178:A:ASN:N	1:178:A:ASN:CA	1:178:A:ASN:C	1:179:A:HIS:N	2	1.8	0.26	1.8
(1,94)	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	1:73:A:ARG:N	2	1.54	0.28	1.54
(1,36)	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	1:23:A:LEU:N	2	1.4	0.09	1.4
(1,171)	1:128:A:PRO:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	2	1.26	0.05	1.26
(1,219)	1:153:A:ALA:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	2	1.21	0.15	1.21
(1,209)	1:148:A:PHE:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	2	1.19	0.19	1.19
(1,24)	1:15:A:VAL:N	1:15:A:VAL:CA	1:15:A:VAL:C	1:16:A:GLU:N	2	1.19	0.11	1.19

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 (°)
(1,132)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:GLY:N	3	23.16
(1,132)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:GLY:N	4	20.73
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	5	19.58
(1,132)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:GLY:N	8	17.91
(1,132)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:GLY:N	2	14.94
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	2	14.6
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	9	14.06
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	6	13.92
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	8	13.5
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	10	13.17
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	7	13.06
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	1	12.24
(1,131)	1:94:A:HIS:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	5	11.74
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	2	11.64
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	6	11.15
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	5	11.13
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	4	11.03
(1,132)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:GLY:N	9	10.96
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	9	10.9
(1,239)	1:163:A:ALA:C	1:164:A:MET:N	1:164:A:MET:CA	1:164:A:MET:C	5	10.72
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	10	10.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	8	10.17
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	1	10.15
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	3	9.64
(1,262)	1:176:A:LYS:N	1:176:A:LYS:CA	1:176:A:LYS:C	1:177:A:ALA:N	4	9.49
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	9	9.46
(1,131)	1:94:A:HIS:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	7	9.38
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	7	9.18
(1,344)	1:228:A:ARG:N	1:228:A:ARG:CA	1:228:A:ARG:C	1:229:A:TRP:N	9	9.04
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	8	9.01
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	1	8.83
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	9	8.77
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	2	8.74
(1,76)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLU:N	8	8.73
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	7	8.45
(1,76)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLU:N	4	8.39
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	2	8.33
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	10	8.31
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	6	8.28
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	5	8.18
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	3	8.14
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1	8.12
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	9	8.1
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	8	8.04
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	2	7.99
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	6	7.89
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	5	7.87
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	7	7.86
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	3	7.62
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	10	7.6
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	2	7.59
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	6	7.58
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	9	7.47
(1,4)	1:5:A:HIS:N	1:5:A:HIS:CA	1:5:A:HIS:C	1:6:A:GLU:N	4	7.46
(1,290)	1:197:A:ASP:N	1:197:A:ASP:CA	1:197:A:ASP:C	1:198:A:SER:N	5	7.45
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	8	7.45
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	8	7.38
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	4	7.36
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	7	7.3
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	3	7.3
(1,90)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:THR:N	6	7.3
(1,294)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:200:A:ASP:N	4	7.24
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	10	7.21
(1,131)	1:94:A:HIS:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1	7.17
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	4	7.15
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	6	7.14
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	7	7.1
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	5	7.1
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	7	7.05
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	1	7.0
(1,67)	1:48:A:SER:C	1:49:A:PHE:N	1:49:A:PHE:CA	1:49:A:PHE:C	5	6.99
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	2	6.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	10	6.95
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	9	6.93
(1,170)	1:128:A:PRO:N	1:128:A:PRO:CA	1:128:A:PRO:C	1:129:A:THR:N	4	6.89
(1,52)	1:36:A:LYS:N	1:36:A:LYS:CA	1:36:A:LYS:C	1:37:A:VAL:N	10	6.87
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	5	6.83
(1,131)	1:94:A:HIS:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	6	6.77
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	9	6.58
(1,190)	1:139:A:ASP:N	1:139:A:ASP:CA	1:139:A:ASP:C	1:140:A:PRO:N	8	6.53
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	4	6.34
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	3	6.33
(1,76)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLU:N	7	6.3
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	1	6.18
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	10	6.09
(1,246)	1:167:A:LEU:N	1:167:A:LEU:CA	1:167:A:LEU:C	1:168:A:LEU:N	5	6.07
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	8	6.04
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	3	6.04
(1,191)	1:139:A:ASP:C	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	4	5.99
(1,128)	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	1:93:A:PHE:N	10	5.93
(1,131)	1:94:A:HIS:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	10	5.92
(1,128)	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	1:93:A:PHE:N	7	5.83
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	5	5.79
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	4	5.7
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	9	5.62
(1,33)	1:20:A:PRO:C	1:21:A:ASP:N	1:21:A:ASP:CA	1:21:A:ASP:C	5	5.58
(1,227)	1:157:A:SER:C	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	3	5.55
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	6	5.55
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	5	5.53
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	8	5.47
(1,346)	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	1:230:A:PHE:N	8	5.4
(1,290)	1:197:A:ASP:N	1:197:A:ASP:CA	1:197:A:ASP:C	1:198:A:SER:N	9	5.4
(1,66)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:PHE:N	10	5.37
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	6	5.34
(1,27)	1:16:A:GLU:C	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	4	5.34
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	4	5.32
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	8	5.32
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	3	5.31
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	7	5.29
(1,66)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:PHE:N	9	5.29
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	6	5.22
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	2	5.22
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	1	5.18
(1,227)	1:157:A:SER:C	1:158:A:GLU:N	1:158:A:GLU:CA	1:158:A:GLU:C	4	5.18
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	1	5.11
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	4	5.01
(1,133)	1:96:A:GLY:C	1:97:A:SER:N	1:97:A:SER:CA	1:97:A:SER:C	5	5.01
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	9	4.89
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	10	4.88
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	6	4.85
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	10	4.84
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	6	4.83
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	2	4.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1	4.77
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	4	4.76
(1,252)	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	1:171:A:ASP:N	5	4.76
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	2	4.71
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	5	4.71
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	4	4.7
(1,356)	1:239:A:ARG:N	1:239:A:ARG:CA	1:239:A:ARG:C	1:240:A:PHE:N	6	4.66
(1,347)	1:232:A:GLY:C	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	8	4.66
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	7	4.55
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	5	4.52
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	1	4.48
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	5	4.47
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	6	4.47
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	9	4.46
(1,225)	1:156:A:THR:C	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	3	4.38
(1,116)	1:85:A:PHE:N	1:85:A:PHE:CA	1:85:A:PHE:C	1:86:A:GLN:N	4	4.36
(1,33)	1:20:A:PRO:C	1:21:A:ASP:N	1:21:A:ASP:CA	1:21:A:ASP:C	4	4.35
(1,224)	1:156:A:THR:N	1:156:A:THR:CA	1:156:A:THR:C	1:157:A:SER:N	3	4.34
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	10	4.34
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	2	4.29
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	6	4.26
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	2	4.24
(1,128)	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	1:93:A:PHE:N	1	4.24
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	2	4.22
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	4	4.21
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	10	4.2
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	10	4.18
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	7	4.18
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	9	4.18
(1,356)	1:239:A:ARG:N	1:239:A:ARG:CA	1:239:A:ARG:C	1:240:A:PHE:N	5	4.11
(1,92)	1:71:A:ALA:N	1:71:A:ALA:CA	1:71:A:ALA:C	1:72:A:LYS:N	8	4.11
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	3	4.1
(1,90)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:THR:N	5	4.07
(1,93)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	8	4.05
(1,200)	1:144:A:ARG:N	1:144:A:ARG:CA	1:144:A:ARG:C	1:145:A:GLY:N	1	4.04
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	6	4.02
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	7	4.01
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	3	4.0
(1,356)	1:239:A:ARG:N	1:239:A:ARG:CA	1:239:A:ARG:C	1:240:A:PHE:N	1	3.98
(1,95)	1:72:A:LYS:C	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	7	3.98
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	3	3.96
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	5	3.95
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	4	3.94
(1,294)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:200:A:ASP:N	6	3.93
(1,301)	1:205:A:ALA:C	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	6	3.92
(1,167)	1:126:A:ASP:C	1:127:A:ILE:N	1:127:A:ILE:CA	1:127:A:ILE:C	10	3.85
(1,90)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:THR:N	4	3.84
(1,29)	1:17:A:ALA:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	4	3.84
(1,285)	1:194:A:THR:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	2	3.78
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	1	3.78
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	10	3.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	7	3.75
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	7	3.74
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	8	3.71
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	6	3.7
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	8	3.69
(1,134)	1:97:A:SER:N	1:97:A:SER:CA	1:97:A:SER:C	1:98:A:VAL:N	5	3.69
(1,142)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	1:104:A:LEU:N	4	3.65
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	2	3.62
(1,288)	1:196:A:GLN:N	1:196:A:GLN:CA	1:196:A:GLN:C	1:197:A:ASP:N	2	3.58
(1,92)	1:71:A:ALA:N	1:71:A:ALA:CA	1:71:A:ALA:C	1:72:A:LYS:N	6	3.58
(1,341)	1:226:A:VAL:C	1:227:A:ALA:N	1:227:A:ALA:CA	1:227:A:ALA:C	9	3.55
(1,244)	1:166:A:ASP:N	1:166:A:ASP:CA	1:166:A:ASP:C	1:167:A:LEU:N	5	3.53
(1,340)	1:226:A:VAL:N	1:226:A:VAL:CA	1:226:A:VAL:C	1:227:A:ALA:N	5	3.52
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	8	3.52
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	9	3.51
(1,4)	1:5:A:HIS:N	1:5:A:HIS:CA	1:5:A:HIS:C	1:6:A:GLU:N	7	3.51
(1,192)	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	1:141:A:ILE:N	4	3.5
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	4	3.48
(1,346)	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	1:230:A:PHE:N	5	3.48
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	2	3.45
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	8	3.43
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	2	3.43
(1,301)	1:205:A:ALA:C	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	2	3.37
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	10	3.25
(1,208)	1:148:A:PHE:N	1:148:A:PHE:CA	1:148:A:PHE:C	1:149:A:MET:N	6	3.23
(1,222)	1:155:A:VAL:N	1:155:A:VAL:CA	1:155:A:VAL:C	1:156:A:THR:N	1	3.21
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	9	3.21
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	10	3.19
(1,302)	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	1:207:A:GLY:N	1	3.15
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	9	3.15
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	7	3.14
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	5	3.13
(1,347)	1:232:A:GLY:C	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	3	3.1
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	10	3.1
(1,349)	1:233:A:ALA:C	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	7	3.09
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	2	3.03
(1,294)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:200:A:ASP:N	9	3.02
(1,202)	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	1:146:A:SER:N	4	3.01
(1,346)	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	1:230:A:PHE:N	2	3.0
(1,81)	1:62:A:ILE:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	7	2.98
(1,302)	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	1:207:A:GLY:N	10	2.97
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	10	2.97
(1,90)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:THR:N	1	2.97
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	4	2.95
(1,294)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:200:A:ASP:N	3	2.89
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	1	2.88
(1,72)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:HIS:N	9	2.86
(1,142)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	1:104:A:LEU:N	6	2.83
(1,5)	1:5:A:HIS:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	4	2.81
(1,89)	1:66:A:VAL:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	9	2.79
(1,95)	1:72:A:LYS:C	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	2	2.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	6	2.73
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	9	2.72
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	4	2.7
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	3	2.69
(1,27)	1:16:A:GLU:C	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	5	2.69
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	9	2.68
(1,129)	1:93:A:PHE:C	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	7	2.68
(1,27)	1:16:A:GLU:C	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	10	2.65
(1,93)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	6	2.64
(1,385)	1:253:A:ARG:C	1:254:A:ALA:N	1:254:A:ALA:CA	1:254:A:ALA:C	3	2.63
(1,231)	1:159:A:GLU:C	1:160:A:GLN:N	1:160:A:GLN:CA	1:160:A:GLN:C	6	2.63
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	7	2.63
(1,208)	1:148:A:PHE:N	1:148:A:PHE:CA	1:148:A:PHE:C	1:149:A:MET:N	5	2.63
(1,153)	1:108:A:ASP:C	1:109:A:GLY:N	1:109:A:GLY:CA	1:109:A:GLY:C	3	2.62
(1,33)	1:20:A:PRO:C	1:21:A:ASP:N	1:21:A:ASP:CA	1:21:A:ASP:C	8	2.62
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	7	2.61
(1,66)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:PHE:N	7	2.6
(1,231)	1:159:A:GLU:C	1:160:A:GLN:N	1:160:A:GLN:CA	1:160:A:GLN:C	2	2.59
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	5	2.57
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	9	2.56
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	8	2.56
(1,116)	1:85:A:PHE:N	1:85:A:PHE:CA	1:85:A:PHE:C	1:86:A:GLN:N	3	2.56
(1,69)	1:49:A:PHE:C	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	5	2.56
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	7	2.55
(1,277)	1:186:A:ILE:C	1:187:A:LYS:N	1:187:A:LYS:CA	1:187:A:LYS:C	5	2.54
(1,346)	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	1:230:A:PHE:N	1	2.53
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	2	2.53
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	5	2.5
(1,252)	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	1:171:A:ASP:N	4	2.48
(1,142)	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	1:104:A:LEU:N	3	2.48
(1,346)	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	1:230:A:PHE:N	9	2.46
(1,70)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:THR:N	3	2.46
(1,354)	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	1:239:A:ARG:N	6	2.44
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	1	2.44
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	8	2.4
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	9	2.4
(1,353)	1:237:A:PRO:C	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	4	2.38
(1,302)	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	1:207:A:GLY:N	9	2.38
(1,66)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:PHE:N	8	2.38
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	1	2.37
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	7	2.36
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	6	2.36
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	3	2.35
(1,96)	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	1:74:A:ASP:N	8	2.32
(1,346)	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	1:230:A:PHE:N	6	2.3
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	2	2.3
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1	2.29
(1,55)	1:42:A:TYR:C	1:43:A:MET:N	1:43:A:MET:CA	1:43:A:MET:C	5	2.28
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	8	2.26
(1,82)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:VAL:N	7	2.24
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	4	2.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	10	2.22
(1,202)	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	1:146:A:SER:N	10	2.22
(1,322)	1:216:A:ILE:N	1:216:A:ILE:CA	1:216:A:ILE:C	1:217:A:MET:N	5	2.2
(1,277)	1:186:A:ILE:C	1:187:A:LYS:N	1:187:A:LYS:CA	1:187:A:LYS:C	8	2.18
(1,153)	1:108:A:ASP:C	1:109:A:GLY:N	1:109:A:GLY:CA	1:109:A:GLY:C	6	2.17
(1,198)	1:143:A:ASP:N	1:143:A:ASP:CA	1:143:A:ASP:C	1:144:A:ARG:N	8	2.16
(1,26)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:ALA:N	4	2.16
(1,158)	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1:112:A:TYR:N	4	2.14
(1,350)	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	1:235:A:ILE:N	2	2.13
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	10	2.13
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	2	2.13
(1,341)	1:226:A:VAL:C	1:227:A:ALA:N	1:227:A:ALA:CA	1:227:A:ALA:C	10	2.12
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	5	2.12
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	2	2.09
(1,89)	1:66:A:VAL:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	4	2.09
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	8	2.07
(1,130)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:ARG:N	5	2.07
(1,264)	1:178:A:ASN:N	1:178:A:ASN:CA	1:178:A:ASN:C	1:179:A:HIS:N	3	2.06
(1,128)	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	1:93:A:PHE:N	6	2.06
(1,280)	1:188:A:GLN:N	1:188:A:GLN:CA	1:188:A:GLN:C	1:189:A:ASP:N	2	2.05
(1,208)	1:148:A:PHE:N	1:148:A:PHE:CA	1:148:A:PHE:C	1:149:A:MET:N	3	2.03
(1,69)	1:49:A:PHE:C	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	9	2.03
(1,321)	1:215:A:THR:C	1:216:A:ILE:N	1:216:A:ILE:CA	1:216:A:ILE:C	5	2.01
(1,129)	1:93:A:PHE:C	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	6	1.98
(1,357)	1:239:A:ARG:C	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	8	1.97
(1,283)	1:193:A:ALA:C	1:194:A:THR:N	1:194:A:THR:CA	1:194:A:THR:C	9	1.97
(1,35)	1:21:A:ASP:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	9	1.95
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	10	1.94
(1,244)	1:166:A:ASP:N	1:166:A:ASP:CA	1:166:A:ASP:C	1:167:A:LEU:N	9	1.93
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	1	1.92
(1,176)	1:131:A:PRO:N	1:131:A:PRO:CA	1:131:A:PRO:C	1:132:A:PHE:N	1	1.92
(1,27)	1:16:A:GLU:C	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	2	1.91
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	6	1.89
(1,230)	1:159:A:GLU:N	1:159:A:GLU:CA	1:159:A:GLU:C	1:160:A:GLN:N	6	1.88
(1,186)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:ALA:N	7	1.88
(1,95)	1:72:A:LYS:C	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	3	1.87
(1,35)	1:21:A:ASP:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	8	1.87
(1,218)	1:153:A:ALA:N	1:153:A:ALA:CA	1:153:A:ALA:C	1:154:A:HIS:N	8	1.86
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	3	1.85
(1,308)	1:209:A:ARG:N	1:209:A:ARG:CA	1:209:A:ARG:C	1:210:A:MET:N	5	1.85
(1,48)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:VAL:N	8	1.85
(1,288)	1:196:A:GLN:N	1:196:A:GLN:CA	1:196:A:GLN:C	1:197:A:ASP:N	3	1.83
(1,134)	1:97:A:SER:N	1:97:A:SER:CA	1:97:A:SER:C	1:98:A:VAL:N	2	1.83
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	6	1.81
(1,222)	1:155:A:VAL:N	1:155:A:VAL:CA	1:155:A:VAL:C	1:156:A:THR:N	10	1.81
(1,94)	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	1:73:A:ARG:N	1	1.81
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	10	1.8
(1,291)	1:197:A:ASP:C	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	8	1.77
(1,170)	1:128:A:PRO:N	1:128:A:PRO:CA	1:128:A:PRO:C	1:129:A:THR:N	8	1.77
(1,350)	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	1:235:A:ILE:N	5	1.75
(1,89)	1:66:A:VAL:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	10	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:ALA:N	1	1.74
(1,214)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:ALA:N	6	1.72
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	9	1.71
(1,204)	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	1:147:A:THR:N	3	1.7
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	2	1.68
(1,238)	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	1:164:A:MET:N	6	1.68
(1,90)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:THR:N	9	1.67
(1,357)	1:239:A:ARG:C	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	7	1.66
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	5	1.66
(1,256)	1:173:A:LYS:N	1:173:A:LYS:CA	1:173:A:LYS:C	1:174:A:MET:N	2	1.64
(1,102)	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1:79:A:LYS:N	9	1.63
(1,238)	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	1:164:A:MET:N	5	1.62
(1,305)	1:207:A:GLY:C	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	9	1.61
(1,294)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:200:A:ASP:N	5	1.61
(1,179)	1:132:A:PHE:C	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	5	1.61
(1,348)	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	1:234:A:HIS:N	5	1.6
(1,202)	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	1:146:A:SER:N	2	1.6
(1,3)	1:4:A:ASP:C	1:5:A:HIS:N	1:5:A:HIS:CA	1:5:A:HIS:C	4	1.6
(1,378)	1:250:A:ALA:N	1:250:A:ALA:CA	1:250:A:ALA:C	1:251:A:VAL:N	1	1.57
(1,35)	1:21:A:ASP:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	10	1.57
(1,204)	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	1:147:A:THR:N	10	1.56
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	1	1.55
(1,264)	1:178:A:ASN:N	1:178:A:ASN:CA	1:178:A:ASN:C	1:179:A:HIS:N	5	1.54
(1,204)	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	1:147:A:THR:N	7	1.54
(1,181)	1:133:A:GLU:C	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	6	1.52
(1,181)	1:133:A:GLU:C	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	8	1.52
(1,137)	1:100:A:LEU:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	6	1.52
(1,127)	1:91:A:SER:C	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	3	1.52
(1,35)	1:21:A:ASP:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	6	1.5
(1,268)	1:180:A:VAL:N	1:180:A:VAL:CA	1:180:A:VAL:C	1:181:A:MET:N	7	1.49
(1,226)	1:157:A:SER:N	1:157:A:SER:CA	1:157:A:SER:C	1:158:A:GLU:N	10	1.49
(1,36)	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	1:23:A:LEU:N	5	1.49
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	1	1.48
(1,301)	1:205:A:ALA:C	1:206:A:ALA:N	1:206:A:ALA:CA	1:206:A:ALA:C	1	1.48
(1,186)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:ALA:N	6	1.48
(1,153)	1:108:A:ASP:C	1:109:A:GLY:N	1:109:A:GLY:CA	1:109:A:GLY:C	2	1.48
(1,144)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:THR:N	6	1.46
(1,48)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:VAL:N	5	1.46
(1,41)	1:27:A:GLN:C	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	4	1.46
(1,35)	1:21:A:ASP:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	2	1.46
(1,354)	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	1:239:A:ARG:N	1	1.45
(1,201)	1:144:A:ARG:C	1:145:A:GLY:N	1:145:A:GLY:CA	1:145:A:GLY:C	8	1.45
(1,357)	1:239:A:ARG:C	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	3	1.44
(1,378)	1:250:A:ALA:N	1:250:A:ALA:CA	1:250:A:ALA:C	1:251:A:VAL:N	10	1.43
(1,353)	1:237:A:PRO:C	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	9	1.43
(1,292)	1:198:A:SER:N	1:198:A:SER:CA	1:198:A:SER:C	1:199:A:ASP:N	2	1.43
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	8	1.42
(1,82)	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	1:64:A:VAL:N	1	1.42
(1,48)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:VAL:N	3	1.42
(1,209)	1:148:A:PHE:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	7	1.39
(1,304)	1:207:A:GLY:N	1:207:A:GLY:CA	1:207:A:GLY:C	1:208:A:SER:N	1	1.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,364)	1:243:A:ILE:N	1:243:A:ILE:CA	1:243:A:ILE:C	1:244:A:ASN:N	7	1.37
(1,181)	1:133:A:GLU:C	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	9	1.37
(1,387)	1:254:A:ALA:C	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	7	1.36
(1,275)	1:185:A:ARG:C	1:186:A:ILE:N	1:186:A:ILE:CA	1:186:A:ILE:C	8	1.36
(1,219)	1:153:A:ALA:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	3	1.36
(1,295)	1:202:A:GLY:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	8	1.35
(1,89)	1:66:A:VAL:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	3	1.35
(1,48)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:VAL:N	9	1.35
(1,66)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:PHE:N	4	1.34
(1,289)	1:196:A:GLN:C	1:197:A:ASP:N	1:197:A:ASP:CA	1:197:A:ASP:C	2	1.33
(1,238)	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	1:164:A:MET:N	3	1.33
(1,231)	1:159:A:GLU:C	1:160:A:GLN:N	1:160:A:GLN:CA	1:160:A:GLN:C	7	1.33
(1,222)	1:155:A:VAL:N	1:155:A:VAL:CA	1:155:A:VAL:C	1:156:A:THR:N	8	1.33
(1,353)	1:237:A:PRO:C	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	6	1.32
(1,231)	1:159:A:GLU:C	1:160:A:GLN:N	1:160:A:GLN:CA	1:160:A:GLN:C	1	1.32
(1,171)	1:128:A:PRO:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	8	1.31
(1,27)	1:16:A:GLU:C	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	7	1.31
(1,36)	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	1:23:A:LEU:N	7	1.3
(1,24)	1:15:A:VAL:N	1:15:A:VAL:CA	1:15:A:VAL:C	1:16:A:GLU:N	4	1.3
(1,340)	1:226:A:VAL:N	1:226:A:VAL:CA	1:226:A:VAL:C	1:227:A:ALA:N	3	1.28
(1,35)	1:21:A:ASP:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	1	1.28
(1,231)	1:159:A:GLU:C	1:160:A:GLN:N	1:160:A:GLN:CA	1:160:A:GLN:C	9	1.27
(1,350)	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	1:235:A:ILE:N	1	1.26
(1,284)	1:194:A:THR:N	1:194:A:THR:CA	1:194:A:THR:C	1:195:A:TYR:N	2	1.26
(1,277)	1:186:A:ILE:C	1:187:A:LYS:N	1:187:A:LYS:CA	1:187:A:LYS:C	4	1.26
(1,94)	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	1:73:A:ARG:N	4	1.26
(1,345)	1:228:A:ARG:C	1:229:A:TRP:N	1:229:A:TRP:CA	1:229:A:TRP:C	9	1.25
(1,196)	1:142:A:THR:N	1:142:A:THR:CA	1:142:A:THR:C	1:143:A:ASP:N	1	1.25
(1,29)	1:17:A:ALA:C	1:18:A:ILE:N	1:18:A:ILE:CA	1:18:A:ILE:C	5	1.25
(1,353)	1:237:A:PRO:C	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	3	1.23
(1,48)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:VAL:N	7	1.23
(1,171)	1:128:A:PRO:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	5	1.21
(1,326)	1:218:A:ASP:N	1:218:A:ASP:CA	1:218:A:ASP:C	1:219:A:VAL:N	3	1.2
(1,222)	1:155:A:VAL:N	1:155:A:VAL:CA	1:155:A:VAL:C	1:156:A:THR:N	6	1.2
(1,134)	1:97:A:SER:N	1:97:A:SER:CA	1:97:A:SER:C	1:98:A:VAL:N	10	1.2
(1,90)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:THR:N	3	1.18
(1,272)	1:184:A:TRP:N	1:184:A:TRP:CA	1:184:A:TRP:C	1:185:A:ARG:N	4	1.15
(1,92)	1:71:A:ALA:N	1:71:A:ALA:CA	1:71:A:ALA:C	1:72:A:LYS:N	3	1.15
(1,388)	1:255:A:GLY:N	1:255:A:GLY:CA	1:255:A:GLY:C	1:256:A:PHE:N	5	1.14
(1,132)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:GLY:N	10	1.12
(1,378)	1:250:A:ALA:N	1:250:A:ALA:CA	1:250:A:ALA:C	1:251:A:VAL:N	9	1.1
(1,186)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:ALA:N	5	1.1
(1,358)	1:240:A:PHE:N	1:240:A:PHE:CA	1:240:A:PHE:C	1:241:A:LYS:N	8	1.08
(1,81)	1:62:A:ILE:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	3	1.08
(1,24)	1:15:A:VAL:N	1:15:A:VAL:CA	1:15:A:VAL:C	1:16:A:GLU:N	5	1.08
(1,350)	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	1:235:A:ILE:N	8	1.07
(1,89)	1:66:A:VAL:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	2	1.07
(1,353)	1:237:A:PRO:C	1:238:A:ASP:N	1:238:A:ASP:CA	1:238:A:ASP:C	5	1.06
(1,347)	1:232:A:GLY:C	1:233:A:ALA:N	1:233:A:ALA:CA	1:233:A:ALA:C	7	1.06
(1,219)	1:153:A:ALA:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	6	1.06
(1,350)	1:234:A:HIS:N	1:234:A:HIS:CA	1:234:A:HIS:C	1:235:A:ILE:N	10	1.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,277)	1:186:A:ILE:C	1:187:A:LYS:N	1:187:A:LYS:CA	1:187:A:LYS:C	3	1.04
(1,48)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:VAL:N	6	1.04
(1,231)	1:159:A:GLU:C	1:160:A:GLN:N	1:160:A:GLN:CA	1:160:A:GLN:C	5	1.03
(1,203)	1:145:A:GLY:C	1:146:A:SER:N	1:146:A:SER:CA	1:146:A:SER:C	3	1.03
(1,76)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:GLU:N	6	1.03
(1,378)	1:250:A:ALA:N	1:250:A:ALA:CA	1:250:A:ALA:C	1:251:A:VAL:N	8	1.02
(1,73)	1:52:A:HIS:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	6	1.02
(1,222)	1:155:A:VAL:N	1:155:A:VAL:CA	1:155:A:VAL:C	1:156:A:THR:N	2	1.0
(1,209)	1:148:A:PHE:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	10	1.0
(1,92)	1:71:A:ALA:N	1:71:A:ALA:CA	1:71:A:ALA:C	1:72:A:LYS:N	1	1.0