



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:28 PM UTC

PDB ID : 2MHQ / pdb_00002mhq
BMRB ID : 19646
Title : Solution structure of the major factor VIII binding region on von Willebrand factor
Authors : Shiltagh, N.; Kirkpatrick, J.; Cabrita, L.D.; McKinnon, T.A.J.; Thalassinou, K.; Tuddenham, E.G.D.; Hansen, D.F.
Deposited on : 2013-12-02

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

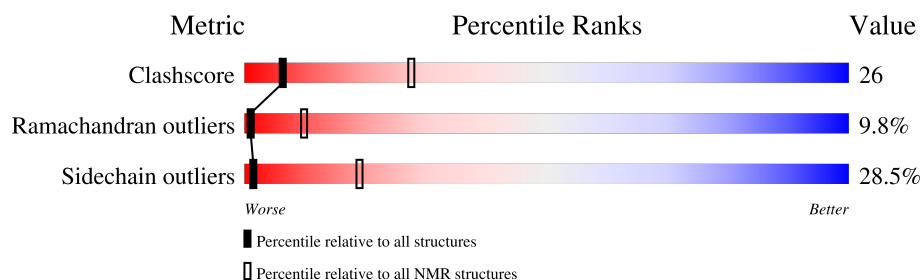
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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	103	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *not applicable*.

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:6-A:103 (98)	2.21	5

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1507 atoms, of which 733 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called von Willebrand factor.

Mol	Chain	Residues	Atoms						Trace
1	A	103	Total	C	H	N	O	S	0
			1507	465	733	143	145	21	

There are 5 discrepancies between the modelled and reference sequences:

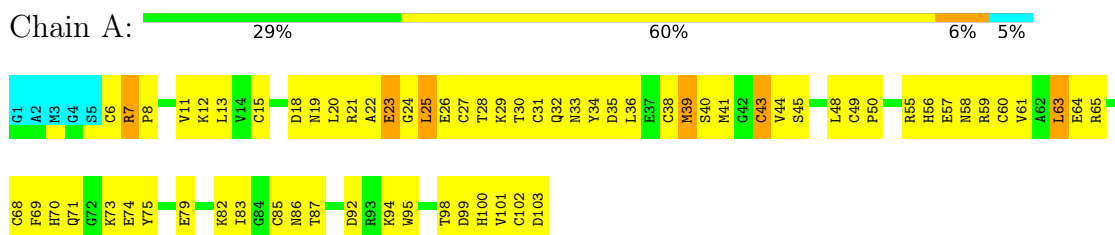
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P04275
A	2	ALA	-	expression tag	UNP P04275
A	3	MET	-	expression tag	UNP P04275
A	4	GLY	-	expression tag	UNP P04275
A	91	ARG	GLN	SEE REMARK 999	UNP P04275

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: von Willebrand factor

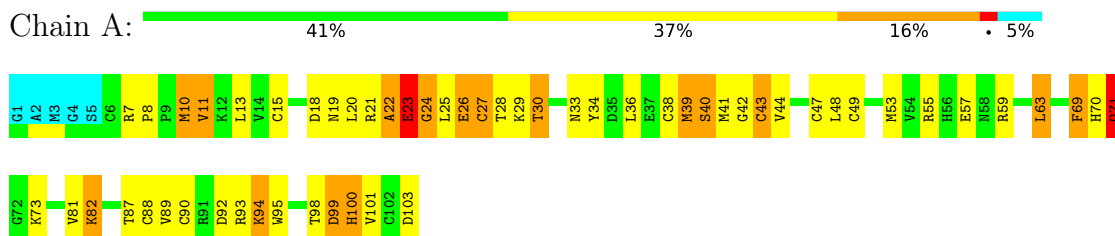


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

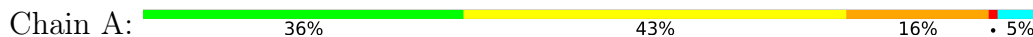
4.2.1 Score per residue for model 1

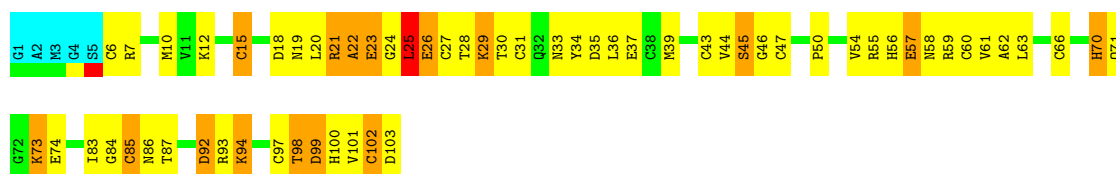
- Molecule 1: von Willebrand factor



4.2.2 Score per residue for model 2

- Molecule 1: von Willebrand factor

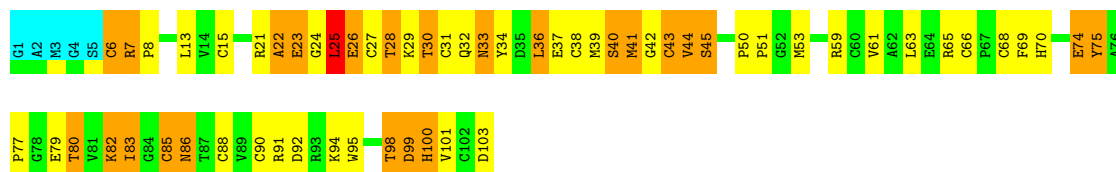




4.2.3 Score per residue for model 3

- Molecule 1: von Willebrand factor

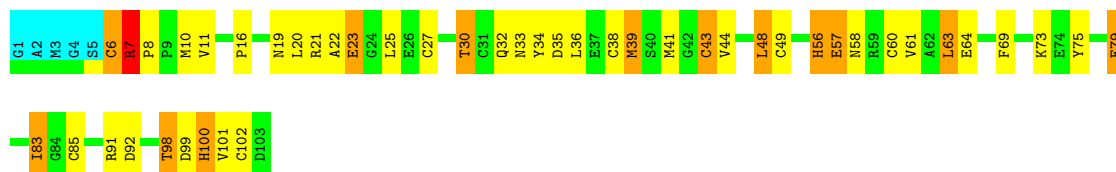
Chain A: 37% 34% 23% 5%



4.2.4 Score per residue for model 4

- Molecule 1: von Willebrand factor

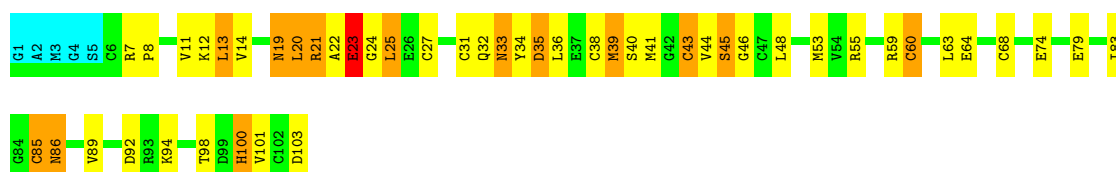
Chain A: 50% 31% 13% 5%



4.2.5 Score per residue for model 5 (medoid)

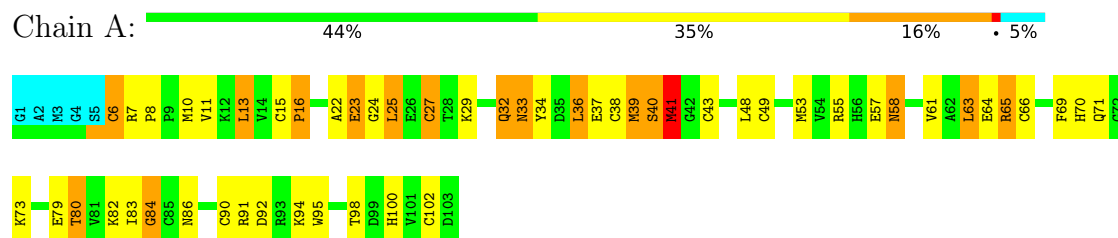
- Molecule 1: von Willebrand factor

Chain A: 49% 32% 14% 5%



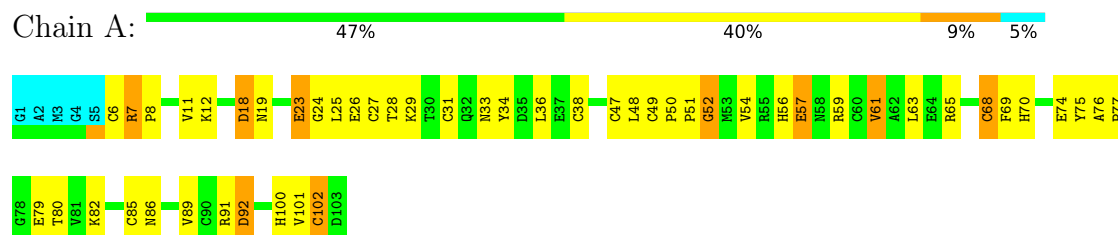
4.2.6 Score per residue for model 6

- Molecule 1: von Willebrand factor



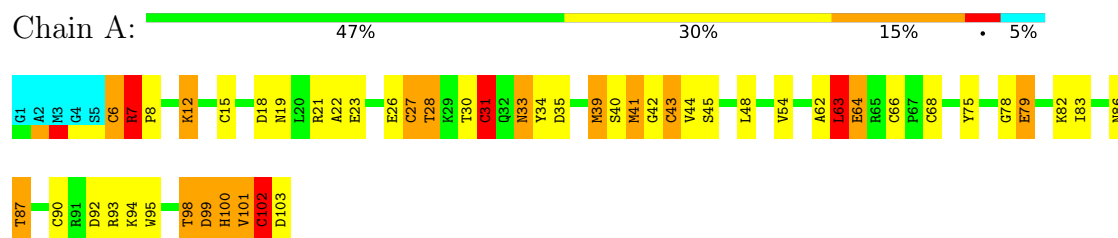
4.2.7 Score per residue for model 7

- Molecule 1: von Willebrand factor



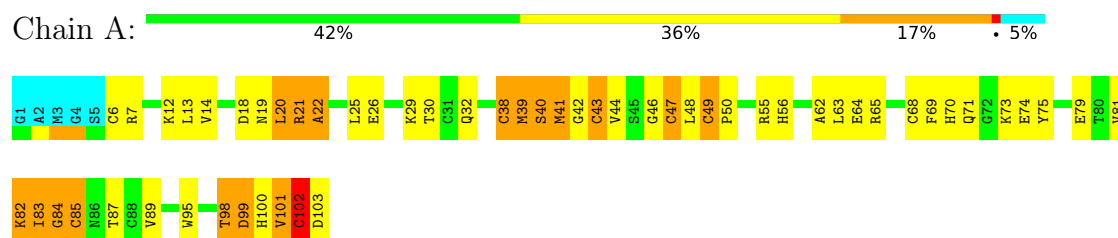
4.2.8 Score per residue for model 8

- Molecule 1: von Willebrand factor



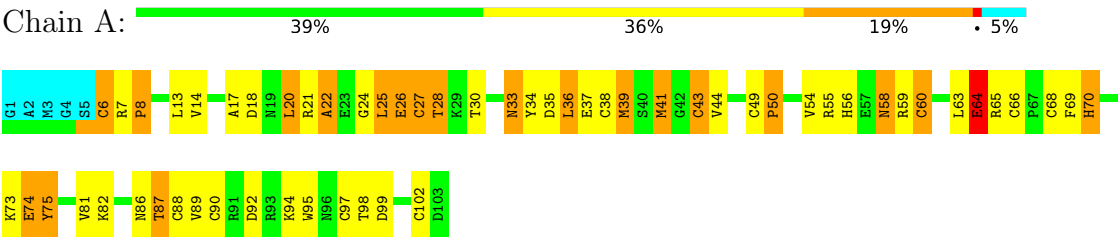
4.2.9 Score per residue for model 9

- Molecule 1: von Willebrand factor



4.2.10 Score per residue for model 10

• Molecule 1: von Willebrand factor



5 Refinement protocol and experimental data overview

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

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
Xplor-NIH	structure solution	
Xplor-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	959
Number of shifts mapped to atoms	959
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	747	706	706	37±6
All	All	7470	7060	7060	372

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:H	1:A:13:LEU:HD22	0.90	1.23	5	1
1:A:20:LEU:H	1:A:20:LEU:HD23	0.88	1.27	2	1
1:A:63:LEU:HD22	1:A:63:LEU:N	0.76	1.94	4	1
1:A:36:LEU:H	1:A:36:LEU:HD12	0.75	1.40	3	1
1:A:13:LEU:HD22	1:A:13:LEU:N	0.74	1.97	5	1
1:A:20:LEU:HD23	1:A:21:ARG:N	0.72	1.98	9	1
1:A:33:ASN:OD1	1:A:36:LEU:HD22	0.72	1.83	5	1
1:A:23:GLU:H	1:A:23:GLU:CD	0.71	1.93	6	1
1:A:17:ALA:H	1:A:20:LEU:HD21	0.69	1.46	10	1
1:A:6:CYS:N	1:A:7:ARG:HH12	0.66	1.88	3	1
1:A:20:LEU:HD23	1:A:20:LEU:N	0.65	2.04	2	1
1:A:30:THR:HG22	1:A:31:CYS:H	0.64	1.52	2	1
1:A:13:LEU:HD12	1:A:13:LEU:N	0.64	2.08	6	1
1:A:20:LEU:H	1:A:20:LEU:CD2	0.63	2.03	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:H	1:A:63:LEU:HD13	0.63	1.53	4	1
1:A:20:LEU:O	1:A:22:ALA:N	0.63	2.32	4	1
1:A:98:THR:C	1:A:100:HIS:H	0.63	2.00	4	2
1:A:6:CYS:SG	1:A:6:CYS:O	0.62	2.57	9	2
1:A:58:ASN:HD22	1:A:58:ASN:C	0.62	2.02	6	1
1:A:90:CYS:SG	1:A:95:TRP:CE2	0.62	2.93	3	1
1:A:63:LEU:HD22	1:A:63:LEU:H	0.62	1.55	4	1
1:A:30:THR:N	1:A:33:ASN:ND2	0.62	2.47	8	1
1:A:90:CYS:SG	1:A:95:TRP:CZ2	0.61	2.94	3	2
1:A:27:CYS:O	1:A:28:THR:O	0.61	2.18	10	2
1:A:6:CYS:SG	1:A:47:CYS:N	0.61	2.74	7	1
1:A:7:ARG:N	1:A:8:PRO:CD	0.60	2.63	6	6
1:A:36:LEU:HD12	1:A:36:LEU:N	0.60	2.09	3	2
1:A:56:HIS:N	1:A:59:ARG:O	0.60	2.34	10	1
1:A:11:VAL:HG23	1:A:13:LEU:HD11	0.60	1.72	6	1
1:A:57:GLU:O	1:A:58:ASN:ND2	0.59	2.35	6	1
1:A:83:ILE:O	1:A:85:CYS:N	0.59	2.35	2	1
1:A:25:LEU:H	1:A:25:LEU:HD12	0.59	1.58	5	1
1:A:68:CYS:O	1:A:75:TYR:O	0.59	2.20	3	1
1:A:78:GLY:N	1:A:90:CYS:O	0.59	2.35	8	1
1:A:81:VAL:HG22	1:A:95:TRP:CH2	0.59	2.33	9	1
1:A:22:ALA:O	1:A:23:GLU:O	0.59	2.20	2	2
1:A:90:CYS:SG	1:A:95:TRP:CH2	0.59	2.96	10	1
1:A:42:GLY:O	1:A:43:CYS:CB	0.58	2.51	3	2
1:A:21:ARG:O	1:A:22:ALA:HB3	0.58	1.98	5	1
1:A:68:CYS:SG	1:A:95:TRP:NE1	0.58	2.76	3	1
1:A:68:CYS:N	1:A:75:TYR:O	0.58	2.37	3	1
1:A:12:LYS:H	1:A:12:LYS:CD	0.58	2.10	8	1
1:A:53:MET:SD	1:A:60:CYS:SG	0.58	3.01	5	1
1:A:40:SER:OG	1:A:41:MET:N	0.57	2.36	6	1
1:A:98:THR:C	1:A:100:HIS:N	0.57	2.61	4	2
1:A:79:GLU:OE1	1:A:79:GLU:N	0.57	2.38	9	2
1:A:82:LYS:NZ	1:A:87:THR:HG23	0.57	2.15	9	1
1:A:58:ASN:C	1:A:58:ASN:ND2	0.56	2.61	6	1
1:A:43:CYS:SG	1:A:43:CYS:O	0.56	2.63	6	4
1:A:25:LEU:H	1:A:25:LEU:CD1	0.56	2.13	5	1
1:A:98:THR:HG1	1:A:100:HIS:CE1	0.56	2.18	3	1
1:A:22:ALA:O	1:A:23:GLU:C	0.56	2.49	1	1
1:A:92:ASP:C	1:A:94:LYS:H	0.56	2.09	8	4
1:A:98:THR:OG1	1:A:100:HIS:CD2	0.56	2.59	5	1
1:A:10:MET:SD	1:A:11:VAL:N	0.55	2.80	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:GLU:N	1:A:23:GLU:CD	0.55	2.64	7	1
1:A:44:VAL:O	1:A:46:GLY:N	0.55	2.38	5	2
1:A:13:LEU:C	1:A:13:LEU:HD13	0.55	2.26	1	1
1:A:98:THR:OG1	1:A:100:HIS:CE1	0.55	2.59	3	1
1:A:100:HIS:ND1	1:A:100:HIS:C	0.55	2.64	1	1
1:A:30:THR:H	1:A:33:ASN:HD21	0.55	1.44	3	1
1:A:42:GLY:O	1:A:43:CYS:C	0.55	2.50	1	1
1:A:32:GLN:C	1:A:34:TYR:H	0.55	2.08	3	2
1:A:64:GLU:OE1	1:A:65:ARG:N	0.55	2.39	10	1
1:A:30:THR:OG1	1:A:33:ASN:ND2	0.55	2.39	4	1
1:A:22:ALA:O	1:A:23:GLU:CB	0.55	2.55	5	1
1:A:95:TRP:CD1	1:A:95:TRP:N	0.54	2.74	10	2
1:A:17:ALA:H	1:A:20:LEU:CD2	0.54	2.15	10	1
1:A:40:SER:O	1:A:41:MET:C	0.54	2.51	9	3
1:A:30:THR:H	1:A:33:ASN:ND2	0.54	2.01	8	2
1:A:33:ASN:O	1:A:36:LEU:O	0.54	2.26	3	1
1:A:20:LEU:C	1:A:22:ALA:H	0.54	2.10	4	1
1:A:27:CYS:O	1:A:27:CYS:SG	0.54	2.66	10	1
1:A:22:ALA:O	1:A:24:GLY:N	0.54	2.41	1	1
1:A:92:ASP:OD1	1:A:92:ASP:O	0.54	2.25	3	1
1:A:98:THR:O	1:A:100:HIS:N	0.54	2.40	4	2
1:A:7:ARG:CZ	1:A:7:ARG:N	0.54	2.71	3	1
1:A:18:ASP:O	1:A:19:ASN:ND2	0.54	2.40	7	2
1:A:44:VAL:HG13	1:A:44:VAL:O	0.54	2.02	10	2
1:A:83:ILE:O	1:A:84:GLY:O	0.53	2.27	9	2
1:A:13:LEU:C	1:A:13:LEU:HD12	0.53	2.28	9	1
1:A:30:THR:O	1:A:34:TYR:N	0.53	2.42	1	1
1:A:39:MET:O	1:A:40:SER:C	0.53	2.50	1	1
1:A:38:CYS:O	1:A:39:MET:O	0.53	2.27	9	2
1:A:70:HIS:O	1:A:73:LYS:N	0.53	2.42	1	1
1:A:91:ARG:N	1:A:94:LYS:O	0.53	2.42	6	1
1:A:25:LEU:O	1:A:27:CYS:N	0.53	2.41	3	2
1:A:41:MET:C	1:A:41:MET:SD	0.53	2.91	10	1
1:A:86:ASN:ND2	1:A:88:CYS:SG	0.53	2.82	3	1
1:A:102:CYS:O	1:A:102:CYS:SG	0.53	2.66	9	1
1:A:21:ARG:O	1:A:22:ALA:C	0.52	2.52	1	5
1:A:70:HIS:O	1:A:73:LYS:O	0.52	2.27	6	1
1:A:74:GLU:C	1:A:75:TYR:CD1	0.52	2.87	9	2
1:A:42:GLY:O	1:A:44:VAL:N	0.52	2.43	9	2
1:A:63:LEU:N	1:A:63:LEU:CD2	0.52	2.64	4	1
1:A:16:PRO:O	1:A:19:ASN:N	0.52	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:THR:O	1:A:99:ASP:CB	0.51	2.59	9	5
1:A:25:LEU:HD12	1:A:25:LEU:N	0.51	2.21	5	1
1:A:27:CYS:SG	1:A:38:CYS:O	0.51	2.68	6	1
1:A:101:VAL:O	1:A:102:CYS:C	0.51	2.53	7	1
1:A:6:CYS:O	1:A:7:ARG:CB	0.51	2.59	7	1
1:A:63:LEU:N	1:A:63:LEU:HD13	0.51	2.20	4	1
1:A:100:HIS:C	1:A:100:HIS:HD1	0.51	2.14	5	1
1:A:58:ASN:N	1:A:58:ASN:OD1	0.51	2.42	10	1
1:A:33:ASN:N	1:A:33:ASN:OD1	0.51	2.44	3	1
1:A:63:LEU:H	1:A:63:LEU:CD1	0.51	2.13	4	1
1:A:39:MET:N	1:A:39:MET:SD	0.51	2.83	6	1
1:A:36:LEU:HD13	1:A:37:GLU:N	0.51	2.21	10	1
1:A:24:GLY:O	1:A:25:LEU:C	0.50	2.53	2	1
1:A:73:LYS:O	1:A:75:TYR:CZ	0.50	2.64	10	1
1:A:32:GLN:O	1:A:34:TYR:N	0.50	2.45	3	1
1:A:18:ASP:OD1	1:A:18:ASP:N	0.50	2.36	10	2
1:A:62:ALA:O	1:A:64:GLU:N	0.50	2.44	8	1
1:A:100:HIS:NE2	1:A:102:CYS:O	0.50	2.44	8	1
1:A:86:ASN:OD1	1:A:88:CYS:SG	0.50	2.69	10	2
1:A:76:ALA:HB1	1:A:77:PRO:HD2	0.50	1.82	7	1
1:A:68:CYS:SG	1:A:95:TRP:CE2	0.50	3.05	3	1
1:A:59:ARG:NH1	1:A:61:VAL:HG22	0.50	2.21	7	1
1:A:70:HIS:O	1:A:75:TYR:OH	0.50	2.29	10	1
1:A:101:VAL:O	1:A:102:CYS:CB	0.50	2.59	9	2
1:A:100:HIS:CE1	1:A:102:CYS:O	0.50	2.65	8	1
1:A:86:ASN:OD1	1:A:97:CYS:SG	0.50	2.69	10	1
1:A:63:LEU:H	1:A:63:LEU:CD2	0.49	2.15	4	1
1:A:13:LEU:O	1:A:46:GLY:O	0.49	2.30	9	1
1:A:87:THR:C	1:A:88:CYS:SG	0.49	2.95	1	1
1:A:86:ASN:CG	1:A:87:THR:N	0.49	2.69	10	1
1:A:24:GLY:O	1:A:25:LEU:CB	0.49	2.60	6	1
1:A:56:HIS:O	1:A:59:ARG:O	0.49	2.30	7	1
1:A:87:THR:HG23	1:A:98:THR:OG1	0.49	2.07	8	1
1:A:28:THR:HG22	1:A:29:LYS:H	0.49	1.67	1	1
1:A:32:GLN:C	1:A:34:TYR:N	0.49	2.70	3	2
1:A:26:GLU:C	1:A:27:CYS:SG	0.49	2.96	8	1
1:A:56:HIS:O	1:A:59:ARG:N	0.49	2.44	2	2
1:A:27:CYS:SG	1:A:38:CYS:C	0.49	2.96	6	1
1:A:92:ASP:O	1:A:94:LYS:N	0.49	2.46	2	3
1:A:68:CYS:SG	1:A:75:TYR:O	0.48	2.70	7	1
1:A:13:LEU:HD12	1:A:13:LEU:H	0.48	1.65	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:O	1:A:66:CYS:SG	0.48	2.72	2	1
1:A:102:CYS:O	1:A:103:ASP:C	0.48	2.56	9	2
1:A:98:THR:OG1	1:A:100:HIS:NE2	0.48	2.44	3	1
1:A:100:HIS:O	1:A:101:VAL:C	0.48	2.56	8	1
1:A:32:GLN:OE1	1:A:69:PHE:CD1	0.48	2.67	4	1
1:A:79:GLU:O	1:A:89:VAL:HG13	0.48	2.08	7	1
1:A:23:GLU:N	1:A:23:GLU:OE1	0.48	2.46	7	1
1:A:21:ARG:O	1:A:22:ALA:O	0.48	2.32	9	2
1:A:57:GLU:O	1:A:58:ASN:CG	0.47	2.57	6	1
1:A:54:VAL:HG21	1:A:63:LEU:CD1	0.47	2.39	7	1
1:A:70:HIS:O	1:A:71:GLN:C	0.47	2.56	1	4
1:A:98:THR:O	1:A:99:ASP:CG	0.47	2.56	2	2
1:A:91:ARG:O	1:A:92:ASP:OD1	0.47	2.33	3	2
1:A:56:HIS:O	1:A:57:GLU:CG	0.47	2.62	4	1
1:A:33:ASN:O	1:A:34:TYR:C	0.47	2.58	6	5
1:A:6:CYS:N	1:A:7:ARG:NH1	0.47	2.59	3	1
1:A:103:ASP:N	1:A:103:ASP:OD1	0.47	2.48	3	1
1:A:11:VAL:O	1:A:13:LEU:HD13	0.47	2.09	5	1
1:A:63:LEU:C	1:A:65:ARG:N	0.47	2.73	6	3
1:A:13:LEU:HD12	1:A:13:LEU:O	0.47	2.10	9	1
1:A:40:SER:O	1:A:41:MET:O	0.47	2.33	6	2
1:A:86:ASN:OD1	1:A:86:ASN:N	0.47	2.43	8	1
1:A:92:ASP:C	1:A:94:LYS:N	0.47	2.73	10	3
1:A:19:ASN:O	1:A:19:ASN:CG	0.47	2.58	5	2
1:A:100:HIS:CE1	1:A:101:VAL:O	0.47	2.68	4	2
1:A:7:ARG:H	1:A:8:PRO:CD	0.46	2.24	8	3
1:A:100:HIS:C	1:A:100:HIS:ND1	0.46	2.73	5	1
1:A:101:VAL:O	1:A:101:VAL:HG13	0.46	2.10	5	1
1:A:23:GLU:CD	1:A:23:GLU:N	0.46	2.70	6	1
1:A:63:LEU:O	1:A:63:LEU:HD13	0.46	2.10	1	1
1:A:71:GLN:C	1:A:73:LYS:H	0.46	2.19	2	2
1:A:35:ASP:C	1:A:36:LEU:HD12	0.46	2.36	4	1
1:A:21:ARG:O	1:A:22:ALA:CB	0.46	2.63	5	1
1:A:18:ASP:O	1:A:19:ASN:CB	0.46	2.62	2	1
1:A:35:ASP:O	1:A:35:ASP:OD1	0.46	2.34	2	1
1:A:63:LEU:C	1:A:65:ARG:H	0.46	2.19	10	2
1:A:79:GLU:CD	1:A:79:GLU:O	0.46	2.58	5	1
1:A:46:GLY:C	1:A:47:CYS:SG	0.46	2.98	9	1
1:A:20:LEU:C	1:A:22:ALA:N	0.46	2.72	4	1
1:A:56:HIS:O	1:A:58:ASN:N	0.46	2.49	2	1
1:A:37:GLU:N	1:A:37:GLU:OE1	0.46	2.48	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ASP:C	1:A:20:LEU:H	0.46	2.19	9	1
1:A:13:LEU:N	1:A:13:LEU:CD2	0.46	2.68	5	1
1:A:36:LEU:N	1:A:36:LEU:CD1	0.45	2.77	3	1
1:A:18:ASP:O	1:A:19:ASN:CG	0.45	2.58	1	1
1:A:25:LEU:HD22	1:A:25:LEU:N	0.45	2.26	2	1
1:A:91:ARG:O	1:A:92:ASP:CG	0.45	2.59	4	1
1:A:75:TYR:CD1	1:A:75:TYR:N	0.45	2.85	9	1
1:A:23:GLU:C	1:A:25:LEU:N	0.45	2.74	6	1
1:A:23:GLU:CD	1:A:23:GLU:C	0.45	2.85	7	1
1:A:24:GLY:O	1:A:25:LEU:O	0.45	2.35	10	1
1:A:44:VAL:O	1:A:44:VAL:CG1	0.45	2.65	10	1
1:A:69:PHE:CD1	1:A:69:PHE:N	0.45	2.84	9	2
1:A:15:CYS:O	1:A:15:CYS:SG	0.45	2.74	2	1
1:A:86:ASN:HD22	1:A:87:THR:H	0.45	1.53	2	1
1:A:68:CYS:SG	1:A:95:TRP:CZ2	0.45	3.10	3	1
1:A:13:LEU:N	1:A:13:LEU:HD13	0.45	2.26	5	1
1:A:21:ARG:O	1:A:21:ARG:CG	0.45	2.65	8	1
1:A:26:GLU:N	1:A:26:GLU:OE2	0.45	2.50	10	1
1:A:33:ASN:C	1:A:35:ASP:N	0.45	2.75	5	1
1:A:62:ALA:O	1:A:63:LEU:C	0.45	2.61	8	2
1:A:84:GLY:O	1:A:85:CYS:CB	0.45	2.63	9	1
1:A:69:PHE:O	1:A:69:PHE:CG	0.45	2.69	10	1
1:A:23:GLU:C	1:A:23:GLU:OE1	0.44	2.60	5	1
1:A:13:LEU:N	1:A:13:LEU:CD1	0.44	2.75	6	1
1:A:34:TYR:OH	1:A:54:VAL:HG21	0.44	2.12	8	1
1:A:18:ASP:O	1:A:18:ASP:OD1	0.44	2.36	9	1
1:A:26:GLU:O	1:A:26:GLU:CG	0.44	2.64	2	1
1:A:50:PRO:O	1:A:52:GLY:N	0.44	2.49	7	1
1:A:12:LYS:CD	1:A:12:LYS:N	0.44	2.79	8	1
1:A:18:ASP:C	1:A:20:LEU:N	0.44	2.76	9	1
1:A:7:ARG:CA	1:A:7:ARG:NE	0.44	2.80	3	1
1:A:98:THR:O	1:A:99:ASP:OD2	0.44	2.35	3	1
1:A:83:ILE:O	1:A:84:GLY:C	0.44	2.61	6	2
1:A:56:HIS:O	1:A:57:GLU:C	0.44	2.60	7	2
1:A:98:THR:C	1:A:99:ASP:CG	0.44	2.86	2	1
1:A:23:GLU:C	1:A:25:LEU:H	0.44	2.20	6	1
1:A:100:HIS:O	1:A:100:HIS:CG	0.44	2.70	8	1
1:A:101:VAL:O	1:A:102:CYS:O	0.44	2.36	8	1
1:A:28:THR:OG1	1:A:29:LYS:N	0.44	2.45	3	1
1:A:92:ASP:OD1	1:A:92:ASP:N	0.44	2.50	6	1
1:A:85:CYS:SG	1:A:103:ASP:OD1	0.44	2.76	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:HIS:ND1	1:A:101:VAL:N	0.44	2.65	7	1
1:A:98:THR:O	1:A:99:ASP:HB2	0.43	2.12	3	1
1:A:62:ALA:C	1:A:64:GLU:N	0.43	2.76	8	1
1:A:99:ASP:OD1	1:A:100:HIS:ND1	0.43	2.51	2	1
1:A:61:VAL:HG22	1:A:62:ALA:N	0.43	2.28	2	1
1:A:56:HIS:O	1:A:57:GLU:HG3	0.43	2.12	4	1
1:A:19:ASN:O	1:A:20:LEU:C	0.43	2.61	5	1
1:A:54:VAL:O	1:A:60:CYS:SG	0.43	2.77	10	1
1:A:55:ARG:HH21	1:A:58:ASN:C	0.43	2.22	10	1
1:A:81:VAL:O	1:A:88:CYS:O	0.43	2.36	10	1
1:A:70:HIS:CB	1:A:95:TRP:CZ2	0.43	3.01	3	1
1:A:18:ASP:C	1:A:19:ASN:ND2	0.43	2.76	1	1
1:A:29:LYS:C	1:A:30:THR:HG1	0.43	2.22	2	1
1:A:79:GLU:OE1	1:A:79:GLU:C	0.43	2.62	4	1
1:A:85:CYS:SG	1:A:103:ASP:CG	0.43	3.02	5	1
1:A:30:THR:HG23	1:A:54:VAL:HG11	0.43	1.90	2	1
1:A:48:LEU:O	1:A:49:CYS:C	0.43	2.61	7	1
1:A:77:PRO:C	1:A:79:GLU:H	0.43	2.22	7	1
1:A:44:VAL:O	1:A:45:SER:C	0.43	2.61	5	2
1:A:69:PHE:CD1	1:A:69:PHE:O	0.43	2.72	6	1
1:A:21:ARG:CZ	1:A:21:ARG:H	0.42	2.27	5	1
1:A:59:ARG:NH1	1:A:60:CYS:O	0.42	2.51	5	1
1:A:86:ASN:HD22	1:A:87:THR:N	0.42	2.12	2	1
1:A:16:PRO:C	1:A:19:ASN:H	0.42	2.22	4	1
1:A:19:ASN:O	1:A:19:ASN:OD1	0.42	2.36	7	1
1:A:87:THR:O	1:A:98:THR:OG1	0.42	2.37	8	1
1:A:91:ARG:O	1:A:94:LYS:O	0.42	2.38	3	1
1:A:15:CYS:O	1:A:16:PRO:O	0.42	2.38	6	1
1:A:82:LYS:HZ1	1:A:87:THR:HG23	0.42	1.73	9	1
1:A:30:THR:O	1:A:31:CYS:C	0.42	2.62	8	1
1:A:27:CYS:O	1:A:28:THR:C	0.42	2.62	2	1
1:A:12:LYS:C	1:A:13:LEU:HD13	0.42	2.39	5	1
1:A:23:GLU:OE1	1:A:24:GLY:N	0.42	2.53	5	1
1:A:81:VAL:HG22	1:A:82:LYS:N	0.42	2.30	1	1
1:A:51:PRO:C	1:A:53:MET:H	0.42	2.23	3	1
1:A:98:THR:C	1:A:99:ASP:OD1	0.42	2.63	9	1
1:A:11:VAL:O	1:A:48:LEU:O	0.42	2.38	4	1
1:A:24:GLY:O	1:A:26:GLU:OE1	0.42	2.37	7	1
1:A:74:GLU:O	1:A:74:GLU:OE1	0.41	2.37	3	1
1:A:91:ARG:C	1:A:92:ASP:CG	0.41	2.88	4	1
1:A:7:ARG:H	1:A:8:PRO:HD3	0.41	1.75	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:GLU:C	1:A:59:ARG:H	0.41	2.23	7	2
1:A:26:GLU:OE2	1:A:40:SER:OG	0.41	2.38	9	1
1:A:86:ASN:ND2	1:A:86:ASN:N	0.41	2.68	5	1
1:A:81:VAL:HG12	1:A:95:TRP:CH2	0.41	2.50	1	1
1:A:63:LEU:O	1:A:65:ARG:N	0.41	2.53	6	1
1:A:83:ILE:O	1:A:86:ASN:OD1	0.41	2.38	8	1
1:A:49:CYS:O	1:A:50:PRO:C	0.41	2.64	9	1
1:A:98:THR:OG1	1:A:99:ASP:OD1	0.41	2.37	9	1
1:A:82:LYS:C	1:A:83:ILE:HD13	0.41	2.40	3	1
1:A:25:LEU:CD1	1:A:25:LEU:N	0.41	2.82	5	1
1:A:34:TYR:O	1:A:34:TYR:CG	0.41	2.72	5	1
1:A:63:LEU:N	1:A:63:LEU:HD23	0.41	2.31	6	1
1:A:84:GLY:O	1:A:86:ASN:N	0.41	2.51	6	1
1:A:26:GLU:O	1:A:27:CYS:C	0.41	2.63	1	1
1:A:83:ILE:O	1:A:83:ILE:HG23	0.41	2.15	4	1
1:A:49:CYS:O	1:A:50:PRO:O	0.41	2.38	10	1
1:A:86:ASN:OD1	1:A:100:HIS:O	0.41	2.38	7	1
1:A:73:LYS:O	1:A:75:TYR:CE1	0.41	2.74	10	1
1:A:91:ARG:O	1:A:94:LYS:N	0.41	2.49	3	1
1:A:56:HIS:O	1:A:56:HIS:CG	0.41	2.73	10	1
1:A:85:CYS:SG	1:A:102:CYS:O	0.41	2.79	4	1
1:A:6:CYS:O	1:A:7:ARG:C	0.41	2.64	9	1
1:A:21:ARG:O	1:A:23:GLU:N	0.40	2.54	2	1
1:A:91:ARG:O	1:A:92:ASP:CB	0.40	2.68	7	1
1:A:39:MET:CG	1:A:40:SER:N	0.40	2.84	8	1
1:A:103:ASP:OXT	1:A:103:ASP:OD1	0.40	2.40	8	1
1:A:30:THR:N	1:A:33:ASN:HD21	0.40	2.14	3	1
1:A:79:GLU:C	1:A:80:THR:CG2	0.40	2.95	6	2
1:A:43:CYS:O	1:A:43:CYS:SG	0.40	2.80	9	1
1:A:18:ASP:O	1:A:20:LEU:N	0.40	2.55	9	1
1:A:33:ASN:ND2	1:A:36:LEU:HD12	0.40	2.31	2	1
1:A:71:GLN:O	1:A:73:LYS:N	0.40	2.54	2	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.40	2.83	4	1
1:A:33:ASN:C	1:A:36:LEU:H	0.40	2.24	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	97/103 (94%)	72±3 (74±4%)	15±3 (16±3%)	10±3 (10±3%)	1	10
All	All	970/1030 (94%)	721 (74%)	154 (16%)	95 (10%)	1	10

All 37 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	39	MET	7
1	A	22	ALA	6
1	A	23	GLU	6
1	A	6	CYS	6
1	A	99	ASP	5
1	A	27	CYS	4
1	A	43	CYS	4
1	A	41	MET	4
1	A	102	CYS	4
1	A	40	SER	3
1	A	93	ARG	3
1	A	25	LEU	3
1	A	45	SER	3
1	A	50	PRO	3
1	A	84	GLY	3
1	A	28	THR	3
1	A	7	ARG	3
1	A	8	PRO	3
1	A	24	GLY	2
1	A	101	VAL	2
1	A	64	GLU	2
1	A	71	GLN	1
1	A	57	GLU	1
1	A	26	GLU	1
1	A	33	ASN	1
1	A	77	PRO	1
1	A	85	CYS	1
1	A	21	ARG	1
1	A	16	PRO	1
1	A	90	CYS	1
1	A	51	PRO	1
1	A	52	GLY	1
1	A	92	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	31	CYS	1
1	A	63	LEU	1
1	A	79	GLU	1
1	A	19	ASN	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	87/89 (98%)	62±3 (71±3%)	25±3 (29±3%)	1	19
All	All	870/890 (98%)	622 (71%)	248 (29%)	1	19

All 72 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	25	LEU	8
1	A	82	LYS	7
1	A	38	CYS	6
1	A	48	LEU	6
1	A	63	LEU	6
1	A	100	HIS	6
1	A	98	THR	6
1	A	23	GLU	5
1	A	30	THR	5
1	A	36	LEU	5
1	A	55	ARG	5
1	A	7	ARG	5
1	A	74	GLU	5
1	A	85	CYS	5
1	A	64	GLU	5
1	A	68	CYS	5
1	A	10	MET	4
1	A	15	CYS	4
1	A	20	LEU	4
1	A	26	GLU	4
1	A	39	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	41	MET	4
1	A	49	CYS	4
1	A	89	VAL	4
1	A	12	LYS	4
1	A	29	LYS	4
1	A	43	CYS	4
1	A	60	CYS	4
1	A	102	CYS	4
1	A	13	LEU	4
1	A	31	CYS	4
1	A	61	VAL	4
1	A	66	CYS	4
1	A	75	TYR	4
1	A	83	ILE	4
1	A	33	ASN	4
1	A	47	CYS	3
1	A	69	PHE	3
1	A	94	LYS	3
1	A	21	ARG	3
1	A	70	HIS	3
1	A	73	LYS	3
1	A	65	ARG	3
1	A	80	THR	3
1	A	27	CYS	3
1	A	58	ASN	3
1	A	14	VAL	3
1	A	32	GLN	3
1	A	35	ASP	3
1	A	11	VAL	2
1	A	53	MET	2
1	A	101	VAL	2
1	A	37	GLU	2
1	A	45	SER	2
1	A	92	ASP	2
1	A	44	VAL	2
1	A	86	ASN	2
1	A	56	HIS	2
1	A	57	GLU	2
1	A	79	GLU	2
1	A	19	ASN	2
1	A	18	ASP	2
1	A	28	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	87	THR	2
1	A	99	ASP	2
1	A	71	GLN	1
1	A	90	CYS	1
1	A	103	ASP	1
1	A	34	TYR	1
1	A	97	CYS	1
1	A	40	SER	1
1	A	59	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	959
Number of shifts mapped to atoms	959
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	90	-0.04 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	84	-0.05 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	77	-0.09 ± 0.56	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 75%, i.e. 941 atoms were assigned a chemical shift out of a possible 1254. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	337/483 (70%)	172/196 (88%)	88/196 (45%)	77/91 (85%)
Sidechain	554/710 (78%)	378/458 (83%)	169/219 (77%)	7/33 (21%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	50/61 (82%)	25/31 (81%)	24/26 (92%)	1/4 (25%)
Overall	941/1254 (75%)	575/685 (84%)	281/441 (64%)	85/128 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 959 atoms were assigned a chemical shift out of a possible 1298. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	341/510 (67%)	174/208 (84%)	90/206 (44%)	77/96 (80%)
Sidechain	568/727 (78%)	388/470 (83%)	173/224 (77%)	7/33 (21%)
Aromatic	50/61 (82%)	25/31 (81%)	24/26 (92%)	1/4 (25%)
Overall	959/1298 (74%)	587/709 (83%)	287/456 (63%)	85/133 (64%)

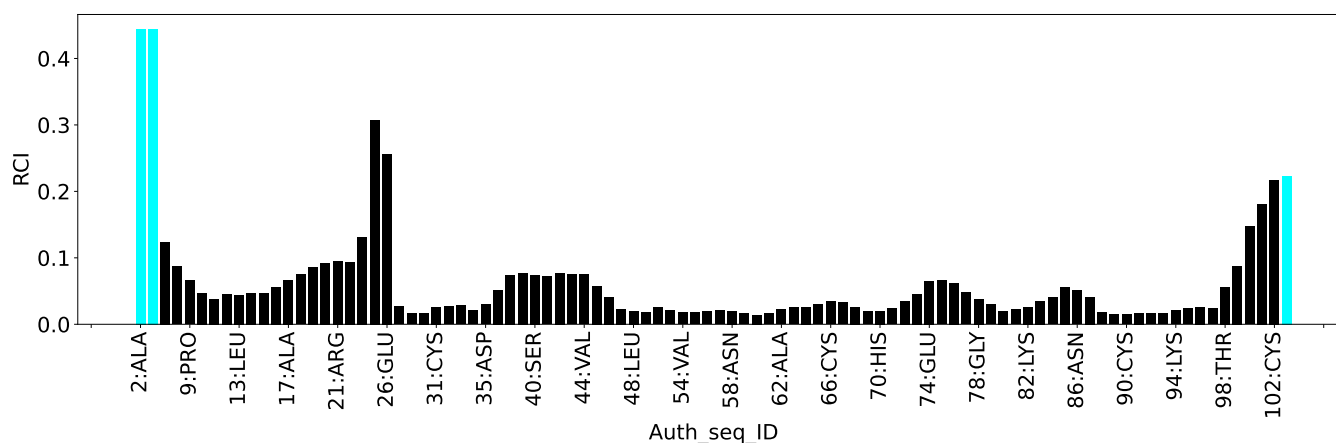
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1177
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	515
Medium range ($ i-j >1$ and $ i-j <5$)	187
Long range ($ i-j \geq 5$)	475
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	135
Number of unmapped restraints	0
Number of restraints per residue	12.7
Number of long range restraints per residue ¹	4.6

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	16.2	0.2
0.2-0.5 (Medium)	39.3	0.5
>0.5 (Large)	130.0	12.87

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)	9.0	8.59
10.0-20.0 (Medium)	0.5	17.96
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

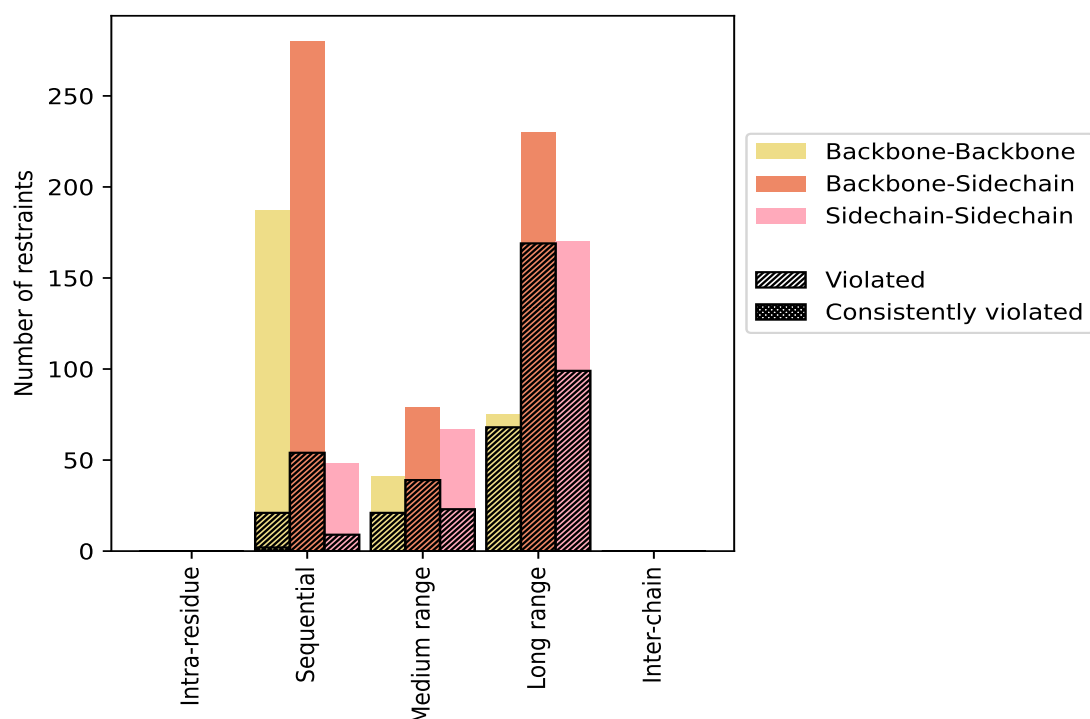
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	515	43.8	84	16.3	7.1	2	0.4	0.2
Backbone-Backbone	187	15.9	21	11.2	1.8	2	1.1	0.2
Backbone-Sidechain	280	23.8	54	19.3	4.6	0	0.0	0.0
Sidechain-Sidechain	48	4.1	9	18.8	0.8	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	187	15.9	83	44.4	7.1	0	0.0	0.0
Backbone-Backbone	41	3.5	21	51.2	1.8	0	0.0	0.0
Backbone-Sidechain	79	6.7	39	49.4	3.3	0	0.0	0.0
Sidechain-Sidechain	67	5.7	23	34.3	2.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	475	40.4	336	70.7	28.5	0	0.0	0.0
Backbone-Backbone	75	6.4	68	90.7	5.8	0	0.0	0.0
Backbone-Sidechain	230	19.5	169	73.5	14.4	0	0.0	0.0
Sidechain-Sidechain	170	14.4	99	58.2	8.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	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	1177	100.0	503	42.7	42.7	2	0.2	0.2
Backbone-Backbone	303	25.7	110	36.3	9.3	2	0.7	0.2
Backbone-Sidechain	589	50.0	262	44.5	22.3	0	0.0	0.0
Sidechain-Sidechain	285	24.2	131	46.0	11.1	0	0.0	0.0

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

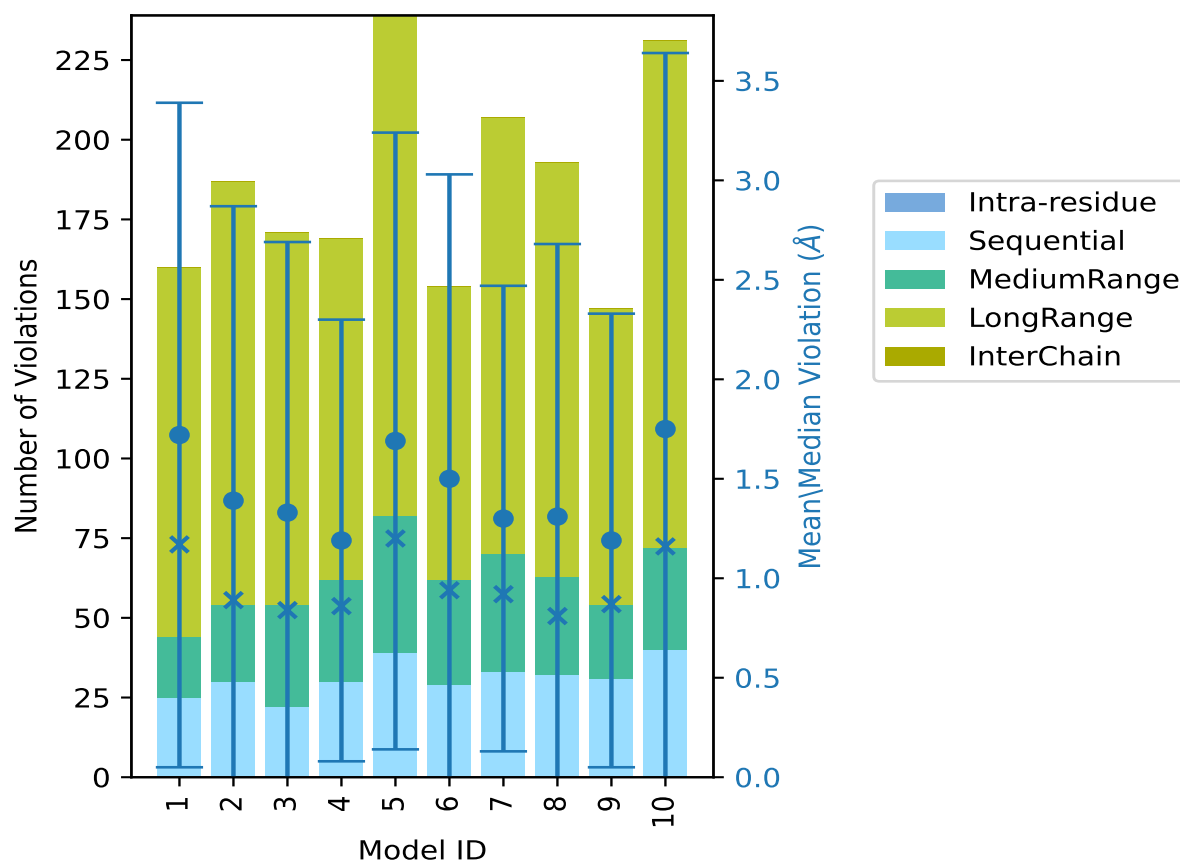
9.2 Distance violation statistics for each model [i](#)

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	0	25	19	116	0	160	1.72	10.53	1.67	1.17
2	0	30	24	133	0	187	1.39	9.82	1.48	0.89
3	0	22	32	117	0	171	1.33	8.38	1.36	0.84
4	0	30	32	107	0	169	1.19	8.7	1.11	0.86
5	0	39	43	157	0	239	1.69	9.17	1.55	1.2
6	0	29	33	92	0	154	1.5	8.59	1.53	0.94
7	0	33	37	137	0	207	1.3	6.17	1.17	0.92
8	0	32	31	130	0	193	1.31	9.5	1.37	0.81
9	0	31	23	93	0	147	1.19	5.6	1.14	0.87
10	0	40	32	159	0	231	1.75	12.87	1.89	1.16

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, 674(IR:0, SQ:431, MR:104, LR:139, 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	%
0	12	28	82	0	122	1	10.0
0	17	7	60	0	84	2	20.0
0	14	11	43	0	68	3	30.0

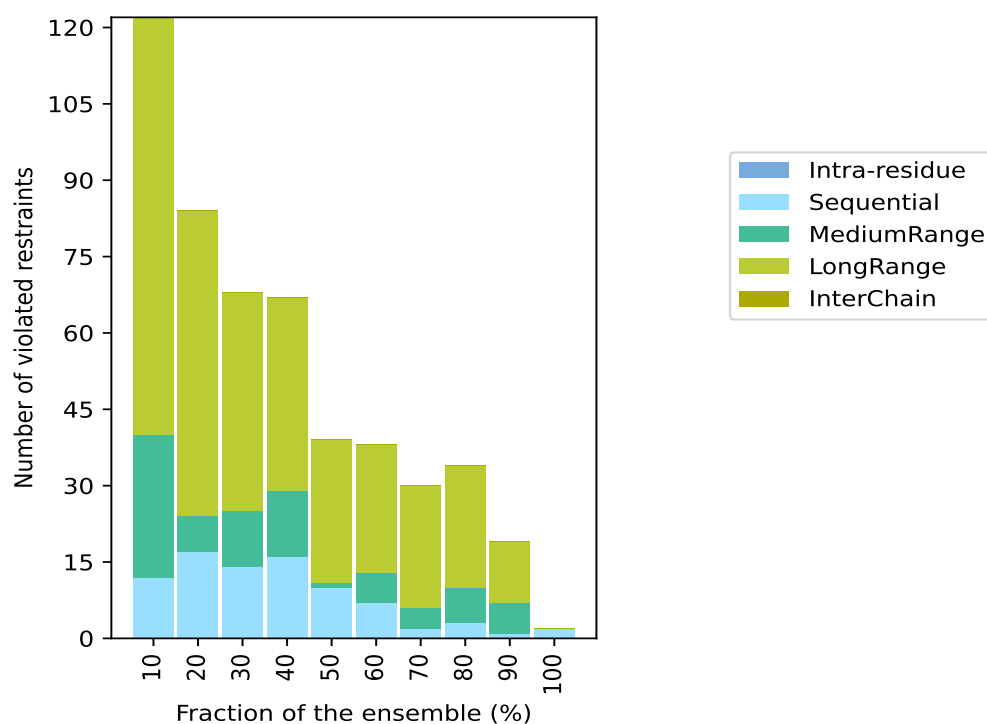
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	16	13	38	0	67	4	40.0
0	10	1	28	0	39	5	50.0
0	7	6	25	0	38	6	60.0
0	2	4	24	0	30	7	70.0
0	3	7	24	0	34	8	80.0
0	1	6	12	0	19	9	90.0
0	2	0	0	0	2	10	100.0

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 ⓘ

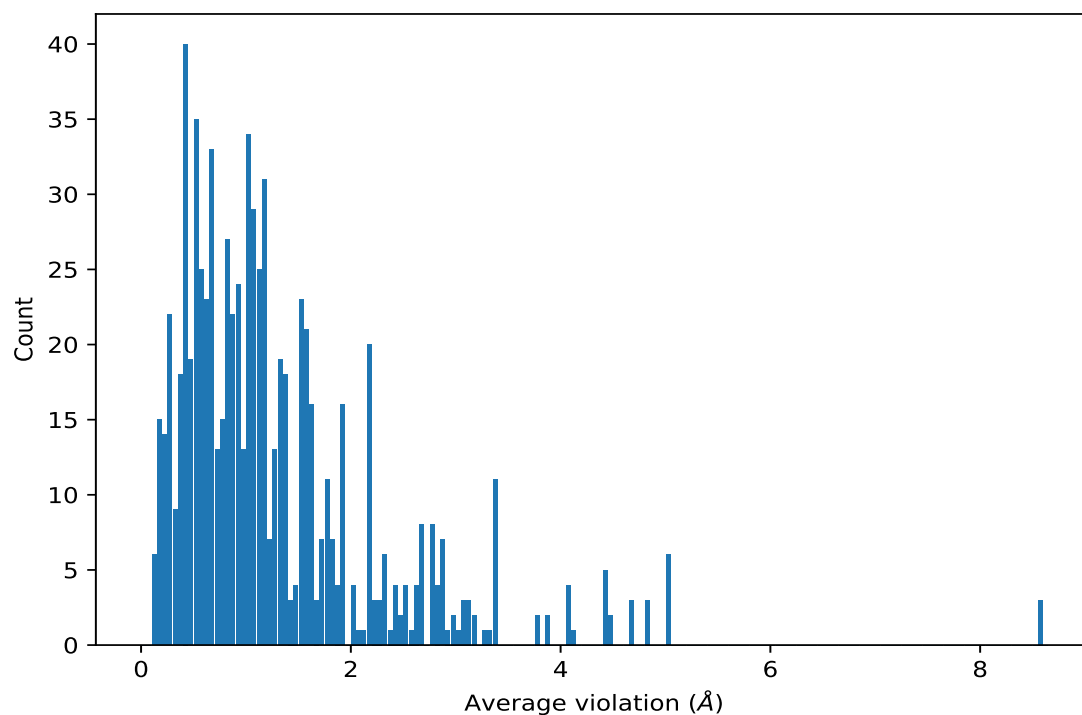


9.4 Most violated distance restraints in the ensemble ⓘ

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)
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	10	0.32	0.08	0.33
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	10	0.32	0.08	0.33
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	9	8.56	2.34	9.17
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	9	8.56	2.34	9.17
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	9	8.56	2.34	9.17
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	9	4.47	0.91	4.96
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	9	4.47	0.91	4.96
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	9	4.44	0.68	4.43
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	9	4.44	0.68	4.43
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	9	4.44	0.68	4.43
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	9	4.44	0.68	4.43
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	9	4.13	1.42	4.6
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	9	4.08	1.8	4.58
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	9	4.06	1.79	3.78
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	9	3.36	1.72	3.93

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	9	3.36	1.72	3.93
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	9	3.36	1.72	3.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	9	3.36	1.72	3.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	9	3.36	1.72	3.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	9	3.36	1.72	3.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	9	3.36	1.72	3.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	9	3.36	1.72	3.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	9	3.36	1.72	3.93
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	9	3.26	1.43	3.14
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	9	2.89	1.35	2.52
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	9	2.86	0.83	3.1
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	9	2.86	0.83	3.1
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	9	2.81	1.64	3.54
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	9	2.81	1.64	3.54
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	9	1.89	1.06	1.9
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	9	1.82	0.58	1.8
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	9	1.42	0.65	1.33
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	9	1.2	0.66	1.07
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	9	1.2	0.66	1.07
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	9	0.5	0.24	0.43
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	9	0.27	0.1	0.29
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	8	5.05	2.01	4.48
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	8	5.05	2.01	4.48
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	8	5.05	2.01	4.48
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	8	5.05	2.01	4.48
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	8	5.05	2.01	4.48
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	8	5.05	2.01	4.48
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	8	4.41	4.05	3.17
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	8	4.06	1.1	3.8
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	8	4.06	1.1	3.8
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	8	3.89	1.75	4.26
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	8	3.89	1.75	4.26
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	8	3.34	1.11	3.34
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	8	3.09	1.36	3.26
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	8	3.09	1.36	3.26
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	8	3.07	1.24	3.22
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	8	3.02	0.85	3.16
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	8	2.92	1.13	2.92
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	8	2.9	1.9	2.88
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	8	2.9	1.9	2.88
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	8	2.9	1.9	2.88
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	8	2.9	1.9	2.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	8	2.63	1.31	2.28
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	8	2.44	1.95	1.68
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	8	2.42	0.94	2.49
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	8	2.42	0.94	2.49
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	8	2.42	0.94	2.49
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	8	2.38	0.94	2.51
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	8	2.32	0.9	2.34
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	8	2.32	0.9	2.34
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	8	2.25	1.47	2.38
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	8	2.25	1.47	2.38
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	8	2.22	1.03	2.15
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	8	2.22	1.03	2.15
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	8	2.18	0.99	2.2
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	8	2.18	0.99	2.2
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	8	2.18	0.99	2.2
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	8	2.18	0.99	2.2
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	8	2.18	0.99	2.2
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	8	2.18	0.99	2.2
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	8	2.09	1.04	2.22
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	8	1.46	1.17	1.1
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	8	1.36	0.83	1.37
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	8	1.29	0.81	1.12
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	8	1.24	0.62	1.34
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	8	1.24	0.62	1.34
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	8	1.17	0.72	0.82
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	8	1.14	0.42	1.06
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	8	1.14	0.42	1.06
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	8	1.13	1.15	0.72
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	8	1.13	0.65	1.17
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	8	1.13	1.15	0.72
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	8	1.08	0.68	0.96
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	8	0.97	0.59	0.86
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	8	0.88	0.34	0.86
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	8	0.65	0.28	0.57
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	8	0.65	0.28	0.57
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	7	4.82	1.88	4.41
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	7	4.82	1.88	4.41
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	7	4.82	1.88	4.41
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	7	4.66	1.55	4.47
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	7	4.66	1.55	4.47
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	7	4.66	1.55	4.47
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	7	3.1	1.41	2.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	7	3.1	1.41	2.86
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	7	3.1	1.41	2.86
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	7	2.95	1.37	2.86
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	7	2.95	1.37	2.86
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	7	2.81	1.42	3.11
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	7	2.81	1.42	3.11
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	7	2.66	1.01	2.62
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	7	2.66	1.01	2.62
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	7	2.21	1.2	1.99
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	7	2.13	1.32	1.42
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	7	2.05	0.83	1.83
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	7	2.05	0.83	1.83
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	7	2.05	0.83	1.83
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	7	1.95	0.92	1.9
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	7	1.77	1.12	1.73
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	7	1.77	1.1	1.58
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	7	1.77	1.1	1.58
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	7	1.77	1.1	1.58
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	7	1.76	0.79	1.99
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	7	1.65	0.56	1.59
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	7	1.65	1.03	1.44
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	7	1.64	0.74	1.6
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	7	1.59	0.81	1.82
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	7	1.54	1.1	1.58
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	7	1.52	0.84	1.53
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	7	1.52	0.84	1.53
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	7	1.52	0.84	1.53
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	7	1.52	0.84	1.53
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	7	1.52	0.84	1.53
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	7	1.52	0.84	1.53
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	7	1.5	1.05	1.67
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	7	1.18	0.94	0.77
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	7	1.1	0.52	1.04
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	7	1.1	0.52	1.04
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	7	1.1	0.52	1.04
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	7	1.08	0.43	1.04
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	7	1.08	0.53	1.29
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	7	1.08	0.53	1.29
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	7	1.04	0.2	1.02
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	7	0.84	0.54	0.74
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	7	0.72	0.41	0.7
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	7	0.72	0.49	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	7	0.57	0.5	0.32
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	7	0.57	0.5	0.32
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE1	6	3.78	3.27	2.53
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE2	6	3.78	3.27	2.53
(1,38)	1:11:A:VAL:HB	1:48:A:LEU:H	6	2.57	1.16	2.68
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE1	6	2.52	1.63	2.19
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE2	6	2.52	1.63	2.19
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE1	6	2.52	1.63	2.19
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE2	6	2.52	1.63	2.19
(1,384)	1:67:A:PRO:HG2	1:69:A:PHE:HZ	6	2.47	1.18	2.25
(1,384)	1:67:A:PRO:HG3	1:69:A:PHE:HZ	6	2.47	1.18	2.25
(1,839)	1:14:A:VAL:HG11	1:45:A:SER:H	6	2.34	1.04	2.49
(1,839)	1:14:A:VAL:HG12	1:45:A:SER:H	6	2.34	1.04	2.49
(1,839)	1:14:A:VAL:HG13	1:45:A:SER:H	6	2.34	1.04	2.49
(1,553)	1:80:A:THR:HB	1:88:A:CYS:H	6	2.26	0.51	2.06
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB2	6	2.18	1.57	2.0
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB3	6	2.18	1.57	2.0
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB2	6	2.18	1.57	2.0
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB3	6	2.18	1.57	2.0
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB2	6	2.18	1.57	2.0
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB3	6	2.18	1.57	2.0
(1,68)	1:13:A:LEU:HB2	1:48:A:LEU:HG	6	2.15	0.65	1.98
(1,68)	1:13:A:LEU:HB3	1:48:A:LEU:HG	6	2.15	0.65	1.98
(1,441)	1:70:A:HIS:HD2	1:81:A:VAL:HB	6	2.03	0.97	2.01
(1,831)	1:11:A:VAL:H	1:48:A:LEU:H	6	1.95	0.35	2.01
(1,977)	1:69:A:PHE:H	1:95:A:TRP:HE1	6	1.66	1.03	1.38
(1,647)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	6	1.65	0.95	1.66
(1,647)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	6	1.65	0.95	1.66
(1,647)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	6	1.65	0.95	1.66
(1,1072)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	6	1.65	0.95	1.66
(1,1072)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	6	1.65	0.95	1.66
(1,1072)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	6	1.65	0.95	1.66
(1,333)	1:61:A:VAL:HB	1:65:A:ARG:HA	6	1.57	0.83	1.68
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG2	6	1.51	1.54	0.91
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG3	6	1.51	1.54	0.91
(1,565)	1:80:A:THR:HA	1:95:A:TRP:HZ3	6	1.45	0.95	1.4
(1,148)	1:30:A:THR:HA	1:54:A:VAL:HB	6	1.34	0.84	1.26
(1,149)	1:30:A:THR:HB	1:54:A:VAL:HB	6	1.33	0.78	1.18
(1,144)	1:30:A:THR:H	1:54:A:VAL:HB	6	1.3	0.6	1.23
(1,865)	1:30:A:THR:H	1:54:A:VAL:HB	6	1.3	0.6	1.23
(1,173)	1:32:A:GLN:HG2	1:33:A:ASN:HA	6	1.22	0.36	1.32
(1,173)	1:32:A:GLN:HG3	1:33:A:ASN:HA	6	1.22	0.36	1.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB1	6	1.19	0.51	1.01
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB2	6	1.19	0.51	1.01
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB3	6	1.19	0.51	1.01
(1,421)	1:69:A:PHE:H	1:95:A:TRP:HD1	6	1.17	0.74	1.12
(1,979)	1:69:A:PHE:H	1:95:A:TRP:HD1	6	1.17	0.74	1.12
(1,237)	1:53:A:MET:HA	1:62:A:ALA:HA	6	1.06	0.62	1.01
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG11	6	1.0	0.47	0.99
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG12	6	1.0	0.47	0.99
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG13	6	1.0	0.47	0.99
(1,575)	1:81:A:VAL:HB	1:82:A:LYS:H	6	0.88	0.14	0.86
(1,1050)	1:81:A:VAL:HB	1:82:A:LYS:H	6	0.88	0.14	0.86
(1,1060)	1:81:A:VAL:H	1:89:A:VAL:HA	6	0.71	0.37	0.68
(1,792)	1:98:A:THR:HB	1:99:A:ASP:H	6	0.7	0.15	0.7
(1,1160)	1:98:A:THR:HB	1:99:A:ASP:H	6	0.7	0.15	0.7
(1,554)	1:80:A:THR:H	1:89:A:VAL:HA	6	0.68	0.27	0.73
(1,1045)	1:80:A:THR:H	1:89:A:VAL:HA	6	0.68	0.27	0.73
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD2	6	0.47	0.35	0.33
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD3	6	0.47	0.35	0.33
(1,692)	1:88:A:CYS:HA	1:96:A:ASN:HA	6	0.41	0.19	0.46
(1,827)	1:11:A:VAL:HB	1:12:A:LYS:H	6	0.28	0.09	0.29
(1,845)	1:17:A:ALA:H	1:18:A:ASP:HA	6	0.28	0.12	0.26
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE1	5	3.39	1.4	3.59
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE2	5	3.39	1.4	3.59
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB2	5	2.75	1.28	3.51
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB3	5	2.75	1.28	3.51
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB2	5	2.75	1.28	3.51
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB3	5	2.75	1.28	3.51
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB2	5	2.75	1.28	3.51
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB3	5	2.75	1.28	3.51
(1,13)	1:10:A:MET:HE1	1:47:A:CYS:HA	5	2.18	1.37	1.41
(1,13)	1:10:A:MET:HE2	1:47:A:CYS:HA	5	2.18	1.37	1.41
(1,13)	1:10:A:MET:HE3	1:47:A:CYS:HA	5	2.18	1.37	1.41
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD2	5	1.95	1.52	2.2
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD3	5	1.95	1.52	2.2
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG11	5	1.88	0.85	2.04
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG12	5	1.88	0.85	2.04
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG13	5	1.88	0.85	2.04
(1,74)	1:14:A:VAL:HG11	1:45:A:SER:HA	5	1.76	0.67	1.78
(1,74)	1:14:A:VAL:HG12	1:45:A:SER:HA	5	1.76	0.67	1.78
(1,74)	1:14:A:VAL:HG13	1:45:A:SER:HA	5	1.76	0.67	1.78
(1,1122)	1:90:A:CYS:H	1:95:A:TRP:HZ3	5	1.67	1.67	1.05
(1,559)	1:80:A:THR:HB	1:89:A:VAL:HB	5	1.42	1.05	1.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,178)	1:32:A:GLN:HG2	1:69:A:PHE:HZ	5	1.37	0.55	1.33
(1,178)	1:32:A:GLN:HG3	1:69:A:PHE:HZ	5	1.37	0.55	1.33
(1,156)	1:30:A:THR:HG21	1:55:A:ARG:HA	5	1.35	0.86	1.91
(1,156)	1:30:A:THR:HG22	1:55:A:ARG:HA	5	1.35	0.86	1.91
(1,156)	1:30:A:THR:HG23	1:55:A:ARG:HA	5	1.35	0.86	1.91
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA2	5	1.34	0.63	1.41
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA3	5	1.34	0.63	1.41
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA2	5	1.34	0.63	1.41
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA3	5	1.34	0.63	1.41
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA2	5	1.34	0.63	1.41
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA3	5	1.34	0.63	1.41
(1,1090)	1:87:A:THR:HB	1:98:A:THR:H	5	1.32	1.29	0.75
(1,1163)	1:98:A:THR:HB	1:100:A:HIS:H	5	1.32	0.93	0.95
(1,152)	1:30:A:THR:HA	1:55:A:ARG:H	5	1.25	0.8	0.97
(1,866)	1:30:A:THR:HA	1:55:A:ARG:H	5	1.25	0.8	0.97
(1,724)	1:89:A:VAL:HB	1:95:A:TRP:HE3	5	1.25	1.03	1.03
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG11	5	1.23	0.88	0.89
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG12	5	1.23	0.88	0.89
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG13	5	1.23	0.88	0.89
(1,11)	1:53:A:MET:HE1	1:63:A:LEU:H	5	1.11	0.85	0.79
(1,11)	1:53:A:MET:HE2	1:63:A:LEU:H	5	1.11	0.85	0.79
(1,11)	1:53:A:MET:HE3	1:63:A:LEU:H	5	1.11	0.85	0.79
(1,243)	1:53:A:MET:HA	1:63:A:LEU:HA	5	1.11	0.74	0.9
(1,539)	1:79:A:GLU:H	1:89:A:VAL:HA	5	1.06	0.81	0.77
(1,415)	1:69:A:PHE:HE1	1:74:A:GLU:HA	5	1.03	0.45	0.99
(1,415)	1:69:A:PHE:HE2	1:74:A:GLU:HA	5	1.03	0.45	0.99
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD2	5	1.02	0.79	0.83
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD3	5	1.02	0.79	0.83
(1,604)	1:81:A:VAL:HA	1:88:A:CYS:H	5	0.88	0.33	0.9
(1,1099)	1:88:A:CYS:H	1:98:A:THR:H	5	0.87	1.08	0.29
(1,3)	1:53:A:MET:HE1	1:60:A:CYS:HA	5	0.84	0.63	0.55
(1,3)	1:53:A:MET:HE2	1:60:A:CYS:HA	5	0.84	0.63	0.55
(1,3)	1:53:A:MET:HE3	1:60:A:CYS:HA	5	0.84	0.63	0.55
(1,379)	1:66:A:CYS:HB2	1:93:A:ARG:HA	5	0.83	0.81	0.55
(1,379)	1:66:A:CYS:HB3	1:93:A:ARG:HA	5	0.83	0.81	0.55
(1,687)	1:88:A:CYS:HA	1:95:A:TRP:HA	5	0.67	0.31	0.65
(1,563)	1:80:A:THR:HG21	1:89:A:VAL:HB	5	0.56	0.48	0.32
(1,563)	1:80:A:THR:HG22	1:89:A:VAL:HB	5	0.56	0.48	0.32
(1,563)	1:80:A:THR:HG23	1:89:A:VAL:HB	5	0.56	0.48	0.32
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB2	5	0.56	0.25	0.68
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB3	5	0.56	0.25	0.68
(1,600)	1:81:A:VAL:HG21	1:87:A:THR:HB	5	0.52	0.2	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,600)	1:81:A:VAL:HG22	1:87:A:THR:HB	5	0.52	0.2	0.6
(1,600)	1:81:A:VAL:HG23	1:87:A:THR:HB	5	0.52	0.2	0.6
(1,793)	1:98:A:THR:HB	1:99:A:ASP:HA	5	0.48	0.17	0.52
(1,670)	1:87:A:THR:HB	1:88:A:CYS:H	5	0.4	0.06	0.42
(1,1171)	1:101:A:VAL:HB	1:102:A:CYS:H	5	0.36	0.09	0.38
(1,819)	1:102:A:CYS:HA	1:103:A:ASP:H	5	0.25	0.11	0.29
(1,1176)	1:102:A:CYS:HA	1:103:A:ASP:H	5	0.25	0.11	0.29
(1,201)	1:35:A:ASP:HA	1:36:A:LEU:H	5	0.2	0.08	0.19
(1,207)	1:39:A:MET:HA	1:40:A:SER:H	5	0.2	0.05	0.22
(1,888)	1:39:A:MET:HA	1:40:A:SER:H	5	0.2	0.05	0.22
(1,92)	1:17:A:ALA:HA	1:18:A:ASP:HA	5	0.16	0.04	0.14
(1,170)	1:31:A:CYS:HB2	1:69:A:PHE:HZ	4	3.18	1.33	2.95
(1,170)	1:31:A:CYS:HB3	1:69:A:PHE:HZ	4	3.18	1.33	2.95
(1,40)	1:11:A:VAL:HG21	1:48:A:LEU:H	4	2.67	1.05	2.96
(1,40)	1:11:A:VAL:HG22	1:48:A:LEU:H	4	2.67	1.05	2.96
(1,40)	1:11:A:VAL:HG23	1:48:A:LEU:H	4	2.67	1.05	2.96
(1,644)	1:83:A:ILE:HD11	1:95:A:TRP:HE3	4	2.18	0.77	2.4
(1,644)	1:83:A:ILE:HD12	1:95:A:TRP:HE3	4	2.18	0.77	2.4
(1,644)	1:83:A:ILE:HD13	1:95:A:TRP:HE3	4	2.18	0.77	2.4
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD11	4	1.91	1.27	1.7
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD12	4	1.91	1.27	1.7
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD13	4	1.91	1.27	1.7
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB2	4	1.74	0.45	1.9
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB3	4	1.74	0.45	1.9
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB2	4	1.74	0.45	1.9
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB3	4	1.74	0.45	1.9
(1,723)	1:89:A:VAL:HB	1:95:A:TRP:HZ3	4	1.7	1.53	1.17
(1,36)	1:11:A:VAL:HG21	1:47:A:CYS:HA	4	1.59	0.88	1.76
(1,36)	1:11:A:VAL:HG22	1:47:A:CYS:HA	4	1.59	0.88	1.76
(1,36)	1:11:A:VAL:HG23	1:47:A:CYS:HA	4	1.59	0.88	1.76
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG21	4	1.59	0.98	1.78
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG22	4	1.59	0.98	1.78
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG23	4	1.59	0.98	1.78
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG21	4	1.59	0.98	1.78
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG22	4	1.59	0.98	1.78
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG23	4	1.59	0.98	1.78
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE1	4	1.58	0.88	1.62
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE2	4	1.58	0.88	1.62
(1,39)	1:11:A:VAL:HG11	1:48:A:LEU:H	4	1.56	0.85	1.84
(1,39)	1:11:A:VAL:HG12	1:48:A:LEU:H	4	1.56	0.85	1.84
(1,39)	1:11:A:VAL:HG13	1:48:A:LEU:H	4	1.56	0.85	1.84
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE1	4	1.54	1.31	1.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE2	4	1.54	1.31	1.18
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE1	4	1.54	1.31	1.18
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE2	4	1.54	1.31	1.18
(1,253)	1:54:A:VAL:HG21	1:61:A:VAL:HB	4	1.49	0.8	1.46
(1,253)	1:54:A:VAL:HG22	1:61:A:VAL:HB	4	1.49	0.8	1.46
(1,253)	1:54:A:VAL:HG23	1:61:A:VAL:HB	4	1.49	0.8	1.46
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE1	4	1.36	1.21	1.19
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE2	4	1.36	1.21	1.19
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG21	4	1.35	1.33	0.89
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG22	4	1.35	1.33	0.89
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG23	4	1.35	1.33	0.89
(1,674)	1:87:A:THR:HB	1:97:A:CYS:HA	4	1.32	0.53	1.18
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD2	4	1.18	0.81	1.11
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD3	4	1.18	0.81	1.11
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB2	4	1.14	0.56	1.3
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB3	4	1.14	0.56	1.3
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB2	4	1.14	0.56	1.3
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB3	4	1.14	0.56	1.3
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB2	4	1.14	0.56	1.3
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB3	4	1.14	0.56	1.3
(1,803)	1:98:A:THR:HG21	1:100:A:HIS:HE1	4	1.08	0.64	0.98
(1,803)	1:98:A:THR:HG22	1:100:A:HIS:HE1	4	1.08	0.64	0.98
(1,803)	1:98:A:THR:HG23	1:100:A:HIS:HE1	4	1.08	0.64	0.98
(1,818)	1:101:A:VAL:HG11	1:103:A:ASP:H	4	1.03	0.43	0.96
(1,818)	1:101:A:VAL:HG12	1:103:A:ASP:H	4	1.03	0.43	0.96
(1,818)	1:101:A:VAL:HG13	1:103:A:ASP:H	4	1.03	0.43	0.96
(1,1174)	1:101:A:VAL:HG11	1:103:A:ASP:H	4	1.03	0.43	0.96
(1,1174)	1:101:A:VAL:HG12	1:103:A:ASP:H	4	1.03	0.43	0.96
(1,1174)	1:101:A:VAL:HG13	1:103:A:ASP:H	4	1.03	0.43	0.96
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG21	4	1.03	0.56	0.88
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG22	4	1.03	0.56	0.88
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG23	4	1.03	0.56	0.88
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG21	4	1.03	0.56	0.88
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG22	4	1.03	0.56	0.88
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG23	4	1.03	0.56	0.88
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG11	4	0.99	0.54	0.8
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG12	4	0.99	0.54	0.8
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG13	4	0.99	0.54	0.8
(1,1134)	1:91:A:ARG:H	1:95:A:TRP:HE3	4	0.92	0.82	0.6
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE1	4	0.92	0.36	1.04
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE2	4	0.92	0.36	1.04
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB2	4	0.91	0.42	0.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB3	4	0.91	0.42	0.84
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB2	4	0.91	0.42	0.84
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB3	4	0.91	0.42	0.84
(1,732)	1:89:A:VAL:HB	1:96:A:ASN:H	4	0.91	0.34	0.96
(1,1111)	1:89:A:VAL:HB	1:96:A:ASN:H	4	0.91	0.34	0.96
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE1	4	0.88	0.33	0.72
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE2	4	0.88	0.33	0.72
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE1	4	0.88	0.33	0.72
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE2	4	0.88	0.33	0.72
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG21	4	0.86	0.49	0.82
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG22	4	0.86	0.49	0.82
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG23	4	0.86	0.49	0.82
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG21	4	0.86	0.49	0.82
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG22	4	0.86	0.49	0.82
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG23	4	0.86	0.49	0.82
(1,815)	1:101:A:VAL:HA	1:103:A:ASP:H	4	0.86	0.03	0.86
(1,490)	1:75:A:TYR:HE1	1:81:A:VAL:HA	4	0.85	0.56	0.84
(1,490)	1:75:A:TYR:HE2	1:81:A:VAL:HA	4	0.85	0.56	0.84
(1,968)	1:68:A:CYS:HA	1:95:A:TRP:HE1	4	0.74	0.77	0.38
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG11	4	0.73	0.38	0.74
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG12	4	0.73	0.38	0.74
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG13	4	0.73	0.38	0.74
(1,636)	1:82:A:LYS:HD2	1:88:A:CYS:H	4	0.72	0.3	0.82
(1,636)	1:82:A:LYS:HD3	1:88:A:CYS:H	4	0.72	0.3	0.82
(1,329)	1:61:A:VAL:HB	1:62:A:ALA:H	4	0.7	0.22	0.71
(1,935)	1:61:A:VAL:HB	1:62:A:ALA:H	4	0.7	0.22	0.71
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB1	4	0.69	0.47	0.52
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB2	4	0.69	0.47	0.52
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB3	4	0.69	0.47	0.52
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD11	4	0.68	0.54	0.47
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD12	4	0.68	0.54	0.47
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD13	4	0.68	0.54	0.47
(1,628)	1:82:A:LYS:HA	1:87:A:THR:HA	4	0.66	0.36	0.5
(1,1132)	1:91:A:ARG:H	1:94:A:LYS:H	4	0.65	0.31	0.61
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD21	4	0.62	0.35	0.5
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD22	4	0.62	0.35	0.5
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD23	4	0.62	0.35	0.5
(1,794)	1:98:A:THR:HG21	1:99:A:ASP:HA	4	0.6	0.06	0.63
(1,794)	1:98:A:THR:HG22	1:99:A:ASP:HA	4	0.6	0.06	0.63
(1,794)	1:98:A:THR:HG23	1:99:A:ASP:HA	4	0.6	0.06	0.63
(1,281)	1:55:A:ARG:HA	1:61:A:VAL:H	4	0.6	0.28	0.55
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG2	4	0.6	0.24	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG3	4	0.6	0.24	0.56
(1,991)	1:70:A:HIS:HB2	1:95:A:TRP:HE1	4	0.56	0.29	0.53
(1,991)	1:70:A:HIS:HB3	1:95:A:TRP:HE1	4	0.56	0.29	0.53
(1,802)	1:98:A:THR:HG21	1:100:A:HIS:HD2	4	0.53	0.21	0.48
(1,802)	1:98:A:THR:HG22	1:100:A:HIS:HD2	4	0.53	0.21	0.48
(1,802)	1:98:A:THR:HG23	1:100:A:HIS:HD2	4	0.53	0.21	0.48
(1,621)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	4	0.53	0.24	0.53
(1,621)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	4	0.53	0.24	0.53
(1,621)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	4	0.53	0.24	0.53
(1,756)	1:91:A:ARG:HA	1:93:A:ARG:H	4	0.51	0.31	0.44
(1,1130)	1:91:A:ARG:HA	1:93:A:ARG:H	4	0.51	0.31	0.44
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG21	4	0.44	0.09	0.45
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG22	4	0.44	0.09	0.45
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG23	4	0.44	0.09	0.45
(1,721)	1:89:A:VAL:HA	1:95:A:TRP:HA	4	0.44	0.24	0.3
(1,81)	1:15:A:CYS:HB2	1:45:A:SER:HA	4	0.42	0.2	0.45
(1,81)	1:15:A:CYS:HB3	1:45:A:SER:HA	4	0.42	0.2	0.45
(1,135)	1:30:A:THR:HB	1:31:A:CYS:H	4	0.42	0.2	0.36
(1,860)	1:30:A:THR:HB	1:31:A:CYS:H	4	0.42	0.2	0.36
(1,1142)	1:92:A:ASP:HA	1:94:A:LYS:H	4	0.39	0.06	0.4
(1,1066)	1:82:A:LYS:HG2	1:83:A:ILE:H	4	0.37	0.22	0.32
(1,1066)	1:82:A:LYS:HG3	1:83:A:ILE:H	4	0.37	0.22	0.32
(1,420)	1:69:A:PHE:HA	1:75:A:TYR:H	4	0.31	0.08	0.32
(1,248)	1:54:A:VAL:HB	1:55:A:ARG:H	4	0.2	0.05	0.22
(1,669)	1:87:A:THR:HB	1:88:A:CYS:HA	4	0.2	0.06	0.2
(1,372)	1:65:A:ARG:HD2	1:66:A:CYS:H	4	0.19	0.05	0.18
(1,372)	1:65:A:ARG:HD3	1:66:A:CYS:H	4	0.19	0.05	0.18
(1,771)	1:93:A:ARG:HA	1:94:A:LYS:H	4	0.19	0.03	0.18
(1,1145)	1:93:A:ARG:HA	1:94:A:LYS:H	4	0.19	0.03	0.18
(1,806)	1:99:A:ASP:HA	1:100:A:HIS:H	4	0.18	0.06	0.16
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD2	3	2.76	0.8	2.32
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD3	3	2.76	0.8	2.32
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG11	3	1.95	1.2	2.58
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG12	3	1.95	1.2	2.58
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG13	3	1.95	1.2	2.58
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG11	3	1.95	1.2	2.58
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG12	3	1.95	1.2	2.58
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG13	3	1.95	1.2	2.58
(1,499)	1:75:A:TYR:HE1	1:95:A:TRP:HH2	3	1.84	1.45	1.14
(1,499)	1:75:A:TYR:HE2	1:95:A:TRP:HH2	3	1.84	1.45	1.14
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB2	3	1.6	0.73	1.9
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB3	3	1.6	0.73	1.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB2	3	1.6	0.73	1.9
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB3	3	1.6	0.73	1.9
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB2	3	1.6	0.73	1.9
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB3	3	1.6	0.73	1.9
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB2	3	1.59	0.32	1.69
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB3	3	1.59	0.32	1.69
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD1	3	1.57	0.8	1.77
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD2	3	1.57	0.8	1.77
(1,1116)	1:89:A:VAL:H	1:98:A:THR:H	3	1.55	1.34	0.76
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD2	3	1.52	0.98	0.95
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD3	3	1.52	0.98	0.95
(1,335)	1:61:A:VAL:HB	1:65:A:ARG:H	3	1.51	0.37	1.45
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG21	3	1.25	0.75	1.14
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG22	3	1.25	0.75	1.14
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG23	3	1.25	0.75	1.14
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG11	3	1.2	0.44	0.99
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG12	3	1.2	0.44	0.99
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG13	3	1.2	0.44	0.99
(1,738)	1:89:A:VAL:H	1:97:A:CYS:HA	3	1.18	1.22	0.41
(1,1114)	1:89:A:VAL:H	1:97:A:CYS:HA	3	1.18	1.22	0.41
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG21	3	1.18	0.87	0.86
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG22	3	1.18	0.87	0.86
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG23	3	1.18	0.87	0.86
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG11	3	1.17	0.89	1.09
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG12	3	1.17	0.89	1.09
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG13	3	1.17	0.89	1.09
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG11	3	1.17	0.89	1.09
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG12	3	1.17	0.89	1.09
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG13	3	1.17	0.89	1.09
(1,746)	1:90:A:CYS:HA	1:95:A:TRP:HE3	3	1.15	0.98	0.72
(1,617)	1:81:A:VAL:HG21	1:95:A:TRP:HZ2	3	1.09	1.02	0.6
(1,617)	1:81:A:VAL:HG22	1:95:A:TRP:HZ2	3	1.09	1.02	0.6
(1,617)	1:81:A:VAL:HG23	1:95:A:TRP:HZ2	3	1.09	1.02	0.6
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD2	3	1.09	1.03	0.58
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD3	3	1.09	1.03	0.58
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD2	3	1.09	1.03	0.58
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD3	3	1.09	1.03	0.58
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD21	3	1.06	0.33	1.26
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD22	3	1.06	0.33	1.26
(1,750)	1:90:A:CYS:HA	1:96:A:ASN:H	3	1.06	0.8	0.55
(1,1123)	1:90:A:CYS:HA	1:96:A:ASN:H	3	1.06	0.8	0.55
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD1	3	1.03	0.64	1.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD2	3	1.03	0.64	1.38
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD21	3	0.97	0.45	0.98
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD22	3	0.97	0.45	0.98
(1,835)	1:13:A:LEU:H	1:46:A:GLY:H	3	0.96	0.36	0.94
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA2	3	0.95	0.37	0.98
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA3	3	0.95	0.37	0.98
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA2	3	0.95	0.37	0.98
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA3	3	0.95	0.37	0.98
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA2	3	0.95	0.37	0.98
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA3	3	0.95	0.37	0.98
(1,158)	1:30:A:THR:HG21	1:55:A:ARG:H	3	0.93	0.21	0.88
(1,158)	1:30:A:THR:HG22	1:55:A:ARG:H	3	0.93	0.21	0.88
(1,158)	1:30:A:THR:HG23	1:55:A:ARG:H	3	0.93	0.21	0.88
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD1	3	0.9	1.0	0.25
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD2	3	0.9	1.0	0.25
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG21	3	0.89	0.56	1.03
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG22	3	0.89	0.56	1.03
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG23	3	0.89	0.56	1.03
(1,5)	1:53:A:MET:HE1	1:61:A:VAL:H	3	0.87	0.28	0.89
(1,5)	1:53:A:MET:HE2	1:61:A:VAL:H	3	0.87	0.28	0.89
(1,5)	1:53:A:MET:HE3	1:61:A:VAL:H	3	0.87	0.28	0.89
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG21	3	0.8	0.13	0.79
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG22	3	0.8	0.13	0.79
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG23	3	0.8	0.13	0.79
(1,656)	1:85:A:CYS:HB2	1:102:A:CYS:HA	3	0.79	0.04	0.81
(1,656)	1:85:A:CYS:HB3	1:102:A:CYS:HA	3	0.79	0.04	0.81
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG21	3	0.79	0.36	0.8
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG22	3	0.79	0.36	0.8
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG23	3	0.79	0.36	0.8
(1,552)	1:80:A:THR:HA	1:88:A:CYS:H	3	0.76	0.5	0.63
(1,967)	1:68:A:CYS:H	1:75:A:TYR:H	3	0.74	0.63	0.42
(1,858)	1:29:A:LYS:HB2	1:34:A:TYR:H	3	0.66	0.38	0.43
(1,858)	1:29:A:LYS:HB3	1:34:A:TYR:H	3	0.66	0.38	0.43
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD2	3	0.63	0.27	0.56
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD3	3	0.63	0.27	0.56
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG21	3	0.63	0.14	0.62
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG22	3	0.63	0.14	0.62
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG23	3	0.63	0.14	0.62
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG21	3	0.62	0.16	0.73
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG22	3	0.62	0.16	0.73
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG23	3	0.62	0.16	0.73
(1,686)	1:88:A:CYS:H	1:95:A:TRP:HE3	3	0.61	0.34	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1094)	1:88:A:CYS:H	1:95:A:TRP:HE3	3	0.61	0.34	0.4
(1,1162)	1:98:A:THR:HA	1:100:A:HIS:H	3	0.56	0.22	0.57
(1,1109)	1:89:A:VAL:H	1:96:A:ASN:H	3	0.56	0.2	0.57
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB2	3	0.56	0.43	0.44
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB3	3	0.56	0.43	0.44
(1,641)	1:83:A:ILE:H	1:87:A:THR:HA	3	0.56	0.42	0.35
(1,1063)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	3	0.54	0.16	0.43
(1,1063)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	3	0.54	0.16	0.43
(1,1063)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	3	0.54	0.16	0.43
(1,1175)	1:102:A:CYS:H	1:103:A:ASP:H	3	0.53	0.13	0.61
(1,327)	1:61:A:VAL:HB	1:62:A:ALA:HA	3	0.51	0.01	0.51
(1,616)	1:81:A:VAL:HG11	1:95:A:TRP:HZ2	3	0.51	0.21	0.4
(1,616)	1:81:A:VAL:HG12	1:95:A:TRP:HZ2	3	0.51	0.21	0.4
(1,616)	1:81:A:VAL:HG13	1:95:A:TRP:HZ2	3	0.51	0.21	0.4
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB1	3	0.51	0.15	0.5
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB2	3	0.51	0.15	0.5
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB3	3	0.51	0.15	0.5
(1,1076)	1:85:A:CYS:H	1:86:A:ASN:H	3	0.51	0.12	0.59
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG11	3	0.49	0.32	0.34
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG12	3	0.49	0.32	0.34
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG13	3	0.49	0.32	0.34
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG2	3	0.48	0.09	0.47
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG3	3	0.48	0.09	0.47
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD11	3	0.46	0.13	0.51
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD12	3	0.46	0.13	0.51
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD13	3	0.46	0.13	0.51
(1,558)	1:80:A:THR:HA	1:89:A:VAL:HA	3	0.44	0.1	0.49
(1,536)	1:79:A:GLU:HG2	1:80:A:THR:HB	3	0.44	0.17	0.37
(1,536)	1:79:A:GLU:HG3	1:80:A:THR:HB	3	0.44	0.17	0.37
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD2	3	0.41	0.3	0.22
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD3	3	0.41	0.3	0.22
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD2	3	0.41	0.3	0.22
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD3	3	0.41	0.3	0.22
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD2	3	0.41	0.3	0.22
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD3	3	0.41	0.3	0.22
(1,359)	1:63:A:LEU:HA	1:66:A:CYS:H	3	0.41	0.2	0.55
(1,576)	1:81:A:VAL:HB	1:82:A:LYS:HA	3	0.4	0.04	0.42
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG11	3	0.39	0.32	0.24
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG12	3	0.39	0.32	0.24
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG13	3	0.39	0.32	0.24
(1,261)	1:54:A:VAL:HG21	1:63:A:LEU:H	3	0.39	0.18	0.49
(1,261)	1:54:A:VAL:HG22	1:63:A:LEU:H	3	0.39	0.18	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,261)	1:54:A:VAL:HG23	1:63:A:LEU:H	3	0.39	0.18	0.49
(1,408)	1:69:A:PHE:HA	1:73:A:LYS:H	3	0.33	0.14	0.3
(1,974)	1:69:A:PHE:HA	1:73:A:LYS:H	3	0.33	0.14	0.3
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG11	3	0.26	0.04	0.26
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG12	3	0.26	0.04	0.26
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG13	3	0.26	0.04	0.26
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG21	3	0.24	0.03	0.23
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG22	3	0.24	0.03	0.23
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG23	3	0.24	0.03	0.23
(1,57)	1:13:A:LEU:HA	1:14:A:VAL:HB	3	0.24	0.11	0.18
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG21	3	0.23	0.04	0.23
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG22	3	0.23	0.04	0.23
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG23	3	0.23	0.04	0.23
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB2	3	0.19	0.02	0.19
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB3	3	0.19	0.02	0.19
(1,1085)	1:87:A:THR:HB	1:88:A:CYS:H	3	0.14	0.02	0.13
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD11	2	2.68	1.68	2.68
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD12	2	2.68	1.68	2.68
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD13	2	2.68	1.68	2.68
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG21	2	2.64	0.9	2.64
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG22	2	2.64	0.9	2.64
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG23	2	2.64	0.9	2.64
(1,613)	1:81:A:VAL:HB	1:95:A:TRP:HH2	2	2.32	0.69	2.32
(1,521)	1:77:A:PRO:HA	1:90:A:CYS:H	2	1.94	0.08	1.94
(1,126)	1:29:A:LYS:HE2	1:34:A:TYR:HA	2	1.93	0.31	1.93
(1,126)	1:29:A:LYS:HE3	1:34:A:TYR:HA	2	1.93	0.31	1.93
(1,1024)	1:77:A:PRO:HA	1:90:A:CYS:H	2	1.84	0.08	1.84
(1,615)	1:81:A:VAL:HG21	1:95:A:TRP:HE1	2	1.82	0.96	1.82
(1,615)	1:81:A:VAL:HG22	1:95:A:TRP:HE1	2	1.82	0.96	1.82
(1,615)	1:81:A:VAL:HG23	1:95:A:TRP:HE1	2	1.82	0.96	1.82
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG21	2	1.78	0.94	1.78
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG22	2	1.78	0.94	1.78
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG23	2	1.78	0.94	1.78
(1,1064)	1:81:A:VAL:HG21	1:95:A:TRP:HE1	2	1.72	0.96	1.72
(1,1064)	1:81:A:VAL:HG22	1:95:A:TRP:HE1	2	1.72	0.96	1.72
(1,1064)	1:81:A:VAL:HG23	1:95:A:TRP:HE1	2	1.72	0.96	1.72
(1,841)	1:15:A:CYS:H	1:45:A:SER:HA	2	1.63	0.72	1.63
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG11	2	1.52	0.03	1.52
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG12	2	1.52	0.03	1.52
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG13	2	1.52	0.03	1.52
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG11	2	1.52	0.03	1.52
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG12	2	1.52	0.03	1.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG13	2	1.52	0.03	1.52
(1,361)	1:63:A:LEU:HD11	1:93:A:ARG:HD2	2	1.4	0.94	1.4
(1,361)	1:63:A:LEU:HD11	1:93:A:ARG:HD3	2	1.4	0.94	1.4
(1,361)	1:63:A:LEU:HD12	1:93:A:ARG:HD2	2	1.4	0.94	1.4
(1,361)	1:63:A:LEU:HD12	1:93:A:ARG:HD3	2	1.4	0.94	1.4
(1,361)	1:63:A:LEU:HD13	1:93:A:ARG:HD2	2	1.4	0.94	1.4
(1,361)	1:63:A:LEU:HD13	1:93:A:ARG:HD3	2	1.4	0.94	1.4
(1,423)	1:69:A:PHE:HA	1:95:A:TRP:HZ2	2	1.38	0.76	1.38
(1,465)	1:73:A:LYS:HB2	1:75:A:TYR:HE1	2	1.34	0.1	1.34
(1,465)	1:73:A:LYS:HB2	1:75:A:TYR:HE2	2	1.34	0.1	1.34
(1,465)	1:73:A:LYS:HB3	1:75:A:TYR:HE1	2	1.34	0.1	1.34
(1,465)	1:73:A:LYS:HB3	1:75:A:TYR:HE2	2	1.34	0.1	1.34
(1,429)	1:70:A:HIS:H	1:75:A:TYR:HD1	2	1.3	0.33	1.3
(1,429)	1:70:A:HIS:H	1:75:A:TYR:HD2	2	1.3	0.33	1.3
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG21	2	1.28	0.39	1.28
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG22	2	1.28	0.39	1.28
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG23	2	1.28	0.39	1.28
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG21	2	1.28	0.39	1.28
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG22	2	1.28	0.39	1.28
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG23	2	1.28	0.39	1.28
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG11	2	1.2	1.06	1.2
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG12	2	1.2	1.06	1.2
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG13	2	1.2	1.06	1.2
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD21	2	1.16	0.56	1.16
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD22	2	1.16	0.56	1.16
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD23	2	1.16	0.56	1.16
(1,731)	1:89:A:VAL:HB	1:96:A:ASN:HB2	2	1.12	0.2	1.12
(1,731)	1:89:A:VAL:HB	1:96:A:ASN:HB3	2	1.12	0.2	1.12
(1,119)	1:29:A:LYS:HB2	1:34:A:TYR:HE1	2	1.1	0.18	1.1
(1,119)	1:29:A:LYS:HB2	1:34:A:TYR:HE2	2	1.1	0.18	1.1
(1,119)	1:29:A:LYS:HB3	1:34:A:TYR:HE1	2	1.1	0.18	1.1
(1,119)	1:29:A:LYS:HB3	1:34:A:TYR:HE2	2	1.1	0.18	1.1
(1,574)	1:87:A:THR:HG21	1:82:A:LYS:HE2	2	1.08	0.4	1.08
(1,574)	1:87:A:THR:HG21	1:82:A:LYS:HE3	2	1.08	0.4	1.08
(1,574)	1:87:A:THR:HG22	1:82:A:LYS:HE2	2	1.08	0.4	1.08
(1,574)	1:87:A:THR:HG22	1:82:A:LYS:HE3	2	1.08	0.4	1.08
(1,574)	1:87:A:THR:HG23	1:82:A:LYS:HE2	2	1.08	0.4	1.08
(1,574)	1:87:A:THR:HG23	1:82:A:LYS:HE3	2	1.08	0.4	1.08
(1,1107)	1:89:A:VAL:H	1:95:A:TRP:HE3	2	1.08	0.6	1.08
(1,422)	1:69:A:PHE:H	1:95:A:TRP:HZ2	2	1.08	0.87	1.08
(1,978)	1:69:A:PHE:H	1:95:A:TRP:HZ2	2	1.08	0.87	1.08
(1,9)	1:53:A:MET:HE1	1:62:A:ALA:H	2	1.04	0.24	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,9)	1:53:A:MET:HE2	1:62:A:ALA:H	2	1.04	0.24	1.04
(1,9)	1:53:A:MET:HE3	1:62:A:ALA:H	2	1.04	0.24	1.04
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG11	2	1.04	0.09	1.04
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG12	2	1.04	0.09	1.04
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG13	2	1.04	0.09	1.04
(1,598)	1:81:A:VAL:H	1:87:A:THR:HA	2	1.03	0.35	1.03
(1,63)	1:13:A:LEU:HD11	1:46:A:GLY:H	2	1.02	0.18	1.02
(1,63)	1:13:A:LEU:HD12	1:46:A:GLY:H	2	1.02	0.18	1.02
(1,63)	1:13:A:LEU:HD13	1:46:A:GLY:H	2	1.02	0.18	1.02
(1,103)	1:22:A:ALA:HA	1:23:A:GLU:HG2	2	1.01	0.09	1.01
(1,103)	1:22:A:ALA:HA	1:23:A:GLU:HG3	2	1.01	0.09	1.01
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG11	2	0.97	0.44	0.97
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG12	2	0.97	0.44	0.97
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG13	2	0.97	0.44	0.97
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG21	2	0.96	0.8	0.96
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG22	2	0.96	0.8	0.96
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG23	2	0.96	0.8	0.96
(1,801)	1:98:A:THR:HB	1:100:A:HIS:H	2	0.93	0.61	0.93
(1,1054)	1:81:A:VAL:H	1:87:A:THR:HA	2	0.93	0.35	0.93
(1,958)	1:66:A:CYS:HB2	1:93:A:ARG:H	2	0.9	0.5	0.9
(1,958)	1:66:A:CYS:HB3	1:93:A:ARG:H	2	0.9	0.5	0.9
(1,734)	1:89:A:VAL:HG11	1:96:A:ASN:H	2	0.85	0.23	0.85
(1,734)	1:89:A:VAL:HG12	1:96:A:ASN:H	2	0.85	0.23	0.85
(1,734)	1:89:A:VAL:HG13	1:96:A:ASN:H	2	0.85	0.23	0.85
(1,1095)	1:88:A:CYS:HB2	1:95:A:TRP:H	2	0.84	0.49	0.84
(1,1095)	1:88:A:CYS:HB3	1:95:A:TRP:H	2	0.84	0.49	0.84
(1,747)	1:90:A:CYS:HA	1:95:A:TRP:HA	2	0.81	0.35	0.81
(1,383)	1:67:A:PRO:HG2	1:69:A:PHE:HE1	2	0.8	0.25	0.8
(1,383)	1:67:A:PRO:HG2	1:69:A:PHE:HE2	2	0.8	0.25	0.8
(1,383)	1:67:A:PRO:HG3	1:69:A:PHE:HE1	2	0.8	0.25	0.8
(1,383)	1:67:A:PRO:HG3	1:69:A:PHE:HE2	2	0.8	0.25	0.8
(1,567)	1:80:A:THR:HG21	1:95:A:TRP:HH2	2	0.8	0.08	0.8
(1,567)	1:80:A:THR:HG22	1:95:A:TRP:HH2	2	0.8	0.08	0.8
(1,567)	1:80:A:THR:HG23	1:95:A:TRP:HH2	2	0.8	0.08	0.8
(1,1047)	1:80:A:THR:HG21	1:90:A:CYS:H	2	0.8	0.55	0.8
(1,1047)	1:80:A:THR:HG22	1:90:A:CYS:H	2	0.8	0.55	0.8
(1,1047)	1:80:A:THR:HG23	1:90:A:CYS:H	2	0.8	0.55	0.8
(1,157)	1:30:A:THR:HG21	1:55:A:ARG:HG2	2	0.78	0.43	0.78
(1,157)	1:30:A:THR:HG21	1:55:A:ARG:HG3	2	0.78	0.43	0.78
(1,157)	1:30:A:THR:HG22	1:55:A:ARG:HG2	2	0.78	0.43	0.78
(1,157)	1:30:A:THR:HG22	1:55:A:ARG:HG3	2	0.78	0.43	0.78
(1,157)	1:30:A:THR:HG23	1:55:A:ARG:HG2	2	0.78	0.43	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,157)	1:30:A:THR:HG23	1:55:A:ARG:HG3	2	0.78	0.43	0.78
(1,1039)	1:79:A:GLU:H	1:90:A:CYS:H	2	0.78	0.56	0.78
(1,586)	1:81:A:VAL:HB	1:83:A:ILE:HG12	2	0.76	0.57	0.76
(1,586)	1:81:A:VAL:HB	1:83:A:ILE:HG13	2	0.76	0.57	0.76
(1,4)	1:53:A:MET:HE1	1:61:A:VAL:HA	2	0.74	0.14	0.74
(1,4)	1:53:A:MET:HE2	1:61:A:VAL:HA	2	0.74	0.14	0.74
(1,4)	1:53:A:MET:HE3	1:61:A:VAL:HA	2	0.74	0.14	0.74
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG21	2	0.7	0.02	0.7
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG22	2	0.7	0.02	0.7
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG23	2	0.7	0.02	0.7
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG21	2	0.67	0.15	0.67
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG22	2	0.67	0.15	0.67
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG23	2	0.67	0.15	0.67
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG11	2	0.67	0.2	0.67
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG12	2	0.67	0.2	0.67
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG13	2	0.67	0.2	0.67
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG11	2	0.67	0.2	0.67
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG12	2	0.67	0.2	0.67
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG13	2	0.67	0.2	0.67
(1,642)	1:83:A:ILE:HB	1:88:A:CYS:HB2	2	0.66	0.29	0.66
(1,642)	1:83:A:ILE:HB	1:88:A:CYS:HB3	2	0.66	0.29	0.66
(1,147)	1:30:A:THR:HA	1:54:A:VAL:HA	2	0.62	0.32	0.62
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG11	2	0.62	0.46	0.62
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG12	2	0.62	0.46	0.62
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG13	2	0.62	0.46	0.62
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG11	2	0.61	0.16	0.61
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG12	2	0.61	0.16	0.61
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG13	2	0.61	0.16	0.61
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG11	2	0.61	0.16	0.61
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG12	2	0.61	0.16	0.61
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG13	2	0.61	0.16	0.61
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG11	2	0.59	0.36	0.59
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG12	2	0.59	0.36	0.59
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG13	2	0.59	0.36	0.59
(1,729)	1:89:A:VAL:H	1:96:A:ASN:HA	2	0.57	0.3	0.57
(1,564)	1:80:A:THR:HA	1:90:A:CYS:H	2	0.57	0.03	0.57
(1,736)	1:89:A:VAL:HG11	1:96:A:ASN:HA	2	0.54	0.06	0.54
(1,736)	1:89:A:VAL:HG12	1:96:A:ASN:HA	2	0.54	0.06	0.54
(1,736)	1:89:A:VAL:HG13	1:96:A:ASN:HA	2	0.54	0.06	0.54
(1,245)	1:53:A:MET:HG2	1:63:A:LEU:H	2	0.54	0.07	0.54
(1,245)	1:53:A:MET:HG3	1:63:A:LEU:H	2	0.54	0.07	0.54
(1,341)	1:61:A:VAL:HG21	1:66:A:CYS:H	2	0.5	0.24	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,341)	1:61:A:VAL:HG22	1:66:A:CYS:H	2	0.5	0.24	0.5
(1,341)	1:61:A:VAL:HG23	1:66:A:CYS:H	2	0.5	0.24	0.5
(1,607)	1:81:A:VAL:HG21	1:88:A:CYS:HA	2	0.5	0.19	0.5
(1,607)	1:81:A:VAL:HG22	1:88:A:CYS:HA	2	0.5	0.19	0.5
(1,607)	1:81:A:VAL:HG23	1:88:A:CYS:HA	2	0.5	0.19	0.5
(1,1017)	1:76:A:ALA:H	1:79:A:GLU:H	2	0.49	0.25	0.49
(1,409)	1:69:A:PHE:HA	1:74:A:GLU:HA	2	0.45	0.19	0.45
(1,605)	1:81:A:VAL:HG11	1:88:A:CYS:H	2	0.45	0.28	0.45
(1,605)	1:81:A:VAL:HG12	1:88:A:CYS:H	2	0.45	0.28	0.45
(1,605)	1:81:A:VAL:HG13	1:88:A:CYS:H	2	0.45	0.28	0.45
(1,1058)	1:81:A:VAL:HG11	1:88:A:CYS:H	2	0.45	0.28	0.45
(1,1058)	1:81:A:VAL:HG12	1:88:A:CYS:H	2	0.45	0.28	0.45
(1,1058)	1:81:A:VAL:HG13	1:88:A:CYS:H	2	0.45	0.28	0.45
(1,264)	1:54:A:VAL:HG21	1:63:A:LEU:HA	2	0.44	0.34	0.44
(1,264)	1:54:A:VAL:HG22	1:63:A:LEU:HA	2	0.44	0.34	0.44
(1,264)	1:54:A:VAL:HG23	1:63:A:LEU:HA	2	0.44	0.34	0.44
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG11	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG12	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG13	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG11	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG12	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG13	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG11	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG12	2	0.44	0.15	0.44
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG13	2	0.44	0.15	0.44
(1,134)	1:30:A:THR:HB	1:31:A:CYS:HA	2	0.42	0.05	0.42
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD21	2	0.4	0.05	0.4
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD22	2	0.4	0.05	0.4
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD23	2	0.4	0.05	0.4
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD21	2	0.4	0.05	0.4
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD22	2	0.4	0.05	0.4
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD23	2	0.4	0.05	0.4
(1,460)	1:73:A:LYS:HG2	1:74:A:GLU:H	2	0.38	0.04	0.38
(1,460)	1:73:A:LYS:HG3	1:74:A:GLU:H	2	0.38	0.04	0.38
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG11	2	0.37	0.0	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG12	2	0.37	0.0	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG13	2	0.37	0.0	0.37
(1,102)	1:22:A:ALA:HA	1:23:A:GLU:H	2	0.36	0.01	0.36
(1,853)	1:22:A:ALA:HA	1:23:A:GLU:H	2	0.36	0.01	0.36
(1,625)	1:82:A:LYS:HA	1:83:A:ILE:HB	2	0.36	0.05	0.36
(1,278)	1:55:A:ARG:HA	1:60:A:CYS:HA	2	0.33	0.03	0.33
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG21	2	0.32	0.2	0.32

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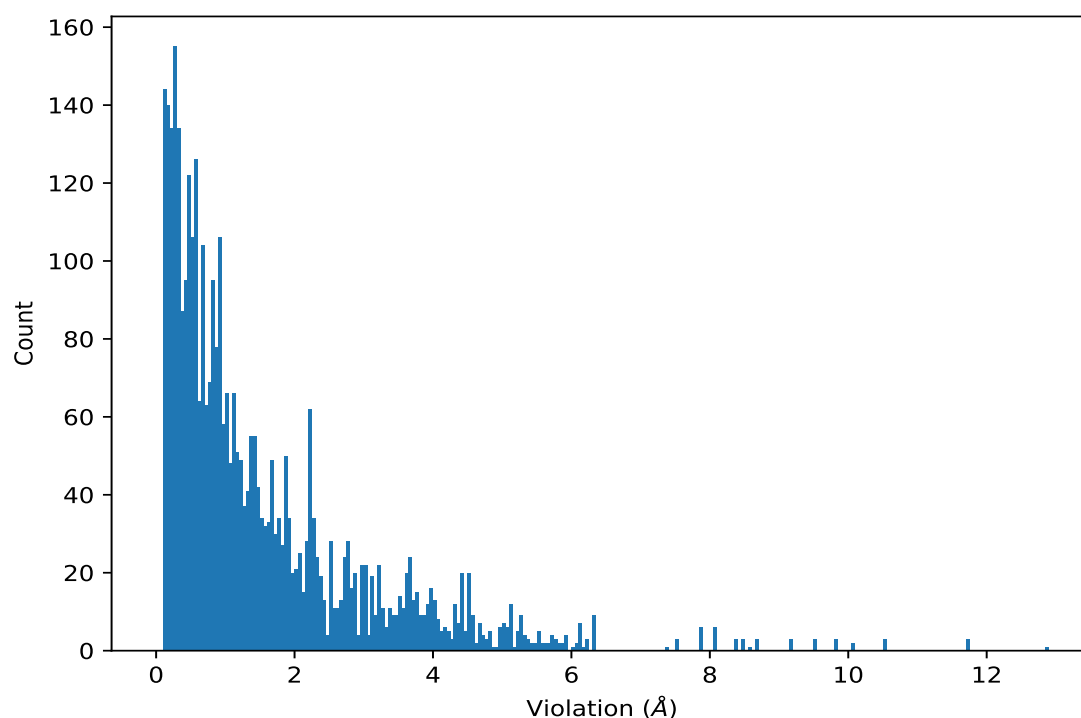
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG22	2	0.32	0.2	0.32
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG23	2	0.32	0.2	0.32
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG21	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG22	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG23	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG21	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG22	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG23	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG21	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG22	2	0.3	0.05	0.3
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG23	2	0.3	0.05	0.3
(1,984)	1:70:A:HIS:H	1:74:A:GLU:HA	2	0.29	0.17	0.29
(1,1170)	1:101:A:VAL:HA	1:102:A:CYS:H	2	0.26	0.06	0.26
(1,58)	1:13:A:LEU:HD11	1:14:A:VAL:H	2	0.26	0.09	0.26
(1,58)	1:13:A:LEU:HD12	1:14:A:VAL:H	2	0.26	0.09	0.26
(1,58)	1:13:A:LEU:HD13	1:14:A:VAL:H	2	0.26	0.09	0.26
(1,1165)	1:99:A:ASP:H	1:100:A:HIS:H	2	0.2	0.01	0.2
(1,1169)	1:100:A:HIS:H	1:99:A:ASP:H	2	0.2	0.01	0.2
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG11	2	0.19	0.01	0.19
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG12	2	0.19	0.01	0.19
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG13	2	0.19	0.01	0.19
(1,480)	1:75:A:TYR:HD1	1:76:A:ALA:H	2	0.18	0.02	0.18
(1,480)	1:75:A:TYR:HD2	1:76:A:ALA:H	2	0.18	0.02	0.18
(1,1011)	1:75:A:TYR:HD1	1:76:A:ALA:H	2	0.18	0.02	0.18
(1,1011)	1:75:A:TYR:HD2	1:76:A:ALA:H	2	0.18	0.02	0.18
(1,223)	1:48:A:LEU:HD21	1:49:A:CYS:H	2	0.14	0.04	0.14
(1,223)	1:48:A:LEU:HD22	1:49:A:CYS:H	2	0.14	0.04	0.14
(1,223)	1:48:A:LEU:HD23	1:49:A:CYS:H	2	0.14	0.04	0.14
(1,461)	1:73:A:LYS:HD2	1:74:A:GLU:H	2	0.14	0.0	0.14
(1,461)	1:73:A:LYS:HD3	1:74:A:GLU:H	2	0.14	0.0	0.14

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)
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	10	12.87
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	10	11.74
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	10	11.74
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	10	11.74
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	1	10.53
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	1	10.53
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	1	10.53
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE1	10	10.05
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE2	10	10.05
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	2	9.82
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	2	9.82
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	2	9.82
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	8	9.5
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	8	9.5
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	8	9.5
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	5	9.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	5	9.17
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	5	9.17
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	4	8.7
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	4	8.7
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	4	8.7
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	6	8.59
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	10	8.47
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	10	8.47
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	10	8.47
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	3	8.38
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	3	8.38
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	3	8.38
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	2	8.05
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	2	8.05
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	2	8.05
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	2	8.05
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	2	8.05
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	2	8.05
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	10	7.88
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	10	7.88
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	10	7.88
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	10	7.88
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	10	7.88
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	10	7.88
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	10	7.5
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	10	7.5
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	10	7.5
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	3	7.37
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	2	6.32
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	2	6.32
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	2	6.32
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	2	6.32
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	2	6.32
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	2	6.32
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	2	6.32
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	2	6.32
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	2	6.32
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	1	6.24
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	1	6.24
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	1	6.24
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	7	6.17
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	6	6.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	6	6.12
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	6	6.12
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	6	6.12
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	6	6.12
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	6	6.12
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	1	6.11
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	5	6.06
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	5	6.06
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	5	6.02
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	5	5.91
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	5	5.91
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	5	5.91
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	5	5.91
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	1	5.86
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	1	5.86
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE1	6	5.84
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE2	6	5.84
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE1	5	5.78
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE2	5	5.78
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	10	5.77
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	1	5.72
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	1	5.72
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	2	5.71
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	2	5.71
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	10	5.67
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	10	5.67
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	10	5.62
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	10	5.62
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	9	5.6
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	9	5.6
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	10	5.52
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	5	5.5
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	5	5.5
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	5	5.5
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	5	5.5
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	8	5.48
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	8	5.47
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	10	5.44
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	2	5.43
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	2	5.38
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	2	5.38
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	2	5.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	1	5.32
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	2	5.31
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	10	5.31
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	10	5.31
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	8	5.28
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	8	5.28
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	8	5.28
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	8	5.28
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	8	5.28
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	8	5.28
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	2	5.27
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	2	5.27
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	2	5.27
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	9	5.23
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	9	5.23
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	9	5.23
(1,170)	1:31:A:CYS:HB2	1:69:A:PHE:HZ	5	5.21
(1,170)	1:31:A:CYS:HB3	1:69:A:PHE:HZ	5	5.21
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	5	5.19
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	6	5.13
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	6	5.13
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	6	5.13
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	6	5.13
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	7	5.12
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	7	5.12
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	1	5.12
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	1	5.12
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	1	5.12
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	1	5.11
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	1	5.11
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	1	5.11
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	9	5.07
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	9	5.07
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	9	5.07
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	9	5.07
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	5	5.06
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	5	5.06
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	3	5.05
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	4	5.04
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	4	5.04
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	8	5.02
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	8	5.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	3	5.01
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	3	5.01
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	10	4.99
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	10	4.99
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	10	4.99
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	10	4.99
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	5	4.96
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	5	4.96
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	7	4.9
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	10	4.86
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	8	4.85
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	8	4.85
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	6	4.84
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	6	4.84
(1,1122)	1:90:A:CYS:H	1:95:A:TRP:HZ3	5	4.83
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	2	4.8
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	5	4.77
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	5	4.77
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE1	5	4.72
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE2	5	4.72
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE1	5	4.72
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE2	5	4.72
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG2	10	4.69
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG3	10	4.69
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	3	4.69
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	3	4.69
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	3	4.69
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	3	4.69
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	7	4.67
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	7	4.63
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	1	4.61
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	6	4.6
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	5	4.58
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB2	1	4.58
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB3	1	4.58
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB2	1	4.58
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB3	1	4.58
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB2	1	4.58
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB3	1	4.58
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	5	4.56
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE1	6	4.53
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE2	6	4.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE1	6	4.53
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE2	6	4.53
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	1	4.51
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	1	4.51
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	10	4.51
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	10	4.51
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	10	4.51
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	10	4.51
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	10	4.51
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	10	4.51
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	10	4.51
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	10	4.51
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	10	4.51
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	8	4.51
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	7	4.51
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	7	4.51
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	3	4.5
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	3	4.5
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	6	4.47
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	6	4.47
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	6	4.47
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	6	4.47
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	6	4.47
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	6	4.43
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	6	4.43
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	9	4.43
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	6	4.43
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	6	4.43
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	5	4.43
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	5	4.43
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	5	4.43
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	5	4.43
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	5	4.43
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	5	4.43
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	5	4.43
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	5	4.43
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	5	4.43
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	10	4.41
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	6	4.41
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	6	4.41
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	6	4.41
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD2	10	4.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD3	10	4.4
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	5	4.39
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD11	10	4.36
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD12	10	4.36
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD13	10	4.36
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	3	4.36
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	3	4.36
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	3	4.36
(1,384)	1:67:A:PRO:HG2	1:69:A:PHE:HZ	6	4.34
(1,384)	1:67:A:PRO:HG3	1:69:A:PHE:HZ	6	4.34
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	8	4.33
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	8	4.33
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	8	4.33
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	8	4.33
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	8	4.33
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	8	4.33
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	8	4.33
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	8	4.33
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	8	4.33
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	1	4.3
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	7	4.27
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	7	4.27
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	5	4.26
(1,723)	1:89:A:VAL:HB	1:95:A:TRP:HZ3	5	4.23
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	4	4.22
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	4	4.22
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	4	4.22
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	4	4.22
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	8	4.19
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	8	4.19
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	8	4.19
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	8	4.18
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	8	4.18
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	8	4.18
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	5	4.14
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	6	4.13
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	8	4.12
(1,448)	1:70:A:HIS:HE1	1:83:A:ILE:HG12	10	4.12
(1,448)	1:70:A:HIS:HE1	1:83:A:ILE:HG13	10	4.12
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	5	4.1
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	5	4.1
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB2	1	4.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB3	1	4.08
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB2	1	4.08
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB3	1	4.08
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB2	1	4.08
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB3	1	4.08
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	7	4.04
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	7	4.04
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	3	4.03
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	3	4.03
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	3	4.03
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	3	4.03
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	7	4.03
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	7	4.03
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	7	4.03
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	2	4.02
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	2	4.02
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	10	4.01
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	10	4.01
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	5	3.99
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	5	3.99
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	5	3.99
(1,38)	1:11:A:VAL:HB	1:48:A:LEU:H	10	3.98
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	8	3.97
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	7	3.96
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	7	3.96
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	8	3.96
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	8	3.96
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	7	3.96
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	7	3.96
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	8	3.96
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	8	3.96
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	3	3.96
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	3	3.96
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	1	3.95
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	6	3.93
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	6	3.93
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	6	3.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	6	3.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	6	3.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	6	3.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	6	3.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	6	3.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	6	3.93
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG11	6	3.93
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG12	6	3.93
(1,17)	1:2:A:ALA:HA	1:14:A:VAL:HG13	6	3.93
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	4	3.89
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	4	3.89
(1,441)	1:70:A:HIS:HD2	1:81:A:VAL:HB	3	3.88
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD2	5	3.88
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD3	5	3.88
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	4	3.88
(1,977)	1:69:A:PHE:H	1:95:A:TRP:HE1	1	3.87
(1,499)	1:75:A:TYR:HE1	1:95:A:TRP:HH2	5	3.86
(1,499)	1:75:A:TYR:HE2	1:95:A:TRP:HH2	5	3.86
(1,13)	1:10:A:MET:HE1	1:47:A:CYS:HA	2	3.83
(1,13)	1:10:A:MET:HE2	1:47:A:CYS:HA	2	3.83
(1,13)	1:10:A:MET:HE3	1:47:A:CYS:HA	2	3.83
(1,13)	1:10:A:MET:HE1	1:47:A:CYS:HA	10	3.83
(1,13)	1:10:A:MET:HE2	1:47:A:CYS:HA	10	3.83
(1,13)	1:10:A:MET:HE3	1:47:A:CYS:HA	10	3.83
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	1	3.82
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	7	3.81
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	7	3.81
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	5	3.8
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	5	3.8
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	5	3.8
(1,40)	1:11:A:VAL:HG21	1:48:A:LEU:H	1	3.8
(1,40)	1:11:A:VAL:HG22	1:48:A:LEU:H	1	3.8
(1,40)	1:11:A:VAL:HG23	1:48:A:LEU:H	1	3.8
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	6	3.78
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	9	3.77
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD11	2	3.77
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD12	2	3.77
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD13	2	3.77
(1,1090)	1:87:A:THR:HB	1:98:A:THR:H	10	3.76
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	9	3.76
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	9	3.76
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	2	3.76
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB2	5	3.72
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB3	5	3.72
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB2	5	3.72
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB3	5	3.72
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB2	5	3.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB3	5	3.72
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	8	3.71
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	8	3.71
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	1	3.71
(1,839)	1:14:A:VAL:HG11	1:45:A:SER:H	2	3.7
(1,839)	1:14:A:VAL:HG12	1:45:A:SER:H	2	3.7
(1,839)	1:14:A:VAL:HG13	1:45:A:SER:H	2	3.7
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	1	3.7
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	5	3.68
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	5	3.68
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	5	3.68
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	5	3.68
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	5	3.68
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	5	3.68
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	7	3.68
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	7	3.68
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	7	3.68
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	7	3.68
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	7	3.68
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	7	3.68
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE1	5	3.66
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE2	5	3.66
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE1	5	3.66
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE2	5	3.66
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	2	3.66
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	2	3.66
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	10	3.66
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	10	3.66
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	10	3.66
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	10	3.66
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	10	3.66
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	10	3.66
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	5	3.65
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	7	3.65
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	7	3.65
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB2	10	3.64
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB3	10	3.64
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB2	10	3.64
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB3	10	3.64
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB2	10	3.64
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB3	10	3.64
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	5	3.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	1	3.63
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	1	3.63
(1,38)	1:11:A:VAL:HB	1:48:A:LEU:H	5	3.63
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	2	3.62
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE1	3	3.61
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE2	3	3.61
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	3	3.61
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	3	3.61
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	2	3.61
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	2	3.61
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE1	6	3.59
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE2	6	3.59
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	9	3.59
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	9	3.59
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	8	3.59
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	1	3.56
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	1	3.56
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	1	3.56
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	1	3.56
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	1	3.56
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	1	3.56
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG21	10	3.54
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG22	10	3.54
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG23	10	3.54
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	10	3.54
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	10	3.54
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	6	3.54
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	6	3.54
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	1	3.54
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB2	5	3.51
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB3	5	3.51
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB2	5	3.51
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB3	5	3.51
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB2	5	3.51
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB3	5	3.51
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	1	3.47
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	9	3.47
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	9	3.47
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG21	10	3.47
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG22	10	3.47
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG23	10	3.47
(1,384)	1:67:A:PRO:HG2	1:69:A:PHE:HZ	10	3.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:67:A:PRO:HG3	1:69:A:PHE:HZ	10	3.46
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	6	3.45
(1,1116)	1:89:A:VAL:H	1:98:A:THR:H	10	3.44
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	7	3.44
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	7	3.44
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	1	3.42
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	1	3.42
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	4	3.41
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	4	3.41
(1,68)	1:13:A:LEU:HB2	1:48:A:LEU:HG	1	3.41
(1,68)	1:13:A:LEU:HB3	1:48:A:LEU:HG	1	3.41
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	3	3.39
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	3	3.39
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	3	3.38
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	8	3.38
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	8	3.38
(1,170)	1:31:A:CYS:HB2	1:69:A:PHE:HZ	6	3.37
(1,170)	1:31:A:CYS:HB3	1:69:A:PHE:HZ	6	3.37
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	10	3.36
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	7	3.36
(1,553)	1:80:A:THR:HB	1:88:A:CYS:H	2	3.35
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	10	3.35
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	7	3.33
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	9	3.33
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	3	3.32
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	8	3.32
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	8	3.32
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	8	3.32
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	7	3.3
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	7	3.3
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	7	3.3
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	8	3.29
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	8	3.29
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	8	3.29
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	8	3.29
(1,839)	1:14:A:VAL:HG11	1:45:A:SER:H	1	3.27
(1,839)	1:14:A:VAL:HG12	1:45:A:SER:H	1	3.27
(1,839)	1:14:A:VAL:HG13	1:45:A:SER:H	1	3.27
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	10	3.25
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	5	3.24
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	4	3.23
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	4	3.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	1	3.23
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	1	3.23
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	1	3.23
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	1	3.23
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	1	3.23
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	1	3.23
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	3	3.23
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	3	3.23
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	3	3.23
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	1	3.22
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG11	3	3.22
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG12	3	3.22
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG13	3	3.22
(1,724)	1:89:A:VAL:HB	1:95:A:TRP:HE3	5	3.21
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	2	3.21
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	8	3.21
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	8	3.21
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	7	3.2
(1,565)	1:80:A:THR:HA	1:95:A:TRP:HZ3	5	3.2
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	6	3.19
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	7	3.16
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	9	3.16
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	4	3.16
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	1	3.16
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	1	3.16
(1,40)	1:11:A:VAL:HG21	1:48:A:LEU:H	5	3.16
(1,40)	1:11:A:VAL:HG22	1:48:A:LEU:H	5	3.16
(1,40)	1:11:A:VAL:HG23	1:48:A:LEU:H	5	3.16
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	4	3.15
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	4	3.15
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	4	3.15
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	5	3.14
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	1	3.14
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	1	3.14
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG2	1	3.12
(1,857)	1:29:A:LYS:H	1:32:A:GLN:HG3	1	3.12
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG2	1	3.12
(1,116)	1:29:A:LYS:H	1:32:A:GLN:HG3	1	3.12
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	8	3.11
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	4	3.11
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	4	3.11
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	1	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	1	3.11
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	8	3.1
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	8	3.1
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	1	3.1
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	1	3.1
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	7	3.09
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	5	3.08
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	6	3.08
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	6	3.08
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	3	3.04
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	7	3.04
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	7	3.04
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	7	3.04
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	7	3.04
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	7	3.04
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	7	3.04
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	7	3.04
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	7	3.04
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	7	3.04
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	6	3.03
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	6	3.03
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	6	3.03
(1,1099)	1:88:A:CYS:H	1:98:A:THR:H	10	3.02
(1,613)	1:81:A:VAL:HB	1:95:A:TRP:HH2	6	3.01
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	8	3.01
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG11	2	3.0
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG12	2	3.0
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG13	2	3.0
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG11	2	3.0
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG12	2	3.0
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG13	2	3.0
(1,38)	1:11:A:VAL:HB	1:48:A:LEU:H	1	2.99
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	8	2.98
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	8	2.98
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	5	2.98
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	9	2.98
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	8	2.98
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	8	2.98
(1,644)	1:83:A:ILE:HD11	1:95:A:TRP:HE3	10	2.97
(1,644)	1:83:A:ILE:HD12	1:95:A:TRP:HE3	10	2.97
(1,644)	1:83:A:ILE:HD13	1:95:A:TRP:HE3	10	2.97
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE1	5	2.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE2	5	2.97
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	2	2.97
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	2	2.97
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	2	2.97
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	2	2.97
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	2	2.97
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	2	2.97
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	9	2.96
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE1	5	2.95
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE2	5	2.95
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	3	2.95
(1,1163)	1:98:A:THR:HB	1:100:A:HIS:H	10	2.94
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	9	2.94
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	2	2.94
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	5	2.91
(1,1114)	1:89:A:VAL:H	1:97:A:CYS:HA	10	2.9
(1,738)	1:89:A:VAL:H	1:97:A:CYS:HA	10	2.9
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	3	2.9
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD2	10	2.9
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD3	10	2.9
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	8	2.9
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG11	10	2.88
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG12	10	2.88
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG13	10	2.88
(1,493)	1:75:A:TYR:HE1	1:81:A:VAL:HB	5	2.88
(1,493)	1:75:A:TYR:HE2	1:81:A:VAL:HB	5	2.88
(1,148)	1:30:A:THR:HA	1:54:A:VAL:HB	8	2.87
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	4	2.86
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	4	2.86
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	4	2.86
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	1	2.86
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	1	2.86
(1,839)	1:14:A:VAL:HG11	1:45:A:SER:H	5	2.85
(1,839)	1:14:A:VAL:HG12	1:45:A:SER:H	5	2.85
(1,839)	1:14:A:VAL:HG13	1:45:A:SER:H	5	2.85
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	9	2.83
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	6	2.83
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	2	2.83
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	2	2.83
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	2	2.83
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	2	2.83
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	2	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	2	2.83
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	5	2.83
(1,1072)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	10	2.82
(1,1072)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	10	2.82
(1,1072)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	10	2.82
(1,647)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	10	2.82
(1,647)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	10	2.82
(1,647)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	10	2.82
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	7	2.82
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	10	2.8
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	10	2.8
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	10	2.8
(1,615)	1:81:A:VAL:HG21	1:95:A:TRP:HE1	7	2.78
(1,615)	1:81:A:VAL:HG22	1:95:A:TRP:HE1	7	2.78
(1,615)	1:81:A:VAL:HG23	1:95:A:TRP:HE1	7	2.78
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	3	2.78
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	3	2.78
(1,11)	1:53:A:MET:HE1	1:63:A:LEU:H	7	2.78
(1,11)	1:53:A:MET:HE2	1:63:A:LEU:H	7	2.78
(1,11)	1:53:A:MET:HE3	1:63:A:LEU:H	7	2.78
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	4	2.77
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	4	2.77
(1,866)	1:30:A:THR:HA	1:55:A:ARG:H	2	2.77
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	4	2.77
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	4	2.77
(1,152)	1:30:A:THR:HA	1:55:A:ARG:H	2	2.77
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	7	2.76
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	7	2.76
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	7	2.76
(1,384)	1:67:A:PRO:HG2	1:69:A:PHE:HZ	5	2.76
(1,384)	1:67:A:PRO:HG3	1:69:A:PHE:HZ	5	2.76
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	7	2.75
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	7	2.75
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	7	2.75
(1,40)	1:11:A:VAL:HG21	1:48:A:LEU:H	10	2.75
(1,40)	1:11:A:VAL:HG22	1:48:A:LEU:H	10	2.75
(1,40)	1:11:A:VAL:HG23	1:48:A:LEU:H	10	2.75
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	10	2.74
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	10	2.74
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	5	2.73
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	5	2.73
(1,74)	1:14:A:VAL:HG11	1:45:A:SER:HA	1	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:14:A:VAL:HG12	1:45:A:SER:HA	1	2.73
(1,74)	1:14:A:VAL:HG13	1:45:A:SER:HA	1	2.73
(1,1072)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	4	2.72
(1,1072)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	4	2.72
(1,1072)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	4	2.72
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	3	2.72
(1,647)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	4	2.72
(1,647)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	4	2.72
(1,647)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	4	2.72
(1,559)	1:80:A:THR:HB	1:89:A:VAL:HB	2	2.72
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE1	6	2.72
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE2	6	2.72
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG21	2	2.72
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG22	2	2.72
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG23	2	2.72
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	1	2.71
(1,14)	1:10:A:MET:HE1	1:59:A:ARG:HA	5	2.7
(1,14)	1:10:A:MET:HE2	1:59:A:ARG:HA	5	2.7
(1,14)	1:10:A:MET:HE3	1:59:A:ARG:HA	5	2.7
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	9	2.69
(1,1064)	1:81:A:VAL:HG21	1:95:A:TRP:HE1	7	2.68
(1,1064)	1:81:A:VAL:HG22	1:95:A:TRP:HE1	7	2.68
(1,1064)	1:81:A:VAL:HG23	1:95:A:TRP:HE1	7	2.68
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	7	2.68
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG21	1	2.68
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG22	1	2.68
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG23	1	2.68
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG21	1	2.68
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG22	1	2.68
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG23	1	2.68
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	2	2.67
(1,149)	1:30:A:THR:HB	1:54:A:VAL:HB	8	2.66
(1,36)	1:11:A:VAL:HG21	1:47:A:CYS:HA	1	2.64
(1,36)	1:11:A:VAL:HG22	1:47:A:CYS:HA	1	2.64
(1,36)	1:11:A:VAL:HG23	1:47:A:CYS:HA	1	2.64
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	7	2.63
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	7	2.63
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	7	2.63
(1,644)	1:83:A:ILE:HD11	1:95:A:TRP:HE3	7	2.62
(1,644)	1:83:A:ILE:HD12	1:95:A:TRP:HE3	7	2.62
(1,644)	1:83:A:ILE:HD13	1:95:A:TRP:HE3	7	2.62
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	2	2.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	2	2.62
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	4	2.59
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	5	2.58
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	5	2.58
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG11	3	2.58
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG12	3	2.58
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG13	3	2.58
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG11	3	2.58
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG12	3	2.58
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG13	3	2.58
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	8	2.57
(1,539)	1:79:A:GLU:H	1:89:A:VAL:HA	9	2.56
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	6	2.55
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	6	2.55
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	6	2.55
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	6	2.55
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	2	2.54
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	4	2.54
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE1	3	2.53
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE2	3	2.53
(1,745)	1:90:A:CYS:H	1:95:A:TRP:HZ3	5	2.53
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE1	3	2.53
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE2	3	2.53
(1,170)	1:31:A:CYS:HB2	1:69:A:PHE:HZ	3	2.53
(1,170)	1:31:A:CYS:HB3	1:69:A:PHE:HZ	3	2.53
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	5	2.53
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	5	2.53
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	10	2.52
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD2	8	2.52
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD3	8	2.52
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD2	8	2.52
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD3	8	2.52
(1,333)	1:61:A:VAL:HB	1:65:A:ARG:HA	5	2.52
(1,617)	1:81:A:VAL:HG21	1:95:A:TRP:HZ2	7	2.51
(1,617)	1:81:A:VAL:HG22	1:95:A:TRP:HZ2	7	2.51
(1,617)	1:81:A:VAL:HG23	1:95:A:TRP:HZ2	7	2.51
(1,746)	1:90:A:CYS:HA	1:95:A:TRP:HE3	5	2.5
(1,253)	1:54:A:VAL:HG21	1:61:A:VAL:HB	2	2.5
(1,253)	1:54:A:VAL:HG22	1:61:A:VAL:HB	2	2.5
(1,253)	1:54:A:VAL:HG23	1:61:A:VAL:HB	2	2.5
(1,425)	1:70:A:HIS:HE1	1:71:A:GLN:HG2	10	2.48
(1,425)	1:70:A:HIS:HE1	1:71:A:GLN:HG3	10	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD2	5	2.45
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD3	5	2.45
(1,68)	1:13:A:LEU:HB2	1:48:A:LEU:HG	2	2.44
(1,68)	1:13:A:LEU:HB3	1:48:A:LEU:HG	2	2.44
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD1	5	2.43
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD2	5	2.43
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	1	2.43
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD2	4	2.43
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD3	4	2.43
(1,379)	1:66:A:CYS:HB2	1:93:A:ARG:HA	10	2.42
(1,379)	1:66:A:CYS:HB3	1:93:A:ARG:HA	10	2.42
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	9	2.41
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD2	6	2.41
(1,291)	1:56:A:HIS:HE1	1:59:A:ARG:HD3	6	2.41
(1,243)	1:53:A:MET:HA	1:63:A:LEU:HA	7	2.41
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	6	2.4
(1,831)	1:11:A:VAL:H	1:48:A:LEU:H	10	2.4
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	10	2.4
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	10	2.4
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	4	2.39
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	9	2.38
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	3	2.38
(1,38)	1:11:A:VAL:HB	1:48:A:LEU:H	7	2.38
(1,333)	1:61:A:VAL:HB	1:65:A:ARG:HA	10	2.37
(1,979)	1:69:A:PHE:H	1:95:A:TRP:HD1	1	2.36
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG21	7	2.36
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG22	7	2.36
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG23	7	2.36
(1,421)	1:69:A:PHE:H	1:95:A:TRP:HD1	1	2.36
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	2	2.36
(1,841)	1:15:A:CYS:H	1:45:A:SER:HA	1	2.35
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD11	4	2.35
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD12	4	2.35
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD13	4	2.35
(1,559)	1:80:A:THR:HB	1:89:A:VAL:HB	5	2.34
(1,361)	1:63:A:LEU:HD11	1:93:A:ARG:HD2	5	2.34
(1,361)	1:63:A:LEU:HD11	1:93:A:ARG:HD3	5	2.34
(1,361)	1:63:A:LEU:HD12	1:93:A:ARG:HD2	5	2.34
(1,361)	1:63:A:LEU:HD12	1:93:A:ARG:HD3	5	2.34
(1,361)	1:63:A:LEU:HD13	1:93:A:ARG:HD2	5	2.34
(1,361)	1:63:A:LEU:HD13	1:93:A:ARG:HD3	5	2.34
(1,39)	1:11:A:VAL:HG11	1:48:A:LEU:H	7	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:11:A:VAL:HG12	1:48:A:LEU:H	7	2.34
(1,39)	1:11:A:VAL:HG13	1:48:A:LEU:H	7	2.34
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	3	2.33
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	5	2.33
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	5	2.33
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	8	2.33
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	1	2.32
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB1	1	2.32
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB2	1	2.32
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB3	1	2.32
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD2	2	2.32
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD3	2	2.32
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD1	5	2.31
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD2	5	2.31
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD2	4	2.31
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD3	4	2.31
(1,553)	1:80:A:THR:HB	1:88:A:CYS:H	7	2.3
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB2	2	2.3
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB3	2	2.3
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB2	2	2.3
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB3	2	2.3
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB2	2	2.3
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB3	2	2.3
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG11	1	2.29
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG12	1	2.29
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG13	1	2.29
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG11	1	2.29
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG12	1	2.29
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG13	1	2.29
(1,1134)	1:91:A:ARG:H	1:95:A:TRP:HE3	5	2.28
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA2	1	2.27
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA3	1	2.27
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA2	1	2.27
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA3	1	2.27
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA2	1	2.27
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA3	1	2.27
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG11	5	2.26
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG12	5	2.26
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG13	5	2.26
(1,491)	1:75:A:TYR:HE1	1:81:A:VAL:HG11	5	2.25
(1,491)	1:75:A:TYR:HE1	1:81:A:VAL:HG12	5	2.25
(1,491)	1:75:A:TYR:HE1	1:81:A:VAL:HG13	5	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:75:A:TYR:HE2	1:81:A:VAL:HG11	5	2.25
(1,491)	1:75:A:TYR:HE2	1:81:A:VAL:HG12	5	2.25
(1,491)	1:75:A:TYR:HE2	1:81:A:VAL:HG13	5	2.25
(1,178)	1:32:A:GLN:HG2	1:69:A:PHE:HZ	2	2.25
(1,178)	1:32:A:GLN:HG3	1:69:A:PHE:HZ	2	2.25
(1,39)	1:11:A:VAL:HG11	1:48:A:LEU:H	1	2.25
(1,39)	1:11:A:VAL:HG12	1:48:A:LEU:H	1	2.25
(1,39)	1:11:A:VAL:HG13	1:48:A:LEU:H	1	2.25
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	8	2.24
(1,441)	1:70:A:HIS:HD2	1:81:A:VAL:HB	5	2.24
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	4	2.24
(1,156)	1:30:A:THR:HG21	1:55:A:ARG:HA	9	2.24
(1,156)	1:30:A:THR:HG22	1:55:A:ARG:HA	9	2.24
(1,156)	1:30:A:THR:HG23	1:55:A:ARG:HA	9	2.24
(1,127)	1:29:A:LYS:HE2	1:53:A:MET:HA	7	2.24
(1,127)	1:29:A:LYS:HE3	1:53:A:MET:HA	7	2.24
(1,126)	1:29:A:LYS:HE2	1:34:A:TYR:HA	7	2.24
(1,126)	1:29:A:LYS:HE3	1:34:A:TYR:HA	7	2.24
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	6	2.23
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	4	2.23
(1,333)	1:61:A:VAL:HB	1:65:A:ARG:HA	2	2.23
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	6	2.23
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	6	2.23
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	6	2.23
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	6	2.23
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	6	2.23
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	6	2.23
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	4	2.23
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	4	2.23
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	4	2.23
(1,74)	1:14:A:VAL:HG11	1:45:A:SER:HA	2	2.23
(1,74)	1:14:A:VAL:HG12	1:45:A:SER:HA	2	2.23
(1,74)	1:14:A:VAL:HG13	1:45:A:SER:HA	2	2.23
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB2	10	2.23
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB3	10	2.23
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB2	10	2.23
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB3	10	2.23
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB2	10	2.23
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB3	10	2.23
(1,865)	1:30:A:THR:H	1:54:A:VAL:HB	8	2.22
(1,831)	1:11:A:VAL:H	1:48:A:LEU:H	2	2.22
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	5	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG21	2	2.22
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG22	2	2.22
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG23	2	2.22
(1,271)	1:54:A:VAL:HG21	1:66:A:CYS:H	2	2.22
(1,271)	1:54:A:VAL:HG22	1:66:A:CYS:H	2	2.22
(1,271)	1:54:A:VAL:HG23	1:66:A:CYS:H	2	2.22
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG11	4	2.22
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG12	4	2.22
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG13	4	2.22
(1,144)	1:30:A:THR:H	1:54:A:VAL:HB	8	2.22
(1,68)	1:13:A:LEU:HB2	1:48:A:LEU:HG	10	2.22
(1,68)	1:13:A:LEU:HB3	1:48:A:LEU:HG	10	2.22
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD2	2	2.2
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD3	2	2.2
(1,831)	1:11:A:VAL:H	1:48:A:LEU:H	7	2.2
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	10	2.2
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	10	2.2
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	10	2.2
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	10	2.2
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	10	2.2
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	10	2.2
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	5	2.2
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG21	5	2.2
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG22	5	2.2
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG23	5	2.2
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG21	5	2.2
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG22	5	2.2
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG23	5	2.2
(1,1123)	1:90:A:CYS:HA	1:96:A:ASN:H	10	2.18
(1,750)	1:90:A:CYS:HA	1:96:A:ASN:H	10	2.18
(1,644)	1:83:A:ILE:HD11	1:95:A:TRP:HE3	4	2.18
(1,644)	1:83:A:ILE:HD12	1:95:A:TRP:HE3	4	2.18
(1,644)	1:83:A:ILE:HD13	1:95:A:TRP:HE3	4	2.18
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	10	2.18
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD2	9	2.17
(1,15)	1:10:A:MET:HE1	1:55:A:ARG:HD3	9	2.17
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD2	9	2.17
(1,15)	1:10:A:MET:HE2	1:55:A:ARG:HD3	9	2.17
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD2	9	2.17
(1,15)	1:10:A:MET:HE3	1:55:A:ARG:HD3	9	2.17
(1,674)	1:87:A:THR:HB	1:97:A:CYS:HA	10	2.16
(1,237)	1:53:A:MET:HA	1:62:A:ALA:HA	4	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	9	2.16
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	9	2.16
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	9	2.16
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	9	2.16
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	9	2.16
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	9	2.16
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	5	2.15
(1,441)	1:70:A:HIS:HD2	1:81:A:VAL:HB	8	2.15
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB2	1	2.15
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB3	1	2.15
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB2	1	2.15
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB3	1	2.15
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	3	2.15
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	3	2.15
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	8	2.14
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	5	2.13
(1,423)	1:69:A:PHE:HA	1:95:A:TRP:HZ2	1	2.13
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE1	3	2.13
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE2	3	2.13
(1,839)	1:14:A:VAL:HG11	1:45:A:SER:H	10	2.12
(1,839)	1:14:A:VAL:HG12	1:45:A:SER:H	10	2.12
(1,839)	1:14:A:VAL:HG13	1:45:A:SER:H	10	2.12
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	1	2.12
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE1	8	2.12
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE2	8	2.12
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	8	2.12
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	8	2.12
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	5	2.11
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	7	2.1
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	10	2.09
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	7	2.09
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	7	2.09
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	10	2.09
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	10	2.09
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	3	2.08
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE1	9	2.08
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE2	9	2.08
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	10	2.07
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	8	2.07
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	10	2.07
(1,442)	1:70:A:HIS:HD2	1:81:A:VAL:HG11	3	2.07
(1,442)	1:70:A:HIS:HD2	1:81:A:VAL:HG12	3	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:70:A:HIS:HD2	1:81:A:VAL:HG13	3	2.07
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB2	9	2.07
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB3	9	2.07
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB2	9	2.07
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB3	9	2.07
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD2	10	2.07
(1,360)	1:63:A:LEU:HG	1:93:A:ARG:HD3	10	2.07
(1,553)	1:80:A:THR:HB	1:88:A:CYS:H	4	2.06
(1,553)	1:80:A:THR:HB	1:88:A:CYS:H	8	2.06
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	3	2.06
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	3	2.06
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	3	2.06
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	9	2.05
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	5	2.05
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	6	2.04
(1,968)	1:68:A:CYS:HA	1:95:A:TRP:HE1	1	2.04
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	8	2.04
(1,253)	1:54:A:VAL:HG21	1:61:A:VAL:HB	8	2.04
(1,253)	1:54:A:VAL:HG22	1:61:A:VAL:HB	8	2.04
(1,253)	1:54:A:VAL:HG23	1:61:A:VAL:HB	8	2.04
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG11	10	2.04
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG12	10	2.04
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG13	10	2.04
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	2	2.03
(1,803)	1:98:A:THR:HG21	1:100:A:HIS:HE1	10	2.03
(1,803)	1:98:A:THR:HG22	1:100:A:HIS:HE1	10	2.03
(1,803)	1:98:A:THR:HG23	1:100:A:HIS:HE1	10	2.03
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	5	2.02
(1,521)	1:77:A:PRO:HA	1:90:A:CYS:H	9	2.02
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	8	2.01
(1,697)	1:88:A:CYS:HA	1:97:A:CYS:HA	10	2.0
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	1	2.0
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	1	2.0
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	9	1.99
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	8	1.99
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE1	5	1.99
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE2	5	1.99
(1,335)	1:61:A:VAL:HB	1:65:A:ARG:H	5	1.99
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	10	1.99
(1,156)	1:30:A:THR:HG21	1:55:A:ARG:HA	7	1.99
(1,156)	1:30:A:THR:HG22	1:55:A:ARG:HA	7	1.99
(1,156)	1:30:A:THR:HG23	1:55:A:ARG:HA	7	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	7	1.99
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	10	1.99
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	6	1.98
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	9	1.98
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	8	1.98
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	5	1.97
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	8	1.97
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	8	1.97
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	7	1.96
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	7	1.96
(1,149)	1:30:A:THR:HB	1:54:A:VAL:HB	3	1.96
(1,978)	1:69:A:PHE:H	1:95:A:TRP:HZ2	1	1.95
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG2	2	1.95
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG3	2	1.95
(1,422)	1:69:A:PHE:H	1:95:A:TRP:HZ2	1	1.95
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG21	10	1.94
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG22	10	1.94
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG23	10	1.94
(1,744)	1:90:A:CYS:H	1:95:A:TRP:HE3	5	1.94
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG21	10	1.94
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG22	10	1.94
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG23	10	1.94
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	3	1.94
(1,12)	1:10:A:MET:HE1	1:60:A:CYS:H	5	1.94
(1,12)	1:10:A:MET:HE2	1:60:A:CYS:H	5	1.94
(1,12)	1:10:A:MET:HE3	1:60:A:CYS:H	5	1.94
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	3	1.93
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	3	1.93
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	9	1.93
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	6	1.93
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	6	1.93
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB2	2	1.93
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB3	2	1.93
(1,1024)	1:77:A:PRO:HA	1:90:A:CYS:H	9	1.92
(1,38)	1:11:A:VAL:HB	1:48:A:LEU:H	2	1.92
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	2	1.91
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	3	1.91
(1,156)	1:30:A:THR:HG21	1:55:A:ARG:HA	8	1.91
(1,156)	1:30:A:THR:HG22	1:55:A:ARG:HA	8	1.91
(1,156)	1:30:A:THR:HG23	1:55:A:ARG:HA	8	1.91
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	3	1.91
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	3	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:53:A:MET:HE1	1:60:A:CYS:HA	10	1.91
(1,3)	1:53:A:MET:HE2	1:60:A:CYS:HA	10	1.91
(1,3)	1:53:A:MET:HE3	1:60:A:CYS:HA	10	1.91
(1,1072)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	7	1.9
(1,1072)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	7	1.9
(1,1072)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	7	1.9
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	7	1.9
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	7	1.9
(1,647)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	7	1.9
(1,647)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	7	1.9
(1,647)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	7	1.9
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	7	1.9
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB2	5	1.9
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB3	5	1.9
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB2	5	1.9
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB3	5	1.9
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB2	5	1.9
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB3	5	1.9
(1,553)	1:80:A:THR:HB	1:88:A:CYS:H	9	1.89
(1,553)	1:80:A:THR:HB	1:88:A:CYS:H	10	1.89
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG11	10	1.89
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG12	10	1.89
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG13	10	1.89
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	6	1.89
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	6	1.89
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	10	1.89
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	10	1.89
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	6	1.89
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	6	1.89
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	6	1.89
(1,720)	1:89:A:VAL:HA	1:95:A:TRP:HZ3	5	1.88
(1,865)	1:30:A:THR:H	1:54:A:VAL:HB	3	1.87
(1,441)	1:70:A:HIS:HD2	1:81:A:VAL:HB	4	1.87
(1,144)	1:30:A:THR:H	1:54:A:VAL:HB	3	1.87
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE1	4	1.86
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE2	4	1.86
(1,521)	1:77:A:PRO:HA	1:90:A:CYS:H	10	1.86
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE1	4	1.86
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE2	4	1.86
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	5	1.86
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	5	1.86
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	9	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	9	1.85
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	9	1.85
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	9	1.85
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	9	1.85
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	9	1.85
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	9	1.85
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	9	1.85
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	9	1.85
(1,36)	1:11:A:VAL:HG21	1:47:A:CYS:HA	5	1.85
(1,36)	1:11:A:VAL:HG22	1:47:A:CYS:HA	5	1.85
(1,36)	1:11:A:VAL:HG23	1:47:A:CYS:HA	5	1.85
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	5	1.84
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB2	7	1.84
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB3	7	1.84
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB2	7	1.84
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB3	7	1.84
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB2	7	1.84
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB3	7	1.84
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	10	1.83
(1,565)	1:80:A:THR:HA	1:95:A:TRP:HZ3	4	1.83
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	10	1.83
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE1	4	1.83
(1,432)	1:70:A:HIS:HA	1:75:A:TYR:HE2	4	1.83
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	1	1.83
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	1	1.83
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	1	1.83
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	4	1.83
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	4	1.83
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	4	1.83
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	6	1.82
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	7	1.82
(1,831)	1:11:A:VAL:H	1:48:A:LEU:H	1	1.82
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	6	1.82
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	6	1.82
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG11	3	1.81
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG12	3	1.81
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG13	3	1.81
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	4	1.8
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	5	1.79
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	1	1.78
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	1	1.78
(1,74)	1:14:A:VAL:HG11	1:45:A:SER:HA	5	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:14:A:VAL:HG12	1:45:A:SER:HA	5	1.78
(1,74)	1:14:A:VAL:HG13	1:45:A:SER:HA	5	1.78
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	4	1.78
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	4	1.78
(1,1122)	1:90:A:CYS:H	1:95:A:TRP:HZ3	3	1.77
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD1	6	1.77
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD2	6	1.77
(1,979)	1:69:A:PHE:H	1:95:A:TRP:HD1	10	1.77
(1,421)	1:69:A:PHE:H	1:95:A:TRP:HD1	10	1.77
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB2	7	1.77
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB3	7	1.77
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB2	7	1.77
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB3	7	1.77
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB2	7	1.77
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB3	7	1.77
(1,1024)	1:77:A:PRO:HA	1:90:A:CYS:H	10	1.76
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG21	2	1.76
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG22	2	1.76
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG23	2	1.76
(1,148)	1:30:A:THR:HA	1:54:A:VAL:HB	3	1.76
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	8	1.76
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	8	1.76
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	8	1.76
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	7	1.75
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	1	1.75
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	1	1.75
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	1	1.75
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	1	1.75
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	1	1.75
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	1	1.75
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	6	1.74
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG21	1	1.74
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG22	1	1.74
(1,676)	1:87:A:THR:HB	1:98:A:THR:HG23	1	1.74
(1,528)	1:78:A:GLY:HA2	1:89:A:VAL:HB	9	1.74
(1,528)	1:78:A:GLY:HA3	1:89:A:VAL:HB	9	1.74
(1,384)	1:67:A:PRO:HG2	1:69:A:PHE:HZ	9	1.74
(1,384)	1:67:A:PRO:HG3	1:69:A:PHE:HZ	9	1.74
(1,68)	1:13:A:LEU:HB2	1:48:A:LEU:HG	6	1.74
(1,68)	1:13:A:LEU:HB3	1:48:A:LEU:HG	6	1.74
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	1	1.73
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB2	7	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB3	7	1.73
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB2	7	1.73
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB3	7	1.73
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB2	7	1.73
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB3	7	1.73
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB2	6	1.73
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB3	6	1.73
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB2	6	1.73
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB3	6	1.73
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	8	1.73
(1,1163)	1:98:A:THR:HB	1:100:A:HIS:H	5	1.72
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD21	4	1.72
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD22	4	1.72
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD23	4	1.72
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	2	1.71
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	10	1.71
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	9	1.71
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	9	1.71
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA2	8	1.7
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA3	8	1.7
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA2	8	1.7
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA3	8	1.7
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA2	8	1.7
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA3	8	1.7
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	5	1.7
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	5	1.7
(1,1107)	1:89:A:VAL:H	1:95:A:TRP:HE3	5	1.69
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	6	1.69
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	7	1.69
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	7	1.69
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	7	1.69
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	7	1.69
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	7	1.69
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	7	1.69
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB2	5	1.69
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB3	5	1.69
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	4	1.69
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	4	1.69
(1,1174)	1:101:A:VAL:HG11	1:103:A:ASP:H	3	1.68
(1,1174)	1:101:A:VAL:HG12	1:103:A:ASP:H	3	1.68
(1,1174)	1:101:A:VAL:HG13	1:103:A:ASP:H	3	1.68
(1,818)	1:101:A:VAL:HG11	1:103:A:ASP:H	3	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:101:A:VAL:HG12	1:103:A:ASP:H	3	1.68
(1,818)	1:101:A:VAL:HG13	1:103:A:ASP:H	3	1.68
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG21	3	1.68
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG22	3	1.68
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG23	3	1.68
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG21	3	1.68
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG22	3	1.68
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG23	3	1.68
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	7	1.68
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	9	1.67
(1,178)	1:32:A:GLN:HG2	1:69:A:PHE:HZ	3	1.66
(1,178)	1:32:A:GLN:HG3	1:69:A:PHE:HZ	3	1.66
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	6	1.66
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	6	1.66
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	6	1.66
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	10	1.66
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG11	4	1.66
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG12	4	1.66
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG13	4	1.66
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	2	1.66
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	2	1.66
(1,49)	1:12:A:LYS:HA	1:47:A:CYS:HA	2	1.66
(1,36)	1:11:A:VAL:HG21	1:47:A:CYS:HA	10	1.66
(1,36)	1:11:A:VAL:HG22	1:47:A:CYS:HA	10	1.66
(1,36)	1:11:A:VAL:HG23	1:47:A:CYS:HA	10	1.66
(1,831)	1:11:A:VAL:H	1:48:A:LEU:H	5	1.65
(1,728)	1:89:A:VAL:HG21	1:95:A:TRP:HZ3	5	1.65
(1,728)	1:89:A:VAL:HG22	1:95:A:TRP:HZ3	5	1.65
(1,728)	1:89:A:VAL:HG23	1:95:A:TRP:HZ3	5	1.65
(1,977)	1:69:A:PHE:H	1:95:A:TRP:HE1	5	1.64
(1,415)	1:69:A:PHE:HE1	1:74:A:GLU:HA	1	1.64
(1,415)	1:69:A:PHE:HE2	1:74:A:GLU:HA	1	1.64
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	7	1.64
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	7	1.64
(1,967)	1:68:A:CYS:H	1:75:A:TYR:H	1	1.63
(1,613)	1:81:A:VAL:HB	1:95:A:TRP:HH2	7	1.63
(1,429)	1:70:A:HIS:H	1:75:A:TYR:HD1	5	1.63
(1,429)	1:70:A:HIS:H	1:75:A:TYR:HD2	5	1.63
(1,188)	1:34:A:TYR:HE1	1:35:A:ASP:HA	8	1.63
(1,188)	1:34:A:TYR:HE2	1:35:A:ASP:HA	8	1.63
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	10	1.62
(1,559)	1:80:A:THR:HB	1:89:A:VAL:HB	8	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	10	1.62
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	10	1.62
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	10	1.62
(1,126)	1:29:A:LYS:HE2	1:34:A:TYR:HA	9	1.62
(1,126)	1:29:A:LYS:HE3	1:34:A:TYR:HA	9	1.62
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	2	1.61
(1,170)	1:31:A:CYS:HB2	1:69:A:PHE:HZ	10	1.61
(1,170)	1:31:A:CYS:HB3	1:69:A:PHE:HZ	10	1.61
(1,68)	1:13:A:LEU:HB2	1:48:A:LEU:HG	5	1.61
(1,68)	1:13:A:LEU:HB3	1:48:A:LEU:HG	5	1.61
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	3	1.6
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	3	1.6
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	4	1.6
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	2	1.6
(1,173)	1:32:A:GLN:HG2	1:33:A:ASN:HA	8	1.6
(1,173)	1:32:A:GLN:HG3	1:33:A:ASN:HA	8	1.6
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	2	1.59
(1,725)	1:89:A:VAL:HG11	1:95:A:TRP:HE3	5	1.59
(1,725)	1:89:A:VAL:HG12	1:95:A:TRP:HE3	5	1.59
(1,725)	1:89:A:VAL:HG13	1:95:A:TRP:HE3	5	1.59
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD11	9	1.59
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD12	9	1.59
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD13	9	1.59
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	5	1.58
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	5	1.58
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	5	1.58
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	4	1.58
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD1	5	1.58
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD2	5	1.58
(1,384)	1:67:A:PRO:HG2	1:69:A:PHE:HZ	1	1.58
(1,384)	1:67:A:PRO:HG3	1:69:A:PHE:HZ	1	1.58
(1,173)	1:32:A:GLN:HG2	1:33:A:ASN:HA	4	1.58
(1,173)	1:32:A:GLN:HG3	1:33:A:ASN:HA	4	1.58
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	7	1.56
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	7	1.56
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	7	1.56
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB2	4	1.55
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB3	4	1.55
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB2	4	1.55
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB3	4	1.55
(1,490)	1:75:A:TYR:HE1	1:81:A:VAL:HA	5	1.55
(1,490)	1:75:A:TYR:HE2	1:81:A:VAL:HA	5	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG11	10	1.55
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG12	10	1.55
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG13	10	1.55
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG11	10	1.55
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG12	10	1.55
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG13	10	1.55
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	5	1.54
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	9	1.54
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	3	1.54
(1,801)	1:98:A:THR:HB	1:100:A:HIS:H	10	1.54
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD2	9	1.54
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD3	9	1.54
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	7	1.53
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	7	1.53
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	8	1.53
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	8	1.53
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	8	1.53
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	8	1.53
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	8	1.53
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	8	1.53
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	5	1.52
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG21	9	1.52
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG22	9	1.52
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG23	9	1.52
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	5	1.52
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG21	9	1.52
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG22	9	1.52
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG23	9	1.52
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	5	1.52
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD21	9	1.52
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD22	9	1.52
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB2	6	1.52
(1,37)	1:11:A:VAL:HB	1:48:A:LEU:HB3	6	1.52
(1,270)	1:54:A:VAL:HG21	1:66:A:CYS:HB2	2	1.51
(1,270)	1:54:A:VAL:HG21	1:66:A:CYS:HB3	2	1.51
(1,270)	1:54:A:VAL:HG22	1:66:A:CYS:HB2	2	1.51
(1,270)	1:54:A:VAL:HG22	1:66:A:CYS:HB3	2	1.51
(1,270)	1:54:A:VAL:HG23	1:66:A:CYS:HB2	2	1.51
(1,270)	1:54:A:VAL:HG23	1:66:A:CYS:HB3	2	1.51
(1,977)	1:69:A:PHE:H	1:95:A:TRP:HE1	10	1.5
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG21	10	1.49
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG22	10	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG23	10	1.49
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	8	1.49
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	8	1.49
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	8	1.49
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG21	2	1.49
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG22	2	1.49
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG23	2	1.49
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG11	4	1.49
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG12	4	1.49
(1,130)	1:29:A:LYS:HE2	1:54:A:VAL:HG13	4	1.49
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG11	4	1.49
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG12	4	1.49
(1,130)	1:29:A:LYS:HE3	1:54:A:VAL:HG13	4	1.49
(1,68)	1:13:A:LEU:HB2	1:48:A:LEU:HG	9	1.49
(1,68)	1:13:A:LEU:HB3	1:48:A:LEU:HG	9	1.49
(1,574)	1:87:A:THR:HG21	1:82:A:LYS:HE2	3	1.48
(1,574)	1:87:A:THR:HG21	1:82:A:LYS:HE3	3	1.48
(1,574)	1:87:A:THR:HG22	1:82:A:LYS:HE2	3	1.48
(1,574)	1:87:A:THR:HG22	1:82:A:LYS:HE3	3	1.48
(1,574)	1:87:A:THR:HG23	1:82:A:LYS:HE2	3	1.48
(1,574)	1:87:A:THR:HG23	1:82:A:LYS:HE3	3	1.48
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	7	1.48
(1,1090)	1:87:A:THR:HB	1:98:A:THR:H	1	1.47
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	10	1.47
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB1	4	1.47
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB2	4	1.47
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB3	4	1.47
(1,91)	1:16:A:PRO:HD2	1:20:A:LEU:HA	3	1.47
(1,91)	1:16:A:PRO:HD3	1:20:A:LEU:HA	3	1.47
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	10	1.46
(1,1098)	1:88:A:CYS:H	1:97:A:CYS:HA	10	1.46
(1,723)	1:89:A:VAL:HB	1:95:A:TRP:HZ3	3	1.46
(1,696)	1:88:A:CYS:H	1:97:A:CYS:HA	10	1.46
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE1	3	1.46
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE2	3	1.46
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE1	3	1.46
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE2	3	1.46
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	5	1.46
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	5	1.46
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	2	1.46
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE1	6	1.45
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE2	6	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:12:A:LYS:HA	1:48:A:LEU:H	3	1.45
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE1	6	1.45
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE2	6	1.45
(1,465)	1:73:A:LYS:HB2	1:75:A:TYR:HE1	6	1.45
(1,465)	1:73:A:LYS:HB2	1:75:A:TYR:HE2	6	1.45
(1,465)	1:73:A:LYS:HB3	1:75:A:TYR:HE1	6	1.45
(1,465)	1:73:A:LYS:HB3	1:75:A:TYR:HE2	6	1.45
(1,335)	1:61:A:VAL:HB	1:65:A:ARG:H	10	1.45
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	5	1.44
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	7	1.44
(1,865)	1:30:A:THR:H	1:54:A:VAL:HB	2	1.44
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	2	1.44
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	7	1.44
(1,144)	1:30:A:THR:H	1:54:A:VAL:HB	2	1.44
(1,1072)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	5	1.43
(1,1072)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	5	1.43
(1,1072)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	5	1.43
(1,798)	1:98:A:THR:HA	1:100:A:HIS:HD2	3	1.43
(1,647)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	5	1.43
(1,647)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	5	1.43
(1,647)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	5	1.43
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	10	1.43
(1,552)	1:80:A:THR:HA	1:88:A:CYS:H	9	1.43
(1,39)	1:11:A:VAL:HG11	1:48:A:LEU:H	2	1.43
(1,39)	1:11:A:VAL:HG12	1:48:A:LEU:H	2	1.43
(1,39)	1:11:A:VAL:HG13	1:48:A:LEU:H	2	1.43
(1,831)	1:11:A:VAL:H	1:48:A:LEU:H	8	1.42
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	1	1.42
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	1	1.42
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	3	1.42
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG11	10	1.42
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG12	10	1.42
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG13	10	1.42
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	4	1.41
(1,835)	1:13:A:LEU:H	1:46:A:GLY:H	1	1.41
(1,563)	1:80:A:THR:HG21	1:89:A:VAL:HB	7	1.41
(1,563)	1:80:A:THR:HG22	1:89:A:VAL:HB	7	1.41
(1,563)	1:80:A:THR:HG23	1:89:A:VAL:HB	7	1.41
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	1	1.41
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	1	1.41
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG11	3	1.41
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG12	3	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG13	3	1.41
(1,148)	1:30:A:THR:HA	1:54:A:VAL:HB	7	1.41
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA2	3	1.41
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA3	3	1.41
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA2	3	1.41
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA3	3	1.41
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA2	3	1.41
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA3	3	1.41
(1,13)	1:10:A:MET:HE1	1:47:A:CYS:HA	5	1.41
(1,13)	1:10:A:MET:HE2	1:47:A:CYS:HA	5	1.41
(1,13)	1:10:A:MET:HE3	1:47:A:CYS:HA	5	1.41
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	6	1.4
(1,958)	1:66:A:CYS:HB2	1:93:A:ARG:H	10	1.4
(1,958)	1:66:A:CYS:HB3	1:93:A:ARG:H	10	1.4
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	8	1.4
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	2	1.4
(1,565)	1:80:A:THR:HA	1:95:A:TRP:HZ3	7	1.4
(1,565)	1:80:A:THR:HA	1:95:A:TRP:HZ3	8	1.4
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB2	4	1.39
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB3	4	1.39
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB2	4	1.39
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB3	4	1.39
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB2	4	1.39
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB3	4	1.39
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	7	1.39
(1,173)	1:32:A:GLN:HG2	1:33:A:ASN:HA	6	1.39
(1,173)	1:32:A:GLN:HG3	1:33:A:ASN:HA	6	1.39
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	1	1.39
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	1	1.39
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	1	1.39
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA2	3	1.39
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA3	3	1.39
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA2	3	1.39
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA3	3	1.39
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA2	3	1.39
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA3	3	1.39
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	7	1.38
(1,598)	1:81:A:VAL:H	1:87:A:THR:HA	9	1.38
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD1	6	1.38
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD2	6	1.38
(1,268)	1:54:A:VAL:HG21	1:65:A:ARG:H	2	1.38
(1,268)	1:54:A:VAL:HG22	1:65:A:ARG:H	2	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:54:A:VAL:HG23	1:65:A:ARG:H	2	1.38
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	6	1.38
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	8	1.37
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	8	1.37
(1,380)	1:66:A:CYS:HB2	1:93:A:ARG:HG2	10	1.37
(1,380)	1:66:A:CYS:HB2	1:93:A:ARG:HG3	10	1.37
(1,380)	1:66:A:CYS:HB3	1:93:A:ARG:HG2	10	1.37
(1,380)	1:66:A:CYS:HB3	1:93:A:ARG:HG3	10	1.37
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	10	1.36
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	10	1.36
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA2	7	1.36
(1,60)	1:13:A:LEU:HG	1:46:A:GLY:HA3	7	1.36
(1,722)	1:89:A:VAL:HA	1:95:A:TRP:HE3	5	1.35
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	9	1.35
(1,237)	1:53:A:MET:HA	1:62:A:ALA:HA	8	1.35
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	8	1.35
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	8	1.35
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	8	1.35
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG21	10	1.35
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG22	10	1.35
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG23	10	1.35
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG21	10	1.35
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG22	10	1.35
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG23	10	1.35
(1,1047)	1:80:A:THR:HG21	1:90:A:CYS:H	7	1.34
(1,1047)	1:80:A:THR:HG22	1:90:A:CYS:H	7	1.34
(1,1047)	1:80:A:THR:HG23	1:90:A:CYS:H	7	1.34
(1,497)	1:75:A:TYR:HD1	1:95:A:TRP:HZ2	5	1.34
(1,497)	1:75:A:TYR:HD2	1:95:A:TRP:HZ2	5	1.34
(1,415)	1:69:A:PHE:HE1	1:74:A:GLU:HA	6	1.34
(1,415)	1:69:A:PHE:HE2	1:74:A:GLU:HA	6	1.34
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	9	1.34
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	9	1.34
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	9	1.34
(1,76)	1:14:A:VAL:HA	1:46:A:GLY:H	6	1.34
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD21	6	1.33
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD22	6	1.33
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	7	1.33
(1,1039)	1:79:A:GLU:H	1:90:A:CYS:H	9	1.33
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	1	1.33
(1,586)	1:81:A:VAL:HB	1:83:A:ILE:HG12	4	1.33
(1,586)	1:81:A:VAL:HB	1:83:A:ILE:HG13	4	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG11	1	1.33
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG12	1	1.33
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG13	1	1.33
(1,243)	1:53:A:MET:HA	1:63:A:LEU:HA	2	1.33
(1,178)	1:32:A:GLN:HG2	1:69:A:PHE:HZ	5	1.33
(1,178)	1:32:A:GLN:HG3	1:69:A:PHE:HZ	5	1.33
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	8	1.32
(1,1095)	1:88:A:CYS:HB2	1:95:A:TRP:H	4	1.32
(1,1095)	1:88:A:CYS:HB3	1:95:A:TRP:H	4	1.32
(1,989)	1:70:A:HIS:H	1:95:A:TRP:HZ2	1	1.32
(1,449)	1:70:A:HIS:H	1:95:A:TRP:HZ2	1	1.32
(1,731)	1:89:A:VAL:HB	1:96:A:ASN:HB2	4	1.31
(1,731)	1:89:A:VAL:HB	1:96:A:ASN:HB3	4	1.31
(1,604)	1:81:A:VAL:HA	1:88:A:CYS:H	9	1.31
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	10	1.31
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	4	1.3
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	4	1.3
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	5	1.3
(1,748)	1:90:A:CYS:HB2	1:95:A:TRP:HZ3	5	1.3
(1,748)	1:90:A:CYS:HB3	1:95:A:TRP:HZ3	5	1.3
(1,674)	1:87:A:THR:HB	1:97:A:CYS:HA	1	1.3
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	6	1.3
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	6	1.3
(1,1060)	1:81:A:VAL:H	1:89:A:VAL:HA	7	1.29
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	8	1.29
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	8	1.29
(1,119)	1:29:A:LYS:HB2	1:34:A:TYR:HE1	2	1.29
(1,119)	1:29:A:LYS:HB2	1:34:A:TYR:HE2	2	1.29
(1,119)	1:29:A:LYS:HB3	1:34:A:TYR:HE1	2	1.29
(1,119)	1:29:A:LYS:HB3	1:34:A:TYR:HE2	2	1.29
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	5	1.29
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	5	1.29
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	5	1.29
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	5	1.29
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	5	1.29
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	5	1.29
(1,9)	1:53:A:MET:HE1	1:62:A:ALA:H	7	1.29
(1,9)	1:53:A:MET:HE2	1:62:A:ALA:H	7	1.29
(1,9)	1:53:A:MET:HE3	1:62:A:ALA:H	7	1.29
(1,1054)	1:81:A:VAL:H	1:87:A:THR:HA	9	1.28
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	1	1.28
(1,803)	1:98:A:THR:HG21	1:100:A:HIS:HE1	6	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:98:A:THR:HG22	1:100:A:HIS:HE1	6	1.28
(1,803)	1:98:A:THR:HG23	1:100:A:HIS:HE1	6	1.28
(1,628)	1:82:A:LYS:HA	1:87:A:THR:HA	6	1.28
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	2	1.28
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	2	1.28
(1,301)	1:56:A:HIS:HE1	1:67:A:PRO:HG2	7	1.28
(1,301)	1:56:A:HIS:HE1	1:67:A:PRO:HG3	7	1.28
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	3	1.27
(1,977)	1:69:A:PHE:H	1:95:A:TRP:HE1	7	1.27
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD21	5	1.26
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD22	5	1.26
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	4	1.26
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE1	4	1.26
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE2	4	1.26
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	2	1.26
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	1	1.25
(1,1111)	1:89:A:VAL:HB	1:96:A:ASN:H	4	1.25
(1,732)	1:89:A:VAL:HB	1:96:A:ASN:H	4	1.25
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	2	1.24
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	7	1.24
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE1	6	1.24
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE2	6	1.24
(1,465)	1:73:A:LYS:HB2	1:75:A:TYR:HE1	5	1.24
(1,465)	1:73:A:LYS:HB2	1:75:A:TYR:HE2	5	1.24
(1,465)	1:73:A:LYS:HB3	1:75:A:TYR:HE1	5	1.24
(1,465)	1:73:A:LYS:HB3	1:75:A:TYR:HE2	5	1.24
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	2	1.24
(1,173)	1:32:A:GLN:HG2	1:33:A:ASN:HA	3	1.24
(1,173)	1:32:A:GLN:HG3	1:33:A:ASN:HA	3	1.24
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	10	1.23
(1,633)	1:82:A:LYS:HD2	1:87:A:THR:HB	3	1.23
(1,633)	1:82:A:LYS:HD3	1:87:A:THR:HB	3	1.23
(1,490)	1:75:A:TYR:HE1	1:81:A:VAL:HA	7	1.23
(1,490)	1:75:A:TYR:HE2	1:81:A:VAL:HA	7	1.23
(1,13)	1:10:A:MET:HE1	1:47:A:CYS:HA	9	1.23
(1,13)	1:10:A:MET:HE2	1:47:A:CYS:HA	9	1.23
(1,13)	1:10:A:MET:HE3	1:47:A:CYS:HA	9	1.23
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG21	1	1.22
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG22	1	1.22
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG23	1	1.22
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	4	1.22
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	4	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1111)	1:89:A:VAL:HB	1:96:A:ASN:H	10	1.21
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG2	9	1.21
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG3	9	1.21
(1,866)	1:30:A:THR:HA	1:55:A:ARG:H	8	1.21
(1,732)	1:89:A:VAL:HB	1:96:A:ASN:H	10	1.21
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE1	2	1.21
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE2	2	1.21
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG11	4	1.21
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG12	4	1.21
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG13	4	1.21
(1,158)	1:30:A:THR:HG21	1:55:A:ARG:H	7	1.21
(1,158)	1:30:A:THR:HG22	1:55:A:ARG:H	7	1.21
(1,158)	1:30:A:THR:HG23	1:55:A:ARG:H	7	1.21
(1,157)	1:30:A:THR:HG21	1:55:A:ARG:HG2	9	1.21
(1,157)	1:30:A:THR:HG21	1:55:A:ARG:HG3	9	1.21
(1,157)	1:30:A:THR:HG22	1:55:A:ARG:HG2	9	1.21
(1,157)	1:30:A:THR:HG22	1:55:A:ARG:HG3	9	1.21
(1,157)	1:30:A:THR:HG23	1:55:A:ARG:HG2	9	1.21
(1,157)	1:30:A:THR:HG23	1:55:A:ARG:HG3	9	1.21
(1,152)	1:30:A:THR:HA	1:55:A:ARG:H	8	1.21
(1,149)	1:30:A:THR:HB	1:54:A:VAL:HB	10	1.21
(1,66)	1:13:A:LEU:HG	1:47:A:CYS:H	5	1.21
(1,3)	1:53:A:MET:HE1	1:60:A:CYS:HA	2	1.21
(1,3)	1:53:A:MET:HE2	1:60:A:CYS:HA	2	1.21
(1,3)	1:53:A:MET:HE3	1:60:A:CYS:HA	2	1.21
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE1	8	1.2
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE2	8	1.2
(1,858)	1:29:A:LYS:HB2	1:34:A:TYR:H	9	1.2
(1,858)	1:29:A:LYS:HB3	1:34:A:TYR:H	9	1.2
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	5	1.2
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB2	10	1.2
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB3	10	1.2
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB2	10	1.2
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB3	10	1.2
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB2	10	1.2
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB3	10	1.2
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE1	5	1.2
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE2	5	1.2
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE1	8	1.2
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE2	8	1.2
(1,414)	1:69:A:PHE:HE1	1:74:A:GLU:HG2	10	1.2
(1,414)	1:69:A:PHE:HE1	1:74:A:GLU:HG3	10	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:69:A:PHE:HE2	1:74:A:GLU:HG2	10	1.2
(1,414)	1:69:A:PHE:HE2	1:74:A:GLU:HG3	10	1.2
(1,63)	1:13:A:LEU:HD11	1:46:A:GLY:H	3	1.2
(1,63)	1:13:A:LEU:HD12	1:46:A:GLY:H	3	1.2
(1,63)	1:13:A:LEU:HD13	1:46:A:GLY:H	3	1.2
(1,5)	1:53:A:MET:HE1	1:61:A:VAL:H	10	1.2
(1,5)	1:53:A:MET:HE2	1:61:A:VAL:H	10	1.2
(1,5)	1:53:A:MET:HE3	1:61:A:VAL:H	10	1.2
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD21	1	1.19
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD22	1	1.19
(1,85)	1:16:A:PRO:HA	1:20:A:LEU:HD23	1	1.19
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD21	5	1.18
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD22	5	1.18
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD23	5	1.18
(1,539)	1:79:A:GLU:H	1:89:A:VAL:HA	10	1.18
(1,237)	1:53:A:MET:HA	1:62:A:ALA:HA	2	1.18
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD2	5	1.18
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD3	5	1.18
(1,979)	1:69:A:PHE:H	1:95:A:TRP:HD1	7	1.17
(1,421)	1:69:A:PHE:H	1:95:A:TRP:HD1	7	1.17
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	6	1.17
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	6	1.17
(1,1174)	1:101:A:VAL:HG11	1:103:A:ASP:H	5	1.16
(1,1174)	1:101:A:VAL:HG12	1:103:A:ASP:H	5	1.16
(1,1174)	1:101:A:VAL:HG13	1:103:A:ASP:H	5	1.16
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	4	1.16
(1,818)	1:101:A:VAL:HG11	1:103:A:ASP:H	5	1.16
(1,818)	1:101:A:VAL:HG12	1:103:A:ASP:H	5	1.16
(1,818)	1:101:A:VAL:HG13	1:103:A:ASP:H	5	1.16
(1,747)	1:90:A:CYS:HA	1:95:A:TRP:HA	10	1.16
(1,604)	1:81:A:VAL:HA	1:88:A:CYS:H	6	1.16
(1,441)	1:70:A:HIS:HD2	1:81:A:VAL:HB	7	1.16
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB2	1	1.16
(1,73)	1:14:A:VAL:HA	1:45:A:SER:HB3	1	1.16
(1,149)	1:30:A:THR:HB	1:54:A:VAL:HB	7	1.15
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	2	1.14
(1,641)	1:83:A:ILE:H	1:87:A:THR:HA	5	1.14
(1,499)	1:75:A:TYR:HE1	1:95:A:TRP:HH2	4	1.14
(1,499)	1:75:A:TYR:HE2	1:95:A:TRP:HH2	4	1.14
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG21	10	1.14
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG22	10	1.14
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG23	10	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	8	1.14
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	8	1.14
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	8	1.14
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	8	1.14
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	8	1.14
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	8	1.14
(1,1045)	1:80:A:THR:H	1:89:A:VAL:HA	9	1.13
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	1	1.13
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	2	1.13
(1,800)	1:98:A:THR:HB	1:100:A:HIS:HD2	3	1.13
(1,554)	1:80:A:THR:H	1:89:A:VAL:HA	9	1.13
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	1	1.13
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	2	1.13
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE1	2	1.13
(1,419)	1:69:A:PHE:HA	1:75:A:TYR:HE2	2	1.13
(1,333)	1:61:A:VAL:HB	1:65:A:ARG:HA	7	1.13
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG11	7	1.13
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG12	7	1.13
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG13	7	1.13
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB2	9	1.13
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB3	9	1.13
(1,1050)	1:81:A:VAL:HB	1:82:A:LYS:H	5	1.12
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG21	2	1.12
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG22	2	1.12
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG23	2	1.12
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	7	1.12
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	7	1.12
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	6	1.12
(1,575)	1:81:A:VAL:HB	1:82:A:LYS:H	5	1.12
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG21	2	1.12
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG22	2	1.12
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG23	2	1.12
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	7	1.12
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	7	1.12
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	4	1.12
(1,494)	1:75:A:TYR:HA	1:95:A:TRP:HH2	8	1.11
(1,148)	1:30:A:THR:HA	1:54:A:VAL:HB	2	1.11
(1,113)	1:28:A:THR:HG21	1:48:A:LEU:HD11	2	1.11
(1,113)	1:28:A:THR:HG21	1:48:A:LEU:HD12	2	1.11
(1,113)	1:28:A:THR:HG21	1:48:A:LEU:HD13	2	1.11
(1,113)	1:28:A:THR:HG22	1:48:A:LEU:HD11	2	1.11
(1,113)	1:28:A:THR:HG22	1:48:A:LEU:HD12	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:28:A:THR:HG22	1:48:A:LEU:HD13	2	1.11
(1,113)	1:28:A:THR:HG23	1:48:A:LEU:HD11	2	1.11
(1,113)	1:28:A:THR:HG23	1:48:A:LEU:HD12	2	1.11
(1,113)	1:28:A:THR:HG23	1:48:A:LEU:HD13	2	1.11
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	10	1.1
(1,562)	1:80:A:THR:HG21	1:89:A:VAL:HA	7	1.1
(1,562)	1:80:A:THR:HG22	1:89:A:VAL:HA	7	1.1
(1,562)	1:80:A:THR:HG23	1:89:A:VAL:HA	7	1.1
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB1	4	1.1
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB2	4	1.1
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB3	4	1.1
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD2	2	1.1
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD3	2	1.1
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	4	1.1
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	4	1.1
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	10	1.1
(1,1094)	1:88:A:CYS:H	1:95:A:TRP:HE3	4	1.09
(1,724)	1:89:A:VAL:HB	1:95:A:TRP:HE3	4	1.09
(1,686)	1:88:A:CYS:H	1:95:A:TRP:HE3	4	1.09
(1,123)	1:29:A:LYS:HG2	1:34:A:TYR:HE1	2	1.09
(1,123)	1:29:A:LYS:HG2	1:34:A:TYR:HE2	2	1.09
(1,123)	1:29:A:LYS:HG3	1:34:A:TYR:HE1	2	1.09
(1,123)	1:29:A:LYS:HG3	1:34:A:TYR:HE2	2	1.09
(1,103)	1:22:A:ALA:HA	1:23:A:GLU:HG2	5	1.09
(1,103)	1:22:A:ALA:HA	1:23:A:GLU:HG3	5	1.09
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG11	7	1.09
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG12	7	1.09
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG13	7	1.09
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG11	7	1.09
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG12	7	1.09
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG13	7	1.09
(1,734)	1:89:A:VAL:HG11	1:96:A:ASN:H	8	1.08
(1,734)	1:89:A:VAL:HG12	1:96:A:ASN:H	8	1.08
(1,734)	1:89:A:VAL:HG13	1:96:A:ASN:H	8	1.08
(1,335)	1:61:A:VAL:HB	1:65:A:ARG:H	2	1.08
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	1	1.08
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	1	1.07
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	4	1.07
(1,979)	1:69:A:PHE:H	1:95:A:TRP:HD1	5	1.07
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	9	1.07
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	10	1.07
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	4	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:69:A:PHE:H	1:95:A:TRP:HD1	5	1.07
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG11	2	1.07
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG12	2	1.07
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG13	2	1.07
(1,1132)	1:91:A:ARG:H	1:94:A:LYS:H	8	1.06
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	3	1.06
(1,674)	1:87:A:THR:HB	1:97:A:CYS:HA	8	1.06
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG11	2	1.06
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG12	2	1.06
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG13	2	1.06
(1,1122)	1:90:A:CYS:H	1:95:A:TRP:HZ3	8	1.05
(1,443)	1:70:A:HIS:HE1	1:81:A:VAL:HG11	10	1.05
(1,443)	1:70:A:HIS:HE1	1:81:A:VAL:HG12	10	1.05
(1,443)	1:70:A:HIS:HE1	1:81:A:VAL:HG13	10	1.05
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB1	9	1.05
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB2	9	1.05
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB3	9	1.05
(1,383)	1:67:A:PRO:HG2	1:69:A:PHE:HE1	6	1.05
(1,383)	1:67:A:PRO:HG2	1:69:A:PHE:HE2	6	1.05
(1,383)	1:67:A:PRO:HG3	1:69:A:PHE:HE1	6	1.05
(1,383)	1:67:A:PRO:HG3	1:69:A:PHE:HE2	6	1.05
(1,281)	1:55:A:ARG:HA	1:61:A:VAL:H	2	1.05
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	7	1.04
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	10	1.04
(1,839)	1:14:A:VAL:HG11	1:45:A:SER:H	9	1.04
(1,839)	1:14:A:VAL:HG12	1:45:A:SER:H	9	1.04
(1,839)	1:14:A:VAL:HG13	1:45:A:SER:H	9	1.04
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	10	1.04
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	8	1.04
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	8	1.04
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	8	1.04
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD11	8	1.04
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD12	8	1.04
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD13	8	1.04
(1,74)	1:14:A:VAL:HG11	1:45:A:SER:HA	10	1.04
(1,74)	1:14:A:VAL:HG12	1:45:A:SER:HA	10	1.04
(1,74)	1:14:A:VAL:HG13	1:45:A:SER:HA	10	1.04
(1,8)	1:53:A:MET:HE1	1:62:A:ALA:HA	7	1.04
(1,8)	1:53:A:MET:HE2	1:62:A:ALA:HA	7	1.04
(1,8)	1:53:A:MET:HE3	1:62:A:ALA:HA	7	1.04
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG21	1	1.03
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG22	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG23	1	1.03
(1,839)	1:14:A:VAL:HG11	1:45:A:SER:H	8	1.03
(1,839)	1:14:A:VAL:HG12	1:45:A:SER:H	8	1.03
(1,839)	1:14:A:VAL:HG13	1:45:A:SER:H	8	1.03
(1,724)	1:89:A:VAL:HB	1:95:A:TRP:HE3	8	1.03
(1,1060)	1:81:A:VAL:H	1:89:A:VAL:HA	6	1.02
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	3	1.02
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	1	1.02
(1,687)	1:88:A:CYS:HA	1:95:A:TRP:HA	4	1.02
(1,636)	1:82:A:LYS:HD2	1:88:A:CYS:H	3	1.02
(1,636)	1:82:A:LYS:HD3	1:88:A:CYS:H	3	1.02
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	3	1.02
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB2	10	1.02
(1,416)	1:69:A:PHE:HE1	1:74:A:GLU:HB3	10	1.02
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB2	10	1.02
(1,416)	1:69:A:PHE:HE2	1:74:A:GLU:HB3	10	1.02
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	2	1.02
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	10	1.02
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	10	1.02
(1,74)	1:14:A:VAL:HG11	1:45:A:SER:HA	8	1.02
(1,74)	1:14:A:VAL:HG12	1:45:A:SER:HA	8	1.02
(1,74)	1:14:A:VAL:HG13	1:45:A:SER:HA	8	1.02
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	6	1.02
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	6	1.02
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB2	7	1.01
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB3	7	1.01
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	3	1.01
(1,865)	1:30:A:THR:H	1:54:A:VAL:HB	7	1.01
(1,687)	1:88:A:CYS:HA	1:95:A:TRP:HA	8	1.01
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB2	7	1.01
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB3	7	1.01
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	4	1.01
(1,144)	1:30:A:THR:H	1:54:A:VAL:HB	7	1.01
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD21	9	1.01
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD22	9	1.01
(1,95)	1:17:A:ALA:HA	1:20:A:LEU:HD23	9	1.01
(1,1130)	1:91:A:ARG:HA	1:93:A:ARG:H	6	1.0
(1,935)	1:61:A:VAL:HB	1:62:A:ALA:H	5	1.0
(1,830)	1:11:A:VAL:H	1:48:A:LEU:HG	4	1.0
(1,756)	1:91:A:ARG:HA	1:93:A:ARG:H	6	1.0
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD11	7	1.0
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD12	7	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,447)	1:70:A:HIS:HE1	1:83:A:ILE:HD13	7	1.0
(1,329)	1:61:A:VAL:HB	1:62:A:ALA:H	5	1.0
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	3	1.0
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	3	1.0
(1,1050)	1:81:A:VAL:HB	1:82:A:LYS:H	8	0.99
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	10	0.99
(1,799)	1:98:A:THR:HB	1:100:A:HIS:HB2	10	0.99
(1,799)	1:98:A:THR:HB	1:100:A:HIS:HB3	10	0.99
(1,575)	1:81:A:VAL:HB	1:82:A:LYS:H	8	0.99
(1,496)	1:75:A:TYR:HB2	1:95:A:TRP:HH2	5	0.99
(1,496)	1:75:A:TYR:HB3	1:95:A:TRP:HH2	5	0.99
(1,415)	1:69:A:PHE:HE1	1:74:A:GLU:HA	10	0.99
(1,415)	1:69:A:PHE:HE2	1:74:A:GLU:HA	10	0.99
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD2	5	0.99
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD3	5	0.99
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG11	4	0.99
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG12	4	0.99
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG13	4	0.99
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	3	0.98
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	6	0.98
(1,805)	1:99:A:ASP:H	1:100:A:HIS:HD2	9	0.98
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG11	7	0.98
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG12	7	0.98
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG13	7	0.98
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG11	2	0.98
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG12	2	0.98
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG13	2	0.98
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD21	7	0.98
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD22	7	0.98
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA2	4	0.98
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA3	4	0.98
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA2	4	0.98
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA3	4	0.98
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA2	4	0.98
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA3	4	0.98
(1,40)	1:11:A:VAL:HG21	1:48:A:LEU:H	7	0.98
(1,40)	1:11:A:VAL:HG22	1:48:A:LEU:H	7	0.98
(1,40)	1:11:A:VAL:HG23	1:48:A:LEU:H	7	0.98
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	1	0.97
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	1	0.97
(1,866)	1:30:A:THR:HA	1:55:A:ARG:H	4	0.97
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG21	9	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG22	9	0.97
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG23	9	0.97
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	1	0.97
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	1	0.97
(1,429)	1:70:A:HIS:H	1:75:A:TYR:HD1	6	0.97
(1,429)	1:70:A:HIS:H	1:75:A:TYR:HD2	6	0.97
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB1	10	0.97
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB2	10	0.97
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB3	10	0.97
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG2	5	0.97
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG3	5	0.97
(1,152)	1:30:A:THR:HA	1:55:A:ARG:H	4	0.97
(1,977)	1:69:A:PHE:H	1:95:A:TRP:HE1	9	0.96
(1,636)	1:82:A:LYS:HD2	1:88:A:CYS:H	1	0.96
(1,636)	1:82:A:LYS:HD3	1:88:A:CYS:H	1	0.96
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	6	0.96
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG11	8	0.96
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG12	8	0.96
(1,190)	1:34:A:TYR:HA	1:54:A:VAL:HG13	8	0.96
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	3	0.96
(1,1163)	1:98:A:THR:HB	1:100:A:HIS:H	3	0.95
(1,1160)	1:98:A:THR:HB	1:99:A:ASP:H	7	0.95
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG21	9	0.95
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG22	9	0.95
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG23	9	0.95
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	8	0.95
(1,792)	1:98:A:THR:HB	1:99:A:ASP:H	7	0.95
(1,642)	1:83:A:ILE:HB	1:88:A:CYS:HB2	5	0.95
(1,642)	1:83:A:ILE:HB	1:88:A:CYS:HB3	5	0.95
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG21	9	0.95
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG22	9	0.95
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG23	9	0.95
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	8	0.95
(1,470)	1:73:A:LYS:HD2	1:75:A:TYR:HE1	6	0.95
(1,470)	1:73:A:LYS:HD2	1:75:A:TYR:HE2	6	0.95
(1,470)	1:73:A:LYS:HD3	1:75:A:TYR:HE1	6	0.95
(1,470)	1:73:A:LYS:HD3	1:75:A:TYR:HE2	6	0.95
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD2	5	0.95
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD3	5	0.95
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG11	6	0.95
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG12	6	0.95
(1,294)	1:56:A:HIS:H	1:61:A:VAL:HG13	6	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	7	0.95
(1,147)	1:30:A:THR:HA	1:54:A:VAL:HA	2	0.95
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG11	3	0.95
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG12	3	0.95
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG13	3	0.95
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	9	0.94
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	3	0.94
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	4	0.94
(1,991)	1:70:A:HIS:HB2	1:95:A:TRP:HE1	1	0.94
(1,991)	1:70:A:HIS:HB3	1:95:A:TRP:HE1	1	0.94
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	2	0.94
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	6	0.94
(1,835)	1:13:A:LEU:H	1:46:A:GLY:H	10	0.94
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	3	0.94
(1,644)	1:83:A:ILE:HD11	1:95:A:TRP:HE3	8	0.94
(1,644)	1:83:A:ILE:HD12	1:95:A:TRP:HE3	8	0.94
(1,644)	1:83:A:ILE:HD13	1:95:A:TRP:HE3	8	0.94
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	4	0.94
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG11	7	0.94
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG12	7	0.94
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG13	7	0.94
(1,378)	1:66:A:CYS:HB2	1:93:A:ARG:HD2	10	0.93
(1,378)	1:66:A:CYS:HB2	1:93:A:ARG:HD3	10	0.93
(1,378)	1:66:A:CYS:HB3	1:93:A:ARG:HD2	10	0.93
(1,378)	1:66:A:CYS:HB3	1:93:A:ARG:HD3	10	0.93
(1,173)	1:32:A:GLN:HG2	1:33:A:ASN:HA	5	0.93
(1,173)	1:32:A:GLN:HG3	1:33:A:ASN:HA	5	0.93
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	1	0.93
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	1	0.93
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	1	0.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	1	0.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	1	0.93
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	1	0.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	1	0.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	1	0.93
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	1	0.93
(1,731)	1:89:A:VAL:HB	1:96:A:ASN:HB2	10	0.92
(1,731)	1:89:A:VAL:HB	1:96:A:ASN:HB3	10	0.92
(1,384)	1:67:A:PRO:HG2	1:69:A:PHE:HZ	7	0.92
(1,384)	1:67:A:PRO:HG3	1:69:A:PHE:HZ	7	0.92
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	9	0.92
(1,119)	1:29:A:LYS:HB2	1:34:A:TYR:HE1	3	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:29:A:LYS:HB2	1:34:A:TYR:HE2	3	0.92
(1,119)	1:29:A:LYS:HB3	1:34:A:TYR:HE1	3	0.92
(1,119)	1:29:A:LYS:HB3	1:34:A:TYR:HE2	3	0.92
(1,103)	1:22:A:ALA:HA	1:23:A:GLU:HG2	9	0.92
(1,103)	1:22:A:ALA:HA	1:23:A:GLU:HG3	9	0.92
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB1	3	0.92
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB2	3	0.92
(1,59)	1:13:A:LEU:HD11	1:22:A:ALA:HB3	3	0.92
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB1	3	0.92
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB2	3	0.92
(1,59)	1:13:A:LEU:HD12	1:22:A:ALA:HB3	3	0.92
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB1	3	0.92
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB2	3	0.92
(1,59)	1:13:A:LEU:HD13	1:22:A:ALA:HB3	3	0.92
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG11	8	0.92
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG12	8	0.92
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG13	8	0.92
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	10	0.91
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	10	0.91
(1,841)	1:15:A:CYS:H	1:45:A:SER:HA	3	0.91
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG11	9	0.91
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG12	9	0.91
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG13	9	0.91
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB1	8	0.91
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB2	8	0.91
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB3	8	0.91
(1,67)	1:13:A:LEU:HD21	1:47:A:CYS:H	2	0.91
(1,67)	1:13:A:LEU:HD22	1:47:A:CYS:H	2	0.91
(1,67)	1:13:A:LEU:HD23	1:47:A:CYS:H	2	0.91
(1,1050)	1:81:A:VAL:HB	1:82:A:LYS:H	4	0.9
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	7	0.9
(1,815)	1:101:A:VAL:HA	1:103:A:ASP:H	8	0.9
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	10	0.9
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	10	0.9
(1,604)	1:81:A:VAL:HA	1:88:A:CYS:H	7	0.9
(1,575)	1:81:A:VAL:HB	1:82:A:LYS:H	4	0.9
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	7	0.9
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE1	6	0.9
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE2	6	0.9
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE1	6	0.9
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE2	6	0.9
(1,243)	1:53:A:MET:HA	1:63:A:LEU:HA	8	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:34:A:TYR:H	1:36:A:LEU:HG	3	0.89
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG21	10	0.89
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG22	10	0.89
(1,634)	1:82:A:LYS:HE2	1:87:A:THR:HG23	10	0.89
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG21	10	0.89
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG22	10	0.89
(1,634)	1:82:A:LYS:HE3	1:87:A:THR:HG23	10	0.89
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB2	4	0.89
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB3	4	0.89
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG11	9	0.89
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG12	9	0.89
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG13	9	0.89
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE1	3	0.89
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE2	3	0.89
(1,296)	1:56:A:HIS:HA	1:61:A:VAL:HG21	2	0.89
(1,296)	1:56:A:HIS:HA	1:61:A:VAL:HG22	2	0.89
(1,296)	1:56:A:HIS:HA	1:61:A:VAL:HG23	2	0.89
(1,241)	1:53:A:MET:HG2	1:62:A:ALA:HA	2	0.89
(1,241)	1:53:A:MET:HG3	1:62:A:ALA:HA	2	0.89
(1,64)	1:13:A:LEU:H	1:47:A:CYS:HA	2	0.89
(1,5)	1:53:A:MET:HE1	1:61:A:VAL:H	7	0.89
(1,5)	1:53:A:MET:HE2	1:61:A:VAL:H	7	0.89
(1,5)	1:53:A:MET:HE3	1:61:A:VAL:H	7	0.89
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	3	0.88
(1,866)	1:30:A:THR:HA	1:55:A:ARG:H	7	0.88
(1,723)	1:89:A:VAL:HB	1:95:A:TRP:HZ3	6	0.88
(1,567)	1:80:A:THR:HG21	1:95:A:TRP:HH2	7	0.88
(1,567)	1:80:A:THR:HG22	1:95:A:TRP:HH2	7	0.88
(1,567)	1:80:A:THR:HG23	1:95:A:TRP:HH2	7	0.88
(1,253)	1:54:A:VAL:HG21	1:61:A:VAL:HB	10	0.88
(1,253)	1:54:A:VAL:HG22	1:61:A:VAL:HB	10	0.88
(1,253)	1:54:A:VAL:HG23	1:61:A:VAL:HB	10	0.88
(1,158)	1:30:A:THR:HG21	1:55:A:ARG:H	8	0.88
(1,158)	1:30:A:THR:HG22	1:55:A:ARG:H	8	0.88
(1,158)	1:30:A:THR:HG23	1:55:A:ARG:H	8	0.88
(1,152)	1:30:A:THR:HA	1:55:A:ARG:H	7	0.88
(1,1072)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	8	0.87
(1,1072)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	8	0.87
(1,1072)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	8	0.87
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	8	0.87
(1,815)	1:101:A:VAL:HA	1:103:A:ASP:H	9	0.87
(1,729)	1:89:A:VAL:H	1:96:A:ASN:HA	10	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	8	0.87
(1,647)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	8	0.87
(1,647)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	8	0.87
(1,615)	1:81:A:VAL:HG21	1:95:A:TRP:HE1	4	0.87
(1,615)	1:81:A:VAL:HG22	1:95:A:TRP:HE1	4	0.87
(1,615)	1:81:A:VAL:HG23	1:95:A:TRP:HE1	4	0.87
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	5	0.87
(1,441)	1:70:A:HIS:HD2	1:81:A:VAL:HB	10	0.87
(1,415)	1:69:A:PHE:HE1	1:74:A:GLU:HA	9	0.87
(1,415)	1:69:A:PHE:HE2	1:74:A:GLU:HA	9	0.87
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	6	0.87
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	6	0.87
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	6	0.87
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG11	4	0.87
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG12	4	0.87
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG13	4	0.87
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG11	4	0.87
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG12	4	0.87
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG13	4	0.87
(1,4)	1:53:A:MET:HE1	1:61:A:VAL:HA	10	0.87
(1,4)	1:53:A:MET:HE2	1:61:A:VAL:HA	10	0.87
(1,4)	1:53:A:MET:HE3	1:61:A:VAL:HA	10	0.87
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	6	0.86
(1,815)	1:101:A:VAL:HA	1:103:A:ASP:H	5	0.86
(1,802)	1:98:A:THR:HG21	1:100:A:HIS:HD2	2	0.86
(1,802)	1:98:A:THR:HG22	1:100:A:HIS:HD2	2	0.86
(1,802)	1:98:A:THR:HG23	1:100:A:HIS:HD2	2	0.86
(1,621)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	6	0.86
(1,621)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	6	0.86
(1,621)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	6	0.86
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG21	1	0.86
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG22	1	0.86
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG23	1	0.86
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	4	0.86
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	4	0.86
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	4	0.86
(1,721)	1:89:A:VAL:HA	1:95:A:TRP:HA	8	0.85
(1,1134)	1:91:A:ARG:H	1:95:A:TRP:HE3	3	0.84
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG11	7	0.84
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG12	7	0.84
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG13	7	0.84
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	9	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:73:A:LYS:HG2	1:75:A:TYR:HE1	6	0.84
(1,467)	1:73:A:LYS:HG2	1:75:A:TYR:HE2	6	0.84
(1,467)	1:73:A:LYS:HG3	1:75:A:TYR:HE1	6	0.84
(1,467)	1:73:A:LYS:HG3	1:75:A:TYR:HE2	6	0.84
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG21	10	0.84
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG22	10	0.84
(1,300)	1:56:A:HIS:HD2	1:61:A:VAL:HG23	10	0.84
(1,237)	1:53:A:MET:HA	1:62:A:ALA:HA	7	0.84
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD2	4	0.84
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD3	4	0.84
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD2	4	0.84
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD3	4	0.84
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD2	4	0.84
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD3	4	0.84
(1,154)	1:30:A:THR:HG21	1:55:A:ARG:HB2	7	0.84
(1,154)	1:30:A:THR:HG21	1:55:A:ARG:HB3	7	0.84
(1,154)	1:30:A:THR:HG22	1:55:A:ARG:HB2	7	0.84
(1,154)	1:30:A:THR:HG22	1:55:A:ARG:HB3	7	0.84
(1,154)	1:30:A:THR:HG23	1:55:A:ARG:HB2	7	0.84
(1,154)	1:30:A:THR:HG23	1:55:A:ARG:HB3	7	0.84
(1,63)	1:13:A:LEU:HD11	1:46:A:GLY:H	4	0.84
(1,63)	1:13:A:LEU:HD12	1:46:A:GLY:H	4	0.84
(1,63)	1:13:A:LEU:HD13	1:46:A:GLY:H	4	0.84
(1,1162)	1:98:A:THR:HA	1:100:A:HIS:H	3	0.83
(1,1132)	1:91:A:ARG:H	1:94:A:LYS:H	1	0.83
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	8	0.83
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	2	0.83
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD2	10	0.83
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD3	10	0.83
(1,90)	1:16:A:PRO:HD2	1:20:A:LEU:HD21	5	0.83
(1,90)	1:16:A:PRO:HD2	1:20:A:LEU:HD22	5	0.83
(1,90)	1:16:A:PRO:HD2	1:20:A:LEU:HD23	5	0.83
(1,90)	1:16:A:PRO:HD3	1:20:A:LEU:HD21	5	0.83
(1,90)	1:16:A:PRO:HD3	1:20:A:LEU:HD22	5	0.83
(1,90)	1:16:A:PRO:HD3	1:20:A:LEU:HD23	5	0.83
(1,1050)	1:81:A:VAL:HB	1:82:A:LYS:H	7	0.82
(1,656)	1:85:A:CYS:HB2	1:102:A:CYS:HA	6	0.82
(1,656)	1:85:A:CYS:HB3	1:102:A:CYS:HA	6	0.82
(1,575)	1:81:A:VAL:HB	1:82:A:LYS:H	7	0.82
(1,267)	1:54:A:VAL:HG11	1:65:A:ARG:H	2	0.82
(1,267)	1:54:A:VAL:HG12	1:65:A:ARG:H	2	0.82
(1,267)	1:54:A:VAL:HG13	1:65:A:ARG:H	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:32:A:GLN:HG2	1:69:A:PHE:HE1	2	0.82
(1,177)	1:32:A:GLN:HG2	1:69:A:PHE:HE2	2	0.82
(1,177)	1:32:A:GLN:HG3	1:69:A:PHE:HE1	2	0.82
(1,177)	1:32:A:GLN:HG3	1:69:A:PHE:HE2	2	0.82
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG21	10	0.82
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG22	10	0.82
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG23	10	0.82
(1,11)	1:53:A:MET:HE1	1:63:A:LEU:H	6	0.82
(1,11)	1:53:A:MET:HE2	1:63:A:LEU:H	6	0.82
(1,11)	1:53:A:MET:HE3	1:63:A:LEU:H	6	0.82
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	8	0.81
(1,815)	1:101:A:VAL:HA	1:103:A:ASP:H	3	0.81
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	1	0.81
(1,726)	1:89:A:VAL:HG21	1:95:A:TRP:HE3	5	0.81
(1,726)	1:89:A:VAL:HG22	1:95:A:TRP:HE3	5	0.81
(1,726)	1:89:A:VAL:HG23	1:95:A:TRP:HE3	5	0.81
(1,656)	1:85:A:CYS:HB2	1:102:A:CYS:HA	4	0.81
(1,656)	1:85:A:CYS:HB3	1:102:A:CYS:HA	4	0.81
(1,622)	1:81:A:VAL:HG21	1:95:A:TRP:HE3	7	0.81
(1,622)	1:81:A:VAL:HG22	1:95:A:TRP:HE3	7	0.81
(1,622)	1:81:A:VAL:HG23	1:95:A:TRP:HE3	7	0.81
(1,616)	1:81:A:VAL:HG11	1:95:A:TRP:HZ2	6	0.81
(1,616)	1:81:A:VAL:HG12	1:95:A:TRP:HZ2	6	0.81
(1,616)	1:81:A:VAL:HG13	1:95:A:TRP:HZ2	6	0.81
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG21	8	0.81
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG22	8	0.81
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG23	8	0.81
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB1	6	0.81
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB2	6	0.81
(1,386)	1:67:A:PRO:HA	1:76:A:ALA:HB3	6	0.81
(1,178)	1:32:A:GLN:HG2	1:69:A:PHE:HZ	1	0.81
(1,178)	1:32:A:GLN:HG3	1:69:A:PHE:HZ	1	0.81
(1,1109)	1:89:A:VAL:H	1:96:A:ASN:H	4	0.8
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG21	8	0.8
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG22	8	0.8
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG23	8	0.8
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG21	10	0.8
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG22	10	0.8
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG23	10	0.8
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	8	0.8
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG21	8	0.8
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG22	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG23	8	0.8
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	3	0.8
(1,9)	1:53:A:MET:HE1	1:62:A:ALA:H	10	0.8
(1,9)	1:53:A:MET:HE2	1:62:A:ALA:H	10	0.8
(1,9)	1:53:A:MET:HE3	1:62:A:ALA:H	10	0.8
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE1	5	0.79
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE2	5	0.79
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG21	8	0.79
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG22	8	0.79
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG23	8	0.79
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE1	5	0.79
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE2	5	0.79
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG11	10	0.79
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG12	10	0.79
(1,143)	1:30:A:THR:H	1:54:A:VAL:HG13	10	0.79
(1,11)	1:53:A:MET:HE1	1:63:A:LEU:H	10	0.79
(1,11)	1:53:A:MET:HE2	1:63:A:LEU:H	10	0.79
(1,11)	1:53:A:MET:HE3	1:63:A:LEU:H	10	0.79
(1,264)	1:54:A:VAL:HG21	1:63:A:LEU:HA	2	0.78
(1,264)	1:54:A:VAL:HG22	1:63:A:LEU:HA	2	0.78
(1,264)	1:54:A:VAL:HG23	1:63:A:LEU:HA	2	0.78
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	10	0.78
(1,178)	1:32:A:GLN:HG2	1:69:A:PHE:HZ	9	0.78
(1,178)	1:32:A:GLN:HG3	1:69:A:PHE:HZ	9	0.78
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA2	4	0.78
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA3	4	0.78
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA2	4	0.78
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA3	4	0.78
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA2	4	0.78
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA3	4	0.78
(1,11)	1:53:A:MET:HE1	1:63:A:LEU:H	1	0.78
(1,11)	1:53:A:MET:HE2	1:63:A:LEU:H	1	0.78
(1,11)	1:53:A:MET:HE3	1:63:A:LEU:H	1	0.78
(1,1064)	1:81:A:VAL:HG21	1:95:A:TRP:HE1	4	0.77
(1,1064)	1:81:A:VAL:HG22	1:95:A:TRP:HE1	4	0.77
(1,1064)	1:81:A:VAL:HG23	1:95:A:TRP:HE1	4	0.77
(1,1060)	1:81:A:VAL:H	1:89:A:VAL:HA	5	0.77
(1,1045)	1:80:A:THR:H	1:89:A:VAL:HA	3	0.77
(1,1045)	1:80:A:THR:H	1:89:A:VAL:HA	7	0.77
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	4	0.77
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	1	0.77
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	2	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	5	0.77
(1,554)	1:80:A:THR:H	1:89:A:VAL:HA	3	0.77
(1,554)	1:80:A:THR:H	1:89:A:VAL:HA	7	0.77
(1,539)	1:79:A:GLU:H	1:89:A:VAL:HA	3	0.77
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG11	8	0.77
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG12	8	0.77
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG13	8	0.77
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG11	8	0.77
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG12	8	0.77
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG13	8	0.77
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	1	0.76
(1,1116)	1:89:A:VAL:H	1:98:A:THR:H	5	0.76
(1,1063)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	6	0.76
(1,1063)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	6	0.76
(1,1063)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	6	0.76
(1,935)	1:61:A:VAL:HB	1:62:A:ALA:H	10	0.76
(1,563)	1:80:A:THR:HG21	1:89:A:VAL:HB	9	0.76
(1,563)	1:80:A:THR:HG22	1:89:A:VAL:HB	9	0.76
(1,563)	1:80:A:THR:HG23	1:89:A:VAL:HB	9	0.76
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	5	0.76
(1,329)	1:61:A:VAL:HB	1:62:A:ALA:H	10	0.76
(1,1174)	1:101:A:VAL:HG11	1:103:A:ASP:H	8	0.75
(1,1174)	1:101:A:VAL:HG12	1:103:A:ASP:H	8	0.75
(1,1174)	1:101:A:VAL:HG13	1:103:A:ASP:H	8	0.75
(1,1090)	1:87:A:THR:HB	1:98:A:THR:H	6	0.75
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	9	0.75
(1,882)	1:35:A:ASP:H	1:36:A:LEU:HG	7	0.75
(1,818)	1:101:A:VAL:HG11	1:103:A:ASP:H	8	0.75
(1,818)	1:101:A:VAL:HG12	1:103:A:ASP:H	8	0.75
(1,818)	1:101:A:VAL:HG13	1:103:A:ASP:H	8	0.75
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD2	5	0.75
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD3	5	0.75
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	6	0.74
(1,1017)	1:76:A:ALA:H	1:79:A:GLU:H	1	0.74
(1,977)	1:69:A:PHE:H	1:95:A:TRP:HE1	3	0.74
(1,860)	1:30:A:THR:HB	1:31:A:CYS:H	7	0.74
(1,674)	1:87:A:THR:HB	1:97:A:CYS:HA	6	0.74
(1,665)	1:86:A:ASN:HA	1:100:A:HIS:HD2	7	0.74
(1,656)	1:85:A:CYS:HB2	1:102:A:CYS:HA	10	0.74
(1,656)	1:85:A:CYS:HB3	1:102:A:CYS:HA	10	0.74
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG21	1	0.74
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG22	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG23	1	0.74
(1,135)	1:30:A:THR:HB	1:31:A:CYS:H	7	0.74
(1,1160)	1:98:A:THR:HB	1:99:A:ASP:H	5	0.73
(1,1058)	1:81:A:VAL:HG11	1:88:A:CYS:H	9	0.73
(1,1058)	1:81:A:VAL:HG12	1:88:A:CYS:H	9	0.73
(1,1058)	1:81:A:VAL:HG13	1:88:A:CYS:H	9	0.73
(1,1050)	1:81:A:VAL:HB	1:82:A:LYS:H	10	0.73
(1,991)	1:70:A:HIS:HB2	1:95:A:TRP:HE1	7	0.73
(1,991)	1:70:A:HIS:HB3	1:95:A:TRP:HE1	7	0.73
(1,792)	1:98:A:THR:HB	1:99:A:ASP:H	5	0.73
(1,749)	1:90:A:CYS:HB2	1:95:A:TRP:HE3	5	0.73
(1,749)	1:90:A:CYS:HB3	1:95:A:TRP:HE3	5	0.73
(1,605)	1:81:A:VAL:HG11	1:88:A:CYS:H	9	0.73
(1,605)	1:81:A:VAL:HG12	1:88:A:CYS:H	9	0.73
(1,605)	1:81:A:VAL:HG13	1:88:A:CYS:H	9	0.73
(1,600)	1:81:A:VAL:HG21	1:87:A:THR:HB	5	0.73
(1,600)	1:81:A:VAL:HG22	1:87:A:THR:HB	5	0.73
(1,600)	1:81:A:VAL:HG23	1:87:A:THR:HB	5	0.73
(1,575)	1:81:A:VAL:HB	1:82:A:LYS:H	10	0.73
(1,565)	1:80:A:THR:HA	1:95:A:TRP:HZ3	3	0.73
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG21	7	0.73
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG22	7	0.73
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG23	7	0.73
(1,341)	1:61:A:VAL:HG21	1:66:A:CYS:H	4	0.73
(1,341)	1:61:A:VAL:HG22	1:66:A:CYS:H	4	0.73
(1,341)	1:61:A:VAL:HG23	1:66:A:CYS:H	4	0.73
(1,1111)	1:89:A:VAL:HB	1:96:A:ASN:H	8	0.72
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	2	0.72
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	4	0.72
(1,1050)	1:81:A:VAL:HB	1:82:A:LYS:H	1	0.72
(1,746)	1:90:A:CYS:HA	1:95:A:TRP:HE3	3	0.72
(1,732)	1:89:A:VAL:HB	1:96:A:ASN:H	8	0.72
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	2	0.72
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	4	0.72
(1,575)	1:81:A:VAL:HB	1:82:A:LYS:H	1	0.72
(1,567)	1:80:A:THR:HG21	1:95:A:TRP:HH2	5	0.72
(1,567)	1:80:A:THR:HG22	1:95:A:TRP:HH2	5	0.72
(1,567)	1:80:A:THR:HG23	1:95:A:TRP:HH2	5	0.72
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG11	4	0.72
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG12	4	0.72
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG13	4	0.72
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG21	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG22	7	0.72
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG23	7	0.72
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	2	0.72
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB2	5	0.72
(1,50)	1:12:A:LYS:HA	1:47:A:CYS:HB3	5	0.72
(1,1160)	1:98:A:THR:HB	1:99:A:ASP:H	6	0.71
(1,793)	1:98:A:THR:HB	1:99:A:ASP:HA	7	0.71
(1,792)	1:98:A:THR:HB	1:99:A:ASP:H	6	0.71
(1,158)	1:30:A:THR:HG21	1:55:A:ARG:H	9	0.71
(1,158)	1:30:A:THR:HG22	1:55:A:ARG:H	9	0.71
(1,158)	1:30:A:THR:HG23	1:55:A:ARG:H	9	0.71
(1,1160)	1:98:A:THR:HB	1:99:A:ASP:H	4	0.7
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	4	0.7
(1,792)	1:98:A:THR:HB	1:99:A:ASP:H	4	0.7
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	3	0.7
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB2	5	0.7
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB3	5	0.7
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG11	4	0.7
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG12	4	0.7
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG13	4	0.7
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD2	2	0.7
(1,377)	1:66:A:CYS:H	1:93:A:ARG:HD3	2	0.7
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB1	5	0.7
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB2	5	0.7
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB3	5	0.7
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB2	8	0.7
(1,42)	1:11:A:VAL:HG21	1:49:A:CYS:HB3	8	0.7
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB2	8	0.7
(1,42)	1:11:A:VAL:HG22	1:49:A:CYS:HB3	8	0.7
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB2	8	0.7
(1,42)	1:11:A:VAL:HG23	1:49:A:CYS:HB3	8	0.7
(1,574)	1:87:A:THR:HG21	1:82:A:LYS:HE2	10	0.69
(1,574)	1:87:A:THR:HG21	1:82:A:LYS:HE3	10	0.69
(1,574)	1:87:A:THR:HG22	1:82:A:LYS:HE2	10	0.69
(1,574)	1:87:A:THR:HG22	1:82:A:LYS:HE3	10	0.69
(1,574)	1:87:A:THR:HG23	1:82:A:LYS:HE2	10	0.69
(1,574)	1:87:A:THR:HG23	1:82:A:LYS:HE3	10	0.69
(1,511)	1:76:A:ALA:HB1	1:79:A:GLU:HG2	5	0.69
(1,511)	1:76:A:ALA:HB1	1:79:A:GLU:HG3	5	0.69
(1,511)	1:76:A:ALA:HB2	1:79:A:GLU:HG2	5	0.69
(1,511)	1:76:A:ALA:HB2	1:79:A:GLU:HG3	5	0.69
(1,511)	1:76:A:ALA:HB3	1:79:A:GLU:HG2	5	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:76:A:ALA:HB3	1:79:A:GLU:HG3	5	0.69
(1,333)	1:61:A:VAL:HB	1:65:A:ARG:HA	4	0.69
(1,148)	1:30:A:THR:HA	1:54:A:VAL:HB	10	0.69
(1,1066)	1:82:A:LYS:HG2	1:83:A:ILE:H	5	0.68
(1,1066)	1:82:A:LYS:HG3	1:83:A:ILE:H	5	0.68
(1,1056)	1:81:A:VAL:H	1:88:A:CYS:H	3	0.68
(1,1045)	1:80:A:THR:H	1:89:A:VAL:HA	2	0.68
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	10	0.68
(1,724)	1:89:A:VAL:HB	1:95:A:TRP:HE3	3	0.68
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	6	0.68
(1,607)	1:81:A:VAL:HG21	1:88:A:CYS:HA	7	0.68
(1,607)	1:81:A:VAL:HG22	1:88:A:CYS:HA	7	0.68
(1,607)	1:81:A:VAL:HG23	1:88:A:CYS:HA	7	0.68
(1,598)	1:81:A:VAL:H	1:87:A:THR:HA	10	0.68
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB2	7	0.68
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB3	7	0.68
(1,554)	1:80:A:THR:H	1:89:A:VAL:HA	2	0.68
(1,536)	1:79:A:GLU:HG2	1:80:A:THR:HB	6	0.68
(1,536)	1:79:A:GLU:HG3	1:80:A:THR:HB	6	0.68
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG21	10	0.68
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG22	10	0.68
(1,444)	1:70:A:HIS:HE1	1:81:A:VAL:HG23	10	0.68
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD2	2	0.68
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD3	2	0.68
(1,269)	1:54:A:VAL:HG11	1:66:A:CYS:HA	2	0.68
(1,269)	1:54:A:VAL:HG12	1:66:A:CYS:HA	2	0.68
(1,269)	1:54:A:VAL:HG13	1:66:A:CYS:HA	2	0.68
(1,243)	1:53:A:MET:HA	1:63:A:LEU:HA	1	0.68
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	4	0.67
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	8	0.67
(1,803)	1:98:A:THR:HG21	1:100:A:HIS:HE1	4	0.67
(1,803)	1:98:A:THR:HG22	1:100:A:HIS:HE1	4	0.67
(1,803)	1:98:A:THR:HG23	1:100:A:HIS:HE1	4	0.67
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	5	0.67
(1,636)	1:82:A:LYS:HD2	1:88:A:CYS:H	7	0.67
(1,636)	1:82:A:LYS:HD3	1:88:A:CYS:H	7	0.67
(1,81)	1:15:A:CYS:HB2	1:45:A:SER:HA	3	0.67
(1,81)	1:15:A:CYS:HB3	1:45:A:SER:HA	3	0.67
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG11	6	0.67
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG12	6	0.67
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG13	6	0.67
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB2	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB3	3	0.66
(1,935)	1:61:A:VAL:HB	1:62:A:ALA:H	2	0.66
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	10	0.66
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	2	0.66
(1,727)	1:89:A:VAL:HG21	1:95:A:TRP:HH2	5	0.66
(1,727)	1:89:A:VAL:HG22	1:95:A:TRP:HH2	5	0.66
(1,727)	1:89:A:VAL:HG23	1:95:A:TRP:HH2	5	0.66
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB2	3	0.66
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB3	3	0.66
(1,329)	1:61:A:VAL:HB	1:62:A:ALA:H	2	0.66
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	9	0.66
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	8	0.65
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	3	0.65
(1,865)	1:30:A:THR:H	1:54:A:VAL:HB	4	0.65
(1,794)	1:98:A:THR:HG21	1:99:A:ASP:HA	8	0.65
(1,794)	1:98:A:THR:HG22	1:99:A:ASP:HA	8	0.65
(1,794)	1:98:A:THR:HG23	1:99:A:ASP:HA	8	0.65
(1,687)	1:88:A:CYS:HA	1:95:A:TRP:HA	1	0.65
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG21	2	0.65
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG22	2	0.65
(1,541)	1:79:A:GLU:H	1:89:A:VAL:HG23	2	0.65
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	8	0.65
(1,338)	1:61:A:VAL:HG21	1:65:A:ARG:HD2	7	0.65
(1,338)	1:61:A:VAL:HG21	1:65:A:ARG:HD3	7	0.65
(1,338)	1:61:A:VAL:HG22	1:65:A:ARG:HD2	7	0.65
(1,338)	1:61:A:VAL:HG22	1:65:A:ARG:HD3	7	0.65
(1,338)	1:61:A:VAL:HG23	1:65:A:ARG:HD2	7	0.65
(1,338)	1:61:A:VAL:HG23	1:65:A:ARG:HD3	7	0.65
(1,237)	1:53:A:MET:HA	1:62:A:ALA:HA	9	0.65
(1,144)	1:30:A:THR:H	1:54:A:VAL:HB	4	0.65
(1,55)	1:12:A:LYS:HA	1:48:A:LEU:HG	3	0.65
(1,1175)	1:102:A:CYS:H	1:103:A:ASP:H	8	0.64
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE1	3	0.64
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE2	3	0.64
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE1	4	0.64
(1,1002)	1:74:A:GLU:H	1:75:A:TYR:HE2	4	0.64
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD21	4	0.64
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD22	4	0.64
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD23	4	0.64
(1,794)	1:98:A:THR:HG21	1:99:A:ASP:HA	6	0.64
(1,794)	1:98:A:THR:HG22	1:99:A:ASP:HA	6	0.64
(1,794)	1:98:A:THR:HG23	1:99:A:ASP:HA	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:88:A:CYS:HB2	1:97:A:CYS:HA	10	0.64
(1,700)	1:88:A:CYS:HB3	1:97:A:CYS:HA	10	0.64
(1,600)	1:81:A:VAL:HG21	1:87:A:THR:HB	10	0.64
(1,600)	1:81:A:VAL:HG22	1:87:A:THR:HB	10	0.64
(1,600)	1:81:A:VAL:HG23	1:87:A:THR:HB	10	0.64
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE1	3	0.64
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE2	3	0.64
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE1	4	0.64
(1,471)	1:74:A:GLU:H	1:75:A:TYR:HE2	4	0.64
(1,409)	1:69:A:PHE:HA	1:74:A:GLU:HA	8	0.64
(1,286)	1:56:A:HIS:HD2	1:57:A:GLU:HG2	9	0.64
(1,286)	1:56:A:HIS:HD2	1:57:A:GLU:HG3	9	0.64
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	7	0.64
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	7	0.64
(1,89)	1:16:A:PRO:HG2	1:20:A:LEU:HD21	5	0.64
(1,89)	1:16:A:PRO:HG2	1:20:A:LEU:HD22	5	0.64
(1,89)	1:16:A:PRO:HG2	1:20:A:LEU:HD23	5	0.64
(1,89)	1:16:A:PRO:HG3	1:20:A:LEU:HD21	5	0.64
(1,89)	1:16:A:PRO:HG3	1:20:A:LEU:HD22	5	0.64
(1,89)	1:16:A:PRO:HG3	1:20:A:LEU:HD23	5	0.64
(1,84)	1:16:A:PRO:HG2	1:19:A:ASN:HB2	2	0.64
(1,84)	1:16:A:PRO:HG2	1:19:A:ASN:HB3	2	0.64
(1,84)	1:16:A:PRO:HG3	1:19:A:ASN:HB2	2	0.64
(1,84)	1:16:A:PRO:HG3	1:19:A:ASN:HB3	2	0.64
(1,552)	1:80:A:THR:HA	1:88:A:CYS:H	2	0.63
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB1	8	0.63
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB2	8	0.63
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB3	8	0.63
(1,1160)	1:98:A:THR:HB	1:99:A:ASP:H	9	0.62
(1,794)	1:98:A:THR:HG21	1:99:A:ASP:HA	3	0.62
(1,794)	1:98:A:THR:HG22	1:99:A:ASP:HA	3	0.62
(1,794)	1:98:A:THR:HG23	1:99:A:ASP:HA	3	0.62
(1,792)	1:98:A:THR:HB	1:99:A:ASP:H	9	0.62
(1,734)	1:89:A:VAL:HG11	1:96:A:ASN:H	5	0.62
(1,734)	1:89:A:VAL:HG12	1:96:A:ASN:H	5	0.62
(1,734)	1:89:A:VAL:HG13	1:96:A:ASN:H	5	0.62
(1,692)	1:88:A:CYS:HA	1:96:A:ASN:HA	8	0.62
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG21	5	0.62
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG22	5	0.62
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG23	5	0.62
(1,423)	1:69:A:PHE:HA	1:95:A:TRP:HZ2	5	0.62
(1,1175)	1:102:A:CYS:H	1:103:A:ASP:H	3	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	6	0.61
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG2	5	0.61
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG3	5	0.61
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	7	0.61
(1,692)	1:88:A:CYS:HA	1:96:A:ASN:HA	10	0.61
(1,604)	1:81:A:VAL:HA	1:88:A:CYS:H	3	0.61
(1,245)	1:53:A:MET:HG2	1:63:A:LEU:H	2	0.61
(1,245)	1:53:A:MET:HG3	1:63:A:LEU:H	2	0.61
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD21	2	0.61
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD22	2	0.61
(1,110)	1:28:A:THR:HB	1:48:A:LEU:HD23	2	0.61
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	2	0.6
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD21	7	0.6
(1,1151)	1:94:A:LYS:H	1:96:A:ASN:HD22	7	0.6
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	2	0.6
(1,1076)	1:85:A:CYS:H	1:86:A:ASN:H	9	0.6
(1,1060)	1:81:A:VAL:H	1:89:A:VAL:HA	3	0.6
(1,865)	1:30:A:THR:H	1:54:A:VAL:HB	10	0.6
(1,736)	1:89:A:VAL:HG11	1:96:A:ASN:HA	8	0.6
(1,736)	1:89:A:VAL:HG12	1:96:A:ASN:HA	8	0.6
(1,736)	1:89:A:VAL:HG13	1:96:A:ASN:HA	8	0.6
(1,617)	1:81:A:VAL:HG21	1:95:A:TRP:HZ2	6	0.6
(1,617)	1:81:A:VAL:HG22	1:95:A:TRP:HZ2	6	0.6
(1,617)	1:81:A:VAL:HG23	1:95:A:TRP:HZ2	6	0.6
(1,600)	1:81:A:VAL:HG21	1:87:A:THR:HB	4	0.6
(1,600)	1:81:A:VAL:HG22	1:87:A:THR:HB	4	0.6
(1,600)	1:81:A:VAL:HG23	1:87:A:THR:HB	4	0.6
(1,564)	1:80:A:THR:HA	1:90:A:CYS:H	7	0.6
(1,498)	1:75:A:TYR:HD1	1:95:A:TRP:HH2	5	0.6
(1,498)	1:75:A:TYR:HD2	1:95:A:TRP:HH2	5	0.6
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG2	8	0.6
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG3	8	0.6
(1,176)	1:32:A:GLN:HA	1:69:A:PHE:HZ	1	0.6
(1,173)	1:32:A:GLN:HG2	1:33:A:ASN:HA	9	0.6
(1,173)	1:32:A:GLN:HG3	1:33:A:ASN:HA	9	0.6
(1,144)	1:30:A:THR:H	1:54:A:VAL:HB	10	0.6
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB2	1	0.6
(1,75)	1:14:A:VAL:HG11	1:45:A:SER:HB3	1	0.6
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB2	1	0.6
(1,75)	1:14:A:VAL:HG12	1:45:A:SER:HB3	1	0.6
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB2	1	0.6
(1,75)	1:14:A:VAL:HG13	1:45:A:SER:HB3	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:12:A:LYS:HB2	1:47:A:CYS:HA	2	0.6
(1,51)	1:12:A:LYS:HB3	1:47:A:CYS:HA	2	0.6
(1,13)	1:10:A:MET:HE1	1:47:A:CYS:HA	4	0.6
(1,13)	1:10:A:MET:HE2	1:47:A:CYS:HA	4	0.6
(1,13)	1:10:A:MET:HE3	1:47:A:CYS:HA	4	0.6
(1,4)	1:53:A:MET:HE1	1:61:A:VAL:HA	7	0.6
(1,4)	1:53:A:MET:HE2	1:61:A:VAL:HA	7	0.6
(1,4)	1:53:A:MET:HE3	1:61:A:VAL:HA	7	0.6
(1,1122)	1:90:A:CYS:H	1:95:A:TRP:HZ3	4	0.59
(1,1076)	1:85:A:CYS:H	1:86:A:ASN:H	6	0.59
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	7	0.59
(1,968)	1:68:A:CYS:HA	1:95:A:TRP:HE1	10	0.59
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	7	0.59
(1,379)	1:66:A:CYS:HB2	1:93:A:ARG:HA	9	0.59
(1,379)	1:66:A:CYS:HB3	1:93:A:ARG:HA	9	0.59
(1,200)	1:34:A:TYR:HE1	1:63:A:LEU:HD11	5	0.59
(1,200)	1:34:A:TYR:HE1	1:63:A:LEU:HD12	5	0.59
(1,200)	1:34:A:TYR:HE1	1:63:A:LEU:HD13	5	0.59
(1,200)	1:34:A:TYR:HE2	1:63:A:LEU:HD11	5	0.59
(1,200)	1:34:A:TYR:HE2	1:63:A:LEU:HD12	5	0.59
(1,200)	1:34:A:TYR:HE2	1:63:A:LEU:HD13	5	0.59
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG2	9	0.59
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG3	9	0.59
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG2	8	0.59
(1,137)	1:30:A:THR:H	1:32:A:GLN:HG3	8	0.59
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG11	10	0.59
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG12	10	0.59
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG13	10	0.59
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG11	10	0.59
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG12	10	0.59
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG13	10	0.59
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG11	10	0.59
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG12	10	0.59
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG13	10	0.59
(1,1054)	1:81:A:VAL:H	1:87:A:THR:HA	10	0.58
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD11	4	0.58
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD12	4	0.58
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD13	4	0.58
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD2	10	0.58
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD3	10	0.58
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD2	10	0.58
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD3	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:56:A:HIS:HE1	1:69:A:PHE:HZ	7	0.58
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD11	5	0.58
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD12	5	0.58
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD13	5	0.58
(1,149)	1:30:A:THR:HB	1:54:A:VAL:HB	2	0.58
(1,1162)	1:98:A:THR:HA	1:100:A:HIS:H	10	0.57
(1,1109)	1:89:A:VAL:H	1:96:A:ASN:H	8	0.57
(1,1028)	1:78:A:GLY:H	1:90:A:CYS:H	9	0.57
(1,609)	1:81:A:VAL:HG21	1:88:A:CYS:HB2	7	0.57
(1,609)	1:81:A:VAL:HG21	1:88:A:CYS:HB3	7	0.57
(1,609)	1:81:A:VAL:HG22	1:88:A:CYS:HB2	7	0.57
(1,609)	1:81:A:VAL:HG22	1:88:A:CYS:HB3	7	0.57
(1,609)	1:81:A:VAL:HG23	1:88:A:CYS:HB2	7	0.57
(1,609)	1:81:A:VAL:HG23	1:88:A:CYS:HB3	7	0.57
(1,52)	1:12:A:LYS:HG2	1:47:A:CYS:HA	6	0.57
(1,52)	1:12:A:LYS:HG3	1:47:A:CYS:HA	6	0.57
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB2	8	0.57
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB3	8	0.57
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB2	8	0.57
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB3	8	0.57
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB2	8	0.57
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB3	8	0.57
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	2	0.56
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	9	0.56
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	2	0.56
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD2	7	0.56
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD3	7	0.56
(1,281)	1:55:A:ARG:HA	1:61:A:VAL:H	10	0.56
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD2	2	0.56
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD3	2	0.56
(1,1174)	1:101:A:VAL:HG11	1:103:A:ASP:H	7	0.55
(1,1174)	1:101:A:VAL:HG12	1:103:A:ASP:H	7	0.55
(1,1174)	1:101:A:VAL:HG13	1:103:A:ASP:H	7	0.55
(1,1123)	1:90:A:CYS:HA	1:96:A:ASN:H	5	0.55
(1,1099)	1:88:A:CYS:H	1:98:A:THR:H	5	0.55
(1,818)	1:101:A:VAL:HG11	1:103:A:ASP:H	7	0.55
(1,818)	1:101:A:VAL:HG12	1:103:A:ASP:H	7	0.55
(1,818)	1:101:A:VAL:HG13	1:103:A:ASP:H	7	0.55
(1,750)	1:90:A:CYS:HA	1:96:A:ASN:H	5	0.55
(1,383)	1:67:A:PRO:HG2	1:69:A:PHE:HE1	10	0.55
(1,383)	1:67:A:PRO:HG2	1:69:A:PHE:HE2	10	0.55
(1,383)	1:67:A:PRO:HG3	1:69:A:PHE:HE1	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:67:A:PRO:HG3	1:69:A:PHE:HE2	10	0.55
(1,379)	1:66:A:CYS:HB2	1:93:A:ARG:HA	3	0.55
(1,379)	1:66:A:CYS:HB3	1:93:A:ARG:HA	3	0.55
(1,359)	1:63:A:LEU:HA	1:66:A:CYS:H	2	0.55
(1,359)	1:63:A:LEU:HA	1:66:A:CYS:H	4	0.55
(1,253)	1:54:A:VAL:HG21	1:61:A:VAL:HB	3	0.55
(1,253)	1:54:A:VAL:HG22	1:61:A:VAL:HB	3	0.55
(1,253)	1:54:A:VAL:HG23	1:61:A:VAL:HB	3	0.55
(1,3)	1:53:A:MET:HE1	1:60:A:CYS:HA	7	0.55
(1,3)	1:53:A:MET:HE2	1:60:A:CYS:HA	7	0.55
(1,3)	1:53:A:MET:HE3	1:60:A:CYS:HA	7	0.55
(1,1110)	1:89:A:VAL:H	1:96:A:ASN:HB2	4	0.54
(1,1110)	1:89:A:VAL:H	1:96:A:ASN:HB3	4	0.54
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	3	0.54
(1,979)	1:69:A:PHE:H	1:95:A:TRP:HD1	3	0.54
(1,793)	1:98:A:THR:HB	1:99:A:ASP:HA	9	0.54
(1,730)	1:89:A:VAL:H	1:96:A:ASN:HB2	4	0.54
(1,730)	1:89:A:VAL:H	1:96:A:ASN:HB3	4	0.54
(1,564)	1:80:A:THR:HA	1:90:A:CYS:H	5	0.54
(1,558)	1:80:A:THR:HA	1:89:A:VAL:HA	7	0.54
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG21	10	0.54
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG22	10	0.54
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG23	10	0.54
(1,421)	1:69:A:PHE:H	1:95:A:TRP:HD1	3	0.54
(1,281)	1:55:A:ARG:HA	1:61:A:VAL:H	9	0.54
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	6	0.54
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	6	0.54
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	6	0.54
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	6	0.54
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	6	0.54
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	6	0.54
(1,835)	1:13:A:LEU:H	1:46:A:GLY:H	5	0.53
(1,802)	1:98:A:THR:HG21	1:100:A:HIS:HD2	6	0.53
(1,802)	1:98:A:THR:HG22	1:100:A:HIS:HD2	6	0.53
(1,802)	1:98:A:THR:HG23	1:100:A:HIS:HD2	6	0.53
(1,621)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	7	0.53
(1,621)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	7	0.53
(1,621)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	7	0.53
(1,621)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	10	0.53
(1,621)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	10	0.53
(1,621)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	10	0.53
(1,327)	1:61:A:VAL:HB	1:62:A:ALA:HA	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE1	8	0.53
(1,303)	1:56:A:HIS:HE1	1:69:A:PHE:HE2	8	0.53
(1,261)	1:54:A:VAL:HG21	1:63:A:LEU:H	4	0.53
(1,261)	1:54:A:VAL:HG22	1:63:A:LEU:H	4	0.53
(1,261)	1:54:A:VAL:HG23	1:63:A:LEU:H	4	0.53
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG11	4	0.53
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG12	4	0.53
(1,189)	1:34:A:TYR:H	1:54:A:VAL:HG13	4	0.53
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG2	4	0.53
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG3	4	0.53
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG21	8	0.52
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG22	8	0.52
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG23	8	0.52
(1,793)	1:98:A:THR:HB	1:99:A:ASP:HA	5	0.52
(1,692)	1:88:A:CYS:HA	1:96:A:ASN:HA	4	0.52
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG21	8	0.52
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG22	8	0.52
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG23	8	0.52
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	4	0.52
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	4	0.52
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG2	8	0.52
(1,417)	1:69:A:PHE:HZ	1:74:A:GLU:HG3	8	0.52
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG21	2	0.52
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG22	2	0.52
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG23	2	0.52
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA2	7	0.52
(1,62)	1:13:A:LEU:HD21	1:46:A:GLY:HA3	7	0.52
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA2	7	0.52
(1,62)	1:13:A:LEU:HD22	1:46:A:GLY:HA3	7	0.52
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA2	7	0.52
(1,62)	1:13:A:LEU:HD23	1:46:A:GLY:HA3	7	0.52
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG21	5	0.52
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG22	5	0.52
(1,26)	1:10:A:MET:HA	1:11:A:VAL:HG23	5	0.52
(1,1130)	1:91:A:ARG:HA	1:93:A:ARG:H	2	0.51
(1,974)	1:69:A:PHE:HA	1:73:A:LYS:H	2	0.51
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	4	0.51
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD11	7	0.51
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD12	7	0.51
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD13	7	0.51
(1,794)	1:98:A:THR:HG21	1:99:A:ASP:HA	2	0.51
(1,794)	1:98:A:THR:HG22	1:99:A:ASP:HA	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:98:A:THR:HG23	1:99:A:ASP:HA	2	0.51
(1,756)	1:91:A:ARG:HA	1:93:A:ARG:H	2	0.51
(1,640)	1:83:A:ILE:H	1:87:A:THR:HB	7	0.51
(1,499)	1:75:A:TYR:HE1	1:95:A:TRP:HH2	1	0.51
(1,499)	1:75:A:TYR:HE2	1:95:A:TRP:HH2	1	0.51
(1,408)	1:69:A:PHE:HA	1:73:A:LYS:H	2	0.51
(1,327)	1:61:A:VAL:HB	1:62:A:ALA:HA	5	0.51
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	4	0.51
(1,35)	1:11:A:VAL:HG11	1:47:A:CYS:HA	7	0.51
(1,35)	1:11:A:VAL:HG12	1:47:A:CYS:HA	7	0.51
(1,35)	1:11:A:VAL:HG13	1:47:A:CYS:HA	7	0.51
(1,5)	1:53:A:MET:HE1	1:61:A:VAL:H	2	0.51
(1,5)	1:53:A:MET:HE2	1:61:A:VAL:H	2	0.51
(1,5)	1:53:A:MET:HE3	1:61:A:VAL:H	2	0.51
(1,1163)	1:98:A:THR:HB	1:100:A:HIS:H	7	0.5
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	6	0.5
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD1	3	0.5
(1,986)	1:70:A:HIS:H	1:75:A:TYR:HD2	3	0.5
(1,862)	1:30:A:THR:H	1:33:A:ASN:HD21	3	0.5
(1,862)	1:30:A:THR:H	1:33:A:ASN:HD22	3	0.5
(1,628)	1:82:A:LYS:HA	1:87:A:THR:HA	9	0.5
(1,427)	1:70:A:HIS:HA	1:73:A:LYS:HB2	4	0.5
(1,427)	1:70:A:HIS:HA	1:73:A:LYS:HB3	4	0.5
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB1	10	0.5
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB2	10	0.5
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB3	10	0.5
(1,327)	1:61:A:VAL:HB	1:62:A:ALA:HA	2	0.5
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG11	3	0.5
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG12	3	0.5
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG13	3	0.5
(1,81)	1:15:A:CYS:HB2	1:45:A:SER:HA	1	0.5
(1,81)	1:15:A:CYS:HB3	1:45:A:SER:HA	1	0.5
(1,38)	1:11:A:VAL:HB	1:48:A:LEU:H	6	0.5
(1,1171)	1:101:A:VAL:HB	1:102:A:CYS:H	8	0.49
(1,1152)	1:94:A:LYS:HG2	1:96:A:ASN:HD21	6	0.49
(1,1152)	1:94:A:LYS:HG2	1:96:A:ASN:HD22	6	0.49
(1,1152)	1:94:A:LYS:HG3	1:96:A:ASN:HD21	6	0.49
(1,1152)	1:94:A:LYS:HG3	1:96:A:ASN:HD22	6	0.49
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	8	0.49
(1,840)	1:14:A:VAL:HA	1:46:A:GLY:H	7	0.49
(1,628)	1:82:A:LYS:HA	1:87:A:THR:HA	3	0.49
(1,608)	1:81:A:VAL:HG11	1:88:A:CYS:HB2	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:81:A:VAL:HG11	1:88:A:CYS:HB3	6	0.49
(1,608)	1:81:A:VAL:HG12	1:88:A:CYS:HB2	6	0.49
(1,608)	1:81:A:VAL:HG12	1:88:A:CYS:HB3	6	0.49
(1,608)	1:81:A:VAL:HG13	1:88:A:CYS:HB2	6	0.49
(1,608)	1:81:A:VAL:HG13	1:88:A:CYS:HB3	6	0.49
(1,558)	1:80:A:THR:HA	1:89:A:VAL:HA	9	0.49
(1,261)	1:54:A:VAL:HG21	1:63:A:LEU:H	10	0.49
(1,261)	1:54:A:VAL:HG22	1:63:A:LEU:H	10	0.49
(1,261)	1:54:A:VAL:HG23	1:63:A:LEU:H	10	0.49
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD11	7	0.49
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD12	7	0.49
(1,111)	1:28:A:THR:HB	1:48:A:LEU:HD13	7	0.49
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB2	5	0.49
(1,107)	1:22:A:ALA:HB1	1:43:A:CYS:HB3	5	0.49
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB2	5	0.49
(1,107)	1:22:A:ALA:HB2	1:43:A:CYS:HB3	5	0.49
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB2	5	0.49
(1,107)	1:22:A:ALA:HB3	1:43:A:CYS:HB3	5	0.49
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA2	1	0.49
(1,61)	1:13:A:LEU:HD11	1:46:A:GLY:HA3	1	0.49
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA2	1	0.49
(1,61)	1:13:A:LEU:HD12	1:46:A:GLY:HA3	1	0.49
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA2	1	0.49
(1,61)	1:13:A:LEU:HD13	1:46:A:GLY:HA3	1	0.49
(1,1163)	1:98:A:THR:HB	1:100:A:HIS:H	9	0.48
(1,1107)	1:89:A:VAL:H	1:95:A:TRP:HE3	6	0.48
(1,1066)	1:82:A:LYS:HG2	1:83:A:ILE:H	10	0.48
(1,1066)	1:82:A:LYS:HG3	1:83:A:ILE:H	10	0.48
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	9	0.48
(1,845)	1:17:A:ALA:H	1:18:A:ASP:HA	4	0.48
(1,736)	1:89:A:VAL:HG11	1:96:A:ASN:HA	5	0.48
(1,736)	1:89:A:VAL:HG12	1:96:A:ASN:HA	5	0.48
(1,736)	1:89:A:VAL:HG13	1:96:A:ASN:HA	5	0.48
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	9	0.48
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG21	3	0.48
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG22	3	0.48
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG23	3	0.48
(1,333)	1:61:A:VAL:HB	1:65:A:ARG:HA	8	0.48
(1,1045)	1:80:A:THR:H	1:89:A:VAL:HA	4	0.47
(1,670)	1:87:A:THR:HB	1:88:A:CYS:H	9	0.47
(1,554)	1:80:A:THR:H	1:89:A:VAL:HA	4	0.47
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG11	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG12	1	0.47
(1,540)	1:79:A:GLU:H	1:89:A:VAL:HG13	1	0.47
(1,379)	1:66:A:CYS:HB2	1:93:A:ARG:HA	8	0.47
(1,379)	1:66:A:CYS:HB3	1:93:A:ARG:HA	8	0.47
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG2	2	0.47
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG3	2	0.47
(1,134)	1:30:A:THR:HB	1:31:A:CYS:HA	7	0.47
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG11	10	0.47
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG12	10	0.47
(1,129)	1:29:A:LYS:HG2	1:54:A:VAL:HG13	10	0.47
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG11	10	0.47
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG12	10	0.47
(1,129)	1:29:A:LYS:HG3	1:54:A:VAL:HG13	10	0.47
(1,1160)	1:98:A:THR:HB	1:99:A:ASP:H	10	0.46
(1,1142)	1:92:A:ASP:HA	1:94:A:LYS:H	4	0.46
(1,1116)	1:89:A:VAL:H	1:98:A:THR:H	3	0.46
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	7	0.46
(1,1060)	1:81:A:VAL:H	1:89:A:VAL:HA	9	0.46
(1,1044)	1:80:A:THR:HA	1:88:A:CYS:H	1	0.46
(1,984)	1:70:A:HIS:H	1:74:A:GLU:HA	8	0.46
(1,792)	1:98:A:THR:HB	1:99:A:ASP:H	10	0.46
(1,747)	1:90:A:CYS:HA	1:95:A:TRP:HA	8	0.46
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	7	0.46
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	2	0.46
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	2	0.46
(1,557)	1:80:A:THR:HA	1:89:A:VAL:HB	8	0.46
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG21	2	0.46
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG22	2	0.46
(1,542)	1:79:A:GLU:HA	1:89:A:VAL:HG23	2	0.46
(1,539)	1:79:A:GLU:H	1:89:A:VAL:HA	2	0.46
(1,490)	1:75:A:TYR:HE1	1:81:A:VAL:HA	4	0.46
(1,490)	1:75:A:TYR:HE2	1:81:A:VAL:HA	4	0.46
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	6	0.46
(1,361)	1:63:A:LEU:HD11	1:93:A:ARG:HD2	10	0.46
(1,361)	1:63:A:LEU:HD11	1:93:A:ARG:HD3	10	0.46
(1,361)	1:63:A:LEU:HD12	1:93:A:ARG:HD2	10	0.46
(1,361)	1:63:A:LEU:HD12	1:93:A:ARG:HD3	10	0.46
(1,361)	1:63:A:LEU:HD13	1:93:A:ARG:HD2	10	0.46
(1,361)	1:63:A:LEU:HD13	1:93:A:ARG:HD3	10	0.46
(1,245)	1:53:A:MET:HG2	1:63:A:LEU:H	6	0.46
(1,245)	1:53:A:MET:HG3	1:63:A:LEU:H	6	0.46
(1,1111)	1:89:A:VAL:HB	1:96:A:ASN:H	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	9	0.45
(1,1090)	1:87:A:THR:HB	1:98:A:THR:H	8	0.45
(1,860)	1:30:A:THR:HB	1:31:A:CYS:H	9	0.45
(1,732)	1:89:A:VAL:HB	1:96:A:ASN:H	1	0.45
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	9	0.45
(1,666)	1:86:A:ASN:HD21	1:100:A:HIS:HB2	8	0.45
(1,666)	1:86:A:ASN:HD21	1:100:A:HIS:HB3	8	0.45
(1,666)	1:86:A:ASN:HD22	1:100:A:HIS:HB2	8	0.45
(1,666)	1:86:A:ASN:HD22	1:100:A:HIS:HB3	8	0.45
(1,600)	1:81:A:VAL:HG21	1:87:A:THR:HB	9	0.45
(1,600)	1:81:A:VAL:HG22	1:87:A:THR:HB	9	0.45
(1,600)	1:81:A:VAL:HG23	1:87:A:THR:HB	9	0.45
(1,369)	1:64:A:GLU:HG2	1:65:A:ARG:H	8	0.45
(1,369)	1:64:A:GLU:HG3	1:65:A:ARG:H	8	0.45
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD2	4	0.45
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD3	4	0.45
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD21	2	0.45
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD22	2	0.45
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD23	2	0.45
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD21	2	0.45
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD22	2	0.45
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD23	2	0.45
(1,135)	1:30:A:THR:HB	1:31:A:CYS:H	9	0.45
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG11	10	0.45
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG12	10	0.45
(1,48)	1:12:A:LYS:HG2	1:14:A:VAL:HG13	10	0.45
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG11	10	0.45
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG12	10	0.45
(1,48)	1:12:A:LYS:HG3	1:14:A:VAL:HG13	10	0.45
(1,1123)	1:90:A:CYS:HA	1:96:A:ASN:H	8	0.44
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	2	0.44
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB2	9	0.44
(1,1038)	1:79:A:GLU:H	1:90:A:CYS:HB3	9	0.44
(1,750)	1:90:A:CYS:HA	1:96:A:ASN:H	8	0.44
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB2	9	0.44
(1,543)	1:79:A:GLU:H	1:90:A:CYS:HB3	9	0.44
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB2	8	0.44
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB3	8	0.44
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	3	0.43
(1,1142)	1:92:A:ASP:HA	1:94:A:LYS:H	9	0.43
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	9	0.43
(1,1063)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	7	0.43
(1,1063)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	7	0.43
(1,1063)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	10	0.43
(1,1063)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	10	0.43
(1,1063)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	10	0.43
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG21	1	0.43
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG22	1	0.43
(1,1055)	1:81:A:VAL:H	1:87:A:THR:HG23	1	0.43
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	5	0.43
(1,866)	1:30:A:THR:HA	1:55:A:ARG:H	5	0.43
(1,858)	1:29:A:LYS:HB2	1:34:A:TYR:H	3	0.43
(1,858)	1:29:A:LYS:HB3	1:34:A:TYR:H	3	0.43
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	3	0.43
(1,670)	1:87:A:THR:HB	1:88:A:CYS:H	4	0.43
(1,604)	1:81:A:VAL:HA	1:88:A:CYS:H	2	0.43
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG21	1	0.43
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG22	1	0.43
(1,597)	1:81:A:VAL:H	1:87:A:THR:HG23	1	0.43
(1,576)	1:81:A:VAL:HB	1:82:A:LYS:HA	7	0.43
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG21	5	0.43
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG22	5	0.43
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG23	5	0.43
(1,152)	1:30:A:THR:HA	1:55:A:ARG:H	5	0.43
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	1	0.42
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	3	0.42
(1,967)	1:68:A:CYS:H	1:75:A:TYR:H	8	0.42
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG2	3	0.42
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG3	3	0.42
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD2	3	0.42
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD3	3	0.42
(1,802)	1:98:A:THR:HG21	1:100:A:HIS:HD2	8	0.42
(1,802)	1:98:A:THR:HG22	1:100:A:HIS:HD2	8	0.42
(1,802)	1:98:A:THR:HG23	1:100:A:HIS:HD2	8	0.42
(1,670)	1:87:A:THR:HB	1:88:A:CYS:H	2	0.42
(1,576)	1:81:A:VAL:HB	1:82:A:LYS:HA	4	0.42
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	1	0.42
(1,460)	1:73:A:LYS:HG2	1:74:A:GLU:H	10	0.42
(1,460)	1:73:A:LYS:HG3	1:74:A:GLU:H	10	0.42
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB1	2	0.42
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB2	2	0.42
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB3	2	0.42
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD21	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:29:A:LYS:HA	1:33:A:ASN:HD22	5	0.42
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	8	0.41
(1,1136)	1:91:A:ARG:H	1:96:A:ASN:H	10	0.41
(1,1114)	1:89:A:VAL:H	1:97:A:CYS:HA	3	0.41
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	2	0.41
(1,983)	1:70:A:HIS:H	1:74:A:GLU:H	8	0.41
(1,793)	1:98:A:THR:HB	1:99:A:ASP:HA	10	0.41
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	8	0.41
(1,738)	1:89:A:VAL:H	1:97:A:CYS:HA	3	0.41
(1,692)	1:88:A:CYS:HA	1:96:A:ASN:HA	1	0.41
(1,625)	1:82:A:LYS:HA	1:83:A:ILE:HB	5	0.41
(1,348)	1:61:A:VAL:HG21	1:63:A:LEU:HA	7	0.41
(1,348)	1:61:A:VAL:HG22	1:63:A:LEU:HA	7	0.41
(1,348)	1:61:A:VAL:HG23	1:63:A:LEU:HA	7	0.41
(1,149)	1:30:A:THR:HB	1:54:A:VAL:HB	5	0.41
(1,1094)	1:88:A:CYS:H	1:95:A:TRP:HE3	8	0.4
(1,958)	1:66:A:CYS:HB2	1:93:A:ARG:H	8	0.4
(1,958)	1:66:A:CYS:HB3	1:93:A:ARG:H	8	0.4
(1,827)	1:11:A:VAL:HB	1:12:A:LYS:H	8	0.4
(1,689)	1:88:A:CYS:HB2	1:95:A:TRP:HA	4	0.4
(1,689)	1:88:A:CYS:HB3	1:95:A:TRP:HA	4	0.4
(1,686)	1:88:A:CYS:H	1:95:A:TRP:HE3	8	0.4
(1,616)	1:81:A:VAL:HG11	1:95:A:TRP:HZ2	10	0.4
(1,616)	1:81:A:VAL:HG12	1:95:A:TRP:HZ2	10	0.4
(1,616)	1:81:A:VAL:HG13	1:95:A:TRP:HZ2	10	0.4
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG21	4	0.4
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG22	4	0.4
(1,548)	1:80:A:THR:HB	1:81:A:VAL:HG23	4	0.4
(1,420)	1:69:A:PHE:HA	1:75:A:TYR:H	1	0.4
(1,252)	1:54:A:VAL:HG21	1:61:A:VAL:HG11	8	0.4
(1,252)	1:54:A:VAL:HG21	1:61:A:VAL:HG12	8	0.4
(1,252)	1:54:A:VAL:HG21	1:61:A:VAL:HG13	8	0.4
(1,252)	1:54:A:VAL:HG22	1:61:A:VAL:HG11	8	0.4
(1,252)	1:54:A:VAL:HG22	1:61:A:VAL:HG12	8	0.4
(1,252)	1:54:A:VAL:HG22	1:61:A:VAL:HG13	8	0.4
(1,252)	1:54:A:VAL:HG23	1:61:A:VAL:HG11	8	0.4
(1,252)	1:54:A:VAL:HG23	1:61:A:VAL:HG12	8	0.4
(1,252)	1:54:A:VAL:HG23	1:61:A:VAL:HG13	8	0.4
(1,81)	1:15:A:CYS:HB2	1:45:A:SER:HA	7	0.4
(1,81)	1:15:A:CYS:HB3	1:45:A:SER:HA	7	0.4
(1,1171)	1:101:A:VAL:HB	1:102:A:CYS:H	10	0.39
(1,1132)	1:91:A:ARG:H	1:94:A:LYS:H	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:79:A:GLU:H	1:89:A:VAL:HG11	10	0.39
(1,1036)	1:79:A:GLU:H	1:89:A:VAL:HG12	10	0.39
(1,1036)	1:79:A:GLU:H	1:89:A:VAL:HG13	10	0.39
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	7	0.39
(1,935)	1:61:A:VAL:HB	1:62:A:ALA:H	4	0.39
(1,687)	1:88:A:CYS:HA	1:95:A:TRP:HA	2	0.39
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	6	0.39
(1,420)	1:69:A:PHE:HA	1:75:A:TYR:H	5	0.39
(1,329)	1:61:A:VAL:HB	1:62:A:ALA:H	4	0.39
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG21	5	0.39
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG22	5	0.39
(1,295)	1:56:A:HIS:H	1:61:A:VAL:HG23	5	0.39
(1,118)	1:29:A:LYS:HA	1:34:A:TYR:HA	3	0.39
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB1	9	0.39
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB2	9	0.39
(1,79)	1:15:A:CYS:HB2	1:22:A:ALA:HB3	9	0.39
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB1	9	0.39
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB2	9	0.39
(1,79)	1:15:A:CYS:HB3	1:22:A:ALA:HB3	9	0.39
(1,57)	1:13:A:LEU:HA	1:14:A:VAL:HB	7	0.39
(1,11)	1:53:A:MET:HE1	1:63:A:LEU:H	9	0.39
(1,11)	1:53:A:MET:HE2	1:63:A:LEU:H	9	0.39
(1,11)	1:53:A:MET:HE3	1:63:A:LEU:H	9	0.39
(1,1176)	1:102:A:CYS:HA	1:103:A:ASP:H	2	0.38
(1,1171)	1:101:A:VAL:HB	1:102:A:CYS:H	5	0.38
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	5	0.38
(1,1130)	1:91:A:ARG:HA	1:93:A:ARG:H	3	0.38
(1,1062)	1:81:A:VAL:H	1:95:A:TRP:HZ3	1	0.38
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	5	0.38
(1,836)	1:13:A:LEU:H	1:47:A:CYS:HA	6	0.38
(1,819)	1:102:A:CYS:HA	1:103:A:ASP:H	2	0.38
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	5	0.38
(1,756)	1:91:A:ARG:HA	1:93:A:ARG:H	3	0.38
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	9	0.38
(1,2)	1:53:A:MET:HE1	1:54:A:VAL:H	10	0.38
(1,2)	1:53:A:MET:HE2	1:54:A:VAL:H	10	0.38
(1,2)	1:53:A:MET:HE3	1:54:A:VAL:H	10	0.38
(1,1142)	1:92:A:ASP:HA	1:94:A:LYS:H	7	0.37
(1,1071)	1:83:A:ILE:H	1:88:A:CYS:H	5	0.37
(1,853)	1:22:A:ALA:HA	1:23:A:GLU:H	5	0.37
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD21	10	0.37
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD22	10	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD23	10	0.37
(1,845)	1:17:A:ALA:H	1:18:A:ASP:HA	6	0.37
(1,642)	1:83:A:ILE:HB	1:88:A:CYS:HB2	8	0.37
(1,642)	1:83:A:ILE:HB	1:88:A:CYS:HB3	8	0.37
(1,628)	1:82:A:LYS:HA	1:87:A:THR:HA	5	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG11	8	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG12	8	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG13	8	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG11	10	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG12	10	0.37
(1,549)	1:80:A:THR:HB	1:81:A:VAL:HG13	10	0.37
(1,536)	1:79:A:GLU:HG2	1:80:A:THR:HB	3	0.37
(1,536)	1:79:A:GLU:HG3	1:80:A:THR:HB	3	0.37
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG2	10	0.37
(1,352)	1:62:A:ALA:H	1:65:A:ARG:HG3	10	0.37
(1,134)	1:30:A:THR:HB	1:31:A:CYS:HA	9	0.37
(1,102)	1:22:A:ALA:HA	1:23:A:GLU:H	5	0.37
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	9	0.36
(1,1134)	1:91:A:ARG:H	1:95:A:TRP:HE3	4	0.36
(1,858)	1:29:A:LYS:HB2	1:34:A:TYR:H	7	0.36
(1,858)	1:29:A:LYS:HB3	1:34:A:TYR:H	7	0.36
(1,853)	1:22:A:ALA:HA	1:23:A:GLU:H	2	0.36
(1,803)	1:98:A:THR:HG21	1:100:A:HIS:HE1	7	0.36
(1,803)	1:98:A:THR:HG22	1:100:A:HIS:HE1	7	0.36
(1,803)	1:98:A:THR:HG23	1:100:A:HIS:HE1	7	0.36
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	9	0.36
(1,657)	1:85:A:CYS:HA	1:103:A:ASP:H	9	0.36
(1,278)	1:55:A:ARG:HA	1:60:A:CYS:HA	9	0.36
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	6	0.36
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	6	0.36
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD11	4	0.36
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD12	4	0.36
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD13	4	0.36
(1,102)	1:22:A:ALA:HA	1:23:A:GLU:H	2	0.36
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG21	7	0.36
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG22	7	0.36
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG23	7	0.36
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG21	7	0.36
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG22	7	0.36
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG23	7	0.36
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG21	7	0.36
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG22	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG23	7	0.36
(1,1175)	1:102:A:CYS:H	1:103:A:ASP:H	5	0.35
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	4	0.35
(1,1095)	1:88:A:CYS:HB2	1:95:A:TRP:H	8	0.35
(1,1095)	1:88:A:CYS:HB3	1:95:A:TRP:H	8	0.35
(1,961)	1:67:A:PRO:HB2	1:75:A:TYR:H	1	0.35
(1,961)	1:67:A:PRO:HB3	1:75:A:TYR:H	1	0.35
(1,670)	1:87:A:THR:HB	1:88:A:CYS:H	3	0.35
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG21	8	0.35
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG22	8	0.35
(1,663)	1:86:A:ASN:HA	1:98:A:THR:HG23	8	0.35
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	2	0.35
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	2	0.35
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	2	0.35
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	2	0.35
(1,641)	1:83:A:ILE:H	1:87:A:THR:HA	3	0.35
(1,566)	1:80:A:THR:HB	1:95:A:TRP:HZ3	3	0.35
(1,385)	1:67:A:PRO:HB2	1:75:A:TYR:H	1	0.35
(1,385)	1:67:A:PRO:HB3	1:75:A:TYR:H	1	0.35
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD21	4	0.35
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD22	4	0.35
(1,199)	1:34:A:TYR:HE1	1:63:A:LEU:HD23	4	0.35
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD21	4	0.35
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD22	4	0.35
(1,199)	1:34:A:TYR:HE2	1:63:A:LEU:HD23	4	0.35
(1,157)	1:30:A:THR:HG21	1:55:A:ARG:HG2	5	0.35
(1,157)	1:30:A:THR:HG21	1:55:A:ARG:HG3	5	0.35
(1,157)	1:30:A:THR:HG22	1:55:A:ARG:HG2	5	0.35
(1,157)	1:30:A:THR:HG22	1:55:A:ARG:HG3	5	0.35
(1,157)	1:30:A:THR:HG23	1:55:A:ARG:HG2	5	0.35
(1,157)	1:30:A:THR:HG23	1:55:A:ARG:HG3	5	0.35
(1,58)	1:13:A:LEU:HD11	1:14:A:VAL:H	7	0.35
(1,58)	1:13:A:LEU:HD12	1:14:A:VAL:H	7	0.35
(1,58)	1:13:A:LEU:HD13	1:14:A:VAL:H	7	0.35
(1,1176)	1:102:A:CYS:HA	1:103:A:ASP:H	6	0.34
(1,1094)	1:88:A:CYS:H	1:95:A:TRP:HE3	5	0.34
(1,1076)	1:85:A:CYS:H	1:86:A:ASN:H	3	0.34
(1,819)	1:102:A:CYS:HA	1:103:A:ASP:H	6	0.34
(1,686)	1:88:A:CYS:H	1:95:A:TRP:HE3	5	0.34
(1,576)	1:81:A:VAL:HB	1:82:A:LYS:HA	1	0.34
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG11	8	0.34
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG12	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:78:A:GLY:H	1:89:A:VAL:HG13	8	0.34
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE1	3	0.34
(1,464)	1:73:A:LYS:HA	1:75:A:TYR:HE2	3	0.34
(1,460)	1:73:A:LYS:HG2	1:74:A:GLU:H	4	0.34
(1,460)	1:73:A:LYS:HG3	1:74:A:GLU:H	4	0.34
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG11	6	0.34
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG12	6	0.34
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG13	6	0.34
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD2	2	0.34
(1,334)	1:61:A:VAL:HB	1:65:A:ARG:HD3	2	0.34
(1,201)	1:35:A:ASP:HA	1:36:A:LEU:H	3	0.34
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	1	0.33
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	2	0.33
(1,1081)	1:86:A:ASN:HB2	1:98:A:THR:H	1	0.33
(1,1081)	1:86:A:ASN:HB3	1:98:A:THR:H	1	0.33
(1,991)	1:70:A:HIS:HB2	1:95:A:TRP:HE1	10	0.33
(1,991)	1:70:A:HIS:HB3	1:95:A:TRP:HE1	10	0.33
(1,990)	1:70:A:HIS:HA	1:95:A:TRP:HE1	6	0.33
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE1	2	0.33
(1,987)	1:70:A:HIS:H	1:75:A:TYR:HE2	2	0.33
(1,827)	1:11:A:VAL:HB	1:12:A:LYS:H	5	0.33
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	1	0.33
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	2	0.33
(1,539)	1:79:A:GLU:H	1:89:A:VAL:HA	4	0.33
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE1	4	0.33
(1,472)	1:74:A:GLU:HA	1:75:A:TYR:HE2	4	0.33
(1,451)	1:70:A:HIS:HA	1:95:A:TRP:HE1	6	0.33
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE1	2	0.33
(1,430)	1:70:A:HIS:H	1:75:A:TYR:HE2	2	0.33
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB1	2	0.33
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB2	2	0.33
(1,328)	1:61:A:VAL:HB	1:62:A:ALA:HB3	2	0.33
(1,168)	1:31:A:CYS:HA	1:63:A:LEU:HD21	4	0.33
(1,168)	1:31:A:CYS:HA	1:63:A:LEU:HD22	4	0.33
(1,168)	1:31:A:CYS:HA	1:63:A:LEU:HD23	4	0.33
(1,1171)	1:101:A:VAL:HB	1:102:A:CYS:H	4	0.32
(1,1170)	1:101:A:VAL:HA	1:102:A:CYS:H	9	0.32
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	4	0.32
(1,1132)	1:91:A:ARG:H	1:94:A:LYS:H	6	0.32
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	8	0.32
(1,801)	1:98:A:THR:HB	1:100:A:HIS:H	5	0.32
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,616)	1:81:A:VAL:HG11	1:95:A:TRP:HZ2	7	0.32
(1,616)	1:81:A:VAL:HG12	1:95:A:TRP:HZ2	7	0.32
(1,616)	1:81:A:VAL:HG13	1:95:A:TRP:HZ2	7	0.32
(1,599)	1:81:A:VAL:HG11	1:87:A:THR:HA	9	0.32
(1,599)	1:81:A:VAL:HG12	1:87:A:THR:HA	9	0.32
(1,599)	1:81:A:VAL:HG13	1:87:A:THR:HA	9	0.32
(1,563)	1:80:A:THR:HG21	1:89:A:VAL:HB	5	0.32
(1,563)	1:80:A:THR:HG22	1:89:A:VAL:HB	5	0.32
(1,563)	1:80:A:THR:HG23	1:89:A:VAL:HB	5	0.32
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG11	8	0.32
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG12	8	0.32
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG13	8	0.32
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	8	0.32
(1,1142)	1:92:A:ASP:HA	1:94:A:LYS:H	5	0.31
(1,1121)	1:90:A:CYS:H	1:95:A:TRP:HE3	2	0.31
(1,1109)	1:89:A:VAL:H	1:96:A:ASN:H	10	0.31
(1,1070)	1:83:A:ILE:H	1:88:A:CYS:HB2	6	0.31
(1,1070)	1:83:A:ILE:H	1:88:A:CYS:HB3	6	0.31
(1,817)	1:101:A:VAL:HG21	1:103:A:ASP:H	3	0.31
(1,817)	1:101:A:VAL:HG22	1:103:A:ASP:H	3	0.31
(1,817)	1:101:A:VAL:HG23	1:103:A:ASP:H	3	0.31
(1,802)	1:98:A:THR:HG21	1:100:A:HIS:HD2	10	0.31
(1,802)	1:98:A:THR:HG22	1:100:A:HIS:HD2	10	0.31
(1,802)	1:98:A:THR:HG23	1:100:A:HIS:HD2	10	0.31
(1,721)	1:89:A:VAL:HA	1:95:A:TRP:HA	4	0.31
(1,717)	1:89:A:VAL:HG11	1:91:A:ARG:H	5	0.31
(1,717)	1:89:A:VAL:HG12	1:91:A:ARG:H	5	0.31
(1,717)	1:89:A:VAL:HG13	1:91:A:ARG:H	5	0.31
(1,670)	1:87:A:THR:HB	1:88:A:CYS:H	5	0.31
(1,625)	1:82:A:LYS:HA	1:83:A:ILE:HB	9	0.31
(1,607)	1:81:A:VAL:HG21	1:88:A:CYS:HA	1	0.31
(1,607)	1:81:A:VAL:HG22	1:88:A:CYS:HA	1	0.31
(1,607)	1:81:A:VAL:HG23	1:88:A:CYS:HA	1	0.31
(1,561)	1:80:A:THR:HG21	1:89:A:VAL:H	7	0.31
(1,561)	1:80:A:THR:HG22	1:89:A:VAL:H	7	0.31
(1,561)	1:80:A:THR:HG23	1:89:A:VAL:H	7	0.31
(1,559)	1:80:A:THR:HB	1:89:A:VAL:HB	7	0.31
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG21	6	0.31
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG22	6	0.31
(1,436)	1:70:A:HIS:H	1:81:A:VAL:HG23	6	0.31
(1,354)	1:62:A:ALA:HB1	1:65:A:ARG:HD2	8	0.31
(1,354)	1:62:A:ALA:HB1	1:65:A:ARG:HD3	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:62:A:ALA:HB2	1:65:A:ARG:HD2	8	0.31
(1,354)	1:62:A:ALA:HB2	1:65:A:ARG:HD3	8	0.31
(1,354)	1:62:A:ALA:HB3	1:65:A:ARG:HD2	8	0.31
(1,354)	1:62:A:ALA:HB3	1:65:A:ARG:HD3	8	0.31
(1,161)	1:31:A:CYS:HA	1:34:A:TYR:HB2	8	0.31
(1,161)	1:31:A:CYS:HA	1:34:A:TYR:HB3	8	0.31
(1,156)	1:30:A:THR:HG21	1:55:A:ARG:HA	5	0.31
(1,156)	1:30:A:THR:HG22	1:55:A:ARG:HA	5	0.31
(1,156)	1:30:A:THR:HG23	1:55:A:ARG:HA	5	0.31
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	3	0.3
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	4	0.3
(1,974)	1:69:A:PHE:HA	1:73:A:LYS:H	1	0.3
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD21	6	0.3
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD22	6	0.3
(1,849)	1:17:A:ALA:H	1:20:A:LEU:HD23	6	0.3
(1,721)	1:89:A:VAL:HA	1:95:A:TRP:HA	10	0.3
(1,635)	1:82:A:LYS:HA	1:88:A:CYS:H	6	0.3
(1,558)	1:80:A:THR:HA	1:89:A:VAL:HA	5	0.3
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG21	8	0.3
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG22	8	0.3
(1,440)	1:70:A:HIS:HD2	1:81:A:VAL:HG23	8	0.3
(1,415)	1:69:A:PHE:HE1	1:74:A:GLU:HA	7	0.3
(1,415)	1:69:A:PHE:HE2	1:74:A:GLU:HA	7	0.3
(1,408)	1:69:A:PHE:HA	1:73:A:LYS:H	1	0.3
(1,278)	1:55:A:ARG:HA	1:60:A:CYS:HA	1	0.3
(1,156)	1:30:A:THR:HG21	1:55:A:ARG:HA	4	0.3
(1,156)	1:30:A:THR:HG22	1:55:A:ARG:HA	4	0.3
(1,156)	1:30:A:THR:HG23	1:55:A:ARG:HA	4	0.3
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG2	2	0.3
(1,153)	1:30:A:THR:HA	1:55:A:ARG:HG3	2	0.3
(1,147)	1:30:A:THR:HA	1:54:A:VAL:HA	8	0.3
(1,1176)	1:102:A:CYS:HA	1:103:A:ASP:H	7	0.29
(1,1162)	1:98:A:THR:HA	1:100:A:HIS:H	5	0.29
(1,1099)	1:88:A:CYS:H	1:98:A:THR:H	2	0.29
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG21	10	0.29
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG22	10	0.29
(1,1027)	1:78:A:GLY:H	1:89:A:VAL:HG23	10	0.29
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE1	7	0.29
(1,1000)	1:73:A:LYS:H	1:75:A:TYR:HE2	7	0.29
(1,827)	1:11:A:VAL:HB	1:12:A:LYS:H	9	0.29
(1,819)	1:102:A:CYS:HA	1:103:A:ASP:H	7	0.29
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	8	0.29
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG21	10	0.29
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG22	10	0.29
(1,524)	1:78:A:GLY:H	1:89:A:VAL:HG23	10	0.29
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	7	0.29
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	7	0.29
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE1	7	0.29
(1,463)	1:73:A:LYS:H	1:75:A:TYR:HE2	7	0.29
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG21	8	0.29
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG22	8	0.29
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG23	8	0.29
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	10	0.28
(1,1112)	1:89:A:VAL:HG11	1:96:A:ASN:H	8	0.28
(1,1112)	1:89:A:VAL:HG12	1:96:A:ASN:H	8	0.28
(1,1112)	1:89:A:VAL:HG13	1:96:A:ASN:H	8	0.28
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	2	0.28
(1,1014)	1:75:A:TYR:H	1:95:A:TRP:HH2	2	0.28
(1,860)	1:30:A:THR:HB	1:31:A:CYS:H	5	0.28
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD11	3	0.28
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD12	3	0.28
(1,850)	1:17:A:ALA:H	1:20:A:LEU:HD13	3	0.28
(1,827)	1:11:A:VAL:HB	1:12:A:LYS:H	3	0.28
(1,806)	1:99:A:ASP:HA	1:100:A:HIS:H	1	0.28
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	10	0.28
(1,729)	1:89:A:VAL:H	1:96:A:ASN:HA	8	0.28
(1,721)	1:89:A:VAL:HA	1:95:A:TRP:HA	1	0.28
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG21	4	0.28
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG22	4	0.28
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG23	4	0.28
(1,340)	1:61:A:VAL:HG21	1:65:A:ARG:H	7	0.28
(1,340)	1:61:A:VAL:HG22	1:65:A:ARG:H	7	0.28
(1,340)	1:61:A:VAL:HG23	1:65:A:ARG:H	7	0.28
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG21	2	0.28
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG22	2	0.28
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG23	2	0.28
(1,193)	1:34:A:TYR:HD1	1:54:A:VAL:HG11	3	0.28
(1,193)	1:34:A:TYR:HD1	1:54:A:VAL:HG12	3	0.28
(1,193)	1:34:A:TYR:HD1	1:54:A:VAL:HG13	3	0.28
(1,193)	1:34:A:TYR:HD2	1:54:A:VAL:HG11	3	0.28
(1,193)	1:34:A:TYR:HD2	1:54:A:VAL:HG12	3	0.28
(1,193)	1:34:A:TYR:HD2	1:54:A:VAL:HG13	3	0.28
(1,135)	1:30:A:THR:HB	1:31:A:CYS:H	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG11	7	0.28
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG12	7	0.28
(1,7)	1:53:A:MET:HE1	1:61:A:VAL:HG13	7	0.28
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG11	7	0.28
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG12	7	0.28
(1,7)	1:53:A:MET:HE2	1:61:A:VAL:HG13	7	0.28
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG11	7	0.28
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG12	7	0.28
(1,7)	1:53:A:MET:HE3	1:61:A:VAL:HG13	7	0.28
(1,3)	1:53:A:MET:HE1	1:60:A:CYS:HA	3	0.28
(1,3)	1:53:A:MET:HE2	1:60:A:CYS:HA	3	0.28
(1,3)	1:53:A:MET:HE3	1:60:A:CYS:HA	3	0.28
(1,1031)	1:78:A:GLY:H	1:91:A:ARG:H	7	0.27
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD2	6	0.27
(1,956)	1:66:A:CYS:H	1:93:A:ARG:HD3	6	0.27
(1,907)	1:54:A:VAL:H	1:61:A:VAL:H	8	0.27
(1,845)	1:17:A:ALA:H	1:18:A:ASP:HA	8	0.27
(1,827)	1:11:A:VAL:HB	1:12:A:LYS:H	1	0.27
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	1	0.27
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB2	1	0.27
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB3	1	0.27
(1,536)	1:79:A:GLU:HG2	1:80:A:THR:HB	7	0.27
(1,536)	1:79:A:GLU:HG3	1:80:A:THR:HB	7	0.27
(1,500)	1:75:A:TYR:HE1	1:95:A:TRP:HZ2	2	0.27
(1,500)	1:75:A:TYR:HE2	1:95:A:TRP:HZ2	2	0.27
(1,399)	1:68:A:CYS:HA	1:95:A:TRP:HE1	3	0.27
(1,1099)	1:88:A:CYS:H	1:98:A:THR:H	3	0.26
(1,888)	1:39:A:MET:HA	1:40:A:SER:H	7	0.26
(1,797)	1:98:A:THR:HA	1:100:A:HIS:H	8	0.26
(1,687)	1:88:A:CYS:HA	1:95:A:TRP:HA	3	0.26
(1,669)	1:87:A:THR:HB	1:88:A:CYS:HA	10	0.26
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB2	10	0.26
(1,573)	1:81:A:VAL:HB	1:82:A:LYS:HB3	10	0.26
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG11	5	0.26
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG12	5	0.26
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG13	5	0.26
(1,409)	1:69:A:PHE:HA	1:74:A:GLU:HA	2	0.26
(1,372)	1:65:A:ARG:HD2	1:66:A:CYS:H	10	0.26
(1,372)	1:65:A:ARG:HD3	1:66:A:CYS:H	10	0.26
(1,341)	1:61:A:VAL:HG21	1:66:A:CYS:H	7	0.26
(1,341)	1:61:A:VAL:HG22	1:66:A:CYS:H	7	0.26
(1,341)	1:61:A:VAL:HG23	1:66:A:CYS:H	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:55:A:ARG:HA	1:61:A:VAL:H	6	0.26
(1,207)	1:39:A:MET:HA	1:40:A:SER:H	7	0.26
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG11	10	0.26
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG12	10	0.26
(1,196)	1:34:A:TYR:HE1	1:54:A:VAL:HG13	10	0.26
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG11	10	0.26
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG12	10	0.26
(1,196)	1:34:A:TYR:HE2	1:54:A:VAL:HG13	10	0.26
(1,3)	1:53:A:MET:HE1	1:60:A:CYS:HA	1	0.26
(1,3)	1:53:A:MET:HE2	1:60:A:CYS:HA	1	0.26
(1,3)	1:53:A:MET:HE3	1:60:A:CYS:HA	1	0.26
(1,1047)	1:80:A:THR:HG21	1:90:A:CYS:H	5	0.25
(1,1047)	1:80:A:THR:HG22	1:90:A:CYS:H	5	0.25
(1,1047)	1:80:A:THR:HG23	1:90:A:CYS:H	5	0.25
(1,1045)	1:80:A:THR:H	1:89:A:VAL:HA	5	0.25
(1,669)	1:87:A:THR:HB	1:88:A:CYS:HA	6	0.25
(1,636)	1:82:A:LYS:HD2	1:88:A:CYS:H	8	0.25
(1,636)	1:82:A:LYS:HD3	1:88:A:CYS:H	8	0.25
(1,627)	1:82:A:LYS:HE2	1:85:A:CYS:HA	1	0.25
(1,627)	1:82:A:LYS:HE3	1:85:A:CYS:HA	1	0.25
(1,554)	1:80:A:THR:H	1:89:A:VAL:HA	5	0.25
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD1	6	0.25
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD2	6	0.25
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE1	2	0.25
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE2	2	0.25
(1,248)	1:54:A:VAL:HB	1:55:A:ARG:H	2	0.25
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB1	9	0.25
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB2	9	0.25
(1,238)	1:53:A:MET:HA	1:62:A:ALA:HB3	9	0.25
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG21	10	0.25
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG22	10	0.25
(1,6)	1:53:A:MET:HE1	1:61:A:VAL:HG23	10	0.25
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG21	10	0.25
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG22	10	0.25
(1,6)	1:53:A:MET:HE2	1:61:A:VAL:HG23	10	0.25
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG21	10	0.25
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG22	10	0.25
(1,6)	1:53:A:MET:HE3	1:61:A:VAL:HG23	10	0.25
(1,1099)	1:88:A:CYS:H	1:98:A:THR:H	9	0.24
(1,1017)	1:76:A:ALA:H	1:79:A:GLU:H	4	0.24
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG11	6	0.24
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG12	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG13	6	0.24
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	8	0.24
(1,845)	1:17:A:ALA:H	1:18:A:ASP:HA	3	0.24
(1,645)	1:83:A:ILE:HD11	1:95:A:TRP:HD1	3	0.24
(1,645)	1:83:A:ILE:HD12	1:95:A:TRP:HD1	3	0.24
(1,645)	1:83:A:ILE:HD13	1:95:A:TRP:HD1	3	0.24
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	2	0.24
(1,532)	1:79:A:GLU:HA	1:80:A:THR:HB	5	0.24
(1,420)	1:69:A:PHE:HA	1:75:A:TYR:H	9	0.24
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG11	2	0.24
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG12	2	0.24
(1,299)	1:56:A:HIS:HD2	1:61:A:VAL:HG13	2	0.24
(1,259)	1:54:A:VAL:HG11	1:63:A:LEU:HA	2	0.24
(1,259)	1:54:A:VAL:HG12	1:63:A:LEU:HA	2	0.24
(1,259)	1:54:A:VAL:HG13	1:63:A:LEU:HA	2	0.24
(1,254)	1:54:A:VAL:HG21	1:61:A:VAL:H	8	0.24
(1,254)	1:54:A:VAL:HG22	1:61:A:VAL:H	8	0.24
(1,254)	1:54:A:VAL:HG23	1:61:A:VAL:H	8	0.24
(1,248)	1:54:A:VAL:HB	1:55:A:ARG:H	3	0.24
(1,185)	1:33:A:ASN:HA	1:37:A:GLU:HA	1	0.24
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG11	5	0.24
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG12	5	0.24
(1,54)	1:12:A:LYS:HA	1:14:A:VAL:HG13	5	0.24
(1,1145)	1:93:A:ARG:HA	1:94:A:LYS:H	1	0.23
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	4	0.23
(1,1114)	1:89:A:VAL:H	1:97:A:CYS:HA	5	0.23
(1,991)	1:70:A:HIS:HB2	1:95:A:TRP:HE1	4	0.23
(1,991)	1:70:A:HIS:HB3	1:95:A:TRP:HE1	4	0.23
(1,912)	1:55:A:ARG:HA	1:59:A:ARG:H	7	0.23
(1,888)	1:39:A:MET:HA	1:40:A:SER:H	6	0.23
(1,771)	1:93:A:ARG:HA	1:94:A:LYS:H	1	0.23
(1,738)	1:89:A:VAL:H	1:97:A:CYS:HA	5	0.23
(1,660)	1:86:A:ASN:HA	1:87:A:THR:HB	7	0.23
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB2	8	0.23
(1,646)	1:83:A:ILE:HD11	1:95:A:TRP:HB3	8	0.23
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB2	8	0.23
(1,646)	1:83:A:ILE:HD12	1:95:A:TRP:HB3	8	0.23
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB2	8	0.23
(1,646)	1:83:A:ILE:HD13	1:95:A:TRP:HB3	8	0.23
(1,632)	1:82:A:LYS:HD2	1:87:A:THR:HA	4	0.23
(1,632)	1:82:A:LYS:HD3	1:87:A:THR:HA	4	0.23
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG21	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG22	7	0.23
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG23	7	0.23
(1,372)	1:65:A:ARG:HD2	1:66:A:CYS:H	6	0.23
(1,372)	1:65:A:ARG:HD3	1:66:A:CYS:H	6	0.23
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG21	5	0.23
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG22	5	0.23
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG23	5	0.23
(1,277)	1:55:A:ARG:HA	1:59:A:ARG:H	7	0.23
(1,207)	1:39:A:MET:HA	1:40:A:SER:H	6	0.23
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG11	4	0.23
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG12	4	0.23
(1,128)	1:29:A:LYS:H	1:54:A:VAL:HG13	4	0.23
(1,92)	1:17:A:ALA:HA	1:18:A:ASP:HA	2	0.23
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	6	0.22
(1,1039)	1:79:A:GLU:H	1:90:A:CYS:H	3	0.22
(1,888)	1:39:A:MET:HA	1:40:A:SER:H	2	0.22
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	6	0.22
(1,746)	1:90:A:CYS:HA	1:95:A:TRP:HE3	8	0.22
(1,724)	1:89:A:VAL:HB	1:95:A:TRP:HE3	1	0.22
(1,552)	1:80:A:THR:HA	1:88:A:CYS:H	10	0.22
(1,420)	1:69:A:PHE:HA	1:75:A:TYR:H	6	0.22
(1,243)	1:53:A:MET:HA	1:63:A:LEU:HA	6	0.22
(1,207)	1:39:A:MET:HA	1:40:A:SER:H	2	0.22
(1,179)	1:33:A:ASN:HA	1:36:A:LEU:HA	8	0.22
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD2	5	0.22
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD3	5	0.22
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD2	5	0.22
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD3	5	0.22
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD2	5	0.22
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD3	5	0.22
(1,39)	1:11:A:VAL:HG11	1:48:A:LEU:H	4	0.22
(1,39)	1:11:A:VAL:HG12	1:48:A:LEU:H	4	0.22
(1,39)	1:11:A:VAL:HG13	1:48:A:LEU:H	4	0.22
(1,1171)	1:101:A:VAL:HB	1:102:A:CYS:H	6	0.21
(1,1170)	1:101:A:VAL:HA	1:102:A:CYS:H	2	0.21
(1,1169)	1:100:A:HIS:H	1:99:A:ASP:H	9	0.21
(1,1165)	1:99:A:ASP:H	1:100:A:HIS:H	9	0.21
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB2	7	0.21
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB3	7	0.21
(1,1043)	1:80:A:THR:HB	1:81:A:VAL:H	5	0.21
(1,978)	1:69:A:PHE:H	1:95:A:TRP:HZ2	5	0.21
(1,860)	1:30:A:THR:HB	1:31:A:CYS:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:89:A:VAL:HB	1:95:A:TRP:HZ3	8	0.21
(1,629)	1:82:A:LYS:HA	1:87:A:THR:HG21	5	0.21
(1,629)	1:82:A:LYS:HA	1:87:A:THR:HG22	5	0.21
(1,629)	1:82:A:LYS:HA	1:87:A:THR:HG23	5	0.21
(1,560)	1:80:A:THR:HB	1:89:A:VAL:HA	3	0.21
(1,550)	1:80:A:THR:HB	1:81:A:VAL:H	5	0.21
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG11	10	0.21
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG12	10	0.21
(1,546)	1:80:A:THR:HA	1:81:A:VAL:HG13	10	0.21
(1,422)	1:69:A:PHE:H	1:95:A:TRP:HZ2	5	0.21
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD2	10	0.21
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD3	10	0.21
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD2	3	0.21
(1,290)	1:56:A:HIS:HD2	1:59:A:ARG:HD3	3	0.21
(1,201)	1:35:A:ASP:HA	1:36:A:LEU:H	6	0.21
(1,148)	1:30:A:THR:HA	1:54:A:VAL:HB	4	0.21
(1,135)	1:30:A:THR:HB	1:31:A:CYS:H	10	0.21
(1,36)	1:11:A:VAL:HG21	1:47:A:CYS:HA	9	0.21
(1,36)	1:11:A:VAL:HG22	1:47:A:CYS:HA	9	0.21
(1,36)	1:11:A:VAL:HG23	1:47:A:CYS:HA	9	0.21
(1,1145)	1:93:A:ARG:HA	1:94:A:LYS:H	8	0.2
(1,1100)	1:88:A:CYS:HA	1:98:A:THR:H	6	0.2
(1,1067)	1:82:A:LYS:HA	1:88:A:CYS:H	8	0.2
(1,1011)	1:75:A:TYR:HD1	1:76:A:ALA:H	5	0.2
(1,1011)	1:75:A:TYR:HD2	1:76:A:ALA:H	5	0.2
(1,1001)	1:73:A:LYS:H	1:75:A:TYR:HD1	6	0.2
(1,1001)	1:73:A:LYS:H	1:75:A:TYR:HD2	6	0.2
(1,982)	1:70:A:HIS:H	1:73:A:LYS:H	10	0.2
(1,869)	1:31:A:CYS:H	1:54:A:VAL:HB	2	0.2
(1,793)	1:98:A:THR:HB	1:99:A:ASP:HA	4	0.2
(1,771)	1:93:A:ARG:HA	1:94:A:LYS:H	8	0.2
(1,701)	1:88:A:CYS:HA	1:98:A:THR:H	6	0.2
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG11	3	0.2
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG12	3	0.2
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG13	3	0.2
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG21	1	0.2
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG22	1	0.2
(1,544)	1:80:A:THR:HA	1:81:A:VAL:HG23	1	0.2
(1,480)	1:75:A:TYR:HD1	1:76:A:ALA:H	5	0.2
(1,480)	1:75:A:TYR:HD2	1:76:A:ALA:H	5	0.2
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG11	1	0.2
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG12	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:70:A:HIS:H	1:81:A:VAL:HG13	1	0.2
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD11	3	0.2
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD12	3	0.2
(1,167)	1:31:A:CYS:HA	1:63:A:LEU:HD13	3	0.2
(1,1169)	1:100:A:HIS:H	1:99:A:ASP:H	10	0.19
(1,1165)	1:99:A:ASP:H	1:100:A:HIS:H	10	0.19
(1,1134)	1:91:A:ARG:H	1:95:A:TRP:HE3	9	0.19
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB2	10	0.19
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB3	10	0.19
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	5	0.19
(1,719)	1:89:A:VAL:H	1:95:A:TRP:HE3	5	0.19
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	10	0.19
(1,621)	1:81:A:VAL:HG11	1:95:A:TRP:HE1	3	0.19
(1,621)	1:81:A:VAL:HG12	1:95:A:TRP:HE1	3	0.19
(1,621)	1:81:A:VAL:HG13	1:95:A:TRP:HE1	3	0.19
(1,610)	1:81:A:VAL:H	1:89:A:VAL:HA	1	0.19
(1,586)	1:81:A:VAL:HB	1:83:A:ILE:HG12	10	0.19
(1,586)	1:81:A:VAL:HB	1:83:A:ILE:HG13	10	0.19
(1,563)	1:80:A:THR:HG21	1:89:A:VAL:HB	2	0.19
(1,563)	1:80:A:THR:HG22	1:89:A:VAL:HB	2	0.19
(1,563)	1:80:A:THR:HG23	1:89:A:VAL:HB	2	0.19
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG21	10	0.19
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG22	10	0.19
(1,323)	1:60:A:CYS:HA	1:61:A:VAL:HG23	10	0.19
(1,248)	1:54:A:VAL:HB	1:55:A:ARG:H	8	0.19
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	5	0.19
(1,237)	1:53:A:MET:HA	1:62:A:ALA:HA	5	0.19
(1,201)	1:35:A:ASP:HA	1:36:A:LEU:H	2	0.19
(1,86)	1:16:A:PRO:HB2	1:20:A:LEU:HD21	5	0.19
(1,86)	1:16:A:PRO:HB2	1:20:A:LEU:HD22	5	0.19
(1,86)	1:16:A:PRO:HB2	1:20:A:LEU:HD23	5	0.19
(1,86)	1:16:A:PRO:HB3	1:20:A:LEU:HD21	5	0.19
(1,86)	1:16:A:PRO:HB3	1:20:A:LEU:HD22	5	0.19
(1,86)	1:16:A:PRO:HB3	1:20:A:LEU:HD23	5	0.19
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB2	2	0.19
(1,41)	1:11:A:VAL:HG21	1:48:A:LEU:HB3	2	0.19
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB2	2	0.19
(1,41)	1:11:A:VAL:HG22	1:48:A:LEU:HB3	2	0.19
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB2	2	0.19
(1,41)	1:11:A:VAL:HG23	1:48:A:LEU:HB3	2	0.19
(1,1072)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	2	0.18
(1,1072)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	2	0.18
(1,974)	1:69:A:PHE:HA	1:73:A:LYS:H	6	0.18
(1,968)	1:68:A:CYS:HA	1:95:A:TRP:HE1	7	0.18
(1,967)	1:68:A:CYS:H	1:75:A:TYR:H	3	0.18
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG2	8	0.18
(1,957)	1:66:A:CYS:H	1:93:A:ARG:HG3	8	0.18
(1,888)	1:39:A:MET:HA	1:40:A:SER:H	8	0.18
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG11	7	0.18
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG12	7	0.18
(1,681)	1:88:A:CYS:HA	1:89:A:VAL:HG13	7	0.18
(1,647)	1:83:A:ILE:HD11	1:95:A:TRP:HE1	2	0.18
(1,647)	1:83:A:ILE:HD12	1:95:A:TRP:HE1	2	0.18
(1,647)	1:83:A:ILE:HD13	1:95:A:TRP:HE1	2	0.18
(1,641)	1:83:A:ILE:H	1:87:A:THR:HA	9	0.18
(1,408)	1:69:A:PHE:HA	1:73:A:LYS:H	6	0.18
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD2	7	0.18
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD3	7	0.18
(1,339)	1:61:A:VAL:HG11	1:65:A:ARG:HD2	5	0.18
(1,339)	1:61:A:VAL:HG11	1:65:A:ARG:HD3	5	0.18
(1,339)	1:61:A:VAL:HG12	1:65:A:ARG:HD2	5	0.18
(1,339)	1:61:A:VAL:HG12	1:65:A:ARG:HD3	5	0.18
(1,339)	1:61:A:VAL:HG13	1:65:A:ARG:HD2	5	0.18
(1,339)	1:61:A:VAL:HG13	1:65:A:ARG:HD3	5	0.18
(1,223)	1:48:A:LEU:HD21	1:49:A:CYS:H	8	0.18
(1,223)	1:48:A:LEU:HD22	1:49:A:CYS:H	8	0.18
(1,223)	1:48:A:LEU:HD23	1:49:A:CYS:H	8	0.18
(1,207)	1:39:A:MET:HA	1:40:A:SER:H	8	0.18
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD2	9	0.18
(1,155)	1:30:A:THR:HG21	1:55:A:ARG:HD3	9	0.18
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD2	9	0.18
(1,155)	1:30:A:THR:HG22	1:55:A:ARG:HD3	9	0.18
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD2	9	0.18
(1,155)	1:30:A:THR:HG23	1:55:A:ARG:HD3	9	0.18
(1,92)	1:17:A:ALA:HA	1:18:A:ASP:HA	4	0.18
(1,72)	1:14:A:VAL:HA	1:45:A:SER:HA	7	0.18
(1,57)	1:13:A:LEU:HA	1:14:A:VAL:HB	3	0.18
(1,53)	1:12:A:LYS:HA	1:48:A:LEU:H	9	0.18
(1,1156)	1:95:A:TRP:HE3	1:96:A:ASN:H	7	0.17
(1,1145)	1:93:A:ARG:HA	1:94:A:LYS:H	6	0.17
(1,1090)	1:87:A:THR:HB	1:98:A:THR:H	7	0.17
(1,1085)	1:87:A:THR:HB	1:88:A:CYS:H	9	0.17
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB2	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:85:A:CYS:H	1:102:A:CYS:HB3	8	0.17
(1,1066)	1:82:A:LYS:HG2	1:83:A:ILE:H	7	0.17
(1,1066)	1:82:A:LYS:HG3	1:83:A:ILE:H	7	0.17
(1,1058)	1:81:A:VAL:HG11	1:88:A:CYS:H	3	0.17
(1,1058)	1:81:A:VAL:HG12	1:88:A:CYS:H	3	0.17
(1,1058)	1:81:A:VAL:HG13	1:88:A:CYS:H	3	0.17
(1,1046)	1:80:A:THR:HA	1:90:A:CYS:H	9	0.17
(1,968)	1:68:A:CYS:HA	1:95:A:TRP:HE1	9	0.17
(1,806)	1:99:A:ASP:HA	1:100:A:HIS:H	6	0.17
(1,771)	1:93:A:ARG:HA	1:94:A:LYS:H	6	0.17
(1,692)	1:88:A:CYS:HA	1:96:A:ASN:HA	5	0.17
(1,605)	1:81:A:VAL:HG11	1:88:A:CYS:H	3	0.17
(1,605)	1:81:A:VAL:HG12	1:88:A:CYS:H	3	0.17
(1,605)	1:81:A:VAL:HG13	1:88:A:CYS:H	3	0.17
(1,600)	1:81:A:VAL:HG21	1:87:A:THR:HB	3	0.17
(1,600)	1:81:A:VAL:HG22	1:87:A:THR:HB	3	0.17
(1,600)	1:81:A:VAL:HG23	1:87:A:THR:HB	3	0.17
(1,527)	1:78:A:GLY:HA2	1:89:A:VAL:HG11	10	0.17
(1,527)	1:78:A:GLY:HA2	1:89:A:VAL:HG12	10	0.17
(1,527)	1:78:A:GLY:HA2	1:89:A:VAL:HG13	10	0.17
(1,527)	1:78:A:GLY:HA3	1:89:A:VAL:HG11	10	0.17
(1,527)	1:78:A:GLY:HA3	1:89:A:VAL:HG12	10	0.17
(1,527)	1:78:A:GLY:HA3	1:89:A:VAL:HG13	10	0.17
(1,437)	1:70:A:HIS:HA	1:81:A:VAL:HG11	7	0.17
(1,437)	1:70:A:HIS:HA	1:81:A:VAL:HG12	7	0.17
(1,437)	1:70:A:HIS:HA	1:81:A:VAL:HG13	7	0.17
(1,201)	1:35:A:ASP:HA	1:36:A:LEU:H	1	0.17
(1,58)	1:13:A:LEU:HD11	1:14:A:VAL:H	8	0.17
(1,58)	1:13:A:LEU:HD12	1:14:A:VAL:H	8	0.17
(1,58)	1:13:A:LEU:HD13	1:14:A:VAL:H	8	0.17
(1,1145)	1:93:A:ARG:HA	1:94:A:LYS:H	10	0.16
(1,1130)	1:91:A:ARG:HA	1:93:A:ARG:H	7	0.16
(1,1066)	1:82:A:LYS:HG2	1:83:A:ILE:H	4	0.16
(1,1066)	1:82:A:LYS:HG3	1:83:A:ILE:H	4	0.16
(1,1030)	1:78:A:GLY:H	1:90:A:CYS:HA	7	0.16
(1,1011)	1:75:A:TYR:HD1	1:76:A:ALA:H	6	0.16
(1,1011)	1:75:A:TYR:HD2	1:76:A:ALA:H	6	0.16
(1,975)	1:69:A:PHE:HD1	1:74:A:GLU:H	1	0.16
(1,975)	1:69:A:PHE:HD2	1:74:A:GLU:H	1	0.16
(1,845)	1:17:A:ALA:H	1:18:A:ASP:HA	7	0.16
(1,806)	1:99:A:ASP:HA	1:100:A:HIS:H	2	0.16
(1,771)	1:93:A:ARG:HA	1:94:A:LYS:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:91:A:ARG:HA	1:93:A:ARG:H	7	0.16
(1,669)	1:87:A:THR:HB	1:88:A:CYS:HA	1	0.16
(1,617)	1:81:A:VAL:HG21	1:95:A:TRP:HZ2	4	0.16
(1,617)	1:81:A:VAL:HG22	1:95:A:TRP:HZ2	4	0.16
(1,617)	1:81:A:VAL:HG23	1:95:A:TRP:HZ2	4	0.16
(1,490)	1:75:A:TYR:HE1	1:81:A:VAL:HA	1	0.16
(1,490)	1:75:A:TYR:HE2	1:81:A:VAL:HA	1	0.16
(1,480)	1:75:A:TYR:HD1	1:76:A:ALA:H	6	0.16
(1,480)	1:75:A:TYR:HD2	1:76:A:ALA:H	6	0.16
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD2	1	0.16
(1,370)	1:64:A:GLU:HG2	1:65:A:ARG:HD3	1	0.16
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD2	1	0.16
(1,370)	1:64:A:GLU:HG3	1:65:A:ARG:HD3	1	0.16
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB2	9	0.16
(1,235)	1:53:A:MET:HA	1:60:A:CYS:HB3	9	0.16
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG11	3	0.16
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG12	3	0.16
(1,165)	1:31:A:CYS:HA	1:54:A:VAL:HG13	3	0.16
(1,1082)	1:86:A:ASN:HD21	1:100:A:HIS:H	8	0.15
(1,1082)	1:86:A:ASN:HD22	1:100:A:HIS:H	8	0.15
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	6	0.15
(1,861)	1:30:A:THR:HG21	1:31:A:CYS:H	2	0.15
(1,861)	1:30:A:THR:HG22	1:31:A:CYS:H	2	0.15
(1,861)	1:30:A:THR:HG23	1:31:A:CYS:H	2	0.15
(1,845)	1:17:A:ALA:H	1:18:A:ASP:HA	10	0.15
(1,702)	1:88:A:CYS:HA	1:98:A:THR:HG21	10	0.15
(1,702)	1:88:A:CYS:HA	1:98:A:THR:HG22	10	0.15
(1,702)	1:88:A:CYS:HA	1:98:A:THR:HG23	10	0.15
(1,565)	1:80:A:THR:HA	1:95:A:TRP:HZ3	2	0.15
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG11	1	0.15
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG12	1	0.15
(1,485)	1:75:A:TYR:HA	1:81:A:VAL:HG13	1	0.15
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB1	2	0.15
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB2	2	0.15
(1,395)	1:68:A:CYS:H	1:76:A:ALA:HB3	2	0.15
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	6	0.15
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG21	7	0.15
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG22	7	0.15
(1,164)	1:31:A:CYS:HA	1:54:A:VAL:HG23	7	0.15
(1,1159)	1:98:A:THR:HA	1:99:A:ASP:H	7	0.14
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG21	4	0.14
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:87:A:THR:H	1:98:A:THR:HG23	4	0.14
(1,1060)	1:81:A:VAL:H	1:89:A:VAL:HA	2	0.14
(1,903)	1:53:A:MET:HA	1:63:A:LEU:H	9	0.14
(1,791)	1:98:A:THR:HA	1:99:A:ASP:H	7	0.14
(1,692)	1:88:A:CYS:HA	1:96:A:ASN:HA	9	0.14
(1,563)	1:80:A:THR:HG21	1:89:A:VAL:HB	8	0.14
(1,563)	1:80:A:THR:HG22	1:89:A:VAL:HB	8	0.14
(1,563)	1:80:A:THR:HG23	1:89:A:VAL:HB	8	0.14
(1,461)	1:73:A:LYS:HD2	1:74:A:GLU:H	2	0.14
(1,461)	1:73:A:LYS:HD3	1:74:A:GLU:H	2	0.14
(1,461)	1:73:A:LYS:HD2	1:74:A:GLU:H	3	0.14
(1,461)	1:73:A:LYS:HD3	1:74:A:GLU:H	3	0.14
(1,453)	1:70:A:HIS:HB2	1:95:A:TRP:HE1	1	0.14
(1,453)	1:70:A:HIS:HB3	1:95:A:TRP:HE1	1	0.14
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG21	1	0.14
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG22	1	0.14
(1,446)	1:70:A:HIS:HE1	1:83:A:ILE:HG23	1	0.14
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD1	3	0.14
(1,431)	1:70:A:HIS:HA	1:75:A:TYR:HD2	3	0.14
(1,372)	1:65:A:ARG:HD2	1:66:A:CYS:H	1	0.14
(1,372)	1:65:A:ARG:HD3	1:66:A:CYS:H	1	0.14
(1,372)	1:65:A:ARG:HD2	1:66:A:CYS:H	9	0.14
(1,372)	1:65:A:ARG:HD3	1:66:A:CYS:H	9	0.14
(1,261)	1:54:A:VAL:HG21	1:63:A:LEU:H	3	0.14
(1,261)	1:54:A:VAL:HG22	1:63:A:LEU:H	3	0.14
(1,261)	1:54:A:VAL:HG23	1:63:A:LEU:H	3	0.14
(1,244)	1:53:A:MET:HA	1:63:A:LEU:H	9	0.14
(1,218)	1:47:A:CYS:HA	1:48:A:LEU:HD21	9	0.14
(1,218)	1:47:A:CYS:HA	1:48:A:LEU:HD22	9	0.14
(1,218)	1:47:A:CYS:HA	1:48:A:LEU:HD23	9	0.14
(1,92)	1:17:A:ALA:HA	1:18:A:ASP:HA	5	0.14
(1,57)	1:13:A:LEU:HA	1:14:A:VAL:HB	1	0.14
(1,1135)	1:91:A:ARG:H	1:96:A:ASN:HD21	5	0.13
(1,1135)	1:91:A:ARG:H	1:96:A:ASN:HD22	5	0.13
(1,1085)	1:87:A:THR:HB	1:88:A:CYS:H	4	0.13
(1,979)	1:69:A:PHE:H	1:95:A:TRP:HD1	9	0.13
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	3	0.13
(1,559)	1:80:A:THR:HB	1:89:A:VAL:HB	3	0.13
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE1	8	0.13
(1,433)	1:70:A:HIS:HB2	1:75:A:TYR:HE2	8	0.13
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE1	8	0.13
(1,433)	1:70:A:HIS:HB3	1:75:A:TYR:HE2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:69:A:PHE:H	1:95:A:TRP:HD1	9	0.13
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD1	3	0.13
(1,418)	1:69:A:PHE:HA	1:75:A:TYR:HD2	3	0.13
(1,379)	1:66:A:CYS:HB2	1:93:A:ARG:HA	5	0.13
(1,379)	1:66:A:CYS:HB3	1:93:A:ARG:HA	5	0.13
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD2	8	0.13
(1,353)	1:62:A:ALA:H	1:65:A:ARG:HD3	8	0.13
(1,92)	1:17:A:ALA:HA	1:18:A:ASP:HA	8	0.13
(1,81)	1:15:A:CYS:HB2	1:45:A:SER:HA	6	0.13
(1,81)	1:15:A:CYS:HB3	1:45:A:SER:HA	6	0.13
(1,1176)	1:102:A:CYS:HA	1:103:A:ASP:H	1	0.12
(1,1085)	1:87:A:THR:HB	1:88:A:CYS:H	2	0.12
(1,1016)	1:76:A:ALA:H	1:79:A:GLU:HG2	4	0.12
(1,1016)	1:76:A:ALA:H	1:79:A:GLU:HG3	4	0.12
(1,984)	1:70:A:HIS:H	1:74:A:GLU:HA	9	0.12
(1,819)	1:102:A:CYS:HA	1:103:A:ASP:H	1	0.12
(1,806)	1:99:A:ASP:HA	1:100:A:HIS:H	4	0.12
(1,585)	1:81:A:VAL:HA	1:83:A:ILE:HD11	4	0.12
(1,585)	1:81:A:VAL:HA	1:83:A:ILE:HD12	4	0.12
(1,585)	1:81:A:VAL:HA	1:83:A:ILE:HD13	4	0.12
(1,509)	1:76:A:ALA:H	1:79:A:GLU:HG2	4	0.12
(1,509)	1:76:A:ALA:H	1:79:A:GLU:HG3	4	0.12
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE1	8	0.12
(1,390)	1:68:A:CYS:HA	1:69:A:PHE:HE2	8	0.12
(1,359)	1:63:A:LEU:HA	1:66:A:CYS:H	3	0.12
(1,258)	1:54:A:VAL:HG11	1:63:A:LEU:H	2	0.12
(1,258)	1:54:A:VAL:HG12	1:63:A:LEU:H	2	0.12
(1,258)	1:54:A:VAL:HG13	1:63:A:LEU:H	2	0.12
(1,248)	1:54:A:VAL:HB	1:55:A:ARG:H	7	0.12
(1,92)	1:17:A:ALA:HA	1:18:A:ASP:HA	3	0.12
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG11	3	0.12
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG12	3	0.12
(1,19)	1:50:A:PRO:HD2	1:11:A:VAL:HG13	3	0.12
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG11	3	0.12
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG12	3	0.12
(1,19)	1:50:A:PRO:HD3	1:11:A:VAL:HG13	3	0.12
(1,1176)	1:102:A:CYS:HA	1:103:A:ASP:H	10	0.11
(1,1122)	1:90:A:CYS:H	1:95:A:TRP:HZ3	6	0.11
(1,1120)	1:90:A:CYS:HA	1:94:A:LYS:H	5	0.11
(1,888)	1:39:A:MET:HA	1:40:A:SER:H	9	0.11
(1,827)	1:11:A:VAL:HB	1:12:A:LYS:H	10	0.11
(1,819)	1:102:A:CYS:HA	1:103:A:ASP:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:101:A:VAL:HG11	1:102:A:CYS:HA	2	0.11
(1,813)	1:101:A:VAL:HG12	1:102:A:CYS:HA	2	0.11
(1,813)	1:101:A:VAL:HG13	1:102:A:CYS:HA	2	0.11
(1,706)	1:89:A:VAL:HB	1:90:A:CYS:H	9	0.11
(1,669)	1:87:A:THR:HB	1:88:A:CYS:HA	8	0.11
(1,652)	1:85:A:CYS:HA	1:86:A:ASN:H	7	0.11
(1,596)	1:81:A:VAL:H	1:87:A:THR:HB	8	0.11
(1,593)	1:81:A:VAL:HG21	1:83:A:ILE:HA	10	0.11
(1,593)	1:81:A:VAL:HG22	1:83:A:ILE:HA	10	0.11
(1,593)	1:81:A:VAL:HG23	1:83:A:ILE:HA	10	0.11
(1,371)	1:64:A:GLU:HA	1:66:A:CYS:H	6	0.11
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG21	10	0.11
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG22	10	0.11
(1,283)	1:55:A:ARG:HA	1:61:A:VAL:HG23	10	0.11
(1,264)	1:54:A:VAL:HG21	1:63:A:LEU:HA	10	0.11
(1,264)	1:54:A:VAL:HG22	1:63:A:LEU:HA	10	0.11
(1,264)	1:54:A:VAL:HG23	1:63:A:LEU:HA	10	0.11
(1,209)	1:43:A:CYS:HA	1:44:A:VAL:HA	1	0.11
(1,207)	1:39:A:MET:HA	1:40:A:SER:H	9	0.11
(1,201)	1:35:A:ASP:HA	1:36:A:LEU:H	8	0.11
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD2	1	0.11
(1,151)	1:30:A:THR:HA	1:55:A:ARG:HD3	1	0.11
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG21	7	0.11
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG22	7	0.11
(1,18)	1:50:A:PRO:HD2	1:11:A:VAL:HG23	7	0.11
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG21	7	0.11
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG22	7	0.11
(1,18)	1:50:A:PRO:HD3	1:11:A:VAL:HG23	7	0.11
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG11	1	0.1
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG12	1	0.1
(1,988)	1:70:A:HIS:H	1:81:A:VAL:HG13	1	0.1
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB2	4	0.1
(1,288)	1:56:A:HIS:HE1	1:57:A:GLU:HB3	4	0.1
(1,223)	1:48:A:LEU:HD21	1:49:A:CYS:H	7	0.1
(1,223)	1:48:A:LEU:HD22	1:49:A:CYS:H	7	0.1
(1,223)	1:48:A:LEU:HD23	1:49:A:CYS:H	7	0.1

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

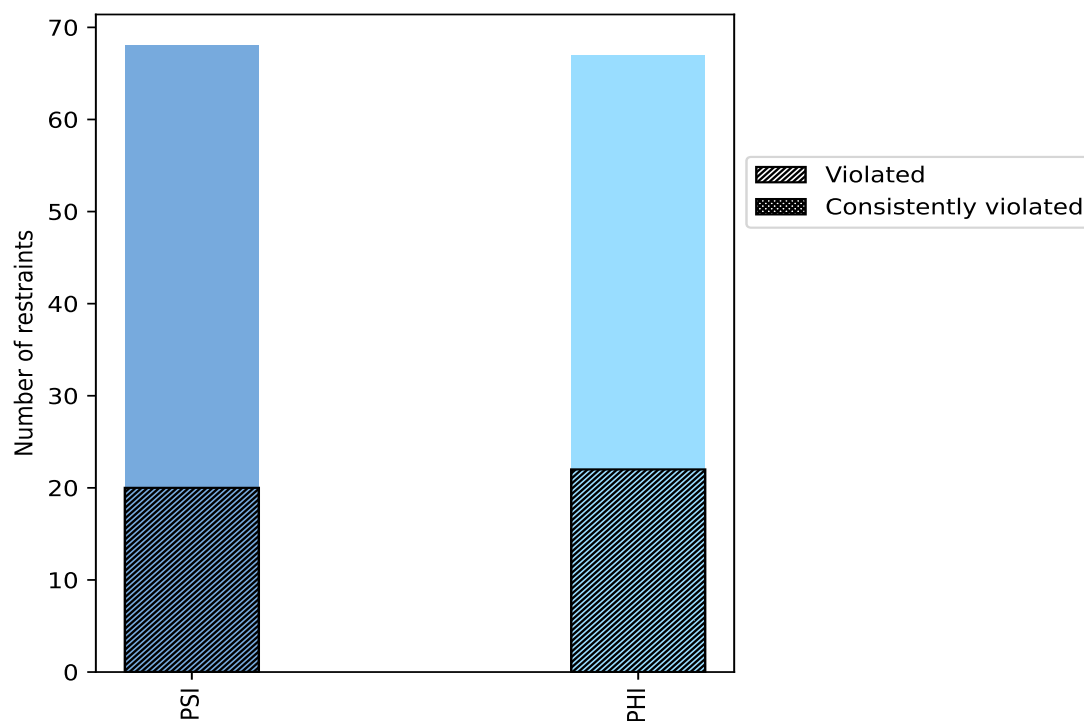
10.1 Summary of dihedral-angle violations [i](#)

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	68	50.4	20	29.4	14.8	0	0.0	0.0
PHI	67	49.6	22	32.8	16.3	0	0.0	0.0
Total	135	100.0	42	31.1	31.1	0	0.0	0.0

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

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



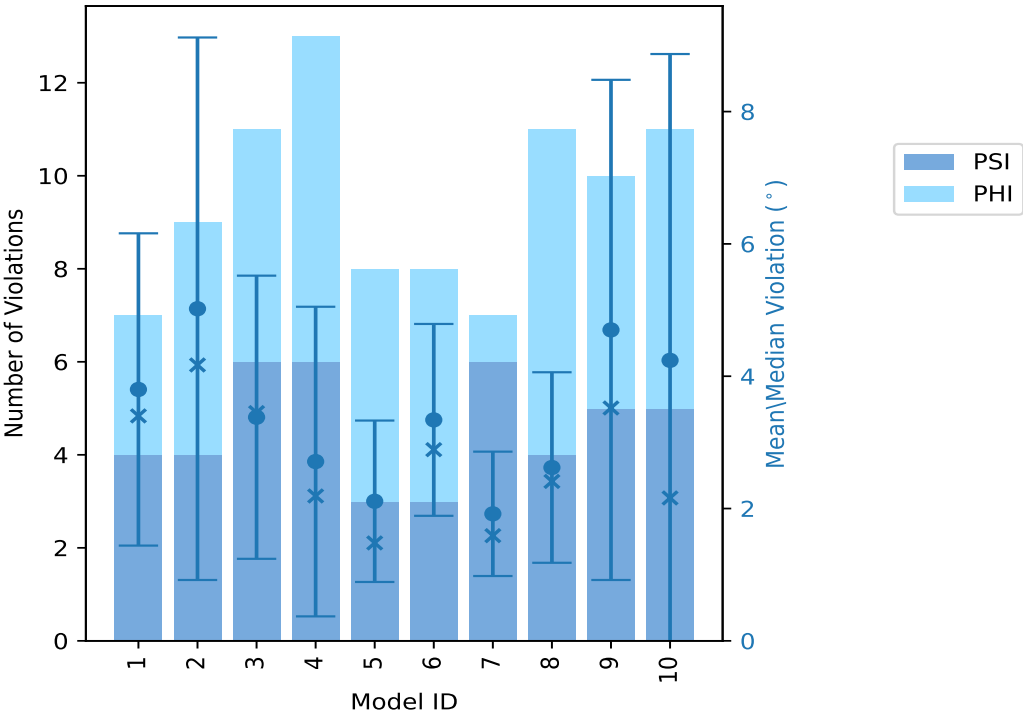
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	4	3	7	3.8	8.44	2.36	3.4
2	4	5	9	5.02	15.72	4.1	4.17
3	6	5	11	3.38	8.59	2.14	3.45
4	6	7	13	2.71	10.41	2.34	2.19
5	3	5	8	2.11	4.98	1.22	1.48
6	3	5	8	3.34	6.54	1.45	2.89
7	6	1	7	1.92	4.02	0.94	1.59
8	4	7	11	2.62	5.9	1.44	2.41
9	5	5	10	4.7	12.98	3.78	3.52
10	5	6	11	4.24	17.96	4.63	2.16

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

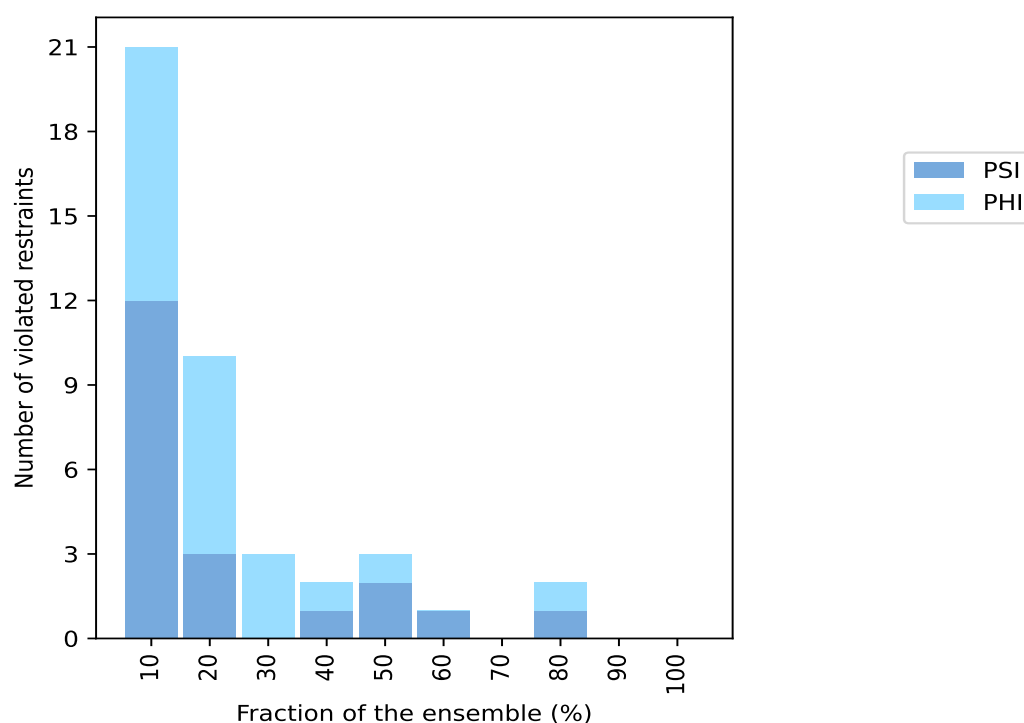
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
12	9	21	1	10.0
3	7	10	2	20.0
0	3	3	3	30.0
1	1	2	4	40.0
2	1	3	5	50.0
1	0	1	6	60.0
0	0	0	7	70.0
1	1	2	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

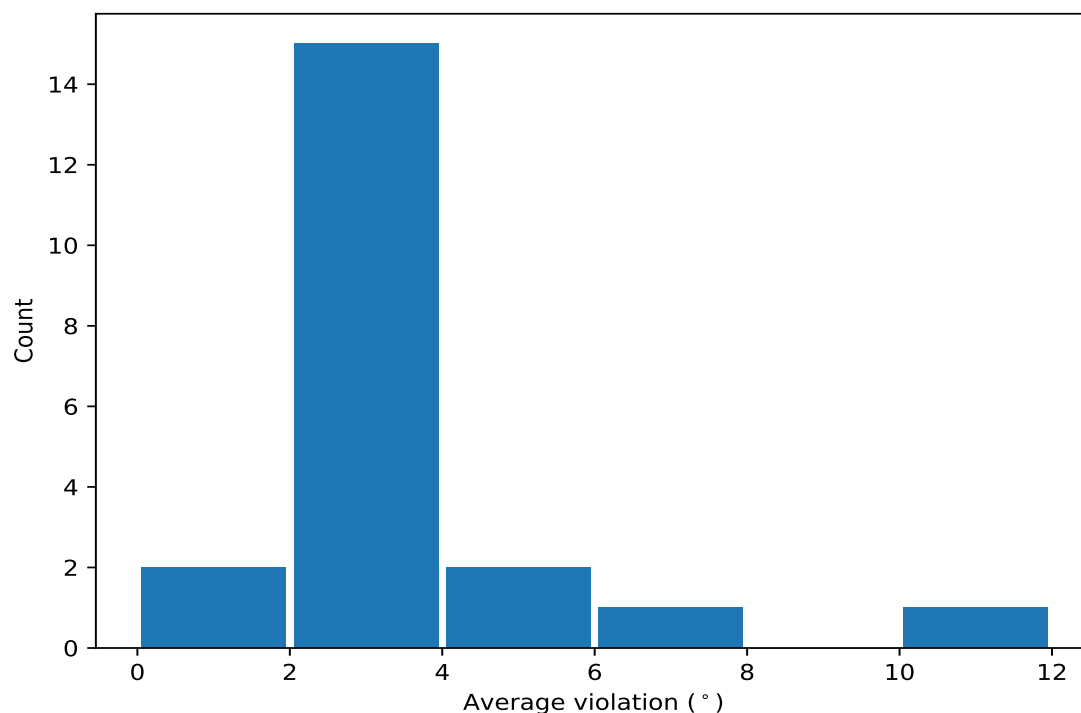
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	8	4.12	1.17	4.66
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	8	2.67	0.86	2.52
(1,133)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:ASP:N	6	10.69	5.09	9.76
(1,48)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:CYS:N	5	4.15	4.5	1.67
(1,79)	1:65:A:ARG:C	1:66:A:CYS:N	1:66:A:CYS:CA	1:66:A:CYS:C	5	2.52	1.16	2.57
(1,2)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	5	1.93	0.67	1.65
(1,19)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:ASP:N	4	3.27	1.72	2.62
(1,57)	1:54:A:VAL:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	4	2.52	1.38	2.28
(1,5)	1:9:A:PRO:C	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	3	3.32	1.83	2.18
(1,118)	1:89:A:VAL:C	1:90:A:CYS:N	1:90:A:CYS:CA	1:90:A:CYS:C	3	3.01	2.5	1.37
(1,112)	1:86:A:ASN:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	3	2.55	0.83	3.14
(1,24)	1:19:A:ASN:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	2	6.0	4.41	6.0
(1,49)	1:46:A:GLY:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	2	3.48	0.91	3.48

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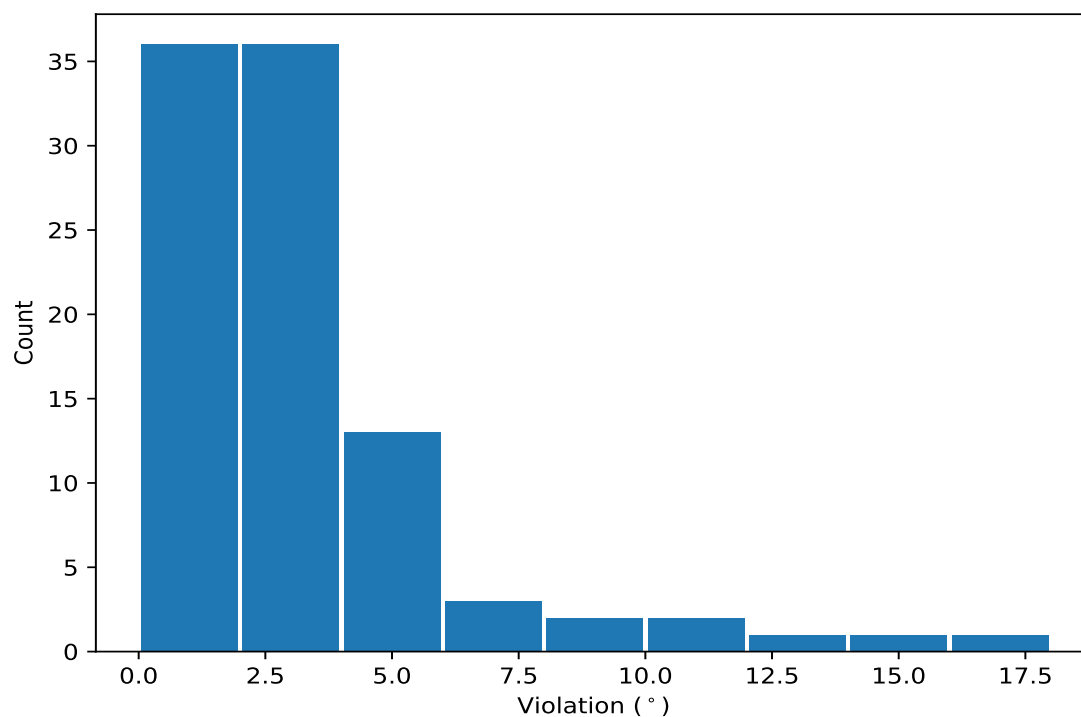
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,109)	1:82:A:LYS:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	2	2.94	1.82	2.94
(1,33)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:ASN:N	2	2.7	1.32	2.7
(1,126)	1:93:A:ARG:C	1:94:A:LYS:N	1:94:A:LYS:CA	1:94:A:LYS:C	2	2.64	0.05	2.64
(1,78)	1:65:A:ARG:N	1:65:A:ARG:CA	1:65:A:ARG:C	1:66:A:CYS:N	2	2.24	0.36	2.24
(1,103)	1:79:A:GLU:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	2	2.17	1.05	2.17
(1,67)	1:59:A:ARG:C	1:60:A:CYS:N	1:60:A:CYS:CA	1:60:A:CYS:C	2	2.09	0.73	2.09
(1,130)	1:95:A:TRP:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	2	2.08	0.33	2.08
(1,104)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:VAL:N	2	1.44	0.32	1.44

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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 (°)
(1,133)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:ASP:N	10	17.96
(1,133)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:ASP:N	2	15.72
(1,48)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:CYS:N	9	12.98
(1,133)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:ASP:N	9	10.94
(1,24)	1:19:A:ASN:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	4	10.41
(1,133)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:ASP:N	3	8.59
(1,133)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:ASP:N	1	8.44
(1,28)	1:28:A:THR:C	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	2	6.89
(1,118)	1:89:A:VAL:C	1:90:A:CYS:N	1:90:A:CYS:CA	1:90:A:CYS:C	6	6.54
(1,19)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:ASP:N	10	6.03
(1,97)	1:75:A:TYR:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	3	5.96
(1,5)	1:9:A:PRO:C	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	8	5.9
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1	5.66
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	5	4.98
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	10	4.92
(1,109)	1:82:A:LYS:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	10	4.76
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	8	4.68
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	2	4.65
(1,57)	1:54:A:VAL:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	2	4.41
(1,49)	1:46:A:GLY:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	9	4.39
(1,96)	1:75:A:TYR:N	1:75:A:TYR:CA	1:75:A:TYR:C	1:76:A:ALA:N	6	4.18
(1,27)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:ALA:N	2	4.17
(1,33)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:ASN:N	7	4.02
(1,79)	1:65:A:ARG:C	1:66:A:CYS:N	1:66:A:CYS:CA	1:66:A:CYS:C	9	3.97
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	9	3.82
(1,30)	1:29:A:LYS:C	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	2	3.77
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	1	3.71
(1,17)	1:16:A:PRO:N	1:16:A:PRO:CA	1:16:A:PRO:C	1:17:A:ALA:N	4	3.7
(1,52)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:CYS:N	3	3.69
(1,106)	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	1:82:A:LYS:N	6	3.68
(1,79)	1:65:A:ARG:C	1:66:A:CYS:N	1:66:A:CYS:CA	1:66:A:CYS:C	3	3.6
(1,48)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:CYS:N	3	3.59
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	3	3.45
(1,19)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:ASP:N	1	3.4
(1,57)	1:54:A:VAL:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	10	3.24
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	9	3.23
(1,103)	1:79:A:GLU:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	4	3.22
(1,112)	1:86:A:ASN:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	6	3.14
(1,112)	1:86:A:ASN:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	8	3.14
(1,2)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	5	3.12
(1,67)	1:59:A:ARG:C	1:60:A:CYS:N	1:60:A:CYS:CA	1:60:A:CYS:C	1	2.82
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	8	2.82
(1,126)	1:93:A:ARG:C	1:94:A:LYS:N	1:94:A:LYS:CA	1:94:A:LYS:C	9	2.69
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	6	2.64
(1,78)	1:65:A:ARG:N	1:65:A:ARG:CA	1:65:A:ARG:C	1:66:A:CYS:N	4	2.61
(1,126)	1:93:A:ARG:C	1:94:A:LYS:N	1:94:A:LYS:CA	1:94:A:LYS:C	6	2.59
(1,79)	1:65:A:ARG:C	1:66:A:CYS:N	1:66:A:CYS:CA	1:66:A:CYS:C	6	2.57
(1,49)	1:46:A:GLY:C	1:47:A:CYS:N	1:47:A:CYS:CA	1:47:A:CYS:C	3	2.57
(1,133)	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	1:99:A:ASP:N	8	2.47
(1,130)	1:95:A:TRP:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	8	2.41
(1,39)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	7	2.39
(1,18)	1:16:A:PRO:C	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	2	2.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:97:A:CYS:C	1:98:A:THR:N	1:98:A:THR:CA	1:98:A:THR:C	4	2.22
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	4	2.22
(1,2)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	4	2.19
(1,5)	1:9:A:PRO:C	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	9	2.18
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	10	2.16
(1,21)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:ASN:N	10	2.06
(1,47)	1:45:A:SER:C	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	8	2.05
(1,78)	1:65:A:ARG:N	1:65:A:ARG:CA	1:65:A:ARG:C	1:66:A:CYS:N	2	1.88
(1,5)	1:9:A:PRO:C	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	4	1.88
(1,19)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:ASP:N	3	1.85
(1,19)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:ASP:N	8	1.8
(1,104)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:VAL:N	5	1.77
(1,130)	1:95:A:TRP:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	4	1.75
(1,48)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:CYS:N	4	1.67
(1,2)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	10	1.65
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	7	1.62
(1,12)	1:13:A:LEU:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	10	1.61
(1,24)	1:19:A:ASN:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	7	1.59
(1,6)	1:10:A:MET:N	1:10:A:MET:CA	1:10:A:MET:C	1:11:A:VAL:N	5	1.55
(1,110)	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	1:84:A:GLY:N	9	1.54
(1,2)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	7	1.41
(1,79)	1:65:A:ARG:C	1:66:A:CYS:N	1:66:A:CYS:CA	1:66:A:CYS:C	5	1.4
(1,33)	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1:33:A:ASN:N	3	1.39
(1,112)	1:86:A:ASN:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	1	1.38
(1,118)	1:89:A:VAL:C	1:90:A:CYS:N	1:90:A:CYS:CA	1:90:A:CYS:C	5	1.37
(1,10)	1:12:A:LYS:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	3	1.37
(1,67)	1:59:A:ARG:C	1:60:A:CYS:N	1:60:A:CYS:CA	1:60:A:CYS:C	5	1.36
(1,48)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:CYS:N	7	1.35
(1,35)	1:33:A:ASN:N	1:33:A:ASN:CA	1:33:A:ASN:C	1:34:A:TYR:N	2	1.34
(1,13)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:CYS:N	6	1.34
(1,1)	1:7:A:ARG:C	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	5	1.34
(1,57)	1:54:A:VAL:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	8	1.31
(1,2)	1:8:A:PRO:N	1:8:A:PRO:CA	1:8:A:PRO:C	1:9:A:PRO:N	9	1.29
(1,131)	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	1:97:A:CYS:N	1	1.18
(1,48)	1:46:A:GLY:N	1:46:A:GLY:CA	1:46:A:GLY:C	1:47:A:CYS:N	8	1.17
(1,83)	1:68:A:CYS:C	1:69:A:PHE:N	1:69:A:PHE:CA	1:69:A:PHE:C	4	1.16
(1,109)	1:82:A:LYS:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	4	1.13
(1,103)	1:79:A:GLU:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	10	1.13
(1,104)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:VAL:N	4	1.12
(1,118)	1:89:A:VAL:C	1:90:A:CYS:N	1:90:A:CYS:CA	1:90:A:CYS:C	10	1.11
(1,57)	1:54:A:VAL:C	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	3	1.1
(1,9)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LEU:N	7	1.08
(1,79)	1:65:A:ARG:C	1:66:A:CYS:N	1:66:A:CYS:CA	1:66:A:CYS:C	8	1.04