



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 04:32 AM UTC

PDB ID : 5W88 / pdb_00005w88
BMRB ID : 30308
Title : NMR structure of the N-domain of troponin C bound to switch region of troponin I and 3-methyldiphenylamine (peptide mode)
Authors : Cai, F.; Hwang, P.M.; Sykes, B.D.
Deposited on : 2017-06-21

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
Mogul : 2022.3.0, CSD as543be (2022)
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

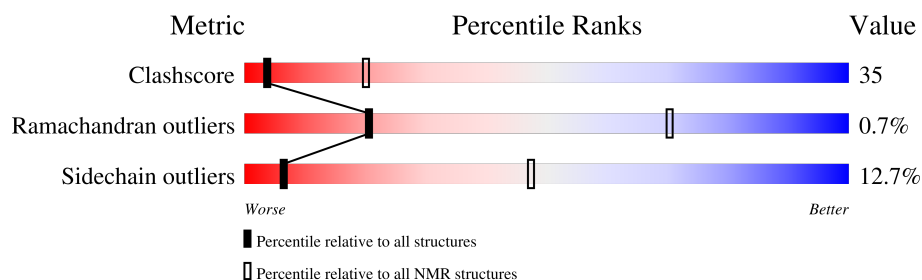
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	120	

2 Ensemble composition and analysis

This entry contains 8 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:84, A:149-A:158 (93)	0.52	4

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

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

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

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1901 atoms, of which 949 are hydrogens and 0 are deuteriums.

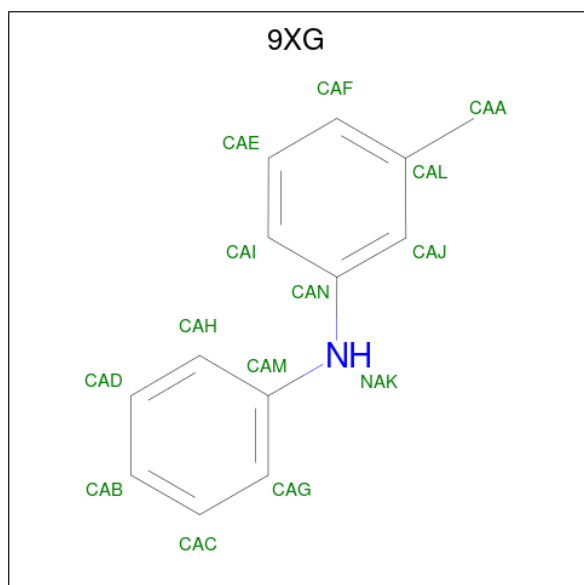
- Molecule 1 is a protein called Troponin C, Troponin I.

Mol	Chain	Residues	Atoms						Trace
1	A	120	Total	C	H	N	O	S	0
			1874	582	936	160	187	9	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	CYS	engineered mutation	UNP P63316
A	84	SER	CYS	engineered mutation	UNP P63316
A	136	GLY	-	linker	UNP P63316
A	137	LYS	-	linker	UNP P63316
A	164	GLY	-	expression tag	UNP P19429
A	165	HIS	-	expression tag	UNP P19429

- Molecule 2 is 3-methyl-N-phenylaniline (CCD ID: 9XG) (formula: C₁₃H₁₃N).



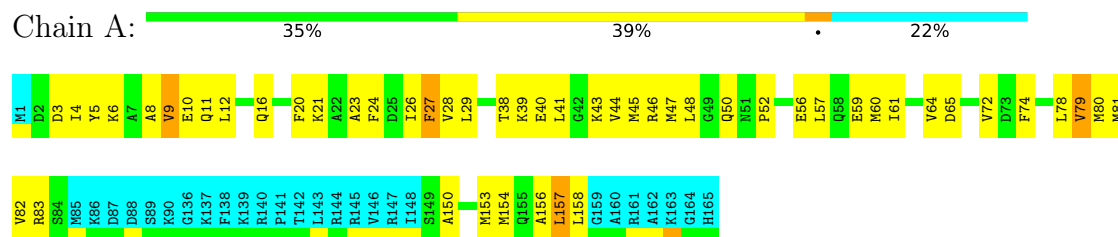
Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	N
			27	13	13	1

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: Troponin C, Troponin I

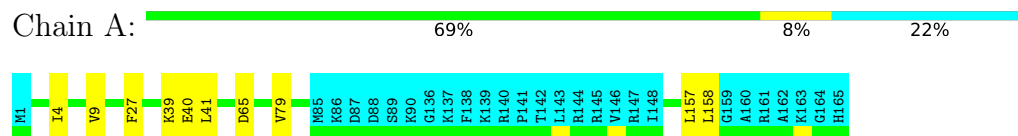


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

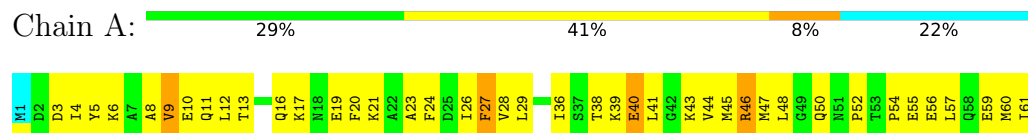
4.2.1 Score per residue for model 1

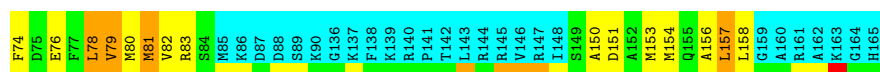
- Molecule 1: Troponin C, Troponin I



4.2.2 Score per residue for model 2

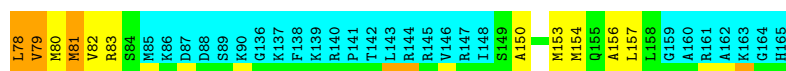
- Molecule 1: Troponin C, Troponin I





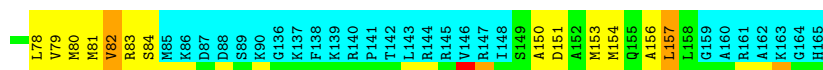
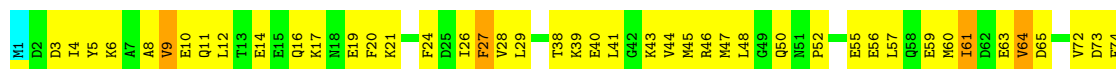
4.2.3 Score per residue for model 3

- Molecule 1: Troponin C, Troponin I



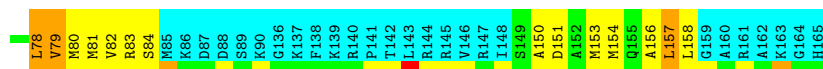
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Troponin C, Troponin I



4.2.5 Score per residue for model 5

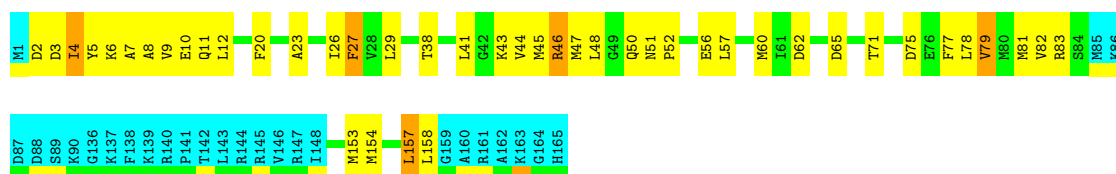
- Molecule 1: Troponin C, Troponin I



4.2.6 Score per residue for model 6

- Molecule 1: Troponin C, Troponin I

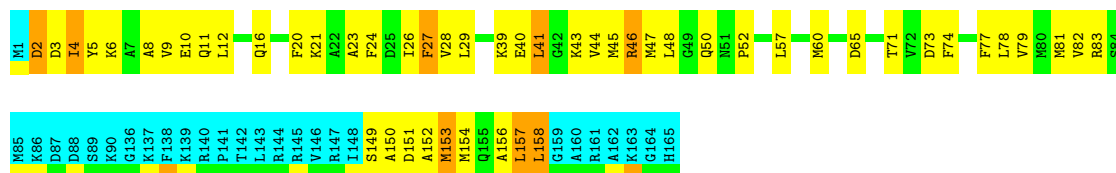




4.2.7 Score per residue for model 7

- Molecule 1: Troponin C, Troponin I

Chain A: 35% 36% 7% 22%



4.2.8 Score per residue for model 8

- Molecule 1: Troponin C, Troponin I

Chain A: 35% 39% • 22%



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 8 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA2	structure calculation	
ARIA2	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	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9XG

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	720	692	692	46±19
2	A	14	13	0	0±0
All	All	5872	5640	4844	370

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:O	1:A:48:LEU:HG	0.78	1.78	7	3
1:A:5:TYR:HB3	1:A:82:VAL:HG13	0.76	1.57	7	2
1:A:61:ILE:HG23	1:A:72:VAL:HG23	0.76	1.57	5	5
1:A:20:PHE:CE2	1:A:81:MET:HE2	0.74	2.18	2	3
1:A:20:PHE:CE1	1:A:81:MET:HE2	0.73	2.18	3	1
1:A:5:TYR:CD1	1:A:83:ARG:HG3	0.73	2.19	2	4
1:A:81:MET:HE1	1:A:150:ALA:HB1	0.71	1.62	4	3
1:A:74:PHE:CZ	1:A:78:LEU:HD22	0.70	2.22	4	3
1:A:5:TYR:CE2	1:A:83:ARG:HG3	0.69	2.22	3	1
1:A:150:ALA:O	1:A:154:MET:HG3	0.69	1.86	5	6
1:A:26:ILE:HG22	1:A:157:LEU:HD12	0.69	1.64	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:TYR:CE1	1:A:83:ARG:HG3	0.69	2.23	2	4
1:A:26:ILE:O	1:A:29:LEU:HG	0.69	1.88	6	6
1:A:27:PHE:HE2	1:A:153:MET:SD	0.69	2.11	7	1
1:A:20:PHE:HE1	1:A:154:MET:SD	0.67	2.13	3	1
1:A:43:LYS:HE3	1:A:47:MET:SD	0.65	2.32	6	4
1:A:57:LEU:HD23	1:A:60:MET:CE	0.65	2.21	7	3
1:A:27:PHE:HE1	1:A:153:MET:SD	0.65	2.15	3	3
1:A:6:LYS:O	1:A:10:GLU:HG3	0.64	1.92	5	4
1:A:157:LEU:HD22	1:A:157:LEU:H	0.64	1.52	4	1
1:A:26:ILE:HG23	1:A:29:LEU:HD11	0.63	1.71	5	6
1:A:26:ILE:CG2	1:A:157:LEU:HB3	0.63	2.24	5	3
1:A:38:THR:O	1:A:57:LEU:HD13	0.63	1.94	3	5
1:A:8:ALA:O	1:A:12:LEU:HG	0.62	1.94	6	5
1:A:46:ARG:HD2	1:A:52:PRO:HD2	0.62	1.72	8	3
1:A:41:LEU:HD21	1:A:60:MET:HE3	0.61	1.71	4	3
1:A:27:PHE:HE1	1:A:41:LEU:HD12	0.61	1.56	4	2
1:A:12:LEU:HB3	1:A:16:GLN:CB	0.61	2.26	8	3
1:A:40:GLU:O	1:A:43:LYS:HB3	0.61	1.95	3	3
1:A:55:GLU:O	1:A:59:GLU:HG2	0.60	1.96	2	2
1:A:9:VAL:CG2	1:A:78:LEU:HD13	0.60	2.27	3	2
1:A:8:ALA:HA	1:A:11:GLN:HB2	0.60	1.74	4	2
1:A:44:VAL:O	1:A:47:MET:HB2	0.60	1.96	8	6
1:A:45:MET:SD	1:A:60:MET:HE1	0.59	2.38	6	3
1:A:48:LEU:HD21	1:A:156:ALA:HB2	0.59	1.75	4	4
1:A:27:PHE:CE2	1:A:41:LEU:HD13	0.58	2.34	8	1
1:A:6:LYS:O	1:A:9:VAL:HG13	0.58	1.98	4	3
1:A:48:LEU:CD2	1:A:156:ALA:HB2	0.58	2.28	2	5
1:A:81:MET:HA	1:A:81:MET:HE2	0.58	1.76	8	1
1:A:27:PHE:CE1	1:A:157:LEU:HD21	0.57	2.34	3	1
1:A:27:PHE:CE2	1:A:153:MET:SD	0.57	2.97	7	1
1:A:79:VAL:O	1:A:83:ARG:HB2	0.57	1.99	2	6
1:A:3:ASP:HA	1:A:6:LYS:HB3	0.57	1.77	5	7
1:A:154:MET:HE2	1:A:158:LEU:HD11	0.57	1.75	2	2
1:A:3:ASP:HA	1:A:6:LYS:CB	0.57	2.29	6	7
1:A:64:VAL:CG1	1:A:80:MET:HB2	0.57	2.30	2	1
1:A:64:VAL:HG11	1:A:80:MET:HB2	0.57	1.75	4	3
1:A:77:PHE:O	1:A:81:MET:HG2	0.57	1.99	7	2
1:A:44:VAL:HA	1:A:47:MET:SD	0.56	2.40	8	1
1:A:12:LEU:HD22	1:A:16:GLN:CG	0.56	2.30	2	3
1:A:26:ILE:HA	1:A:29:LEU:HG	0.56	1.76	3	3
1:A:27:PHE:CE1	1:A:153:MET:SD	0.56	2.99	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:MET:HE3	1:A:81:MET:C	0.56	2.25	2	2
1:A:7:ALA:O	1:A:11:GLN:HG3	0.56	2.00	3	1
1:A:5:TYR:CD2	1:A:83:ARG:HG3	0.56	2.35	7	2
1:A:46:ARG:HA	1:A:50:GLN:O	0.55	2.02	6	6
1:A:27:PHE:HE2	1:A:41:LEU:HD12	0.55	1.61	2	1
1:A:21:LYS:HA	1:A:74:PHE:CE1	0.55	2.36	4	3
1:A:74:PHE:CE1	1:A:78:LEU:HG	0.54	2.38	5	2
1:A:74:PHE:CE2	1:A:78:LEU:HG	0.54	2.38	3	1
1:A:154:MET:HB3	1:A:158:LEU:HD12	0.54	1.80	6	1
1:A:13:THR:OG1	1:A:16:GLN:HB2	0.54	2.03	5	2
1:A:20:PHE:CE1	1:A:154:MET:SD	0.54	3.00	3	1
1:A:12:LEU:HD22	1:A:16:GLN:HG2	0.53	1.79	2	3
1:A:8:ALA:O	1:A:11:GLN:HB3	0.53	2.03	6	1
1:A:41:LEU:O	1:A:45:MET:HG2	0.53	2.04	4	2
1:A:26:ILE:HA	1:A:29:LEU:CG	0.53	2.34	3	3
1:A:21:LYS:O	1:A:24:PHE:HB3	0.53	2.03	2	5
1:A:78:LEU:O	1:A:81:MET:HB2	0.52	2.04	6	2
1:A:9:VAL:HG23	1:A:78:LEU:HD13	0.52	1.80	3	1
1:A:20:PHE:CZ	1:A:81:MET:HE2	0.52	2.40	3	1
1:A:20:PHE:HE2	1:A:154:MET:SD	0.52	2.27	5	3
1:A:157:LEU:N	1:A:157:LEU:HD13	0.52	2.19	4	2
1:A:9:VAL:HB	1:A:78:LEU:HG	0.52	1.82	4	1
1:A:9:VAL:O	1:A:17:LYS:HD3	0.52	2.04	2	4
1:A:26:ILE:CG2	1:A:157:LEU:HD12	0.52	2.35	3	1
1:A:23:ALA:HB1	1:A:157:LEU:HD23	0.51	1.81	2	1
1:A:23:ALA:HA	1:A:157:LEU:HD12	0.51	1.82	7	1
1:A:26:ILE:HB	1:A:157:LEU:CB	0.51	2.35	4	1
1:A:24:PHE:CZ	1:A:73:ASP:HA	0.50	2.41	4	2
1:A:12:LEU:HB3	1:A:16:GLN:HB2	0.50	1.83	8	2
1:A:20:PHE:HD1	1:A:78:LEU:CD1	0.50	2.20	7	1
1:A:8:ALA:HA	1:A:11:GLN:HG3	0.50	1.84	3	1
1:A:45:MET:C	1:A:50:GLN:HB2	0.49	2.31	6	2
1:A:8:ALA:O	1:A:11:GLN:HB2	0.49	2.06	2	1
1:A:8:ALA:HA	1:A:11:GLN:HB3	0.49	1.83	7	1
1:A:20:PHE:CD2	1:A:78:LEU:HD21	0.49	2.43	3	1
1:A:8:ALA:CB	1:A:82:VAL:HG11	0.49	2.37	4	1
1:A:28:VAL:CG1	1:A:36:ILE:HG13	0.49	2.37	5	2
1:A:8:ALA:HA	1:A:11:GLN:CG	0.49	2.37	3	1
1:A:27:PHE:HE2	1:A:41:LEU:HD13	0.49	1.67	3	1
1:A:52:PRO:HA	1:A:56:GLU:OE1	0.49	2.08	5	2
1:A:44:VAL:CG2	1:A:157:LEU:HD11	0.49	2.38	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ALA:CA	1:A:11:GLN:HB2	0.48	2.37	4	2
1:A:46:ARG:HG3	1:A:50:GLN:O	0.48	2.09	6	4
1:A:27:PHE:CE2	1:A:41:LEU:HA	0.48	2.42	8	1
1:A:80:MET:SD	1:A:83:ARG:HD3	0.48	2.48	2	2
1:A:151:ASP:O	1:A:154:MET:HB2	0.48	2.09	2	4
1:A:52:PRO:HB2	1:A:57:LEU:HD11	0.48	1.86	8	4
1:A:41:LEU:CD2	1:A:60:MET:HE3	0.47	2.39	6	2
1:A:41:LEU:HG	1:A:60:MET:HE3	0.47	1.86	7	1
1:A:13:THR:OG1	1:A:16:GLN:HG2	0.47	2.10	8	1
1:A:24:PHE:O	1:A:28:VAL:HG22	0.47	2.08	8	3
1:A:57:LEU:HA	1:A:60:MET:HE2	0.47	1.87	8	1
1:A:78:LEU:HD12	1:A:78:LEU:O	0.47	2.10	8	1
1:A:27:PHE:CE2	1:A:41:LEU:HD12	0.47	2.45	2	1
1:A:46:ARG:HD2	1:A:51:ASN:HA	0.47	1.87	6	1
1:A:27:PHE:CZ	1:A:41:LEU:HD13	0.47	2.44	8	1
1:A:5:TYR:CE2	1:A:83:ARG:HA	0.46	2.45	2	1
1:A:5:TYR:CE1	1:A:83:ARG:HA	0.46	2.45	3	1
1:A:27:PHE:CD1	1:A:157:LEU:HD21	0.46	2.45	6	2
1:A:27:PHE:CE1	1:A:44:VAL:HG11	0.46	2.44	8	1
1:A:41:LEU:HD21	1:A:60:MET:HB2	0.46	1.88	2	1
1:A:4:ILE:HG23	1:A:5:TYR:N	0.46	2.26	3	1
1:A:7:ALA:HA	1:A:10:GLU:HG3	0.46	1.86	6	2
1:A:9:VAL:HA	1:A:12:LEU:HG	0.46	1.87	6	3
1:A:50:GLN:NE2	1:A:50:GLN:HA	0.46	2.25	7	1
1:A:8:ALA:HB1	1:A:82:VAL:HG11	0.46	1.87	4	1
1:A:41:LEU:HD12	1:A:45:MET:CG	0.46	2.41	7	1
1:A:44:VAL:HG22	1:A:157:LEU:HD22	0.46	1.88	7	1
1:A:64:VAL:HG21	1:A:80:MET:HB2	0.46	1.86	8	1
1:A:21:LYS:HA	1:A:74:PHE:CE2	0.46	2.46	7	2
1:A:27:PHE:HE2	1:A:41:LEU:CD1	0.45	2.23	2	1
1:A:9:VAL:HA	1:A:12:LEU:CD1	0.45	2.41	5	1
1:A:5:TYR:HA	1:A:8:ALA:HB3	0.45	1.86	8	3
1:A:44:VAL:CG2	1:A:157:LEU:HD22	0.45	2.42	7	1
1:A:26:ILE:HB	1:A:157:LEU:HB3	0.45	1.89	4	3
1:A:44:VAL:HA	1:A:47:MET:HB2	0.45	1.88	3	3
1:A:8:ALA:HA	1:A:11:GLN:CB	0.45	2.41	7	1
1:A:9:VAL:HA	1:A:12:LEU:HD12	0.45	1.87	5	2
1:A:81:MET:HA	1:A:81:MET:CE	0.45	2.40	8	1
1:A:27:PHE:CE2	1:A:41:LEU:CD1	0.45	3.00	2	1
1:A:151:ASP:HA	1:A:154:MET:SD	0.45	2.52	5	2
1:A:13:THR:OG1	1:A:16:GLN:N	0.44	2.47	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ALA:C	1:A:11:GLN:HB2	0.44	2.38	2	2
1:A:52:PRO:CG	1:A:57:LEU:HD21	0.44	2.43	8	2
1:A:43:LYS:O	1:A:47:MET:HG3	0.44	2.13	5	1
1:A:52:PRO:HB2	1:A:57:LEU:CD1	0.44	2.43	7	1
1:A:63:GLU:HG3	1:A:83:ARG:NH1	0.44	2.27	8	1
1:A:28:VAL:HA	1:A:40:GLU:HG3	0.44	1.89	5	1
1:A:6:LYS:O	1:A:10:GLU:HG2	0.44	2.12	7	1
1:A:5:TYR:CD2	1:A:83:ARG:HA	0.44	2.48	2	1
1:A:153:MET:C	1:A:153:MET:SD	0.44	3.01	8	1
1:A:2:ASP:OD2	1:A:4:ILE:HG22	0.44	2.13	6	1
1:A:41:LEU:HD12	1:A:45:MET:HG2	0.44	1.90	7	1
1:A:12:LEU:HB3	1:A:16:GLN:HB3	0.43	1.90	8	3
1:A:23:ALA:HA	1:A:157:LEU:CD1	0.43	2.43	7	1
1:A:41:LEU:HD12	1:A:41:LEU:C	0.43	2.39	3	1
1:A:17:LYS:HG2	1:A:78:LEU:HD21	0.43	1.89	4	1
1:A:7:ALA:HA	1:A:10:GLU:CG	0.43	2.43	8	1
1:A:45:MET:CB	1:A:52:PRO:HG3	0.43	2.43	7	1
1:A:23:ALA:HA	1:A:26:ILE:HD12	0.43	1.89	2	1
1:A:153:MET:SD	2:A:201:9XG:CAL	0.43	3.07	5	2
1:A:12:LEU:HD13	1:A:20:PHE:HE1	0.43	1.73	8	1
1:A:27:PHE:CD1	1:A:44:VAL:HG21	0.43	2.48	8	1
1:A:54:PRO:HA	1:A:57:LEU:HD12	0.43	1.90	2	1
1:A:26:ILE:CB	1:A:157:LEU:HB3	0.43	2.44	5	1
1:A:2:ASP:O	1:A:6:LYS:HB2	0.43	2.14	7	1
1:A:8:ALA:CB	1:A:82:VAL:HG21	0.43	2.44	7	2
1:A:153:MET:O	1:A:157:LEU:HD22	0.42	2.14	2	1
1:A:79:VAL:O	1:A:82:VAL:HG23	0.42	2.14	4	1
1:A:20:PHE:CD1	1:A:78:LEU:HD21	0.42	2.50	5	2
1:A:5:TYR:O	1:A:9:VAL:HG12	0.42	2.13	4	1
1:A:59:GLU:O	1:A:63:GLU:HG2	0.42	2.14	4	1
1:A:73:ASP:O	1:A:76:GLU:HB2	0.42	2.14	3	1
1:A:78:LEU:O	1:A:78:LEU:HD12	0.42	2.14	6	1
1:A:154:MET:O	1:A:158:LEU:HG	0.42	2.14	2	1
1:A:79:VAL:CG1	1:A:80:MET:N	0.42	2.82	3	1
1:A:27:PHE:CG	1:A:44:VAL:HG21	0.42	2.49	4	1
1:A:26:ILE:C	1:A:29:LEU:HG	0.42	2.39	5	1
1:A:153:MET:SD	1:A:154:MET:N	0.42	2.93	7	1
1:A:23:ALA:O	1:A:27:PHE:HB2	0.42	2.15	5	2
1:A:151:ASP:HA	1:A:154:MET:CG	0.42	2.45	5	1
1:A:64:VAL:CG2	1:A:76:GLU:HB3	0.41	2.45	2	2
1:A:6:LYS:N	1:A:79:VAL:HG23	0.41	2.30	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:CE1	1:A:41:LEU:HD12	0.41	2.50	5	1
1:A:5:TYR:CB	1:A:79:VAL:HG22	0.41	2.45	6	1
1:A:9:VAL:CG2	1:A:78:LEU:HG	0.41	2.45	7	1
1:A:8:ALA:HB1	1:A:82:VAL:HG21	0.41	1.92	8	1
1:A:36:ILE:O	1:A:71:THR:HA	0.41	2.16	3	1
1:A:23:ALA:HB2	1:A:158:LEU:HD11	0.41	1.92	6	1
1:A:5:TYR:HB2	1:A:79:VAL:HG22	0.41	1.90	4	1
1:A:62:ASP:HA	1:A:65:ASP:HB3	0.41	1.91	6	1
1:A:149:SER:HB2	1:A:152:ALA:HB3	0.41	1.92	7	1
1:A:153:MET:SD	1:A:153:MET:C	0.41	3.03	3	1
1:A:26:ILE:HD13	1:A:157:LEU:O	0.41	2.16	5	1
1:A:23:ALA:O	1:A:157:LEU:HD23	0.41	2.16	8	1
1:A:52:PRO:CB	1:A:57:LEU:HD21	0.41	2.46	2	1
1:A:5:TYR:HB3	1:A:82:VAL:CG1	0.41	2.39	7	1
1:A:80:MET:HA	1:A:83:ARG:HB3	0.40	1.92	4	1
1:A:3:ASP:HA	1:A:6:LYS:HB2	0.40	1.93	6	1
1:A:4:ILE:HG23	1:A:5:TYR:CD2	0.40	2.51	7	1
1:A:35:SER:HB2	1:A:71:THR:HB	0.40	1.93	3	1
1:A:6:LYS:O	1:A:9:VAL:HB	0.40	2.17	6	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	93/120 (78%)	88±1 (94±1%)	4±1 (5±2%)	1±0 (1±1%)	20	70
All	All	744/960 (78%)	703 (94%)	36 (5%)	5 (1%)	20	70

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	65	ASP	5

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	79/101 (78%)	69±2 (87±3%)	10±2 (13±3%)	6 47
All	All	632/808 (78%)	552 (87%)	80 (13%)	6 47

All 23 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	4	ILE	7
1	A	27	PHE	7
1	A	79	VAL	7
1	A	39	LYS	6
1	A	40	GLU	6
1	A	157	LEU	6
1	A	9	VAL	5
1	A	64	VAL	5
1	A	41	LEU	4
1	A	46	ARG	4
1	A	78	LEU	3
1	A	81	MET	3
1	A	71	THR	3
1	A	158	LEU	2
1	A	19	GLU	2
1	A	61	ILE	2
1	A	2	ASP	2
1	A	14	GLU	1
1	A	82	VAL	1
1	A	43	LYS	1
1	A	59	GLU	1
1	A	73	ASP	1
1	A	153	MET	1

6.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	9XG	A	201	-	15,15,15	1.63±0.01	3±0 (20±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	9XG	A	201	-	19,19,19	0.48±0.03	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9XG	A	201	-	-	0±0,4,4,4	0±0,2,2,2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	9XG	CAA-CAL	4.02	1.39	1.51	1	8
2	A	201	9XG	CAM-NAK	3.50	1.33	1.40	3	8
2	A	201	9XG	CAN-NAK	3.45	1.33	1.40	5	8

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 87% 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

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	119	-0.13 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	110	0.09 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	114	-0.40 ± 0.12	None needed (< 0.5 ppm)
^{15}N	111	0.03 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1110 atoms were assigned a chemical shift out of a possible 1218. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	463/467 (99%)	188/190 (99%)	186/186 (100%)	89/91 (98%)
Sidechain	617/692 (89%)	422/448 (94%)	195/226 (86%)	0/18 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	30/59 (51%)	15/29 (52%)	15/30 (50%)	0/0 (—%)
Overall	1110/1218 (91%)	625/667 (94%)	396/442 (90%)	89/109 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1420 atoms were assigned a chemical shift out of a possible 1623. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	583/603 (97%)	239/246 (97%)	233/240 (97%)	111/117 (95%)
Sidechain	805/943 (85%)	549/608 (90%)	256/297 (86%)	0/38 (0%)
Aromatic	32/77 (42%)	16/38 (42%)	16/37 (43%)	0/2 (0%)
Overall	1420/1623 (87%)	804/892 (90%)	505/574 (88%)	111/157 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

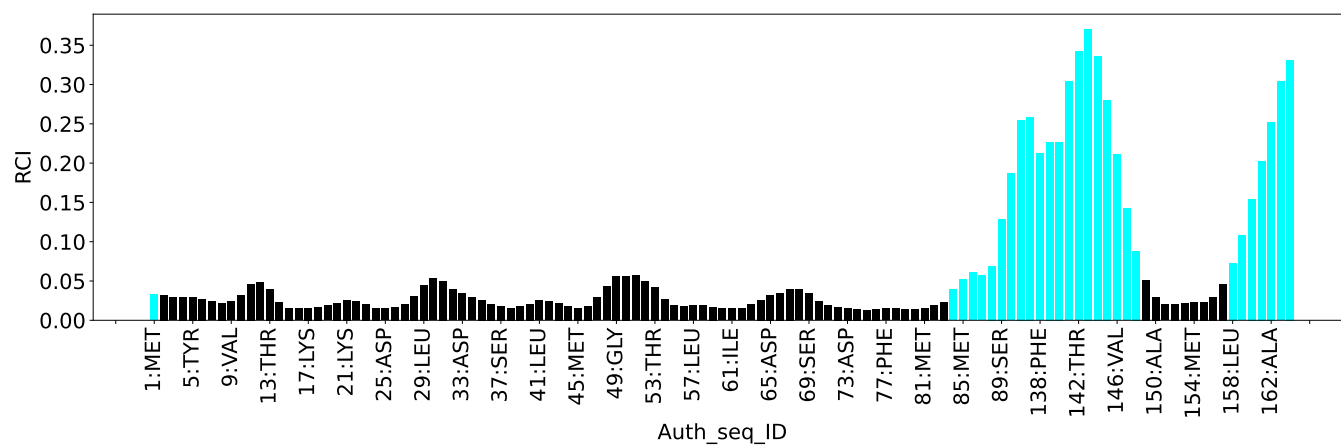
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	21	LYS	HD3	0.46	0.54 – 2.65	-5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1983
Intra-residue ($ i-j =0$)	785
Sequential ($ i-j =1$)	315
Medium range ($ i-j >1$ and $ i-j <5$)	363
Long range ($ i-j \geq 5$)	496
Inter-chain	24
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.4
Number of long range restraints per residue ¹	4.1

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)	75.2	0.2
0.2-0.5 (Medium)	145.8	0.5
>0.5 (Large)	134.9	8.22

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

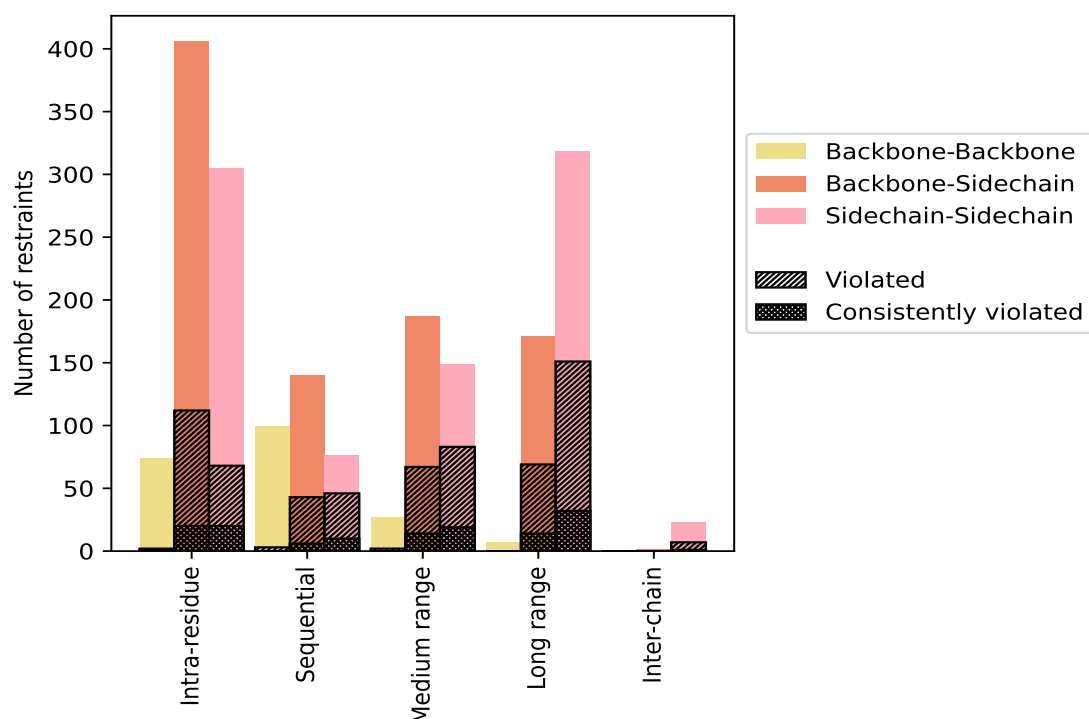
9.1 Summary of distance violations ⓘ

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)	785	39.6	182	23.2	9.2	41	5.2	2.1
Backbone-Backbone	74	3.7	2	2.7	0.1	1	1.4	0.1
Backbone-Sidechain	406	20.5	112	27.6	5.6	20	4.9	1.0
Sidechain-Sidechain	305	15.4	68	22.3	3.4	20	6.6	1.0
Sequential (i-j =1)	315	15.9	92	29.2	4.6	16	5.1	0.8
Backbone-Backbone	99	5.0	3	3.0	0.2	0	0.0	0.0
Backbone-Sidechain	140	7.1	43	30.7	2.2	6	4.3	0.3
Sidechain-Sidechain	76	3.8	46	60.5	2.3	10	13.2	0.5
Medium range (i-j >1 & i-j <5)	363	18.3	152	41.9	7.7	33	9.1	1.7
Backbone-Backbone	27	1.4	2	7.4	0.1	0	0.0	0.0
Backbone-Sidechain	187	9.4	67	35.8	3.4	14	7.5	0.7
Sidechain-Sidechain	149	7.5	83	55.7	4.2	19	12.8	1.0
Long range (i-j ≥5)	496	25.0	220	44.4	11.1	46	9.3	2.3
Backbone-Backbone	7	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	171	8.6	69	40.4	3.5	14	8.2	0.7
Sidechain-Sidechain	318	16.0	151	47.5	7.6	32	10.1	1.6
Inter-chain	24	1.2	7	29.2	0.4	1	4.2	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	23	1.2	7	30.4	0.4	1	4.3	0.1
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	1983	100.0	653	32.9	32.9	137	6.9	6.9
Backbone-Backbone	207	10.4	7	3.4	0.4	1	0.5	0.1
Backbone-Sidechain	905	45.6	291	32.2	14.7	54	6.0	2.7
Sidechain-Sidechain	871	43.9	355	40.8	17.9	82	9.4	4.1

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

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

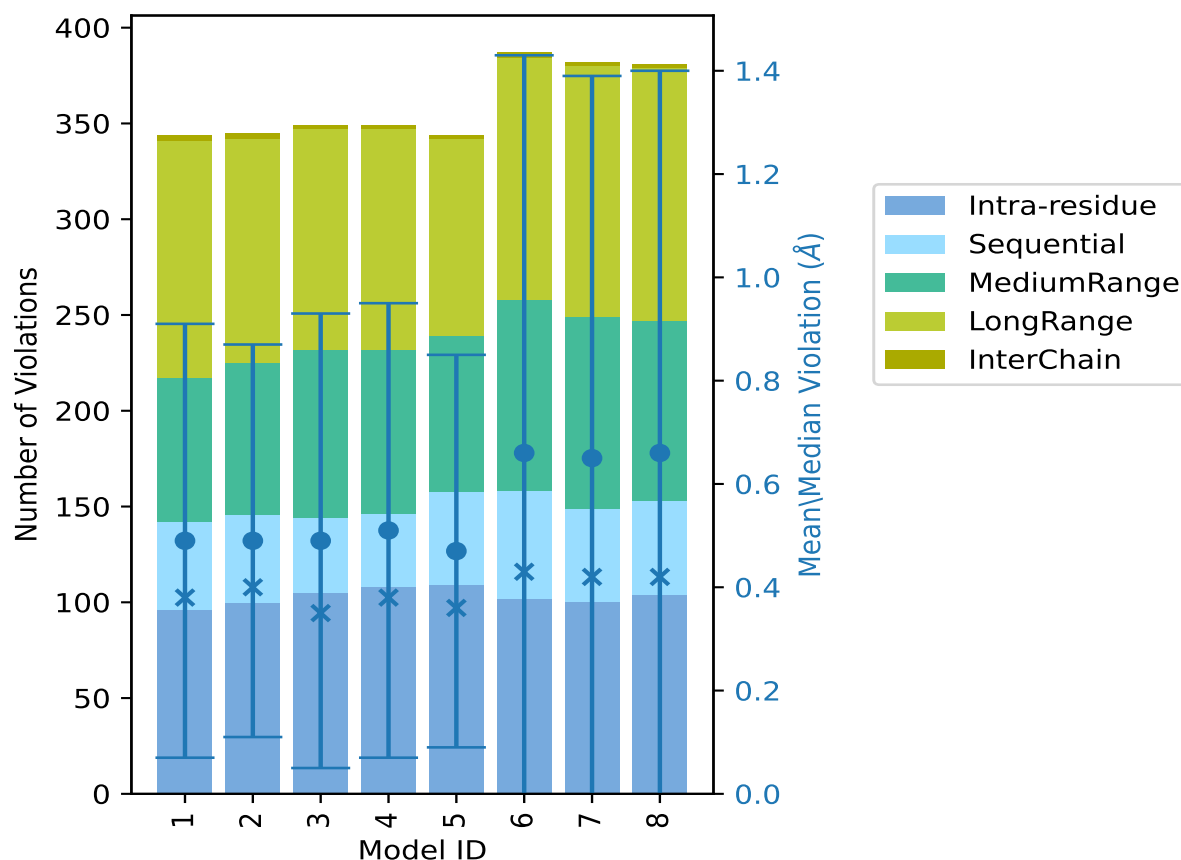
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	96	46	75	124	3	344	0.49	3.35	0.42	0.38
2	100	46	79	117	3	345	0.49	2.72	0.38	0.4
3	105	39	88	115	2	349	0.49	3.5	0.44	0.35
4	108	38	86	115	2	349	0.51	3.67	0.44	0.38
5	109	49	81	103	2	344	0.47	2.77	0.38	0.36
6	102	56	100	126	3	387	0.66	8.22	0.77	0.43
7	100	49	100	131	2	382	0.65	6.99	0.74	0.42
8	104	49	94	132	2	381	0.66	7.7	0.74	0.42

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, 1330(IR:603, SQ:223, MR:211, LR:276, IC:17) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
25	22	24	34	3	108	1	12.5
26	10	20	24	1	81	2	25.0
26	12	21	34	2	95	3	37.5
20	5	14	27	0	66	4	50.0
19	13	20	26	0	78	5	62.5
10	8	7	15	0	40	6	75.0

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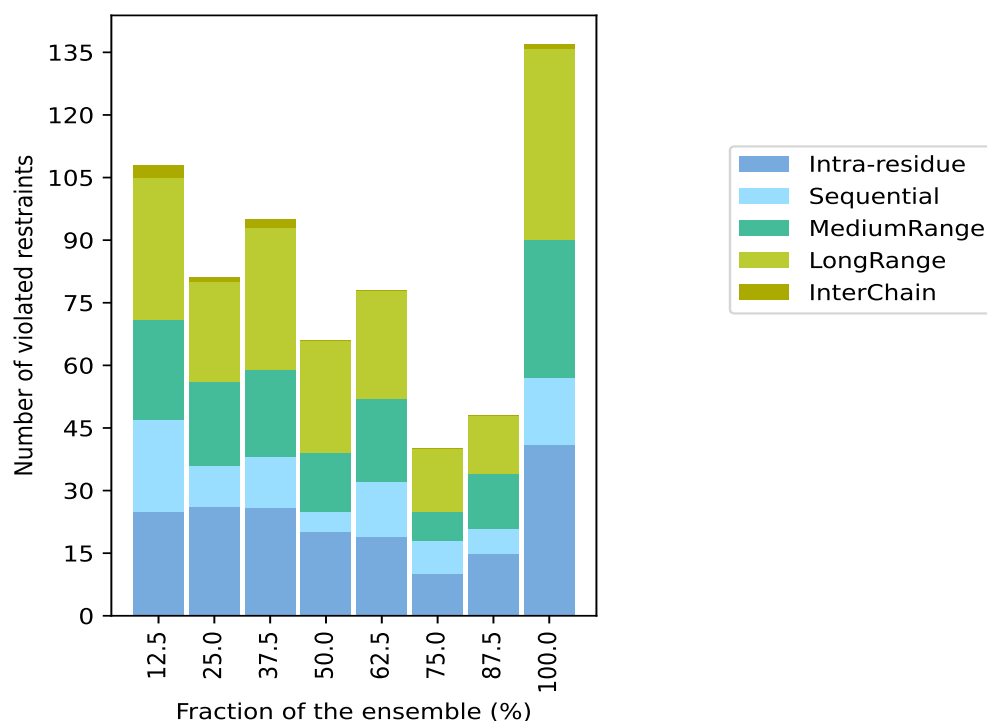
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
15	6	13	14	0	48	7	87.5
41	16	33	46	1	137	8	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

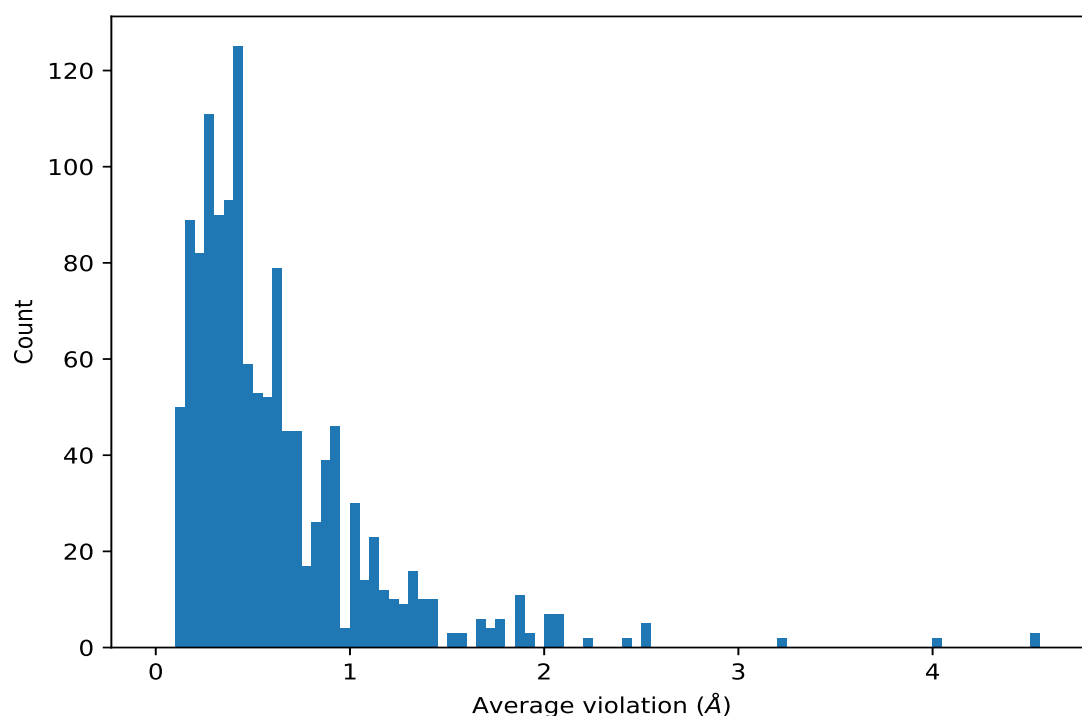
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



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)
(2,1063)	1:145:A:ARG:HD3	1:142:A:THR:HA	8	3.24	3.42	0.73
(2,1063)	1:145:A:ARG:HD2	1:142:A:THR:HA	8	3.24	3.42	0.73
(1,166)	1:158:A:LEU:HD13	1:78:A:LEU:HD13	8	2.05	0.84	2.45
(1,166)	1:158:A:LEU:HD11	1:44:A:VAL:HG13	8	2.05	0.84	2.45
(1,166)	1:158:A:LEU:HD13	1:44:A:VAL:HG12	8	2.05	0.84	2.45
(1,166)	1:158:A:LEU:HD11	1:78:A:LEU:HD12	8	2.05	0.84	2.45
(1,166)	1:158:A:LEU:HD12	1:44:A:VAL:HG12	8	2.05	0.84	2.45
(1,166)	1:158:A:LEU:HD12	1:44:A:VAL:HG13	8	2.05	0.84	2.45
(1,166)	1:158:A:LEU:HD12	1:78:A:LEU:HD13	8	2.05	0.84	2.45
(1,125)	1:160:A:ALA:HB1	1:26:A:ILE:HB	8	1.91	1.46	0.92
(1,125)	1:160:A:ALA:HB3	1:26:A:ILE:HB	8	1.91	1.46	0.92
(1,125)	1:160:A:ALA:HB2	1:26:A:ILE:HB	8	1.91	1.46	0.92
(1,104)	1:4:A:ILE:HG23	1:80:A:MET:HB2	8	1.87	0.28	1.92
(1,104)	1:4:A:ILE:HG22	1:80:A:MET:HB2	8	1.87	0.28	1.92
(1,104)	1:4:A:ILE:HG21	1:80:A:MET:HB2	8	1.87	0.28	1.92
(1,104)	1:4:A:ILE:HG23	1:139:A:LYS:HB3	8	1.87	0.28	1.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,297)	1:4:A:ILE:HD11	1:2:A:ASP:HB2	8	1.78	0.74	1.32
(1,297)	1:4:A:ILE:HD13	1:2:A:ASP:HB2	8	1.78	0.74	1.32
(1,297)	1:4:A:ILE:HD12	1:2:A:ASP:HB2	8	1.78	0.74	1.32
(1,262)	1:151:A:ASP:HB2	1:148:A:ILE:HG22	8	1.7	0.15	1.72
(1,262)	1:151:A:ASP:HB3	1:158:A:LEU:HD22	8	1.7	0.15	1.72
(1,262)	1:151:A:ASP:HB3	1:148:A:ILE:HG23	8	1.7	0.15	1.72
(1,262)	1:151:A:ASP:HB3	1:148:A:ILE:HG21	8	1.7	0.15	1.72
(1,279)	1:60:A:MET:HE1	1:147:A:ARG:HD3	8	1.66	1.0	1.6
(1,279)	1:60:A:MET:HE1	1:145:A:ARG:HD2	8	1.66	1.0	1.6
(1,279)	1:60:A:MET:HE3	1:145:A:ARG:HD2	8	1.66	1.0	1.6
(1,279)	1:60:A:MET:HE3	1:147:A:ARG:HD2	8	1.66	1.0	1.6
(1,279)	1:60:A:MET:HE1	1:147:A:ARG:HD2	8	1.66	1.0	1.6
(1,279)	1:60:A:MET:HE2	1:147:A:ARG:HD2	8	1.66	1.0	1.6
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB2	8	1.54	0.37	1.32
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB3	8	1.54	0.37	1.32
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB1	8	1.54	0.37	1.32
(1,153)	1:41:A:LEU:HD12	1:52:A:PRO:HB3	8	1.44	0.36	1.48
(1,153)	1:41:A:LEU:HD13	1:72:A:VAL:HB	8	1.44	0.36	1.48
(1,153)	1:41:A:LEU:HD12	1:72:A:VAL:HB	8	1.44	0.36	1.48
(1,153)	1:41:A:LEU:HD11	1:72:A:VAL:HB	8	1.44	0.36	1.48
(1,153)	1:41:A:LEU:HD13	1:52:A:PRO:HB3	8	1.44	0.36	1.48
(1,153)	1:41:A:LEU:HD11	1:50:A:GLN:HG3	8	1.44	0.36	1.48
(1,152)	1:41:A:LEU:HD11	1:153:A:MET:HE1	8	1.35	0.46	1.49
(1,152)	1:41:A:LEU:HD12	1:153:A:MET:HE2	8	1.35	0.46	1.49
(1,152)	1:41:A:LEU:HD13	1:153:A:MET:HE3	8	1.35	0.46	1.49
(1,152)	1:41:A:LEU:HD11	1:153:A:MET:HE3	8	1.35	0.46	1.49
(1,152)	1:41:A:LEU:HD13	1:153:A:MET:HE2	8	1.35	0.46	1.49
(1,268)	1:22:A:ALA:HB2	1:20:A:PHE:HD2	8	1.31	0.17	1.34
(1,268)	1:22:A:ALA:HB1	1:20:A:PHE:HD1	8	1.31	0.17	1.34
(1,268)	1:22:A:ALA:HB1	1:20:A:PHE:HD2	8	1.31	0.17	1.34
(2,481)	1:4:A:ILE:HG23	1:7:A:ALA:HB2	8	1.3	0.07	1.28
(2,481)	1:4:A:ILE:HG22	1:7:A:ALA:HB1	8	1.3	0.07	1.28
(2,481)	1:4:A:ILE:HG22	1:7:A:ALA:HB2	8	1.3	0.07	1.28
(2,481)	1:4:A:ILE:HG21	1:7:A:ALA:HB3	8	1.3	0.07	1.28
(2,481)	1:4:A:ILE:HG21	1:7:A:ALA:HB1	8	1.3	0.07	1.28
(1,110)	1:154:A:MET:HE3	1:155:A:GLN:HA	8	1.19	0.14	1.23
(1,110)	1:154:A:MET:HE1	1:155:A:GLN:HA	8	1.19	0.14	1.23
(1,110)	1:154:A:MET:HE2	1:155:A:GLN:HA	8	1.19	0.14	1.23
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD22	8	1.17	0.55	1.36
(1,7)	1:44:A:VAL:HA	1:26:A:ILE:HG23	8	1.17	0.55	1.36
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD23	8	1.17	0.55	1.36
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD21	8	1.17	0.55	1.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	8	1.15	0.15	1.19
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD23	8	1.15	0.15	1.19
(1,181)	1:152:A:ALA:HB1	1:155:A:GLN:HB2	8	1.14	0.16	1.1
(1,181)	1:152:A:ALA:HB2	1:155:A:GLN:HB2	8	1.14	0.16	1.1
(1,181)	1:152:A:ALA:HB3	1:155:A:GLN:HB2	8	1.14	0.16	1.1
(1,181)	1:156:A:ALA:HB3	1:155:A:GLN:HB2	8	1.14	0.16	1.1
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD22	8	1.12	0.66	0.84
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD21	8	1.12	0.66	0.84
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD23	8	1.12	0.66	0.84
(2,1111)	1:153:A:MET:HE1	1:44:A:VAL:HG21	8	1.12	0.47	1.04
(2,1111)	1:153:A:MET:HE3	1:44:A:VAL:HG21	8	1.12	0.47	1.04
(2,1111)	1:153:A:MET:HE3	1:44:A:VAL:HG22	8	1.12	0.47	1.04
(2,1111)	1:153:A:MET:HE1	1:44:A:VAL:HG23	8	1.12	0.47	1.04
(2,1111)	1:153:A:MET:HE2	1:44:A:VAL:HG22	8	1.12	0.47	1.04
(2,1111)	1:153:A:MET:HE2	1:44:A:VAL:HG21	8	1.12	0.47	1.04
(1,116)	1:8:A:ALA:HB3	1:11:A:GLN:HG2	8	1.1	0.32	1.21
(1,116)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	8	1.1	0.32	1.21
(1,116)	1:8:A:ALA:HB2	1:11:A:GLN:HG2	8	1.1	0.32	1.21
(1,107)	1:153:A:MET:HE2	1:23:A:ALA:HA	8	1.09	0.48	1.1
(1,107)	1:153:A:MET:HE3	1:23:A:ALA:HA	8	1.09	0.48	1.1
(1,107)	1:153:A:MET:HE2	1:152:A:ALA:HA	8	1.09	0.48	1.1
(1,107)	1:153:A:MET:HE1	1:23:A:ALA:HA	8	1.09	0.48	1.1
(2,648)	1:48:A:LEU:HD13	1:156:A:ALA:HB1	8	1.03	0.66	0.57
(2,648)	1:48:A:LEU:HD12	1:156:A:ALA:HB2	8	1.03	0.66	0.57
(2,648)	1:48:A:LEU:HD13	1:156:A:ALA:HB2	8	1.03	0.66	0.57
(2,648)	1:48:A:LEU:HD11	1:156:A:ALA:HB3	8	1.03	0.66	0.57
(2,648)	1:48:A:LEU:HD12	1:156:A:ALA:HB1	8	1.03	0.66	0.57
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	8	1.01	0.15	1.0
(2,1059)	1:137:A:LYS:HB2	1:138:A:PHE:HD2	8	1.01	0.15	1.0
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD1	8	1.01	0.15	1.0
(1,123)	1:28:A:VAL:HG22	1:26:A:ILE:HG13	8	1.01	0.07	1.0
(1,123)	1:28:A:VAL:HG22	1:29:A:LEU:HB2	8	1.01	0.07	1.0
(1,123)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	8	1.01	0.07	1.0
(1,123)	1:28:A:VAL:HG21	1:26:A:ILE:HG13	8	1.01	0.07	1.0
(1,123)	1:28:A:VAL:HG23	1:29:A:LEU:HB2	8	1.01	0.07	1.0
(1,265)	1:27:A:PHE:HB3	1:26:A:ILE:HG21	8	1.0	0.41	1.1
(1,265)	1:148:A:ILE:HG21	1:147:A:ARG:HD3	8	1.0	0.41	1.1
(1,265)	1:27:A:PHE:HB3	1:26:A:ILE:HG22	8	1.0	0.41	1.1
(1,265)	1:147:A:ARG:HD2	1:148:A:ILE:HG22	8	1.0	0.41	1.1
(1,265)	1:27:A:PHE:HB3	1:26:A:ILE:HG23	8	1.0	0.41	1.1
(1,265)	1:147:A:ARG:HD2	1:148:A:ILE:HG21	8	1.0	0.41	1.1
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE2	8	0.97	0.95	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE1	8	0.97	0.95	0.42
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE3	8	0.97	0.95	0.42
(1,286)	1:36:A:ILE:HG22	1:71:A:THR:HB	8	0.94	0.35	0.82
(1,286)	1:36:A:ILE:HG23	1:71:A:THR:HB	8	0.94	0.35	0.82
(1,286)	1:36:A:ILE:HG21	1:71:A:THR:HB	8	0.94	0.35	0.82
(2,596)	1:157:A:LEU:HD22	1:157:A:LEU:HA	8	0.94	0.37	0.97
(2,596)	1:157:A:LEU:HD21	1:157:A:LEU:HA	8	0.94	0.37	0.97
(2,596)	1:157:A:LEU:HD23	1:157:A:LEU:HA	8	0.94	0.37	0.97
(2,864)	1:81:A:MET:HE2	1:84:A:SER:HB3	8	0.94	0.9	0.44
(2,864)	1:81:A:MET:HE1	1:84:A:SER:HB3	8	0.94	0.9	0.44
(2,864)	1:81:A:MET:HE3	1:84:A:SER:HB3	8	0.94	0.9	0.44
(2,864)	1:81:A:MET:HE1	1:84:A:SER:HB2	8	0.94	0.9	0.44
(2,1083)	1:148:A:ILE:HG22	1:154:A:MET:HG3	8	0.93	0.1	0.9
(2,1083)	1:148:A:ILE:HG21	1:154:A:MET:HG3	8	0.93	0.1	0.9
(2,1083)	1:148:A:ILE:HG23	1:154:A:MET:HG3	8	0.93	0.1	0.9
(1,142)	1:38:A:THR:HG22	1:60:A:MET:HE2	8	0.93	0.19	0.86
(1,142)	1:38:A:THR:HG21	1:60:A:MET:HE3	8	0.93	0.19	0.86
(1,142)	1:38:A:THR:HG22	1:60:A:MET:HE3	8	0.93	0.19	0.86
(1,142)	1:38:A:THR:HG21	1:60:A:MET:HE2	8	0.93	0.19	0.86
(1,138)	1:13:A:THR:HG21	1:15:A:GLU:HB3	8	0.92	0.31	0.79
(1,138)	1:13:A:THR:HG22	1:15:A:GLU:HB2	8	0.92	0.31	0.79
(1,138)	1:13:A:THR:HG22	1:15:A:GLU:HB3	8	0.92	0.31	0.79
(1,138)	1:13:A:THR:HG23	1:15:A:GLU:HB2	8	0.92	0.31	0.79
(1,138)	1:13:A:THR:HG21	1:15:A:GLU:HB2	8	0.92	0.31	0.79
(1,189)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	8	0.92	0.57	0.7
(1,189)	1:59:A:GLU:HG3	1:61:A:ILE:HG13	8	0.92	0.57	0.7
(1,189)	1:8:A:ALA:HB1	1:10:A:GLU:HG3	8	0.92	0.57	0.7
(1,189)	1:8:A:ALA:HB3	1:10:A:GLU:HG3	8	0.92	0.57	0.7
(2,1152)	1:4:A:ILE:HD12	1:86:A:LYS:HE3	8	0.91	0.15	0.88
(2,1152)	1:4:A:ILE:HD11	1:86:A:LYS:HE3	8	0.91	0.15	0.88
(2,1152)	1:4:A:ILE:HD13	1:86:A:LYS:HE2	8	0.91	0.15	0.88
(2,1152)	1:4:A:ILE:HD13	1:86:A:LYS:HE3	8	0.91	0.15	0.88
(1,248)	1:61:A:ILE:HD12	1:57:A:LEU:HA	8	0.9	0.18	0.9
(1,248)	1:61:A:ILE:HD13	1:57:A:LEU:HA	8	0.9	0.18	0.9
(1,248)	1:61:A:ILE:HD11	1:57:A:LEU:HA	8	0.9	0.18	0.9
(2,502)	1:28:A:VAL:HG22	1:36:A:ILE:HD11	8	0.9	0.19	0.95
(2,502)	1:28:A:VAL:HG23	1:36:A:ILE:HD13	8	0.9	0.19	0.95
(2,502)	1:28:A:VAL:HG22	1:36:A:ILE:HD12	8	0.9	0.19	0.95
(2,502)	1:28:A:VAL:HG23	1:36:A:ILE:HD12	8	0.9	0.19	0.95
(2,502)	1:28:A:VAL:HG23	1:36:A:ILE:HD11	8	0.9	0.19	0.95
(2,502)	1:28:A:VAL:HG21	1:36:A:ILE:HD12	8	0.9	0.19	0.95
(2,1115)	1:162:A:ALA:HB2	1:163:A:LYS:HE2	8	0.89	0.22	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1115)	1:162:A:ALA:HB3	1:163:A:LYS:HE3	8	0.89	0.22	0.8
(2,1115)	1:162:A:ALA:HB1	1:163:A:LYS:HE2	8	0.89	0.22	0.8
(2,1115)	1:162:A:ALA:HB1	1:163:A:LYS:HE3	8	0.89	0.22	0.8
(2,1115)	1:162:A:ALA:HB3	1:163:A:LYS:HE2	8	0.89	0.22	0.8
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG11	8	0.89	0.23	0.92
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG13	8	0.89	0.23	0.92
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG12	8	0.89	0.23	0.92
(1,93)	1:61:A:ILE:HD12	1:38:A:THR:HB	8	0.87	0.18	0.86
(1,93)	1:61:A:ILE:HD11	1:38:A:THR:HB	8	0.87	0.18	0.86
(1,93)	1:61:A:ILE:HD13	1:38:A:THR:HB	8	0.87	0.18	0.86
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD13	8	0.87	0.16	0.9
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD12	8	0.87	0.16	0.9
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD11	8	0.87	0.16	0.9
(1,198)	1:72:A:VAL:HB	1:77:A:PHE:HB3	8	0.87	0.08	0.84
(1,198)	1:50:A:GLN:HG3	1:52:A:PRO:HD2	8	0.87	0.08	0.84
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD11	8	0.85	0.61	0.47
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD13	8	0.85	0.61	0.47
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD12	8	0.85	0.61	0.47
(1,150)	1:48:A:LEU:HD23	1:156:A:ALA:HA	8	0.83	0.41	0.61
(1,150)	1:48:A:LEU:HD22	1:156:A:ALA:HA	8	0.83	0.41	0.61
(1,150)	1:48:A:LEU:HD21	1:156:A:ALA:HA	8	0.83	0.41	0.61
(2,414)	1:61:A:ILE:HD11	1:61:A:ILE:HA	8	0.82	0.14	0.82
(2,414)	1:61:A:ILE:HD13	1:61:A:ILE:HA	8	0.82	0.14	0.82
(2,414)	1:61:A:ILE:HD12	1:61:A:ILE:HA	8	0.82	0.14	0.82
(2,1157)	1:28:A:VAL:HG23	1:24:A:PHE:HD2	8	0.8	0.19	0.82
(2,1157)	1:28:A:VAL:HG21	1:24:A:PHE:HD1	8	0.8	0.19	0.82
(2,1157)	1:28:A:VAL:HG22	1:24:A:PHE:HD2	8	0.8	0.19	0.82
(2,1157)	1:28:A:VAL:HG21	1:24:A:PHE:HD2	8	0.8	0.19	0.82
(2,1157)	1:28:A:VAL:HG22	1:24:A:PHE:HD1	8	0.8	0.19	0.82
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE3	8	0.8	0.42	0.86
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE1	8	0.8	0.42	0.86
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE2	8	0.8	0.42	0.86
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	8	0.76	0.14	0.76
(1,101)	1:85:A:MET:HE2	1:84:A:SER:HB3	8	0.75	0.4	0.66
(1,101)	1:85:A:MET:HE2	1:17:A:LYS:HA	8	0.75	0.4	0.66
(1,101)	1:85:A:MET:HE1	1:84:A:SER:HB3	8	0.75	0.4	0.66
(1,101)	1:85:A:MET:HE3	1:84:A:SER:HB3	8	0.75	0.4	0.66
(1,101)	1:85:A:MET:HE3	1:84:A:SER:HB2	8	0.75	0.4	0.66
(2,432)	1:61:A:ILE:HG21	1:38:A:THR:HG21	8	0.74	0.09	0.7
(2,432)	1:61:A:ILE:HG22	1:38:A:THR:HG23	8	0.74	0.09	0.7
(2,432)	1:61:A:ILE:HG22	1:38:A:THR:HG21	8	0.74	0.09	0.7
(2,432)	1:61:A:ILE:HG21	1:38:A:THR:HG23	8	0.74	0.09	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,564)	1:82:A:VAL:HG21	1:9:A:VAL:HA	8	0.73	0.58	0.4
(2,564)	1:82:A:VAL:HG23	1:9:A:VAL:HA	8	0.73	0.58	0.4
(2,564)	1:82:A:VAL:HG22	1:9:A:VAL:HA	8	0.73	0.58	0.4
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD22	8	0.73	0.21	0.78
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD23	8	0.73	0.21	0.78
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD21	8	0.73	0.21	0.78
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB2	8	0.73	0.2	0.79
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB3	8	0.73	0.2	0.79
(2,487)	1:152:A:ALA:HB2	1:148:A:ILE:HA	8	0.72	0.48	0.47
(2,487)	1:152:A:ALA:HB3	1:148:A:ILE:HA	8	0.72	0.48	0.47
(2,487)	1:152:A:ALA:HB1	1:148:A:ILE:HA	8	0.72	0.48	0.47
(2,448)	1:1:A:MET:HE1	1:5:A:TYR:HB2	8	0.71	0.38	0.53
(2,448)	1:1:A:MET:HE3	1:5:A:TYR:HB2	8	0.71	0.38	0.53
(2,448)	1:1:A:MET:HE2	1:5:A:TYR:HB2	8	0.71	0.38	0.53
(1,105)	1:23:A:ALA:HA	1:26:A:ILE:HG22	8	0.7	0.27	0.75
(1,105)	1:23:A:ALA:HA	1:26:A:ILE:HG21	8	0.7	0.27	0.75
(1,105)	1:23:A:ALA:HA	1:26:A:ILE:HG23	8	0.7	0.27	0.75
(1,105)	1:148:A:ILE:HG22	1:152:A:ALA:HA	8	0.7	0.27	0.75
(1,105)	1:148:A:ILE:HG22	1:149:A:SER:HB3	8	0.7	0.27	0.75
(1,105)	1:148:A:ILE:HG21	1:149:A:SER:HB3	8	0.7	0.27	0.75
(1,202)	1:148:A:ILE:HD11	1:45:A:MET:HG2	8	0.7	0.16	0.64
(1,202)	1:48:A:LEU:HD11	1:45:A:MET:HG2	8	0.7	0.16	0.64
(1,202)	1:48:A:LEU:HD12	1:45:A:MET:HG2	8	0.7	0.16	0.64
(1,202)	1:48:A:LEU:HD13	1:45:A:MET:HG2	8	0.7	0.16	0.64
(1,202)	1:148:A:ILE:HD13	1:45:A:MET:HG2	8	0.7	0.16	0.64
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG22	8	0.68	0.11	0.68
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG23	8	0.68	0.11	0.68
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG21	8	0.68	0.11	0.68
(1,222)	1:6:A:LYS:HB3	1:6:A:LYS:HE2	8	0.66	0.34	0.84
(1,222)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	8	0.66	0.34	0.84
(1,222)	1:90:A:LYS:HB3	1:90:A:LYS:HE3	8	0.66	0.34	0.84
(1,222)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	8	0.66	0.34	0.84
(2,1076)	1:157:A:LEU:HD12	1:27:A:PHE:HB3	8	0.65	0.49	0.45
(2,1076)	1:157:A:LEU:HD11	1:27:A:PHE:HB3	8	0.65	0.49	0.45
(2,1076)	1:157:A:LEU:HD13	1:27:A:PHE:HB3	8	0.65	0.49	0.45
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE1	8	0.65	0.04	0.64
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE2	8	0.65	0.04	0.64
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG23	8	0.64	0.17	0.57
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG21	8	0.64	0.17	0.57
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG22	8	0.64	0.17	0.57
(1,82)	1:17:A:LYS:HE3	1:12:A:LEU:HD12	8	0.64	0.17	0.57
(1,82)	1:17:A:LYS:HE3	1:12:A:LEU:HD11	8	0.64	0.17	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,82)	1:17:A:LYS:HE3	1:12:A:LEU:HD13	8	0.64	0.17	0.57
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD11	8	0.64	0.25	0.66
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD13	8	0.64	0.25	0.66
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD12	8	0.64	0.25	0.66
(1,235)	1:28:A:VAL:HG13	1:43:A:LYS:HD2	8	0.64	0.21	0.62
(1,235)	1:28:A:VAL:HG12	1:43:A:LYS:HD2	8	0.64	0.21	0.62
(1,235)	1:28:A:VAL:HG11	1:43:A:LYS:HD2	8	0.64	0.21	0.62
(1,235)	1:28:A:VAL:HG11	1:43:A:LYS:HD3	8	0.64	0.21	0.62
(1,235)	1:28:A:VAL:HG13	1:43:A:LYS:HD3	8	0.64	0.21	0.62
(1,235)	1:28:A:VAL:HG12	1:43:A:LYS:HD3	8	0.64	0.21	0.62
(2,479)	1:45:A:MET:HE3	1:45:A:MET:HG2	8	0.64	0.04	0.62
(2,479)	1:45:A:MET:HE2	1:45:A:MET:HG2	8	0.64	0.04	0.62
(2,479)	1:45:A:MET:HE1	1:45:A:MET:HG2	8	0.64	0.04	0.62
(2,1190)	1:4:A:ILE:HD13	1:5:A:TYR:HD1	8	0.63	0.43	0.49
(2,1190)	1:4:A:ILE:HD11	1:5:A:TYR:HD1	8	0.63	0.43	0.49
(2,1190)	1:4:A:ILE:HD11	1:5:A:TYR:HD2	8	0.63	0.43	0.49
(2,1190)	1:4:A:ILE:HD13	1:5:A:TYR:HD2	8	0.63	0.43	0.49
(2,1190)	1:4:A:ILE:HD12	1:5:A:TYR:HD1	8	0.63	0.43	0.49
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	8	0.62	0.07	0.6
(2,469)	1:154:A:MET:HE3	1:154:A:MET:HA	8	0.62	0.18	0.54
(2,469)	1:154:A:MET:HE1	1:154:A:MET:HA	8	0.62	0.18	0.54
(2,469)	1:154:A:MET:HE2	1:154:A:MET:HA	8	0.62	0.18	0.54
(2,643)	1:48:A:LEU:HD11	1:48:A:LEU:HA	8	0.6	0.09	0.64
(2,643)	1:48:A:LEU:HD12	1:48:A:LEU:HA	8	0.6	0.09	0.64
(2,643)	1:48:A:LEU:HD13	1:48:A:LEU:HA	8	0.6	0.09	0.64
(2,1019)	1:72:A:VAL:HG23	1:36:A:ILE:HD13	8	0.6	0.23	0.66
(2,1019)	1:72:A:VAL:HG22	1:36:A:ILE:HD12	8	0.6	0.23	0.66
(2,1019)	1:72:A:VAL:HG22	1:36:A:ILE:HD13	8	0.6	0.23	0.66
(2,1019)	1:72:A:VAL:HG21	1:36:A:ILE:HD12	8	0.6	0.23	0.66
(2,1019)	1:72:A:VAL:HG21	1:36:A:ILE:HD11	8	0.6	0.23	0.66
(2,1019)	1:72:A:VAL:HG21	1:36:A:ILE:HD13	8	0.6	0.23	0.66
(2,1019)	1:72:A:VAL:HG23	1:36:A:ILE:HD11	8	0.6	0.23	0.66
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	8	0.59	0.31	0.51
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD1	8	0.58	0.46	0.27
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD2	8	0.58	0.46	0.27
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG21	8	0.58	0.03	0.58
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG23	8	0.58	0.03	0.58
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG22	8	0.58	0.03	0.58
(2,1103)	1:143:A:LEU:HD12	1:143:A:LEU:HA	8	0.57	0.15	0.54
(2,1103)	1:143:A:LEU:HD11	1:143:A:LEU:HA	8	0.57	0.15	0.54
(2,1103)	1:143:A:LEU:HD13	1:143:A:LEU:HA	8	0.57	0.15	0.54
(2,1224)	1:20:A:PHE:HE1	1:20:A:PHE:HB2	8	0.56	0.02	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1224)	1:20:A:PHE:HE2	1:20:A:PHE:HB2	8	0.56	0.02	0.57
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE2	8	0.56	0.26	0.49
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE3	8	0.56	0.26	0.49
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE1	8	0.56	0.26	0.49
(2,580)	1:72:A:VAL:HG22	1:76:A:GLU:HA	8	0.55	0.11	0.52
(2,580)	1:72:A:VAL:HG21	1:76:A:GLU:HA	8	0.55	0.11	0.52
(2,580)	1:72:A:VAL:HG23	1:76:A:GLU:HA	8	0.55	0.11	0.52
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG21	8	0.52	0.03	0.53
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG22	8	0.52	0.03	0.53
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG23	8	0.52	0.03	0.53
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE1	8	0.51	0.11	0.53
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE3	8	0.51	0.11	0.53
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE2	8	0.51	0.11	0.53
(1,157)	1:29:A:LEU:HD23	1:26:A:ILE:HB	8	0.51	0.13	0.55
(1,157)	1:29:A:LEU:HD22	1:26:A:ILE:HB	8	0.51	0.13	0.55
(1,157)	1:29:A:LEU:HD21	1:26:A:ILE:HB	8	0.51	0.13	0.55
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	8	0.51	0.08	0.5
(2,507)	1:162:A:ALA:HB3	1:19:A:GLU:HG3	8	0.5	0.16	0.49
(2,507)	1:162:A:ALA:HB1	1:19:A:GLU:HG3	8	0.5	0.16	0.49
(2,507)	1:162:A:ALA:HB2	1:19:A:GLU:HG3	8	0.5	0.16	0.49
(2,594)	1:41:A:LEU:HD12	1:41:A:LEU:HB3	8	0.5	0.18	0.53
(2,594)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	8	0.5	0.18	0.53
(2,594)	1:41:A:LEU:HD11	1:41:A:LEU:HB3	8	0.5	0.18	0.53
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD1	8	0.5	0.3	0.32
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD2	8	0.5	0.3	0.32
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD11	8	0.49	0.07	0.48
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD12	8	0.49	0.07	0.48
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD13	8	0.49	0.07	0.48
(2,533)	1:72:A:VAL:HG12	1:73:A:ASP:HB3	8	0.48	0.08	0.48
(2,533)	1:72:A:VAL:HG11	1:73:A:ASP:HB3	8	0.48	0.08	0.48
(2,533)	1:72:A:VAL:HG13	1:73:A:ASP:HB3	8	0.48	0.08	0.48
(2,1001)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	8	0.48	0.13	0.5
(2,1001)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	8	0.48	0.13	0.5
(2,1001)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	8	0.48	0.13	0.5
(2,1113)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	8	0.48	0.16	0.42
(2,1113)	1:22:A:ALA:HB3	1:25:A:ASP:HB2	8	0.48	0.16	0.42
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE3	8	0.48	0.22	0.47
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE2	8	0.48	0.22	0.47
(2,1081)	1:26:A:ILE:HD11	1:25:A:ASP:HB2	8	0.47	0.09	0.47
(2,1081)	1:26:A:ILE:HD12	1:25:A:ASP:HB2	8	0.47	0.09	0.47
(2,1081)	1:26:A:ILE:HD13	1:25:A:ASP:HB2	8	0.47	0.09	0.47
(2,424)	1:148:A:ILE:HD13	1:45:A:MET:HB3	8	0.45	0.07	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,424)	1:148:A:ILE:HD12	1:45:A:MET:HB3	8	0.45	0.07	0.44
(2,424)	1:148:A:ILE:HD11	1:45:A:MET:HB3	8	0.45	0.07	0.44
(1,106)	1:36:A:ILE:HG23	1:27:A:PHE:HB2	8	0.44	0.13	0.46
(1,106)	1:36:A:ILE:HG22	1:27:A:PHE:HB2	8	0.44	0.13	0.46
(1,106)	1:36:A:ILE:HG21	1:27:A:PHE:HB2	8	0.44	0.13	0.46
(2,485)	1:150:A:ALA:HB2	1:20:A:PHE:HE2	8	0.43	0.08	0.43
(2,485)	1:150:A:ALA:HB1	1:20:A:PHE:HE2	8	0.43	0.08	0.43
(2,485)	1:150:A:ALA:HB2	1:20:A:PHE:HE1	8	0.43	0.08	0.43
(2,485)	1:150:A:ALA:HB3	1:20:A:PHE:HE2	8	0.43	0.08	0.43
(2,485)	1:150:A:ALA:HB3	1:20:A:PHE:HE1	8	0.43	0.08	0.43
(2,330)	1:145:A:ARG:HD3	1:145:A:ARG:HG2	8	0.43	0.07	0.44
(2,330)	1:145:A:ARG:HD3	1:145:A:ARG:HG3	8	0.43	0.07	0.44
(2,330)	1:145:A:ARG:HD2	1:145:A:ARG:HG3	8	0.43	0.07	0.44
(2,549)	1:79:A:VAL:HG11	1:5:A:TYR:HB3	8	0.42	0.13	0.44
(2,549)	1:79:A:VAL:HG13	1:5:A:TYR:HB3	8	0.42	0.13	0.44
(2,549)	1:79:A:VAL:HG12	1:5:A:TYR:HB3	8	0.42	0.13	0.44
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	8	0.42	0.15	0.38
(1,321)	1:39:A:LYS:H	1:37:A:SER:HB2	8	0.41	0.18	0.36
(1,321)	1:39:A:LYS:H	1:38:A:THR:HB	8	0.41	0.18	0.36
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB1	8	0.41	0.03	0.42
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB3	8	0.41	0.03	0.42
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB2	8	0.41	0.03	0.42
(1,42)	1:16:A:GLN:HA	1:15:A:GLU:HB3	8	0.41	0.15	0.4
(1,42)	1:16:A:GLN:HA	1:19:A:GLU:HB2	8	0.41	0.15	0.4
(1,42)	1:16:A:GLN:HA	1:15:A:GLU:HB2	8	0.41	0.15	0.4
(1,212)	1:6:A:LYS:HB3	1:6:A:LYS:HG2	8	0.4	0.06	0.42
(1,212)	1:90:A:LYS:HG2	1:90:A:LYS:HB3	8	0.4	0.06	0.42
(1,212)	1:90:A:LYS:HG3	1:90:A:LYS:HB3	8	0.4	0.06	0.42
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG22	8	0.4	0.11	0.43
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG21	8	0.4	0.11	0.43
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG23	8	0.4	0.11	0.43
(1,89)	1:6:A:LYS:HE2	1:6:A:LYS:HD3	8	0.4	0.03	0.4
(1,89)	1:86:A:LYS:HE3	1:86:A:LYS:HD2	8	0.4	0.03	0.4
(1,89)	1:6:A:LYS:HE3	1:6:A:LYS:HD2	8	0.4	0.03	0.4
(1,89)	1:86:A:LYS:HE2	1:86:A:LYS:HD2	8	0.4	0.03	0.4
(2,1065)	1:151:A:ASP:HB2	1:152:A:ALA:HA	8	0.4	0.07	0.42
(2,1065)	1:151:A:ASP:HB3	1:152:A:ALA:HA	8	0.4	0.07	0.42
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE3	8	0.39	0.06	0.38
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE1	8	0.39	0.06	0.38
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE2	8	0.39	0.06	0.38
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	8	0.39	0.16	0.3
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD1	8	0.37	0.1	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD2	8	0.37	0.1	0.39
(1,12)	1:24:A:PHE:HA	1:77:A:PHE:HZ	8	0.37	0.1	0.39
(1,113)	1:7:A:ALA:HB2	1:4:A:ILE:HG12	8	0.37	0.06	0.37
(1,113)	1:7:A:ALA:HB1	1:4:A:ILE:HG12	8	0.37	0.06	0.37
(1,113)	1:7:A:ALA:HB3	1:4:A:ILE:HG12	8	0.37	0.06	0.37
(1,113)	1:7:A:ALA:HB2	1:4:A:ILE:HG13	8	0.37	0.06	0.37
(1,113)	1:7:A:ALA:HB1	1:4:A:ILE:HG13	8	0.37	0.06	0.37
(1,139)	1:38:A:THR:HG22	1:57:A:LEU:HA	8	0.35	0.15	0.32
(1,139)	1:38:A:THR:HG21	1:57:A:LEU:HA	8	0.35	0.15	0.32
(1,186)	1:18:A:ASN:HB3	1:19:A:GLU:HB3	8	0.35	0.15	0.36
(1,186)	1:18:A:ASN:HB3	1:21:A:LYS:HB3	8	0.35	0.15	0.36
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB3	8	0.35	0.13	0.35
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB2	8	0.35	0.13	0.35
(1,161)	1:39:A:LYS:HG3	1:39:A:LYS:HB3	8	0.34	0.06	0.32
(1,161)	1:90:A:LYS:HG2	1:90:A:LYS:HB3	8	0.34	0.06	0.32
(1,161)	1:90:A:LYS:HG3	1:90:A:LYS:HB3	8	0.34	0.06	0.32
(1,122)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	8	0.33	0.13	0.36
(1,122)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	8	0.33	0.13	0.36
(1,122)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	8	0.33	0.13	0.36
(1,194)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	8	0.32	0.03	0.32
(1,194)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	8	0.32	0.03	0.32
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	8	0.32	0.06	0.33
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG21	8	0.31	0.07	0.32
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG23	8	0.31	0.07	0.32
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG22	8	0.31	0.07	0.32
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG3	8	0.3	0.09	0.29
(1,17)	1:55:A:GLU:HA	1:55:A:GLU:HG2	8	0.3	0.09	0.29
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG2	8	0.3	0.09	0.29
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	8	0.3	0.04	0.29
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB3	8	0.29	0.02	0.3
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB2	8	0.29	0.02	0.3
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB1	8	0.29	0.02	0.3
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	8	0.29	0.08	0.29
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	8	0.28	0.03	0.29
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE1	8	0.27	0.02	0.28
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE2	8	0.27	0.02	0.28
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB2	8	0.27	0.06	0.26
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB3	8	0.27	0.06	0.26
(1,216)	1:59:A:GLU:HA	1:59:A:GLU:HB2	8	0.27	0.06	0.26
(1,184)	1:163:A:LYS:HD3	1:163:A:LYS:HE2	8	0.26	0.02	0.26
(1,184)	1:163:A:LYS:HD2	1:163:A:LYS:HE3	8	0.26	0.02	0.26
(1,184)	1:86:A:LYS:HE2	1:86:A:LYS:HD2	8	0.26	0.02	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB3	8	0.25	0.01	0.26
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB1	8	0.25	0.01	0.26
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB2	8	0.25	0.01	0.26
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	8	0.25	0.03	0.26
(1,211)	1:9:A:VAL:HG23	1:9:A:VAL:HB	8	0.23	0.03	0.24
(1,211)	1:9:A:VAL:HG11	1:9:A:VAL:HB	8	0.23	0.03	0.24
(1,211)	1:9:A:VAL:HG22	1:9:A:VAL:HB	8	0.23	0.03	0.24
(1,211)	1:9:A:VAL:HG13	1:9:A:VAL:HB	8	0.23	0.03	0.24
(1,211)	1:9:A:VAL:HG12	1:9:A:VAL:HB	8	0.23	0.03	0.24
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB3	8	0.22	0.05	0.22
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB2	8	0.22	0.05	0.22
(1,2)	1:38:A:THR:HB	1:41:A:LEU:HB3	8	0.22	0.05	0.23
(1,2)	1:38:A:THR:HB	1:57:A:LEU:HG	8	0.22	0.05	0.23
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG3	8	0.22	0.05	0.2
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG2	8	0.22	0.05	0.2
(1,83)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	8	0.22	0.05	0.2
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	8	0.21	0.04	0.2
(1,356)	1:57:A:LEU:H	1:57:A:LEU:HA	8	0.21	0.04	0.22
(1,356)	1:155:A:GLN:H	1:155:A:GLN:HA	8	0.21	0.04	0.22
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD1	8	0.2	0.06	0.2
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	8	0.2	0.06	0.2
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	8	0.19	0.01	0.18
(2,489)	1:156:A:ALA:HB2	1:156:A:ALA:HA	8	0.18	0.03	0.18
(2,489)	1:156:A:ALA:HB3	1:156:A:ALA:HA	8	0.18	0.03	0.18
(2,489)	1:156:A:ALA:HB1	1:156:A:ALA:HA	8	0.18	0.03	0.18
(1,129)	1:13:A:THR:HB	1:13:A:THR:HG23	8	0.17	0.0	0.17
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG21	8	0.17	0.0	0.17
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG23	8	0.17	0.0	0.17
(1,129)	1:13:A:THR:HB	1:13:A:THR:HG21	8	0.17	0.0	0.17
(1,129)	1:13:A:THR:HB	1:13:A:THR:HG22	8	0.17	0.0	0.17
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG22	8	0.17	0.0	0.17
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	8	0.16	0.02	0.16
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	8	0.16	0.03	0.16
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB3	8	0.13	0.01	0.13
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB1	8	0.13	0.01	0.13
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB2	8	0.13	0.01	0.13
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	8	0.12	0.01	0.12
(1,296)	1:145:A:ARG:HD2	1:146:A:VAL:HG12	7	1.23	0.98	1.07
(1,296)	1:145:A:ARG:HD3	1:146:A:VAL:HG12	7	1.23	0.98	1.07
(1,296)	1:147:A:ARG:HD2	1:146:A:VAL:HG12	7	1.23	0.98	1.07
(1,296)	1:145:A:ARG:HD3	1:146:A:VAL:HG13	7	1.23	0.98	1.07
(1,296)	1:145:A:ARG:HD2	1:146:A:VAL:HG11	7	1.23	0.98	1.07

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,284)	1:160:A:ALA:HB2	1:163:A:LYS:HE2	7	1.1	0.69	1.24
(1,284)	1:160:A:ALA:HB1	1:163:A:LYS:HE3	7	1.1	0.69	1.24
(1,284)	1:160:A:ALA:HB2	1:43:A:LYS:HE3	7	1.1	0.69	1.24
(1,284)	1:160:A:ALA:HB2	1:163:A:LYS:HE3	7	1.1	0.69	1.24
(1,284)	1:160:A:ALA:HB1	1:163:A:LYS:HE2	7	1.1	0.69	1.24
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD23	7	0.82	0.64	0.72
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD21	7	0.82	0.64	0.72
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG12	7	0.74	0.45	0.53
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG11	7	0.74	0.45	0.53
(2,438)	1:1:A:MET:HE3	1:78:A:LEU:HB2	7	0.71	0.38	0.77
(2,438)	1:1:A:MET:HE2	1:78:A:LEU:HB2	7	0.71	0.38	0.77
(2,438)	1:1:A:MET:HE1	1:78:A:LEU:HB2	7	0.71	0.38	0.77
(2,1047)	1:79:A:VAL:HG11	1:5:A:TYR:HE2	7	0.62	0.25	0.74
(2,1047)	1:79:A:VAL:HG13	1:5:A:TYR:HE1	7	0.62	0.25	0.74
(2,1047)	1:79:A:VAL:HG12	1:5:A:TYR:HE1	7	0.62	0.25	0.74
(2,1047)	1:79:A:VAL:HG11	1:5:A:TYR:HE1	7	0.62	0.25	0.74
(2,1047)	1:79:A:VAL:HG13	1:5:A:TYR:HE2	7	0.62	0.25	0.74
(2,912)	1:82:A:VAL:HG22	1:20:A:PHE:HE1	7	0.62	0.29	0.62
(2,912)	1:82:A:VAL:HG21	1:20:A:PHE:HE1	7	0.62	0.29	0.62
(2,912)	1:82:A:VAL:HG23	1:20:A:PHE:HE2	7	0.62	0.29	0.62
(2,912)	1:82:A:VAL:HG22	1:20:A:PHE:HE2	7	0.62	0.29	0.62
(2,912)	1:82:A:VAL:HG23	1:20:A:PHE:HE1	7	0.62	0.29	0.62
(1,197)	1:155:A:GLN:HG3	1:158:A:LEU:HB2	7	0.61	0.33	0.7
(1,197)	1:8:A:ALA:HB3	1:11:A:GLN:HG2	7	0.61	0.33	0.7
(1,197)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	7	0.61	0.33	0.7
(1,197)	1:8:A:ALA:HB2	1:11:A:GLN:HG2	7	0.61	0.33	0.7
(1,217)	1:12:A:LEU:HD22	1:16:A:GLN:HB2	7	0.58	0.27	0.45
(1,217)	1:12:A:LEU:HD23	1:16:A:GLN:HB2	7	0.58	0.27	0.45
(1,217)	1:56:A:GLU:HB2	1:146:A:VAL:HG21	7	0.58	0.27	0.45
(1,217)	1:12:A:LEU:HD21	1:16:A:GLN:HB2	7	0.58	0.27	0.45
(2,455)	1:148:A:ILE:HG23	1:153:A:MET:HG2	7	0.58	0.2	0.57
(2,455)	1:148:A:ILE:HG21	1:153:A:MET:HG2	7	0.58	0.2	0.57
(2,455)	1:148:A:ILE:HG23	1:153:A:MET:HG3	7	0.58	0.2	0.57
(2,455)	1:148:A:ILE:HG22	1:153:A:MET:HG3	7	0.58	0.2	0.57
(2,517)	1:146:A:VAL:HG23	1:146:A:VAL:HA	7	0.55	0.06	0.57
(2,517)	1:146:A:VAL:HG21	1:146:A:VAL:HA	7	0.55	0.06	0.57
(2,517)	1:146:A:VAL:HG22	1:146:A:VAL:HA	7	0.55	0.06	0.57
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG13	7	0.52	0.12	0.52
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG12	7	0.52	0.12	0.52
(1,132)	1:142:A:THR:HG21	1:140:A:ARG:HD3	7	0.48	0.1	0.53
(1,132)	1:142:A:THR:HG23	1:140:A:ARG:HD2	7	0.48	0.1	0.53
(1,132)	1:142:A:THR:HG21	1:140:A:ARG:HD2	7	0.48	0.1	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,97)	1:148:A:ILE:HD12	1:146:A:VAL:HB	7	0.48	0.17	0.5
(1,97)	1:148:A:ILE:HD11	1:146:A:VAL:HB	7	0.48	0.17	0.5
(1,97)	1:148:A:ILE:HD13	1:146:A:VAL:HB	7	0.48	0.17	0.5
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD12	7	0.47	0.27	0.27
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD13	7	0.47	0.27	0.27
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD11	7	0.47	0.27	0.27
(1,6)	1:38:A:THR:HA	1:57:A:LEU:HD12	7	0.44	0.21	0.51
(1,6)	1:38:A:THR:HA	1:41:A:LEU:HD23	7	0.44	0.21	0.51
(1,6)	1:38:A:THR:HA	1:57:A:LEU:HD11	7	0.44	0.21	0.51
(1,6)	1:38:A:THR:HA	1:41:A:LEU:HD21	7	0.44	0.21	0.51
(1,6)	1:38:A:THR:HA	1:57:A:LEU:HD13	7	0.44	0.21	0.51
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB1	7	0.41	0.06	0.42
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB3	7	0.41	0.06	0.42
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB2	7	0.41	0.06	0.42
(2,1197)	1:4:A:ILE:HD11	1:5:A:TYR:HE2	7	0.41	0.17	0.38
(2,1197)	1:4:A:ILE:HD13	1:5:A:TYR:HE1	7	0.41	0.17	0.38
(2,1197)	1:4:A:ILE:HD12	1:5:A:TYR:HE2	7	0.41	0.17	0.38
(2,1197)	1:4:A:ILE:HD12	1:5:A:TYR:HE1	7	0.41	0.17	0.38
(2,1197)	1:4:A:ILE:HD13	1:5:A:TYR:HE2	7	0.41	0.17	0.38
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD21	7	0.4	0.14	0.38
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD23	7	0.4	0.14	0.38
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD22	7	0.4	0.14	0.38
(1,218)	1:79:A:VAL:HB	1:76:A:GLU:HA	7	0.4	0.08	0.44
(1,218)	1:79:A:VAL:HB	1:6:A:LYS:HA	7	0.4	0.08	0.44
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	7	0.39	0.11	0.39
(2,860)	1:47:A:MET:HE3	1:47:A:MET:HG3	7	0.39	0.02	0.39
(2,860)	1:47:A:MET:HE1	1:47:A:MET:HG3	7	0.39	0.02	0.39
(2,860)	1:47:A:MET:HE2	1:47:A:MET:HG3	7	0.39	0.02	0.39
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD21	7	0.39	0.08	0.38
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD22	7	0.39	0.08	0.38
(2,630)	1:158:A:LEU:HD12	1:158:A:LEU:HA	7	0.38	0.19	0.28
(2,630)	1:158:A:LEU:HD11	1:158:A:LEU:HA	7	0.38	0.19	0.28
(2,630)	1:158:A:LEU:HD13	1:158:A:LEU:HA	7	0.38	0.19	0.28
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB1	7	0.37	0.12	0.4
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB2	7	0.37	0.12	0.4
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB3	7	0.37	0.12	0.4
(2,649)	1:48:A:LEU:HD13	1:44:A:VAL:HG21	7	0.37	0.11	0.38
(2,649)	1:48:A:LEU:HD12	1:44:A:VAL:HG23	7	0.37	0.11	0.38
(2,649)	1:48:A:LEU:HD13	1:44:A:VAL:HG22	7	0.37	0.11	0.38
(2,649)	1:48:A:LEU:HD12	1:44:A:VAL:HG22	7	0.37	0.11	0.38
(2,649)	1:48:A:LEU:HD11	1:44:A:VAL:HG21	7	0.37	0.11	0.38
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE2	7	0.34	0.13	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE1	7	0.34	0.13	0.37
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD13	7	0.33	0.11	0.31
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD12	7	0.33	0.11	0.31
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD11	7	0.33	0.11	0.31
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG22	7	0.33	0.13	0.29
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG21	7	0.33	0.13	0.29
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG23	7	0.33	0.13	0.29
(2,514)	1:31:A:ALA:HB1	1:28:A:VAL:HG21	7	0.31	0.15	0.33
(2,514)	1:31:A:ALA:HB3	1:28:A:VAL:HG22	7	0.31	0.15	0.33
(2,514)	1:31:A:ALA:HB3	1:28:A:VAL:HG21	7	0.31	0.15	0.33
(2,514)	1:31:A:ALA:HB2	1:28:A:VAL:HG22	7	0.31	0.15	0.33
(2,514)	1:31:A:ALA:HB1	1:28:A:VAL:HG23	7	0.31	0.15	0.33
(2,514)	1:31:A:ALA:HB1	1:28:A:VAL:HG22	7	0.31	0.15	0.33
(2,1004)	1:72:A:VAL:HG21	1:65:A:ASP:HB3	7	0.31	0.1	0.25
(2,1004)	1:72:A:VAL:HG23	1:65:A:ASP:HB3	7	0.31	0.1	0.25
(2,1004)	1:72:A:VAL:HG22	1:65:A:ASP:HB3	7	0.31	0.1	0.25
(2,462)	1:36:A:ILE:HG22	1:72:A:VAL:HB	7	0.29	0.13	0.32
(2,462)	1:36:A:ILE:HG23	1:72:A:VAL:HB	7	0.29	0.13	0.32
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE3	7	0.29	0.07	0.28
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE2	7	0.29	0.07	0.28
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE1	7	0.29	0.07	0.28
(1,58)	1:50:A:GLN:HA	1:46:A:ARG:HG3	7	0.28	0.07	0.28
(1,58)	1:50:A:GLN:HA	1:45:A:MET:HE2	7	0.28	0.07	0.28
(1,58)	1:50:A:GLN:HA	1:45:A:MET:HE1	7	0.28	0.07	0.28
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	7	0.26	0.08	0.23
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	7	0.26	0.06	0.26
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB1	7	0.25	0.05	0.26
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	7	0.25	0.05	0.26
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB2	7	0.25	0.05	0.26
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG11	7	0.18	0.03	0.18
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG13	7	0.18	0.03	0.18
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG12	7	0.18	0.03	0.18
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	7	0.18	0.04	0.19
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	7	0.18	0.05	0.16
(2,652)	1:48:A:LEU:HD12	1:48:A:LEU:HG	7	0.17	0.01	0.18
(2,652)	1:48:A:LEU:HD11	1:48:A:LEU:HG	7	0.17	0.01	0.18
(2,652)	1:48:A:LEU:HD13	1:48:A:LEU:HG	7	0.17	0.01	0.18
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD1	7	0.17	0.06	0.16
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD2	7	0.17	0.06	0.16
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HB2	7	0.17	0.02	0.18
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HG	7	0.17	0.02	0.18
(1,274)	1:74:A:PHE:HB3	1:24:A:PHE:HD2	7	0.17	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,274)	1:74:A:PHE:HB3	1:24:A:PHE:HD1	7	0.17	0.03	0.15
(1,274)	1:74:A:PHE:HB3	1:74:A:PHE:HE2	7	0.17	0.03	0.15
(1,274)	1:74:A:PHE:HB3	1:74:A:PHE:HE1	7	0.17	0.03	0.15
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	7	0.16	0.03	0.17
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	7	0.14	0.02	0.16
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD12	7	0.12	0.01	0.13
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD13	7	0.12	0.01	0.13
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD11	7	0.12	0.01	0.13
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	7	0.12	0.01	0.12
(1,10)	1:141:A:PRO:HA	1:143:A:LEU:HB2	6	1.41	0.53	1.58
(1,10)	1:141:A:PRO:HA	1:145:A:ARG:HG3	6	1.41	0.53	1.58
(1,136)	1:146:A:VAL:HG12	1:144:A:ARG:HA	6	1.34	0.64	1.25
(1,136)	1:146:A:VAL:HG12	1:145:A:ARG:HA	6	1.34	0.64	1.25
(1,136)	1:146:A:VAL:HG11	1:144:A:ARG:HA	6	1.34	0.64	1.25
(1,136)	1:146:A:VAL:HG13	1:145:A:ARG:HA	6	1.34	0.64	1.25
(1,136)	1:146:A:VAL:HG11	1:145:A:ARG:HA	6	1.34	0.64	1.25
(2,586)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	6	1.27	1.23	1.02
(2,586)	1:9:A:VAL:HG22	1:10:A:GLU:HG3	6	1.27	1.23	1.02
(2,586)	1:9:A:VAL:HG23	1:10:A:GLU:HG3	6	1.27	1.23	1.02
(2,922)	1:4:A:ILE:HG13	1:5:A:TYR:HE2	6	1.03	0.16	1.06
(2,922)	1:4:A:ILE:HG13	1:5:A:TYR:HE1	6	1.03	0.16	1.06
(2,922)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	6	1.03	0.16	1.06
(1,54)	1:87:A:ASP:HA	1:86:A:LYS:HD3	6	0.92	0.21	1.01
(1,54)	1:2:A:ASP:HA	1:4:A:ILE:HB	6	0.92	0.21	1.01
(1,54)	1:87:A:ASP:HA	1:90:A:LYS:HD2	6	0.92	0.21	1.01
(1,54)	1:2:A:ASP:HA	1:6:A:LYS:HD2	6	0.92	0.21	1.01
(1,54)	1:87:A:ASP:HA	1:90:A:LYS:HD3	6	0.92	0.21	1.01
(2,482)	1:81:A:MET:HE3	1:20:A:PHE:HD2	6	0.79	0.85	0.44
(2,482)	1:81:A:MET:HE2	1:20:A:PHE:HD1	6	0.79	0.85	0.44
(2,482)	1:81:A:MET:HE2	1:20:A:PHE:HD2	6	0.79	0.85	0.44
(1,313)	1:27:A:PHE:HE2	1:36:A:ILE:HG23	6	0.72	0.18	0.68
(1,313)	1:27:A:PHE:HE2	1:36:A:ILE:HG22	6	0.72	0.18	0.68
(1,313)	1:27:A:PHE:HE2	1:41:A:LEU:HD21	6	0.72	0.18	0.68
(1,313)	1:27:A:PHE:HE1	1:36:A:ILE:HG21	6	0.72	0.18	0.68
(2,745)	1:4:A:ILE:HD11	1:4:A:ILE:HB	6	0.64	0.03	0.64
(2,745)	1:4:A:ILE:HD13	1:4:A:ILE:HB	6	0.64	0.03	0.64
(2,745)	1:4:A:ILE:HD12	1:4:A:ILE:HB	6	0.64	0.03	0.64
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD13	6	0.63	0.35	0.64
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD12	6	0.63	0.35	0.64
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD11	6	0.63	0.35	0.64
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD11	6	0.59	0.29	0.65
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD13	6	0.59	0.29	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD12	6	0.59	0.29	0.65
(2,727)	1:11:A:GLN:HB2	1:11:A:GLN:HG2	6	0.53	0.25	0.69
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG21	6	0.5	0.14	0.5
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG23	6	0.5	0.14	0.5
(2,548)	1:79:A:VAL:HG11	1:5:A:TYR:HD2	6	0.49	0.13	0.52
(2,548)	1:79:A:VAL:HG13	1:5:A:TYR:HD1	6	0.49	0.13	0.52
(2,548)	1:79:A:VAL:HG12	1:5:A:TYR:HD1	6	0.49	0.13	0.52
(2,548)	1:79:A:VAL:HG11	1:5:A:TYR:HD1	6	0.49	0.13	0.52
(1,98)	1:85:A:MET:HE1	1:86:A:LYS:HG2	6	0.47	0.21	0.48
(1,98)	1:85:A:MET:HE3	1:86:A:LYS:HG2	6	0.47	0.21	0.48
(1,98)	1:85:A:MET:HE1	1:150:A:ALA:HB2	6	0.47	0.21	0.48
(1,98)	1:85:A:MET:HE3	1:150:A:ALA:HB2	6	0.47	0.21	0.48
(1,98)	1:85:A:MET:HE2	1:150:A:ALA:HB3	6	0.47	0.21	0.48
(2,1139)	1:41:A:LEU:HD22	1:45:A:MET:HG3	6	0.44	0.14	0.38
(2,1139)	1:41:A:LEU:HD21	1:45:A:MET:HG3	6	0.44	0.14	0.38
(2,1139)	1:41:A:LEU:HD23	1:45:A:MET:HG3	6	0.44	0.14	0.38
(2,819)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	6	0.43	0.04	0.43
(2,819)	1:7:A:ALA:HB3	1:10:A:GLU:HB2	6	0.43	0.04	0.43
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG11	6	0.43	0.06	0.42
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG13	6	0.43	0.06	0.42
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG12	6	0.43	0.06	0.42
(1,65)	1:52:A:PRO:HD3	1:57:A:LEU:HD11	6	0.4	0.25	0.36
(1,65)	1:52:A:PRO:HD3	1:146:A:VAL:HG11	6	0.4	0.25	0.36
(1,65)	1:52:A:PRO:HD3	1:146:A:VAL:HG13	6	0.4	0.25	0.36
(1,127)	1:150:A:ALA:HB1	1:85:A:MET:HG2	6	0.4	0.3	0.32
(1,127)	1:150:A:ALA:HB3	1:151:A:ASP:HB2	6	0.4	0.3	0.32
(1,127)	1:150:A:ALA:HB2	1:85:A:MET:HG2	6	0.4	0.3	0.32
(1,127)	1:156:A:ALA:HB2	1:47:A:MET:HG2	6	0.4	0.3	0.32
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG21	6	0.38	0.11	0.36
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG22	6	0.38	0.11	0.36
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG23	6	0.38	0.11	0.36
(2,446)	1:1:A:MET:HE1	1:1:A:MET:HA	6	0.37	0.07	0.38
(2,446)	1:1:A:MET:HE3	1:1:A:MET:HA	6	0.37	0.07	0.38
(2,446)	1:1:A:MET:HE2	1:1:A:MET:HA	6	0.37	0.07	0.38
(1,61)	1:51:A:ASN:HA	1:46:A:ARG:HG2	6	0.36	0.1	0.39
(1,280)	1:22:A:ALA:HB1	1:25:A:ASP:HB3	6	0.35	0.11	0.34
(1,280)	1:22:A:ALA:HB3	1:25:A:ASP:HB3	6	0.35	0.11	0.34
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HB2	6	0.34	0.16	0.32
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HD2	6	0.34	0.16	0.32
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG11	6	0.32	0.17	0.26
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG13	6	0.32	0.17	0.26
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG12	6	0.32	0.17	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE2	6	0.32	0.22	0.22
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE3	6	0.32	0.22	0.22
(1,253)	1:71:A:THR:HB	1:69:A:SER:HB3	6	0.31	0.08	0.31
(1,253)	1:71:A:THR:HB	1:37:A:SER:HB2	6	0.31	0.08	0.31
(1,343)	1:59:A:GLU:H	1:58:A:GLN:HB3	6	0.29	0.06	0.29
(1,343)	1:59:A:GLU:H	1:59:A:GLU:HB3	6	0.29	0.06	0.29
(2,493)	1:151:A:ASP:HB2	1:152:A:ALA:HB3	6	0.28	0.1	0.29
(2,493)	1:151:A:ASP:HB3	1:152:A:ALA:HB1	6	0.28	0.1	0.29
(2,493)	1:151:A:ASP:HB2	1:152:A:ALA:HB2	6	0.28	0.1	0.29
(1,146)	1:12:A:LEU:HD23	1:82:A:VAL:HA	6	0.26	0.09	0.24
(1,146)	1:16:A:GLN:HA	1:12:A:LEU:HD21	6	0.26	0.09	0.24
(1,146)	1:12:A:LEU:HD21	1:82:A:VAL:HA	6	0.26	0.09	0.24
(2,1090)	1:21:A:LYS:HB3	1:74:A:PHE:HZ	6	0.25	0.11	0.24
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD12	6	0.24	0.08	0.28
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD13	6	0.24	0.08	0.28
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD11	6	0.24	0.08	0.28
(2,748)	1:55:A:GLU:HB3	1:55:A:GLU:HG3	6	0.24	0.02	0.24
(2,476)	1:45:A:MET:HE3	1:57:A:LEU:HA	6	0.22	0.05	0.22
(2,476)	1:45:A:MET:HE1	1:57:A:LEU:HA	6	0.22	0.05	0.22
(2,476)	1:45:A:MET:HE2	1:57:A:LEU:HA	6	0.22	0.05	0.22
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB2	6	0.19	0.04	0.18
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB3	6	0.19	0.04	0.18
(2,1393)	1:10:A:GLU:H	1:10:A:GLU:HB2	6	0.16	0.03	0.16
(2,366)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	6	0.15	0.04	0.14
(2,366)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	6	0.15	0.04	0.14
(2,1432)	1:155:A:GLN:H	1:156:A:ALA:H	6	0.15	0.01	0.15
(2,588)	1:9:A:VAL:HG23	1:9:A:VAL:HB	6	0.12	0.01	0.12
(2,588)	1:9:A:VAL:HG21	1:9:A:VAL:HB	6	0.12	0.01	0.12
(2,588)	1:9:A:VAL:HG22	1:9:A:VAL:HB	6	0.12	0.01	0.12
(1,228)	1:43:A:LYS:HA	1:43:A:LYS:HB2	6	0.11	0.0	0.11
(2,772)	1:7:A:ALA:HB3	1:11:A:GLN:HG2	5	2.52	1.3	2.71
(2,772)	1:7:A:ALA:HB1	1:11:A:GLN:HG2	5	2.52	1.3	2.71
(2,772)	1:7:A:ALA:HB2	1:11:A:GLN:HG2	5	2.52	1.3	2.71
(2,641)	1:157:A:LEU:HD13	1:23:A:ALA:HB1	5	2.04	0.19	2.06
(2,641)	1:157:A:LEU:HD11	1:23:A:ALA:HB3	5	2.04	0.19	2.06
(2,641)	1:157:A:LEU:HD13	1:23:A:ALA:HB2	5	2.04	0.19	2.06
(2,641)	1:157:A:LEU:HD13	1:23:A:ALA:HB3	5	2.04	0.19	2.06
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG21	5	1.87	1.34	2.61
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG23	5	1.87	1.34	2.61
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG22	5	1.87	1.34	2.61
(2,1041)	1:78:A:LEU:HD13	1:75:A:ASP:HB3	5	1.56	0.14	1.61
(2,1041)	1:78:A:LEU:HD12	1:75:A:ASP:HB3	5	1.56	0.14	1.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1041)	1:78:A:LEU:HD11	1:75:A:ASP:HB3	5	1.56	0.14	1.61
(2,1073)	1:157:A:LEU:HD23	1:27:A:PHE:HB3	5	1.32	0.43	1.36
(2,1073)	1:157:A:LEU:HD22	1:27:A:PHE:HB3	5	1.32	0.43	1.36
(2,1073)	1:157:A:LEU:HD21	1:27:A:PHE:HB3	5	1.32	0.43	1.36
(2,1049)	1:78:A:LEU:HD12	1:81:A:MET:HE3	5	1.26	0.65	1.77
(2,1049)	1:78:A:LEU:HD11	1:81:A:MET:HE2	5	1.26	0.65	1.77
(2,1049)	1:78:A:LEU:HD12	1:81:A:MET:HE2	5	1.26	0.65	1.77
(2,1049)	1:78:A:LEU:HD13	1:81:A:MET:HE1	5	1.26	0.65	1.77
(2,568)	1:82:A:VAL:HG22	1:86:A:LYS:HD3	5	1.21	1.24	0.68
(2,568)	1:82:A:VAL:HG22	1:86:A:LYS:HD2	5	1.21	1.24	0.68
(2,568)	1:82:A:VAL:HG23	1:86:A:LYS:HD2	5	1.21	1.24	0.68
(2,568)	1:82:A:VAL:HG23	1:86:A:LYS:HD3	5	1.21	1.24	0.68
(2,640)	1:157:A:LEU:HD13	1:153:A:MET:HG2	5	1.05	0.66	0.77
(2,640)	1:157:A:LEU:HD11	1:153:A:MET:HG2	5	1.05	0.66	0.77
(2,443)	1:85:A:MET:HE3	1:86:A:LYS:HE2	5	1.0	0.46	1.14
(2,443)	1:85:A:MET:HE2	1:86:A:LYS:HE3	5	1.0	0.46	1.14
(2,1501)	1:11:A:GLN:H	1:11:A:GLN:HG2	5	0.98	0.46	1.15
(1,39)	1:63:A:GLU:HA	1:143:A:LEU:HD13	5	0.89	0.5	1.18
(1,39)	1:63:A:GLU:HA	1:64:A:VAL:HG21	5	0.89	0.5	1.18
(1,39)	1:63:A:GLU:HA	1:64:A:VAL:HG23	5	0.89	0.5	1.18
(1,39)	1:63:A:GLU:HA	1:143:A:LEU:HD11	5	0.89	0.5	1.18
(2,441)	1:47:A:MET:HE1	1:157:A:LEU:HD22	5	0.86	0.2	0.84
(2,441)	1:47:A:MET:HE1	1:157:A:LEU:HD21	5	0.86	0.2	0.84
(2,441)	1:47:A:MET:HE1	1:157:A:LEU:HD23	5	0.86	0.2	0.84
(2,441)	1:47:A:MET:HE2	1:157:A:LEU:HD21	5	0.86	0.2	0.84
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD21	5	0.85	0.22	0.74
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD22	5	0.85	0.22	0.74
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD23	5	0.85	0.22	0.74
(2,1104)	1:143:A:LEU:HD13	1:63:A:GLU:HG3	5	0.85	0.42	0.88
(2,1104)	1:143:A:LEU:HD12	1:63:A:GLU:HG3	5	0.85	0.42	0.88
(2,1104)	1:143:A:LEU:HD11	1:63:A:GLU:HG3	5	0.85	0.42	0.88
(1,289)	1:146:A:VAL:HG22	1:147:A:ARG:HD2	5	0.84	0.26	0.86
(1,289)	1:146:A:VAL:HG22	1:145:A:ARG:HD2	5	0.84	0.26	0.86
(1,289)	1:146:A:VAL:HG23	1:145:A:ARG:HD2	5	0.84	0.26	0.86
(1,289)	1:146:A:VAL:HG22	1:145:A:ARG:HD3	5	0.84	0.26	0.86
(2,1226)	1:20:A:PHE:HE1	1:78:A:LEU:HD22	5	0.82	0.16	0.75
(2,1226)	1:20:A:PHE:HE2	1:78:A:LEU:HD23	5	0.82	0.16	0.75
(2,1226)	1:20:A:PHE:HE1	1:78:A:LEU:HD21	5	0.82	0.16	0.75
(1,290)	1:64:A:VAL:HG21	1:65:A:ASP:HB3	5	0.71	0.93	0.2
(1,290)	1:64:A:VAL:HG23	1:65:A:ASP:HB3	5	0.71	0.93	0.2
(1,290)	1:146:A:VAL:HG21	1:60:A:MET:HG3	5	0.71	0.93	0.2
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD11	5	0.68	0.25	0.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD12	5	0.68	0.25	0.75
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD13	5	0.68	0.25	0.75
(1,177)	1:41:A:LEU:HD23	1:61:A:ILE:HB	5	0.68	0.57	0.3
(1,177)	1:57:A:LEU:HB2	1:41:A:LEU:HD23	5	0.68	0.57	0.3
(1,177)	1:41:A:LEU:HD22	1:61:A:ILE:HB	5	0.68	0.57	0.3
(1,177)	1:41:A:LEU:HD21	1:61:A:ILE:HB	5	0.68	0.57	0.3
(1,191)	1:64:A:VAL:HG12	1:63:A:GLU:HG2	5	0.62	0.48	0.46
(1,191)	1:64:A:VAL:HG11	1:63:A:GLU:HG2	5	0.62	0.48	0.46
(1,191)	1:64:A:VAL:HG13	1:63:A:GLU:HG2	5	0.62	0.48	0.46
(1,169)	1:157:A:LEU:HD12	1:26:A:ILE:HB	5	0.6	0.49	0.52
(1,169)	1:157:A:LEU:HD13	1:153:A:MET:HE3	5	0.6	0.49	0.52
(1,46)	1:85:A:MET:HA	1:150:A:ALA:HB1	5	0.57	0.2	0.6
(1,46)	1:85:A:MET:HA	1:150:A:ALA:HB3	5	0.57	0.2	0.6
(1,46)	1:85:A:MET:HA	1:150:A:ALA:HB2	5	0.57	0.2	0.6
(1,46)	1:151:A:ASP:HA	1:150:A:ALA:HB2	5	0.57	0.2	0.6
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD11	5	0.56	0.05	0.56
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD13	5	0.56	0.05	0.56
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD12	5	0.56	0.05	0.56
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD13	5	0.56	0.22	0.55
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD11	5	0.56	0.22	0.55
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD12	5	0.56	0.22	0.55
(2,785)	1:60:A:MET:HG3	1:41:A:LEU:HD22	5	0.55	0.43	0.43
(2,785)	1:60:A:MET:HG3	1:41:A:LEU:HD23	5	0.55	0.43	0.43
(2,1044)	1:78:A:LEU:HG	1:74:A:PHE:HE1	5	0.54	0.16	0.57
(2,1044)	1:78:A:LEU:HG	1:74:A:PHE:HE2	5	0.54	0.16	0.57
(2,515)	1:31:A:ALA:HB2	1:28:A:VAL:HG13	5	0.53	0.11	0.59
(2,515)	1:31:A:ALA:HB1	1:28:A:VAL:HG12	5	0.53	0.11	0.59
(2,515)	1:31:A:ALA:HB1	1:28:A:VAL:HG11	5	0.53	0.11	0.59
(2,515)	1:31:A:ALA:HB3	1:28:A:VAL:HG12	5	0.53	0.11	0.59
(2,515)	1:31:A:ALA:HB1	1:28:A:VAL:HG13	5	0.53	0.11	0.59
(2,1088)	1:78:A:LEU:HD13	1:74:A:PHE:HD1	5	0.52	0.08	0.55
(2,1088)	1:78:A:LEU:HD12	1:74:A:PHE:HD1	5	0.52	0.08	0.55
(2,1088)	1:78:A:LEU:HD11	1:74:A:PHE:HD1	5	0.52	0.08	0.55
(2,1088)	1:78:A:LEU:HD13	1:74:A:PHE:HD2	5	0.52	0.08	0.55
(2,1088)	1:78:A:LEU:HD12	1:74:A:PHE:HD2	5	0.52	0.08	0.55
(2,516)	1:64:A:VAL:HA	1:64:A:VAL:HG22	5	0.52	0.16	0.57
(2,516)	1:64:A:VAL:HA	1:64:A:VAL:HG23	5	0.52	0.16	0.57
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	0.49	0.08	0.49
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD12	5	0.49	0.08	0.49
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD11	5	0.49	0.08	0.49
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD23	5	0.49	0.08	0.49
(1,118)	1:150:A:ALA:HB3	1:85:A:MET:HB2	5	0.44	0.2	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,118)	1:150:A:ALA:HB2	1:85:A:MET:HB2	5	0.44	0.2	0.53
(1,118)	1:85:A:MET:HE1	1:150:A:ALA:HB2	5	0.44	0.2	0.53
(1,118)	1:150:A:ALA:HB1	1:85:A:MET:HB2	5	0.44	0.2	0.53
(1,118)	1:85:A:MET:HE2	1:150:A:ALA:HB3	5	0.44	0.2	0.53
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG13	5	0.44	0.12	0.42
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG12	5	0.44	0.12	0.42
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG11	5	0.44	0.12	0.42
(2,1079)	1:164:A:GLY:HA3	1:163:A:LYS:HE2	5	0.43	0.07	0.42
(2,1079)	1:164:A:GLY:HA3	1:163:A:LYS:HE3	5	0.43	0.07	0.42
(2,1079)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	5	0.43	0.07	0.42
(2,513)	1:31:A:ALA:HB2	1:36:A:ILE:HG21	5	0.42	0.21	0.48
(2,513)	1:31:A:ALA:HB1	1:36:A:ILE:HG22	5	0.42	0.21	0.48
(2,513)	1:31:A:ALA:HB3	1:36:A:ILE:HG22	5	0.42	0.21	0.48
(2,513)	1:31:A:ALA:HB1	1:36:A:ILE:HG23	5	0.42	0.21	0.48
(2,1070)	1:148:A:ILE:HD11	1:27:A:PHE:HZ	5	0.39	0.06	0.39
(2,1070)	1:148:A:ILE:HD13	1:27:A:PHE:HZ	5	0.39	0.06	0.39
(2,1070)	1:148:A:ILE:HD12	1:27:A:PHE:HZ	5	0.39	0.06	0.39
(2,1062)	1:145:A:ARG:HD3	1:145:A:ARG:HA	5	0.38	0.32	0.21
(2,538)	1:9:A:VAL:HG12	1:9:A:VAL:HA	5	0.37	0.07	0.36
(2,538)	1:9:A:VAL:HG13	1:9:A:VAL:HA	5	0.37	0.07	0.36
(2,538)	1:9:A:VAL:HG11	1:9:A:VAL:HA	5	0.37	0.07	0.36
(1,167)	1:78:A:LEU:HD12	1:17:A:LYS:HG3	5	0.36	0.12	0.37
(1,167)	1:78:A:LEU:HD11	1:17:A:LYS:HG3	5	0.36	0.12	0.37
(1,167)	1:78:A:LEU:HD13	1:17:A:LYS:HG3	5	0.36	0.12	0.37
(2,1150)	1:148:A:ILE:HD12	1:148:A:ILE:HA	5	0.36	0.15	0.35
(2,1150)	1:148:A:ILE:HD11	1:148:A:ILE:HA	5	0.36	0.15	0.35
(2,1150)	1:148:A:ILE:HD13	1:148:A:ILE:HA	5	0.36	0.15	0.35
(1,109)	1:154:A:MET:HE2	1:19:A:GLU:HA	5	0.36	0.18	0.38
(1,109)	1:154:A:MET:HE3	1:19:A:GLU:HA	5	0.36	0.18	0.38
(1,109)	1:154:A:MET:HE1	1:19:A:GLU:HA	5	0.36	0.18	0.38
(1,53)	1:87:A:ASP:HA	1:86:A:LYS:HB3	5	0.36	0.08	0.33
(1,53)	1:2:A:ASP:HA	1:6:A:LYS:HB2	5	0.36	0.08	0.33
(1,59)	1:160:A:ALA:HA	1:163:A:LYS:HD3	5	0.35	0.19	0.29
(1,59)	1:160:A:ALA:HA	1:163:A:LYS:HD2	5	0.35	0.19	0.29
(1,96)	1:148:A:ILE:HD11	1:45:A:MET:HG2	5	0.35	0.17	0.23
(1,96)	1:148:A:ILE:HD13	1:153:A:MET:HG3	5	0.35	0.17	0.23
(1,96)	1:148:A:ILE:HD12	1:153:A:MET:HG3	5	0.35	0.17	0.23
(1,96)	1:148:A:ILE:HD13	1:45:A:MET:HG2	5	0.35	0.17	0.23
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG22	5	0.35	0.16	0.29
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG21	5	0.35	0.16	0.29
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG23	5	0.35	0.16	0.29
(2,475)	1:45:A:MET:HE2	1:45:A:MET:HA	5	0.35	0.12	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,475)	1:45:A:MET:HE1	1:45:A:MET:HA	5	0.35	0.12	0.36
(2,285)	1:54:A:PRO:HD2	1:53:A:THR:HG22	5	0.33	0.05	0.31
(2,285)	1:54:A:PRO:HD3	1:53:A:THR:HG23	5	0.33	0.05	0.31
(2,285)	1:54:A:PRO:HD2	1:53:A:THR:HG23	5	0.33	0.05	0.31
(2,285)	1:54:A:PRO:HD3	1:53:A:THR:HG21	5	0.33	0.05	0.31
(1,41)	1:16:A:GLN:HA	1:16:A:GLN:HB2	5	0.33	0.11	0.38
(1,145)	1:23:A:ALA:HB2	1:158:A:LEU:HD23	5	0.31	0.11	0.32
(1,145)	1:23:A:ALA:HB1	1:158:A:LEU:HD21	5	0.31	0.11	0.32
(1,145)	1:158:A:LEU:HB3	1:158:A:LEU:HD22	5	0.31	0.11	0.32
(2,617)	1:78:A:LEU:HD21	1:20:A:PHE:HB2	5	0.31	0.19	0.21
(2,617)	1:78:A:LEU:HD22	1:20:A:PHE:HB2	5	0.31	0.19	0.21
(2,617)	1:78:A:LEU:HD23	1:20:A:PHE:HB2	5	0.31	0.19	0.21
(2,660)	1:140:A:ARG:HG2	1:141:A:PRO:HD2	5	0.3	0.12	0.35
(2,660)	1:140:A:ARG:HG3	1:141:A:PRO:HD2	5	0.3	0.12	0.35
(2,189)	1:10:A:GLU:HA	1:10:A:GLU:HG3	5	0.3	0.14	0.24
(1,291)	1:158:A:LEU:HD12	1:155:A:GLN:HA	5	0.29	0.1	0.29
(1,291)	1:158:A:LEU:HD11	1:155:A:GLN:HA	5	0.29	0.1	0.29
(1,291)	1:158:A:LEU:HD13	1:155:A:GLN:HA	5	0.29	0.1	0.29
(2,429)	1:61:A:ILE:HG22	1:58:A:GLN:HA	5	0.29	0.13	0.31
(2,429)	1:61:A:ILE:HG21	1:58:A:GLN:HA	5	0.29	0.13	0.31
(2,1196)	1:4:A:ILE:HG23	1:5:A:TYR:HE2	5	0.29	0.11	0.28
(2,1196)	1:4:A:ILE:HG21	1:5:A:TYR:HE1	5	0.29	0.11	0.28
(2,1196)	1:4:A:ILE:HG22	1:5:A:TYR:HE1	5	0.29	0.11	0.28
(2,1174)	1:145:A:ARG:HG3	1:145:A:ARG:HA	5	0.29	0.14	0.22
(2,1174)	1:145:A:ARG:HG2	1:145:A:ARG:HA	5	0.29	0.14	0.22
(1,276)	1:142:A:THR:HA	1:143:A:LEU:HG	5	0.28	0.1	0.24
(2,1153)	1:12:A:LEU:HB3	1:17:A:LYS:HD3	5	0.28	0.21	0.13
(2,1153)	1:12:A:LEU:HB3	1:17:A:LYS:HD2	5	0.28	0.21	0.13
(2,923)	1:157:A:LEU:HD13	1:27:A:PHE:HD1	5	0.27	0.08	0.24
(2,923)	1:157:A:LEU:HD11	1:27:A:PHE:HD1	5	0.27	0.08	0.24
(2,923)	1:157:A:LEU:HD12	1:27:A:PHE:HD1	5	0.27	0.08	0.24
(2,605)	1:57:A:LEU:HD23	1:45:A:MET:HG2	5	0.27	0.15	0.21
(2,605)	1:57:A:LEU:HD22	1:45:A:MET:HG2	5	0.27	0.15	0.21
(2,152)	1:11:A:GLN:HA	1:11:A:GLN:HB3	5	0.26	0.1	0.33
(2,1014)	1:71:A:THR:HA	1:38:A:THR:HG23	5	0.25	0.07	0.23
(2,1014)	1:71:A:THR:HA	1:38:A:THR:HG21	5	0.25	0.07	0.23
(2,1023)	1:35:A:SER:HB2	1:73:A:ASP:HB3	5	0.25	0.18	0.18
(1,63)	1:52:A:PRO:HD3	1:45:A:MET:HG3	5	0.24	0.06	0.22
(2,56)	1:26:A:ILE:HA	1:26:A:ILE:HG23	5	0.23	0.06	0.24
(2,56)	1:26:A:ILE:HA	1:26:A:ILE:HG21	5	0.23	0.06	0.24
(2,1087)	1:78:A:LEU:HD13	1:74:A:PHE:HE1	5	0.22	0.1	0.19
(2,1087)	1:78:A:LEU:HD12	1:74:A:PHE:HE1	5	0.22	0.1	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1087)	1:78:A:LEU:HD11	1:74:A:PHE:HE2	5	0.22	0.1	0.19
(2,1087)	1:78:A:LEU:HD11	1:74:A:PHE:HE1	5	0.22	0.1	0.19
(2,1087)	1:78:A:LEU:HD12	1:74:A:PHE:HE2	5	0.22	0.1	0.19
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE3	5	0.21	0.12	0.16
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE2	5	0.21	0.12	0.16
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE1	5	0.21	0.12	0.16
(2,197)	1:41:A:LEU:HA	1:44:A:VAL:HB	5	0.19	0.02	0.2
(2,298)	1:51:A:ASN:HA	1:52:A:PRO:HD3	5	0.19	0.05	0.18
(2,818)	1:43:A:LYS:HD2	1:43:A:LYS:HG3	5	0.18	0.09	0.15
(2,818)	1:43:A:LYS:HD3	1:43:A:LYS:HG3	5	0.18	0.09	0.15
(2,270)	1:31:A:ALA:HA	1:32:A:GLU:HB2	5	0.18	0.03	0.17
(1,326)	1:87:A:ASP:H	1:86:A:LYS:HA	5	0.18	0.02	0.18
(2,702)	1:155:A:GLN:HA	1:155:A:GLN:HB3	5	0.16	0.06	0.15
(2,702)	1:155:A:GLN:HA	1:155:A:GLN:HB2	5	0.16	0.06	0.15
(2,826)	1:63:A:GLU:HA	1:63:A:GLU:HB2	5	0.16	0.01	0.16
(2,874)	1:86:A:LYS:HB2	1:86:A:LYS:HA	5	0.15	0.03	0.16
(2,250)	1:7:A:ALA:HA	1:10:A:GLU:HB2	5	0.15	0.02	0.15
(2,967)	1:44:A:VAL:HA	1:27:A:PHE:HZ	5	0.14	0.02	0.14
(2,915)	1:15:A:GLU:HG3	1:15:A:GLU:HB2	5	0.13	0.01	0.14
(2,915)	1:15:A:GLU:HG2	1:15:A:GLU:HB3	5	0.13	0.01	0.14
(2,706)	1:55:A:GLU:HA	1:55:A:GLU:HB3	5	0.12	0.01	0.11
(2,1102)	1:145:A:ARG:HD3	1:143:A:LEU:HD12	4	4.52	0.65	4.71
(2,1102)	1:145:A:ARG:HD2	1:143:A:LEU:HD13	4	4.52	0.65	4.71
(2,1102)	1:145:A:ARG:HD3	1:143:A:LEU:HD13	4	4.52	0.65	4.71
(2,105)	1:84:A:SER:HA	1:88:A:ASP:HB2	4	2.51	2.06	2.38
(2,105)	1:84:A:SER:HA	1:88:A:ASP:HB3	4	2.51	2.06	2.38
(2,216)	1:154:A:MET:HA	1:157:A:LEU:HD13	4	2.01	0.36	1.92
(2,216)	1:154:A:MET:HA	1:157:A:LEU:HD12	4	2.01	0.36	1.92
(2,434)	1:85:A:MET:HE3	1:12:A:LEU:HD22	4	1.76	1.06	2.0
(2,434)	1:85:A:MET:HE2	1:12:A:LEU:HD21	4	1.76	1.06	2.0
(2,434)	1:85:A:MET:HE3	1:12:A:LEU:HD23	4	1.76	1.06	2.0
(2,1184)	1:5:A:TYR:HD2	1:85:A:MET:HG3	4	1.25	0.61	0.94
(2,1184)	1:5:A:TYR:HD1	1:85:A:MET:HG3	4	1.25	0.61	0.94
(1,29)	1:59:A:GLU:HA	1:143:A:LEU:HG	4	1.16	0.5	1.3
(1,29)	1:59:A:GLU:HA	1:143:A:LEU:HB3	4	1.16	0.5	1.3
(2,597)	1:27:A:PHE:HA	1:157:A:LEU:HD23	4	1.07	0.4	1.25
(2,597)	1:27:A:PHE:HA	1:157:A:LEU:HD22	4	1.07	0.4	1.25
(2,597)	1:27:A:PHE:HA	1:157:A:LEU:HD21	4	1.07	0.4	1.25
(1,154)	1:157:A:LEU:HD21	1:26:A:ILE:HB	4	0.88	0.2	0.85
(1,154)	1:157:A:LEU:HD23	1:26:A:ILE:HB	4	0.88	0.2	0.85
(1,154)	1:47:A:MET:HE1	1:157:A:LEU:HD23	4	0.88	0.2	0.85
(2,1214)	1:138:A:PHE:HD2	1:139:A:LYS:HD3	4	0.85	0.49	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1214)	1:138:A:PHE:HD1	1:139:A:LYS:HD3	4	0.85	0.49	0.68
(1,214)	1:19:A:GLU:HB3	1:158:A:LEU:HD11	4	0.75	0.24	0.7
(1,214)	1:19:A:GLU:HB3	1:158:A:LEU:HD12	4	0.75	0.24	0.7
(1,214)	1:19:A:GLU:HB3	1:158:A:LEU:HD13	4	0.75	0.24	0.7
(2,851)	1:161:A:ARG:HB2	1:161:A:ARG:HD2	4	0.74	0.35	0.82
(2,453)	1:2:A:ASP:HB2	1:4:A:ILE:HG21	4	0.7	0.35	0.67
(2,453)	1:2:A:ASP:HB2	1:4:A:ILE:HG23	4	0.7	0.35	0.67
(2,453)	1:2:A:ASP:HB2	1:4:A:ILE:HG22	4	0.7	0.35	0.67
(2,910)	1:41:A:LEU:HD12	1:77:A:PHE:HD2	4	0.68	0.32	0.6
(2,910)	1:41:A:LEU:HD11	1:77:A:PHE:HD1	4	0.68	0.32	0.6
(2,910)	1:41:A:LEU:HD13	1:77:A:PHE:HD2	4	0.68	0.32	0.6
(2,910)	1:41:A:LEU:HD12	1:77:A:PHE:HD1	4	0.68	0.32	0.6
(2,642)	1:157:A:LEU:HD11	1:157:A:LEU:HB2	4	0.68	0.07	0.7
(2,642)	1:157:A:LEU:HD12	1:157:A:LEU:HB2	4	0.68	0.07	0.7
(2,1585)	1:162:A:ALA:HA	1:158:A:LEU:HD12	4	0.67	0.29	0.6
(2,1585)	1:162:A:ALA:HA	1:158:A:LEU:HD11	4	0.67	0.29	0.6
(2,1585)	1:162:A:ALA:HA	1:158:A:LEU:HD13	4	0.67	0.29	0.6
(2,473)	1:154:A:MET:HE2	1:158:A:LEU:HD23	4	0.65	0.27	0.64
(2,547)	1:45:A:MET:HE1	1:146:A:VAL:HG11	4	0.64	0.2	0.7
(2,547)	1:45:A:MET:HE2	1:146:A:VAL:HG13	4	0.64	0.2	0.7
(2,547)	1:45:A:MET:HE1	1:146:A:VAL:HG13	4	0.64	0.2	0.7
(2,1069)	1:148:A:ILE:HD11	1:147:A:ARG:HD2	4	0.61	0.26	0.62
(2,1069)	1:148:A:ILE:HD12	1:147:A:ARG:HD2	4	0.61	0.26	0.62
(2,1177)	1:89:A:SER:HA	1:139:A:LYS:HE2	4	0.57	0.43	0.39
(2,1177)	1:89:A:SER:HA	1:139:A:LYS:HE3	4	0.57	0.43	0.39
(1,14)	1:146:A:VAL:HA	1:45:A:MET:HE1	4	0.54	0.18	0.55
(1,14)	1:146:A:VAL:HA	1:147:A:ARG:HB3	4	0.54	0.18	0.55
(1,275)	1:13:A:THR:HB	1:16:A:GLN:HB2	4	0.52	0.25	0.55
(2,1408)	1:86:A:LYS:H	1:86:A:LYS:HG2	4	0.51	0.15	0.45
(2,1408)	1:86:A:LYS:H	1:86:A:LYS:HG3	4	0.51	0.15	0.45
(2,509)	1:162:A:ALA:HB2	1:158:A:LEU:HD22	4	0.51	0.15	0.56
(2,509)	1:162:A:ALA:HB3	1:158:A:LEU:HD22	4	0.51	0.15	0.56
(2,509)	1:162:A:ALA:HB3	1:158:A:LEU:HD23	4	0.51	0.15	0.56
(1,143)	1:82:A:VAL:HG21	1:5:A:TYR:HB2	4	0.48	0.25	0.44
(1,143)	1:71:A:THR:HG23	1:33:A:ASP:HB3	4	0.48	0.25	0.44
(1,143)	1:71:A:THR:HG22	1:33:A:ASP:HB3	4	0.48	0.25	0.44
(1,266)	1:157:A:LEU:HD12	1:27:A:PHE:HB2	4	0.47	0.17	0.43
(1,266)	1:157:A:LEU:HD11	1:27:A:PHE:HB2	4	0.47	0.17	0.43
(1,192)	1:63:A:GLU:HG2	1:143:A:LEU:HD13	4	0.46	0.14	0.42
(1,192)	1:59:A:GLU:HG2	1:143:A:LEU:HD12	4	0.46	0.14	0.42
(1,192)	1:59:A:GLU:HG2	1:143:A:LEU:HD13	4	0.46	0.14	0.42
(1,192)	1:63:A:GLU:HG2	1:143:A:LEU:HD11	4	0.46	0.14	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,806)	1:80:A:MET:HG3	1:84:A:SER:HB2	4	0.46	0.5	0.2
(2,151)	1:11:A:GLN:HA	1:11:A:GLN:HG2	4	0.44	0.35	0.3
(2,125)	1:19:A:GLU:HA	1:161:A:ARG:HG2	4	0.44	0.16	0.43
(2,125)	1:19:A:GLU:HA	1:161:A:ARG:HG3	4	0.44	0.16	0.43
(1,69)	1:46:A:ARG:HD3	1:46:A:ARG:HG2	4	0.44	0.0	0.44
(2,769)	1:11:A:GLN:HG3	1:11:A:GLN:HB3	4	0.44	0.01	0.44
(1,131)	1:72:A:VAL:HG11	1:24:A:PHE:HD1	4	0.43	0.12	0.48
(1,131)	1:72:A:VAL:HG11	1:24:A:PHE:HD2	4	0.43	0.12	0.48
(1,131)	1:72:A:VAL:HG12	1:24:A:PHE:HD1	4	0.43	0.12	0.48
(1,35)	1:12:A:LEU:HA	1:16:A:GLN:HB2	4	0.42	0.15	0.47
(2,882)	1:83:A:ARG:HA	1:86:A:LYS:HB3	4	0.42	0.22	0.43
(2,1171)	1:13:A:THR:HG23	1:16:A:GLN:HG3	4	0.38	0.08	0.4
(2,1140)	1:41:A:LEU:HD21	1:41:A:LEU:HA	4	0.36	0.15	0.36
(2,1140)	1:41:A:LEU:HD23	1:41:A:LEU:HA	4	0.36	0.15	0.36
(2,1140)	1:41:A:LEU:HD22	1:41:A:LEU:HA	4	0.36	0.15	0.36
(2,1064)	1:142:A:THR:HA	1:141:A:PRO:HD2	4	0.34	0.11	0.32
(2,127)	1:39:A:LYS:HA	1:39:A:LYS:HG3	4	0.33	0.08	0.37
(2,561)	1:37:A:SER:HB2	1:71:A:THR:HG22	4	0.32	0.09	0.34
(2,561)	1:37:A:SER:HB2	1:71:A:THR:HG21	4	0.32	0.09	0.34
(2,561)	1:37:A:SER:HB2	1:71:A:THR:HG23	4	0.32	0.09	0.34
(2,566)	1:82:A:VAL:HG23	1:5:A:TYR:HB3	4	0.32	0.17	0.23
(2,566)	1:82:A:VAL:HG22	1:5:A:TYR:HB3	4	0.32	0.17	0.23
(2,566)	1:82:A:VAL:HG21	1:5:A:TYR:HB3	4	0.32	0.17	0.23
(1,206)	1:85:A:MET:HA	1:85:A:MET:HG2	4	0.32	0.03	0.32
(2,1583)	1:154:A:MET:HE2	1:20:A:PHE:HB3	4	0.31	0.12	0.32
(2,1583)	1:154:A:MET:HE3	1:20:A:PHE:HB3	4	0.31	0.12	0.32
(2,613)	1:29:A:LEU:HD12	1:157:A:LEU:HB3	4	0.31	0.07	0.31
(2,613)	1:29:A:LEU:HD13	1:157:A:LEU:HB3	4	0.31	0.07	0.31
(2,695)	1:41:A:LEU:HB3	1:41:A:LEU:HD21	4	0.3	0.17	0.27
(2,695)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	4	0.3	0.17	0.27
(1,271)	1:61:A:ILE:HD11	1:58:A:GLN:HG3	4	0.27	0.09	0.31
(1,271)	1:61:A:ILE:HD12	1:58:A:GLN:HG3	4	0.27	0.09	0.31
(2,331)	1:46:A:ARG:HA	1:46:A:ARG:HD2	4	0.25	0.05	0.26
(2,100)	1:15:A:GLU:HA	1:18:A:ASN:HB2	4	0.25	0.03	0.24
(2,415)	1:61:A:ILE:HD13	1:72:A:VAL:HB	4	0.25	0.08	0.24
(2,415)	1:61:A:ILE:HD11	1:72:A:VAL:HB	4	0.25	0.08	0.24
(2,415)	1:61:A:ILE:HD12	1:72:A:VAL:HB	4	0.25	0.08	0.24
(2,1407)	1:16:A:GLN:H	1:16:A:GLN:HB3	4	0.25	0.05	0.26
(2,822)	1:12:A:LEU:HB3	1:16:A:GLN:HB2	4	0.24	0.04	0.26
(2,408)	1:138:A:PHE:HB3	1:137:A:LYS:HB2	4	0.24	0.07	0.23
(2,408)	1:138:A:PHE:HB3	1:137:A:LYS:HB3	4	0.24	0.07	0.23
(1,293)	1:36:A:ILE:HD13	1:77:A:PHE:HA	4	0.24	0.06	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,293)	1:36:A:ILE:HD11	1:36:A:ILE:HA	4	0.24	0.06	0.26
(1,293)	1:36:A:ILE:HD12	1:77:A:PHE:HA	4	0.24	0.06	0.26
(2,187)	1:16:A:GLN:HA	1:12:A:LEU:HD23	4	0.24	0.15	0.18
(2,187)	1:16:A:GLN:HA	1:12:A:LEU:HD21	4	0.24	0.15	0.18
(2,187)	1:16:A:GLN:HA	1:12:A:LEU:HD22	4	0.24	0.15	0.18
(2,293)	1:52:A:PRO:HD2	1:46:A:ARG:HD2	4	0.23	0.06	0.22
(2,1175)	1:39:A:LYS:HG2	1:39:A:LYS:HE2	4	0.21	0.05	0.19
(2,1209)	1:27:A:PHE:HA	1:27:A:PHE:HD2	4	0.19	0.03	0.19
(2,1209)	1:27:A:PHE:HA	1:27:A:PHE:HD1	4	0.19	0.03	0.19
(2,531)	1:77:A:PHE:HB3	1:72:A:VAL:HG11	4	0.18	0.05	0.2
(2,531)	1:77:A:PHE:HB3	1:72:A:VAL:HG13	4	0.18	0.05	0.2
(1,151)	1:48:A:LEU:HD22	1:48:A:LEU:HG	4	0.18	0.02	0.18
(1,151)	1:48:A:LEU:HB3	1:48:A:LEU:HD22	4	0.18	0.02	0.18
(1,151)	1:48:A:LEU:HD21	1:48:A:LEU:HG	4	0.18	0.02	0.18
(1,151)	1:48:A:LEU:HD23	1:48:A:LEU:HG	4	0.18	0.02	0.18
(2,114)	1:6:A:LYS:HA	1:1:A:MET:HG3	4	0.17	0.05	0.16
(2,1578)	1:35:A:SER:H	1:28:A:VAL:HG13	4	0.17	0.04	0.17
(2,1578)	1:35:A:SER:H	1:28:A:VAL:HG11	4	0.17	0.04	0.17
(2,180)	1:155:A:GLN:HA	1:155:A:GLN:HG2	4	0.16	0.04	0.15
(2,697)	1:12:A:LEU:HD13	1:12:A:LEU:HA	4	0.15	0.03	0.15
(2,697)	1:12:A:LEU:HD11	1:12:A:LEU:HA	4	0.15	0.03	0.15
(2,25)	1:71:A:THR:HB	1:35:A:SER:HB3	4	0.14	0.03	0.15
(2,117)	1:20:A:PHE:HA	1:154:A:MET:HE2	4	0.14	0.01	0.14
(2,117)	1:20:A:PHE:HA	1:154:A:MET:HE3	4	0.14	0.01	0.14
(2,751)	1:16:A:GLN:HA	1:16:A:GLN:HG3	4	0.14	0.02	0.12
(1,119)	1:150:A:ALA:HA	1:150:A:ALA:HB3	4	0.12	0.02	0.11
(1,119)	1:150:A:ALA:HA	1:150:A:ALA:HB1	4	0.12	0.02	0.11
(1,119)	1:150:A:ALA:HA	1:150:A:ALA:HB2	4	0.12	0.02	0.11
(2,497)	1:81:A:MET:HE1	1:85:A:MET:HB3	3	4.04	0.36	3.85
(2,497)	1:81:A:MET:HE3	1:85:A:MET:HB3	3	4.04	0.36	3.85
(2,817)	1:17:A:LYS:HD2	1:9:A:VAL:HG21	3	2.4	0.07	2.41
(2,817)	1:17:A:LYS:HD2	1:9:A:VAL:HG22	3	2.4	0.07	2.41
(2,1082)	1:26:A:ILE:HD13	1:161:A:ARG:HD2	3	2.23	0.85	2.76
(2,1082)	1:26:A:ILE:HD12	1:161:A:ARG:HD3	3	2.23	0.85	2.76
(2,1333)	1:56:A:GLU:H	1:56:A:GLU:HG3	3	2.01	0.03	2.02
(2,1105)	1:9:A:VAL:HG21	1:10:A:GLU:HA	3	1.89	0.07	1.92
(2,1105)	1:9:A:VAL:HG22	1:10:A:GLU:HA	3	1.89	0.07	1.92
(2,638)	1:78:A:LEU:HD12	1:81:A:MET:HG2	3	1.85	0.19	1.8
(2,638)	1:78:A:LEU:HD13	1:81:A:MET:HG2	3	1.85	0.19	1.8
(2,1007)	1:64:A:VAL:HG22	1:72:A:VAL:HA	3	1.38	0.78	0.94
(2,1007)	1:64:A:VAL:HG23	1:72:A:VAL:HA	3	1.38	0.78	0.94
(2,829)	1:76:A:GLU:HB3	1:64:A:VAL:HG21	3	1.37	0.82	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,829)	1:76:A:GLU:HB3	1:64:A:VAL:HG23	3	1.37	0.82	1.08
(2,829)	1:76:A:GLU:HB3	1:64:A:VAL:HG22	3	1.37	0.82	1.08
(1,21)	1:14:A:GLU:HA	1:18:A:ASN:HB2	3	1.2	0.05	1.24
(1,361)	1:57:A:LEU:H	1:56:A:GLU:HB2	3	1.17	0.09	1.18
(2,567)	1:82:A:VAL:HG21	1:86:A:LYS:HB3	3	1.12	0.81	0.67
(2,567)	1:82:A:VAL:HG23	1:86:A:LYS:HB3	3	1.12	0.81	0.67
(2,1100)	1:142:A:THR:HB	1:143:A:LEU:HD22	3	1.05	0.58	0.88
(2,1100)	1:142:A:THR:HB	1:143:A:LEU:HD23	3	1.05	0.58	0.88
(2,1100)	1:142:A:THR:HB	1:143:A:LEU:HD21	3	1.05	0.58	0.88
(1,70)	1:12:A:LEU:HB2	1:16:A:GLN:HG3	3	1.05	0.07	1.01
(1,70)	1:12:A:LEU:HB2	1:16:A:GLN:HB2	3	1.05	0.07	1.01
(2,183)	1:63:A:GLU:HA	1:64:A:VAL:HG12	3	1.04	0.62	0.7
(2,183)	1:63:A:GLU:HA	1:64:A:VAL:HG13	3	1.04	0.62	0.7
(2,183)	1:63:A:GLU:HA	1:64:A:VAL:HG11	3	1.04	0.62	0.7
(2,845)	1:76:A:GLU:HB2	1:64:A:VAL:HG21	3	1.02	0.81	0.68
(2,845)	1:76:A:GLU:HB2	1:64:A:VAL:HG23	3	1.02	0.81	0.68
(2,845)	1:76:A:GLU:HB2	1:64:A:VAL:HG22	3	1.02	0.81	0.68
(2,1154)	1:10:A:GLU:HG3	1:9:A:VAL:HG12	3	0.91	0.24	0.78
(2,1154)	1:10:A:GLU:HG3	1:9:A:VAL:HG13	3	0.91	0.24	0.78
(1,126)	1:160:A:ALA:HB2	1:26:A:ILE:HD11	3	0.8	0.17	0.81
(1,126)	1:160:A:ALA:HB3	1:26:A:ILE:HD11	3	0.8	0.17	0.81
(1,126)	1:160:A:ALA:HB2	1:26:A:ILE:HD12	3	0.8	0.17	0.81
(2,1592)	2:201:A:9XG:HAE	1:61:A:ILE:HD13	3	0.76	0.16	0.76
(2,1592)	2:201:A:9XG:HAF	1:61:A:ILE:HD11	3	0.76	0.16	0.76
(2,1592)	2:201:A:9XG:HAE	1:61:A:ILE:HD11	3	0.76	0.16	0.76
(2,635)	1:78:A:LEU:HD13	1:78:A:LEU:HA	3	0.69	0.05	0.71
(2,635)	1:78:A:LEU:HD11	1:78:A:LEU:HA	3	0.69	0.05	0.71
(2,749)	1:55:A:GLU:HA	1:55:A:GLU:HG2	3	0.68	0.33	0.83
(1,193)	1:76:A:GLU:HG3	1:66:A:GLU:HB3	3	0.67	0.22	0.69
(2,1189)	1:82:A:VAL:HG12	1:5:A:TYR:HD2	3	0.67	0.05	0.68
(2,1189)	1:82:A:VAL:HG11	1:5:A:TYR:HD2	3	0.67	0.05	0.68
(2,1189)	1:82:A:VAL:HG12	1:5:A:TYR:HD1	3	0.67	0.05	0.68
(1,182)	1:26:A:ILE:HG12	1:157:A:LEU:HB3	3	0.65	0.38	0.5
(2,615)	1:143:A:LEU:HD11	1:59:A:GLU:HB3	3	0.65	0.12	0.58
(2,615)	1:143:A:LEU:HD13	1:59:A:GLU:HB3	3	0.65	0.12	0.58
(2,615)	1:143:A:LEU:HD12	1:59:A:GLU:HB3	3	0.65	0.12	0.58
(2,537)	1:9:A:VAL:HG13	1:6:A:LYS:HA	3	0.64	0.02	0.65
(2,537)	1:9:A:VAL:HG11	1:6:A:LYS:HA	3	0.64	0.02	0.65
(1,147)	1:2:A:ASP:HB2	1:79:A:VAL:HG21	3	0.63	0.24	0.53
(1,147)	1:2:A:ASP:HB2	1:79:A:VAL:HG22	3	0.63	0.24	0.53
(1,147)	1:2:A:ASP:HB2	1:79:A:VAL:HG23	3	0.63	0.24	0.53
(1,16)	1:52:A:PRO:HA	1:56:A:GLU:HB2	3	0.63	0.11	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,381)	1:78:A:LEU:HB2	1:78:A:LEU:HD22	3	0.61	0.02	0.62
(2,381)	1:78:A:LEU:HB2	1:78:A:LEU:HD21	3	0.61	0.02	0.62
(2,1421)	1:10:A:GLU:H	1:9:A:VAL:HG23	3	0.61	0.02	0.62
(2,1421)	1:10:A:GLU:H	1:9:A:VAL:HG21	3	0.61	0.02	0.62
(1,256)	1:78:A:LEU:HD21	1:24:A:PHE:HB2	3	0.57	0.05	0.55
(1,256)	1:78:A:LEU:HD23	1:24:A:PHE:HB2	3	0.57	0.05	0.55
(2,608)	1:21:A:LYS:HE2	1:21:A:LYS:HG2	3	0.57	0.01	0.57
(2,480)	1:26:A:ILE:HD13	1:22:A:ALA:HB3	3	0.57	0.1	0.63
(2,480)	1:26:A:ILE:HD11	1:22:A:ALA:HB3	3	0.57	0.1	0.63
(2,179)	1:63:A:GLU:HA	1:63:A:GLU:HG3	3	0.54	0.28	0.7
(1,15)	1:52:A:PRO:HA	1:146:A:VAL:HG13	3	0.53	0.12	0.55
(1,15)	1:52:A:PRO:HA	1:146:A:VAL:HG21	3	0.53	0.12	0.55
(2,1582)	1:146:A:VAL:HG23	1:52:A:PRO:HA	3	0.51	0.04	0.48
(2,1582)	1:146:A:VAL:HG22	1:52:A:PRO:HA	3	0.51	0.04	0.48
(2,1582)	1:146:A:VAL:HG21	1:52:A:PRO:HA	3	0.51	0.04	0.48
(1,95)	1:26:A:ILE:HD13	1:157:A:LEU:HB3	3	0.48	0.27	0.5
(1,95)	1:26:A:ILE:HD12	1:157:A:LEU:HB3	3	0.48	0.27	0.5
(2,884)	1:163:A:LYS:HB3	1:163:A:LYS:HE3	3	0.48	0.1	0.55
(2,1123)	1:157:A:LEU:HD23	1:44:A:VAL:HG21	3	0.47	0.13	0.49
(2,1123)	1:157:A:LEU:HD22	1:44:A:VAL:HG21	3	0.47	0.13	0.49
(2,1123)	1:157:A:LEU:HD22	1:44:A:VAL:HG23	3	0.47	0.13	0.49
(1,304)	1:155:A:GLN:HG3	1:158:A:LEU:HD11	3	0.43	0.21	0.34
(1,304)	1:155:A:GLN:HG3	1:158:A:LEU:HD12	3	0.43	0.21	0.34
(2,98)	1:40:A:GLU:HA	1:43:A:LYS:HD3	3	0.42	0.04	0.43
(2,98)	1:40:A:GLU:HA	1:43:A:LYS:HD2	3	0.42	0.04	0.43
(2,1230)	1:74:A:PHE:HE1	1:78:A:LEU:HD21	3	0.42	0.06	0.43
(2,1230)	1:74:A:PHE:HE2	1:78:A:LEU:HD23	3	0.42	0.06	0.43
(2,1230)	1:74:A:PHE:HE1	1:78:A:LEU:HD23	3	0.42	0.06	0.43
(2,1602)	2:201:A:9XG:HAG	1:153:A:MET:HE1	3	0.42	0.02	0.41
(2,1602)	2:201:A:9XG:HAG	1:153:A:MET:HE2	3	0.42	0.02	0.41
(2,365)	1:2:A:ASP:HB2	1:79:A:VAL:HG21	3	0.42	0.24	0.32
(2,365)	1:2:A:ASP:HB2	1:79:A:VAL:HG22	3	0.42	0.24	0.32
(2,365)	1:2:A:ASP:HB2	1:79:A:VAL:HG23	3	0.42	0.24	0.32
(2,1130)	1:50:A:GLN:HG3	1:148:A:ILE:HG13	3	0.42	0.15	0.34
(2,909)	1:78:A:LEU:HD21	1:77:A:PHE:HD1	3	0.4	0.15	0.5
(2,909)	1:78:A:LEU:HD22	1:77:A:PHE:HD2	3	0.4	0.15	0.5
(2,909)	1:78:A:LEU:HD23	1:77:A:PHE:HD2	3	0.4	0.15	0.5
(1,204)	1:154:A:MET:HG3	1:152:A:ALA:HB2	3	0.38	0.03	0.38
(1,204)	1:154:A:MET:HG3	1:152:A:ALA:HB1	3	0.38	0.03	0.38
(2,540)	1:9:A:VAL:HG13	1:79:A:VAL:HA	3	0.37	0.09	0.38
(2,540)	1:9:A:VAL:HG11	1:79:A:VAL:HA	3	0.37	0.09	0.38
(1,137)	1:146:A:VAL:HG11	1:50:A:GLN:HG3	3	0.37	0.1	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,137)	1:146:A:VAL:HG11	1:52:A:PRO:HB3	3	0.37	0.1	0.39
(2,1074)	1:158:A:LEU:HD23	1:154:A:MET:HG2	3	0.37	0.21	0.29
(2,1074)	1:158:A:LEU:HD21	1:154:A:MET:HG2	3	0.37	0.21	0.29
(1,221)	1:57:A:LEU:HA	1:60:A:MET:HB2	3	0.36	0.06	0.33
(2,618)	1:78:A:LEU:HD23	1:17:A:LYS:HB3	3	0.36	0.01	0.35
(2,618)	1:78:A:LEU:HD22	1:17:A:LYS:HB3	3	0.36	0.01	0.35
(2,458)	1:148:A:ILE:HG22	1:152:A:ALA:HB1	3	0.34	0.1	0.29
(2,458)	1:148:A:ILE:HG22	1:152:A:ALA:HB2	3	0.34	0.1	0.29
(2,458)	1:148:A:ILE:HG21	1:152:A:ALA:HB2	3	0.34	0.1	0.29
(2,955)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	3	0.33	0.01	0.32
(2,492)	1:79:A:VAL:HA	1:8:A:ALA:HB2	3	0.32	0.08	0.3
(2,492)	1:79:A:VAL:HA	1:8:A:ALA:HB3	3	0.32	0.08	0.3
(1,94)	1:26:A:ILE:HD13	1:159:A:GLY:HA2	3	0.31	0.07	0.31
(1,94)	1:27:A:PHE:HA	1:26:A:ILE:HD13	3	0.31	0.07	0.31
(2,794)	1:148:A:ILE:HD12	1:50:A:GLN:HG3	3	0.31	0.09	0.3
(2,832)	1:141:A:PRO:HD2	1:140:A:ARG:HB3	3	0.3	0.07	0.3
(1,115)	1:156:A:ALA:HB2	1:153:A:MET:HG2	3	0.3	0.08	0.34
(1,115)	1:156:A:ALA:HB3	1:47:A:MET:HB2	3	0.3	0.08	0.34
(1,115)	1:156:A:ALA:HB1	1:47:A:MET:HB2	3	0.3	0.08	0.34
(2,880)	1:163:A:LYS:HA	1:163:A:LYS:HB3	3	0.29	0.01	0.29
(2,135)	1:19:A:GLU:HA	1:158:A:LEU:HD11	3	0.29	0.08	0.33
(2,135)	1:19:A:GLU:HA	1:158:A:LEU:HD12	3	0.29	0.08	0.33
(1,84)	1:2:A:ASP:HB3	1:79:A:VAL:HG22	3	0.28	0.1	0.23
(1,84)	1:2:A:ASP:HB3	1:79:A:VAL:HG21	3	0.28	0.1	0.23
(1,84)	1:2:A:ASP:HB3	1:79:A:VAL:HG23	3	0.28	0.1	0.23
(2,472)	1:154:A:MET:HE3	1:151:A:ASP:HB3	3	0.28	0.11	0.21
(2,472)	1:154:A:MET:HE1	1:151:A:ASP:HB3	3	0.28	0.11	0.21
(2,472)	1:154:A:MET:HE3	1:151:A:ASP:HB2	3	0.28	0.11	0.21
(1,251)	1:9:A:VAL:HG22	1:75:A:ASP:HB3	3	0.27	0.12	0.3
(1,251)	1:9:A:VAL:HG23	1:75:A:ASP:HB3	3	0.27	0.12	0.3
(2,562)	1:82:A:VAL:HG22	1:5:A:TYR:HA	3	0.27	0.11	0.31
(2,562)	1:82:A:VAL:HG21	1:5:A:TYR:HA	3	0.27	0.11	0.31
(2,145)	1:12:A:LEU:HA	1:12:A:LEU:HG	3	0.27	0.03	0.28
(1,267)	1:159:A:GLY:HA3	1:160:A:ALA:HB3	3	0.26	0.02	0.26
(1,267)	1:159:A:GLY:HA3	1:160:A:ALA:HB1	3	0.26	0.02	0.26
(2,680)	1:157:A:LEU:HG	1:157:A:LEU:HB2	3	0.26	0.08	0.3
(1,3)	1:79:A:VAL:HA	1:8:A:ALA:HB2	3	0.25	0.08	0.24
(1,3)	1:79:A:VAL:HA	1:8:A:ALA:HB3	3	0.25	0.08	0.24
(1,23)	1:60:A:MET:HA	1:60:A:MET:HG2	3	0.25	0.11	0.19
(1,344)	1:82:A:VAL:H	1:82:A:VAL:HB	3	0.23	0.04	0.26
(1,344)	1:82:A:VAL:H	1:85:A:MET:HE1	3	0.23	0.04	0.26
(1,85)	1:17:A:LYS:HE2	1:17:A:LYS:HB2	3	0.23	0.04	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,130)	1:13:A:THR:HG22	1:16:A:GLN:HG3	3	0.23	0.06	0.26
(1,130)	1:13:A:THR:HG23	1:16:A:GLN:HG3	3	0.23	0.06	0.26
(1,130)	1:13:A:THR:HG21	1:16:A:GLN:HG3	3	0.23	0.06	0.26
(1,308)	1:5:A:TYR:HE2	1:86:A:LYS:HD2	3	0.23	0.01	0.22
(1,308)	1:5:A:TYR:HE1	1:86:A:LYS:HD2	3	0.23	0.01	0.22
(1,134)	1:9:A:VAL:HA	1:82:A:VAL:HG11	3	0.22	0.08	0.27
(1,134)	1:9:A:VAL:HA	1:82:A:VAL:HG12	3	0.22	0.08	0.27
(2,1293)	1:39:A:LYS:H	1:39:A:LYS:HB3	3	0.22	0.08	0.19
(1,331)	1:83:A:ARG:H	1:82:A:VAL:HB	3	0.21	0.05	0.18
(2,553)	1:34:A:GLY:HA2	1:28:A:VAL:HG11	3	0.21	0.07	0.19
(2,553)	1:34:A:GLY:HA2	1:28:A:VAL:HG13	3	0.21	0.07	0.19
(2,1176)	1:163:A:LYS:HG2	1:163:A:LYS:HA	3	0.21	0.01	0.21
(2,1385)	1:17:A:LYS:H	1:16:A:GLN:HB2	3	0.2	0.07	0.23
(2,310)	1:34:A:GLY:HA3	1:28:A:VAL:HG23	3	0.18	0.04	0.18
(2,310)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	3	0.18	0.04	0.18
(1,49)	1:71:A:THR:HB	1:35:A:SER:HA	3	0.17	0.06	0.14
(1,49)	1:35:A:SER:HA	1:34:A:GLY:HA2	3	0.17	0.06	0.14
(1,44)	1:78:A:LEU:HA	1:78:A:LEU:HB2	3	0.17	0.02	0.16
(1,44)	1:78:A:LEU:HA	1:78:A:LEU:HG	3	0.17	0.02	0.16
(2,525)	1:13:A:THR:HA	1:13:A:THR:HG21	3	0.17	0.03	0.16
(2,1032)	1:77:A:PHE:HB2	1:74:A:PHE:HD2	3	0.16	0.05	0.14
(2,581)	1:9:A:VAL:HA	1:9:A:VAL:HG21	3	0.15	0.03	0.15
(2,581)	1:9:A:VAL:HA	1:9:A:VAL:HG22	3	0.15	0.03	0.15
(2,558)	1:57:A:LEU:HB2	1:38:A:THR:HG22	3	0.15	0.03	0.15
(2,558)	1:57:A:LEU:HB2	1:38:A:THR:HG21	3	0.15	0.03	0.15
(2,1058)	1:149:A:SER:HB2	1:151:A:ASP:HB2	3	0.15	0.04	0.12
(2,1058)	1:149:A:SER:HB2	1:151:A:ASP:HB3	3	0.15	0.04	0.12
(1,329)	1:85:A:MET:H	1:85:A:MET:HA	3	0.14	0.01	0.15
(1,22)	1:14:A:GLU:HA	1:14:A:GLU:HG3	3	0.14	0.04	0.12
(2,1308)	1:56:A:GLU:H	1:52:A:PRO:HA	3	0.14	0.04	0.12
(2,177)	1:32:A:GLU:HA	1:32:A:GLU:HB3	3	0.13	0.01	0.13
(2,177)	1:32:A:GLU:HA	1:32:A:GLU:HB2	3	0.13	0.01	0.13
(2,359)	1:88:A:ASP:HB2	1:88:A:ASP:HA	3	0.13	0.01	0.13
(1,223)	1:79:A:VAL:HB	1:79:A:VAL:HG22	3	0.12	0.01	0.12
(1,223)	1:79:A:VAL:HB	1:79:A:VAL:HG21	3	0.12	0.01	0.12
(1,223)	1:79:A:VAL:HB	1:79:A:VAL:HG23	3	0.12	0.01	0.12
(2,131)	1:39:A:LYS:HA	1:39:A:LYS:HG2	3	0.12	0.01	0.12
(2,1477)	1:48:A:LEU:H	1:48:A:LEU:HG	3	0.11	0.01	0.12
(2,495)	1:156:A:ALA:HB2	1:157:A:LEU:HD23	2	1.42	0.36	1.42
(2,495)	1:156:A:ALA:HB1	1:157:A:LEU:HD23	2	1.42	0.36	1.42
(2,1529)	1:64:A:VAL:H	1:64:A:VAL:HG22	2	0.86	0.01	0.86
(2,1008)	1:64:A:VAL:HG21	1:65:A:ASP:HA	2	0.76	0.47	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1008)	1:64:A:VAL:HG23	1:65:A:ASP:HA	2	0.76	0.47	0.76
(2,1141)	1:57:A:LEU:HA	1:41:A:LEU:HD22	2	0.69	0.41	0.69
(1,77)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	2	0.69	0.17	0.69
(1,77)	1:157:A:LEU:HB2	1:26:A:ILE:HD11	2	0.69	0.17	0.69
(1,209)	1:150:A:ALA:HB1	1:85:A:MET:HG2	2	0.66	0.09	0.66
(1,246)	1:85:A:MET:HG3	1:84:A:SER:HB3	2	0.66	0.08	0.66
(1,168)	1:157:A:LEU:HD12	1:27:A:PHE:HA	2	0.6	0.4	0.6
(1,168)	1:157:A:LEU:HD11	1:153:A:MET:HA	2	0.6	0.4	0.6
(2,506)	1:23:A:ALA:HB2	1:157:A:LEU:HD21	2	0.57	0.01	0.57
(2,506)	1:23:A:ALA:HB3	1:157:A:LEU:HD23	2	0.57	0.01	0.57
(2,573)	1:64:A:VAL:HA	1:64:A:VAL:HG12	2	0.52	0.04	0.52
(2,573)	1:64:A:VAL:HA	1:64:A:VAL:HG11	2	0.52	0.04	0.52
(2,747)	1:55:A:GLU:HG3	1:55:A:GLU:HB2	2	0.48	0.03	0.48
(2,1416)	1:82:A:VAL:H	1:81:A:MET:HB3	2	0.45	0.0	0.45
(1,165)	1:78:A:LEU:HD23	1:17:A:LYS:HG3	2	0.43	0.24	0.43
(1,165)	1:78:A:LEU:HD22	1:17:A:LYS:HG3	2	0.43	0.24	0.43
(2,1142)	1:45:A:MET:HE2	1:147:A:ARG:HA	2	0.42	0.11	0.42
(2,1142)	1:45:A:MET:HE3	1:147:A:ARG:HA	2	0.42	0.11	0.42
(2,634)	1:78:A:LEU:HD12	1:74:A:PHE:HZ	2	0.42	0.08	0.42
(2,634)	1:78:A:LEU:HD11	1:74:A:PHE:HZ	2	0.42	0.08	0.42
(2,1191)	1:83:A:ARG:HA	1:5:A:TYR:HE1	2	0.42	0.01	0.42
(2,1191)	1:83:A:ARG:HA	1:5:A:TYR:HE2	2	0.42	0.01	0.42
(2,262)	1:162:A:ALA:HA	1:161:A:ARG:HG3	2	0.41	0.02	0.41
(2,675)	1:157:A:LEU:HG	1:157:A:LEU:HA	2	0.41	0.03	0.41
(2,1151)	1:4:A:ILE:HA	1:4:A:ILE:HD11	2	0.4	0.07	0.4
(2,1151)	1:4:A:ILE:HA	1:4:A:ILE:HD13	2	0.4	0.07	0.4
(1,215)	1:10:A:GLU:HB3	1:9:A:VAL:HG12	2	0.4	0.01	0.4
(2,600)	1:157:A:LEU:HB2	1:157:A:LEU:HD21	2	0.4	0.14	0.4
(2,600)	1:157:A:LEU:HB2	1:157:A:LEU:HD22	2	0.4	0.14	0.4
(1,244)	1:155:A:GLN:HB2	1:48:A:LEU:HD23	2	0.4	0.17	0.4
(2,1052)	1:82:A:VAL:HG12	1:5:A:TYR:HE2	2	0.38	0.03	0.38
(2,1052)	1:82:A:VAL:HG12	1:5:A:TYR:HE1	2	0.38	0.03	0.38
(2,358)	1:137:A:LYS:HE2	1:137:A:LYS:HG2	2	0.36	0.26	0.36
(2,1606)	2:201:A:9XG:HAB	1:45:A:MET:HE1	2	0.35	0.1	0.35
(2,1606)	2:201:A:9XG:HAA	1:45:A:MET:HE1	2	0.35	0.1	0.35
(2,560)	1:37:A:SER:HB3	1:71:A:THR:HG22	2	0.34	0.05	0.34
(2,560)	1:37:A:SER:HB3	1:71:A:THR:HG21	2	0.34	0.05	0.34
(2,603)	1:57:A:LEU:HD22	1:38:A:THR:HA	2	0.34	0.19	0.34
(2,603)	1:57:A:LEU:HD23	1:38:A:THR:HA	2	0.34	0.19	0.34
(2,477)	1:45:A:MET:HE3	1:60:A:MET:HG3	2	0.32	0.18	0.32
(2,220)	1:85:A:MET:HA	1:85:A:MET:HB3	2	0.31	0.03	0.31
(1,8)	1:9:A:VAL:HA	1:17:A:LYS:HG2	2	0.29	0.01	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,124)	1:23:A:ALA:HB2	1:158:A:LEU:HD23	2	0.29	0.1	0.29
(2,483)	1:81:A:MET:HE2	1:154:A:MET:HG3	2	0.28	0.13	0.28
(2,483)	1:81:A:MET:HE1	1:154:A:MET:HG3	2	0.28	0.13	0.28
(1,31)	1:39:A:LYS:HA	1:57:A:LEU:HD12	2	0.28	0.01	0.28
(1,315)	1:20:A:PHE:HE2	1:19:A:GLU:HB3	2	0.28	0.07	0.28
(2,115)	1:19:A:GLU:HA	1:19:A:GLU:HG2	2	0.28	0.18	0.28
(2,147)	1:12:A:LEU:HA	1:17:A:LYS:HD2	2	0.27	0.02	0.27
(2,694)	1:41:A:LEU:HD21	1:60:A:MET:HB3	2	0.26	0.1	0.26
(2,694)	1:41:A:LEU:HD23	1:60:A:MET:HB3	2	0.26	0.1	0.26
(1,264)	1:26:A:ILE:HG21	1:29:A:LEU:H	2	0.26	0.14	0.26
(1,264)	1:26:A:ILE:HG23	1:29:A:LEU:H	2	0.26	0.14	0.26
(2,1173)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	2	0.26	0.07	0.26
(2,1173)	1:16:A:GLN:HG2	1:12:A:LEU:HD23	2	0.26	0.07	0.26
(2,323)	1:83:A:ARG:HD3	1:79:A:VAL:HG13	2	0.25	0.01	0.25
(2,323)	1:83:A:ARG:HD3	1:79:A:VAL:HG11	2	0.25	0.01	0.25
(2,351)	1:158:A:LEU:HB2	1:158:A:LEU:HD12	2	0.25	0.1	0.25
(2,351)	1:158:A:LEU:HB2	1:158:A:LEU:HD13	2	0.25	0.1	0.25
(2,570)	1:158:A:LEU:HD22	1:161:A:ARG:HD2	2	0.25	0.06	0.25
(2,570)	1:158:A:LEU:HD22	1:161:A:ARG:HD3	2	0.25	0.06	0.25
(2,906)	1:12:A:LEU:HD22	1:20:A:PHE:HE1	2	0.25	0.13	0.25
(2,906)	1:12:A:LEU:HD23	1:20:A:PHE:HE1	2	0.25	0.13	0.25
(2,1237)	1:78:A:LEU:HD23	1:20:A:PHE:HD2	2	0.23	0.01	0.23
(2,1237)	1:78:A:LEU:HD21	1:20:A:PHE:HD1	2	0.23	0.01	0.23
(1,56)	1:8:A:ALA:HA	1:11:A:GLN:HB3	2	0.22	0.02	0.22
(2,388)	1:65:A:ASP:HB3	1:61:A:ILE:HG23	2	0.22	0.02	0.22
(2,444)	1:85:A:MET:HE1	1:85:A:MET:HG3	2	0.22	0.04	0.22
(2,444)	1:85:A:MET:HE2	1:85:A:MET:HG3	2	0.22	0.04	0.22
(2,1072)	1:157:A:LEU:HD23	1:27:A:PHE:HB2	2	0.22	0.02	0.22
(2,879)	1:86:A:LYS:HB3	1:86:A:LYS:HA	2	0.22	0.02	0.22
(2,1061)	1:147:A:ARG:HD3	1:147:A:ARG:HA	2	0.22	0.01	0.22
(2,433)	1:85:A:MET:HE2	1:81:A:MET:HG3	2	0.21	0.04	0.21
(2,433)	1:85:A:MET:HE1	1:81:A:MET:HG3	2	0.21	0.04	0.21
(2,360)	1:2:A:ASP:HB3	1:2:A:ASP:HA	2	0.21	0.08	0.21
(2,523)	1:47:A:MET:HE1	1:44:A:VAL:HG12	2	0.21	0.0	0.21
(2,523)	1:47:A:MET:HE3	1:44:A:VAL:HG11	2	0.21	0.0	0.21
(2,552)	1:28:A:VAL:HG11	1:24:A:PHE:HD2	2	0.2	0.04	0.2
(2,552)	1:28:A:VAL:HG13	1:24:A:PHE:HD1	2	0.2	0.04	0.2
(2,236)	1:86:A:LYS:HA	1:86:A:LYS:HG2	2	0.2	0.02	0.2
(1,128)	1:153:A:MET:HA	1:44:A:VAL:HG12	2	0.2	0.09	0.2
(2,210)	1:58:A:GLN:HA	1:61:A:ILE:HD12	2	0.2	0.04	0.2
(2,210)	1:58:A:GLN:HA	1:61:A:ILE:HD11	2	0.2	0.04	0.2
(1,148)	1:72:A:VAL:HG21	1:65:A:ASP:HB2	2	0.18	0.01	0.18

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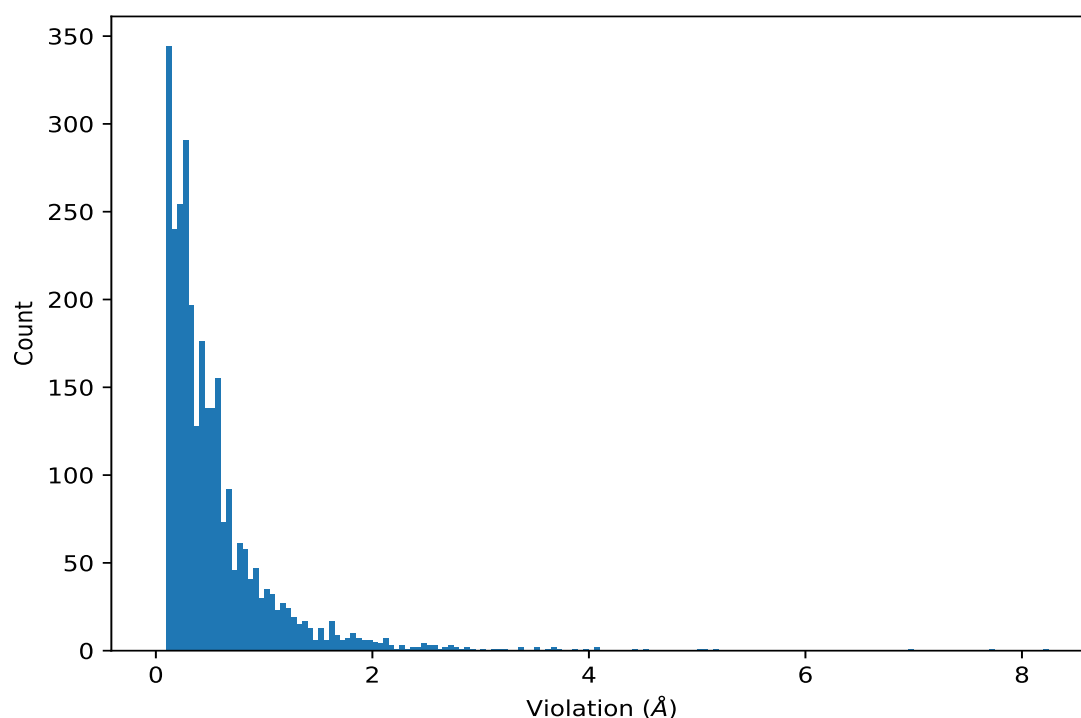
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,148)	1:72:A:VAL:HG22	1:65:A:ASP:HB2	2	0.18	0.01	0.18
(2,1391)	1:59:A:GLU:H	1:59:A:GLU:HG3	2	0.18	0.04	0.18
(2,97)	1:40:A:GLU:HA	1:43:A:LYS:HE2	2	0.17	0.02	0.17
(2,237)	1:86:A:LYS:HA	1:86:A:LYS:HD2	2	0.16	0.06	0.16
(2,908)	1:41:A:LEU:HD13	1:27:A:PHE:HZ	2	0.16	0.01	0.16
(2,908)	1:41:A:LEU:HD12	1:27:A:PHE:HZ	2	0.16	0.01	0.16
(2,510)	1:28:A:VAL:HA	1:31:A:ALA:HB3	2	0.16	0.02	0.16
(2,510)	1:28:A:VAL:HA	1:31:A:ALA:HB1	2	0.16	0.02	0.16
(2,1229)	1:74:A:PHE:HE1	1:20:A:PHE:HB2	2	0.16	0.05	0.16
(2,1229)	1:74:A:PHE:HE2	1:20:A:PHE:HB2	2	0.16	0.05	0.16
(2,21)	1:82:A:VAL:HA	1:85:A:MET:HE3	2	0.15	0.03	0.15
(2,1117)	1:4:A:ILE:HG21	1:4:A:ILE:HG13	2	0.15	0.03	0.15
(2,241)	1:3:A:ASP:HA	1:6:A:LYS:HG2	2	0.15	0.03	0.15
(2,247)	1:158:A:LEU:HA	1:158:A:LEU:HB3	2	0.15	0.0	0.15
(2,705)	1:46:A:ARG:HA	1:46:A:ARG:HG2	2	0.14	0.03	0.14
(2,550)	1:79:A:VAL:HG13	1:5:A:TYR:HB2	2	0.14	0.02	0.14
(2,550)	1:79:A:VAL:HG12	1:5:A:TYR:HB2	2	0.14	0.02	0.14
(2,578)	1:143:A:LEU:HD23	1:59:A:GLU:HB2	2	0.14	0.02	0.14
(2,578)	1:143:A:LEU:HD21	1:59:A:GLU:HB2	2	0.14	0.02	0.14
(2,981)	1:51:A:ASN:HA	1:52:A:PRO:HG3	2	0.14	0.01	0.14
(2,1349)	1:12:A:LEU:H	1:12:A:LEU:HB2	2	0.14	0.01	0.14
(2,1055)	1:84:A:SER:HA	1:84:A:SER:HB2	2	0.12	0.02	0.12
(2,1265)	1:31:A:ALA:H	1:31:A:ALA:HB1	2	0.12	0.02	0.12
(2,231)	1:37:A:SER:HB3	1:37:A:SER:HA	2	0.12	0.0	0.12
(2,768)	1:11:A:GLN:HG3	1:8:A:ALA:HA	2	0.12	0.02	0.12
(2,277)	1:141:A:PRO:HD3	1:141:A:PRO:HB2	2	0.12	0.0	0.12
(2,1438)	1:15:A:GLU:H	1:13:A:THR:HB	2	0.12	0.0	0.12
(2,885)	1:3:A:ASP:HB2	1:6:A:LYS:HB3	2	0.11	0.01	0.11
(2,761)	1:19:A:GLU:HG2	1:19:A:GLU:HB2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1063)	1:145:A:ARG:HD3	1:142:A:THR:HA	6	8.22
(2,1063)	1:145:A:ARG:HD3	1:142:A:THR:HA	8	7.7
(2,1063)	1:145:A:ARG:HD3	1:142:A:THR:HA	7	6.99
(2,1102)	1:145:A:ARG:HD3	1:143:A:LEU:HD13	7	5.16
(2,105)	1:84:A:SER:HA	1:88:A:ASP:HB3	6	5.08
(2,1102)	1:145:A:ARG:HD2	1:143:A:LEU:HD13	6	5.0
(2,497)	1:81:A:MET:HE1	1:85:A:MET:HB3	8	4.54
(2,1102)	1:145:A:ARG:HD3	1:143:A:LEU:HD12	8	4.42
(2,772)	1:7:A:ALA:HB2	1:11:A:GLN:HG2	6	4.06
(1,125)	1:160:A:ALA:HB2	1:26:A:ILE:HB	7	4.06
(2,105)	1:84:A:SER:HA	1:88:A:ASP:HB2	7	3.95
(2,497)	1:81:A:MET:HE1	1:85:A:MET:HB3	7	3.85
(2,497)	1:81:A:MET:HE3	1:85:A:MET:HB3	6	3.72
(2,568)	1:82:A:VAL:HG23	1:86:A:LYS:HD2	4	3.67
(1,125)	1:160:A:ALA:HB2	1:26:A:ILE:HB	8	3.67
(1,125)	1:160:A:ALA:HB3	1:26:A:ILE:HB	6	3.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,772)	1:7:A:ALA:HB1	1:11:A:GLN:HG2	7	3.54
(2,1102)	1:145:A:ARG:HD3	1:143:A:LEU:HD12	3	3.5
(2,586)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	7	3.4
(1,296)	1:145:A:ARG:HD2	1:146:A:VAL:HG12	1	3.35
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG23	7	3.23
(1,279)	1:60:A:MET:HE1	1:147:A:ARG:HD2	7	3.16
(1,297)	1:4:A:ILE:HD13	1:2:A:ASP:HB2	8	3.15
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG21	6	3.01
(1,279)	1:60:A:MET:HE2	1:147:A:ARG:HD2	8	2.93
(2,1082)	1:26:A:ILE:HD13	1:161:A:ARG:HD2	8	2.9
(2,434)	1:85:A:MET:HE3	1:12:A:LEU:HD23	6	2.86
(1,166)	1:158:A:LEU:HD13	1:78:A:LEU:HD13	1	2.83
(1,166)	1:158:A:LEU:HD12	1:44:A:VAL:HG12	5	2.77
(2,1082)	1:26:A:ILE:HD13	1:161:A:ARG:HD2	6	2.76
(1,166)	1:158:A:LEU:HD11	1:44:A:VAL:HG13	2	2.72
(2,772)	1:7:A:ALA:HB3	1:11:A:GLN:HG2	8	2.71
(1,166)	1:158:A:LEU:HD13	1:44:A:VAL:HG12	3	2.7
(2,482)	1:81:A:MET:HE3	1:20:A:PHE:HD2	8	2.68
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE1	7	2.68
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG22	8	2.61
(2,216)	1:154:A:MET:HA	1:157:A:LEU:HD13	3	2.59
(2,434)	1:85:A:MET:HE2	1:12:A:LEU:HD21	7	2.58
(1,297)	1:4:A:ILE:HD11	1:2:A:ASP:HB2	6	2.56
(1,290)	1:64:A:VAL:HG23	1:65:A:ASP:HB3	6	2.54
(2,864)	1:81:A:MET:HE1	1:84:A:SER:HB2	7	2.52
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE3	6	2.52
(2,829)	1:76:A:GLU:HB3	1:64:A:VAL:HG21	8	2.49
(2,1007)	1:64:A:VAL:HG22	1:72:A:VAL:HA	8	2.48
(2,817)	1:17:A:LYS:HD2	1:9:A:VAL:HG22	6	2.48
(1,136)	1:146:A:VAL:HG13	1:145:A:ARG:HA	6	2.48
(2,864)	1:81:A:MET:HE3	1:84:A:SER:HB3	6	2.44
(2,817)	1:17:A:LYS:HD2	1:9:A:VAL:HG22	7	2.41
(1,297)	1:4:A:ILE:HD12	1:2:A:ASP:HB2	7	2.38
(1,189)	1:8:A:ALA:HB3	1:10:A:GLU:HG3	7	2.38
(2,817)	1:17:A:LYS:HD2	1:9:A:VAL:HG21	8	2.32
(2,1184)	1:5:A:TYR:HD2	1:85:A:MET:HG3	8	2.3
(1,284)	1:160:A:ALA:HB2	1:43:A:LYS:HE3	3	2.27
(2,567)	1:82:A:VAL:HG23	1:86:A:LYS:HB3	4	2.25
(2,641)	1:157:A:LEU:HD13	1:23:A:ALA:HB3	4	2.23
(2,641)	1:157:A:LEU:HD11	1:23:A:ALA:HB3	2	2.19
(1,166)	1:158:A:LEU:HD11	1:78:A:LEU:HD12	4	2.19
(1,104)	1:4:A:ILE:HG23	1:80:A:MET:HB2	7	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,845)	1:76:A:GLU:HB2	1:64:A:VAL:HG21	8	2.13
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD23	8	2.13
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB2	6	2.12
(1,279)	1:60:A:MET:HE3	1:147:A:ARG:HD2	6	2.11
(2,638)	1:78:A:LEU:HD12	1:81:A:MET:HG2	2	2.1
(1,279)	1:60:A:MET:HE1	1:145:A:ARG:HD2	4	2.1
(1,153)	1:41:A:LEU:HD11	1:50:A:GLN:HG3	8	2.1
(1,104)	1:4:A:ILE:HG23	1:80:A:MET:HB2	1	2.08
(2,1111)	1:153:A:MET:HE3	1:44:A:VAL:HG22	3	2.07
(1,104)	1:4:A:ILE:HG21	1:80:A:MET:HB2	6	2.07
(2,641)	1:157:A:LEU:HD13	1:23:A:ALA:HB2	3	2.06
(2,640)	1:157:A:LEU:HD13	1:153:A:MET:HG2	3	2.05
(2,1333)	1:56:A:GLU:H	1:56:A:GLU:HG3	6	2.04
(2,641)	1:157:A:LEU:HD13	1:23:A:ALA:HB1	1	2.03
(2,1333)	1:56:A:GLU:H	1:56:A:GLU:HG3	8	2.02
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD13	8	2.02
(2,648)	1:48:A:LEU:HD13	1:156:A:ALA:HB2	8	1.99
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB2	7	1.99
(2,216)	1:154:A:MET:HA	1:157:A:LEU:HD12	2	1.98
(2,1333)	1:56:A:GLU:H	1:56:A:GLU:HG3	7	1.97
(1,104)	1:4:A:ILE:HG22	1:80:A:MET:HB2	5	1.97
(2,1105)	1:9:A:VAL:HG21	1:10:A:GLU:HA	8	1.96
(1,262)	1:151:A:ASP:HB3	1:158:A:LEU:HD22	2	1.95
(2,586)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	6	1.94
(2,1105)	1:9:A:VAL:HG22	1:10:A:GLU:HA	6	1.92
(1,152)	1:41:A:LEU:HD11	1:153:A:MET:HE3	4	1.92
(2,772)	1:7:A:ALA:HB1	1:11:A:GLN:HG2	4	1.91
(2,183)	1:63:A:GLU:HA	1:64:A:VAL:HG12	8	1.91
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB1	8	1.9
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD23	6	1.9
(1,10)	1:141:A:PRO:HA	1:143:A:LEU:HB2	8	1.9
(1,262)	1:151:A:ASP:HB2	1:148:A:ILE:HG22	8	1.89
(2,216)	1:154:A:MET:HA	1:157:A:LEU:HD13	1	1.87
(1,104)	1:4:A:ILE:HG23	1:139:A:LYS:HB3	8	1.86
(2,648)	1:48:A:LEU:HD13	1:156:A:ALA:HB2	6	1.85
(2,1100)	1:142:A:THR:HB	1:143:A:LEU:HD21	5	1.83
(2,1073)	1:157:A:LEU:HD22	1:27:A:PHE:HB3	4	1.83
(2,586)	1:9:A:VAL:HG23	1:10:A:GLU:HG3	8	1.83
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD23	6	1.83
(1,104)	1:4:A:ILE:HG22	1:80:A:MET:HB2	2	1.82
(2,1049)	1:78:A:LEU:HD12	1:81:A:MET:HE2	5	1.81
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD22	5	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1105)	1:9:A:VAL:HG22	1:10:A:GLU:HA	7	1.8
(2,648)	1:48:A:LEU:HD11	1:156:A:ALA:HB3	7	1.8
(2,638)	1:78:A:LEU:HD12	1:81:A:MET:HG2	5	1.8
(1,104)	1:4:A:ILE:HG22	1:80:A:MET:HB2	4	1.79
(2,495)	1:156:A:ALA:HB2	1:157:A:LEU:HD23	8	1.78
(1,152)	1:41:A:LEU:HD11	1:153:A:MET:HE1	1	1.78
(2,1049)	1:78:A:LEU:HD12	1:81:A:MET:HE3	2	1.77
(2,1049)	1:78:A:LEU:HD11	1:81:A:MET:HE2	3	1.77
(1,177)	1:41:A:LEU:HD22	1:61:A:ILE:HB	7	1.75
(1,150)	1:48:A:LEU:HD22	1:156:A:ALA:HA	8	1.75
(1,262)	1:151:A:ASP:HB2	1:148:A:ILE:HG22	5	1.74
(1,262)	1:151:A:ASP:HB3	1:148:A:ILE:HG21	7	1.74
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD23	3	1.74
(1,107)	1:153:A:MET:HE2	1:152:A:ALA:HA	3	1.73
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD22	1	1.73
(2,1073)	1:157:A:LEU:HD23	1:27:A:PHE:HB3	1	1.72
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD13	6	1.7
(1,262)	1:151:A:ASP:HB3	1:148:A:ILE:HG23	3	1.7
(1,152)	1:41:A:LEU:HD13	1:153:A:MET:HE2	5	1.7
(1,29)	1:59:A:GLU:HA	1:143:A:LEU:HB3	7	1.7
(2,641)	1:157:A:LEU:HD13	1:23:A:ALA:HB3	8	1.69
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD22	5	1.69
(1,296)	1:145:A:ARG:HD3	1:146:A:VAL:HG12	3	1.68
(1,152)	1:41:A:LEU:HD12	1:153:A:MET:HE2	2	1.67
(2,1041)	1:78:A:LEU:HD13	1:75:A:ASP:HB3	1	1.66
(2,638)	1:78:A:LEU:HD13	1:81:A:MET:HG2	3	1.65
(2,448)	1:1:A:MET:HE2	1:5:A:TYR:HB2	7	1.65
(1,136)	1:146:A:VAL:HG11	1:145:A:ARG:HA	8	1.65
(2,1214)	1:138:A:PHE:HD2	1:139:A:LYS:HD3	1	1.64
(1,153)	1:41:A:LEU:HD11	1:72:A:VAL:HB	6	1.64
(2,1076)	1:157:A:LEU:HD11	1:27:A:PHE:HB3	6	1.63
(2,1041)	1:78:A:LEU:HD11	1:75:A:ASP:HB3	6	1.63
(2,542)	1:82:A:VAL:HG11	1:5:A:TYR:HB2	4	1.63
(1,153)	1:41:A:LEU:HD12	1:52:A:PRO:HB3	1	1.63
(1,10)	1:141:A:PRO:HA	1:143:A:LEU:HB2	7	1.63
(1,10)	1:141:A:PRO:HA	1:143:A:LEU:HB2	6	1.62
(2,1041)	1:78:A:LEU:HD12	1:75:A:ASP:HB3	4	1.61
(2,1041)	1:78:A:LEU:HD12	1:75:A:ASP:HB3	8	1.61
(2,1190)	1:4:A:ILE:HD13	1:5:A:TYR:HD2	8	1.6
(2,640)	1:157:A:LEU:HD13	1:153:A:MET:HG2	7	1.6
(2,564)	1:82:A:VAL:HG21	1:9:A:VAL:HA	6	1.6
(2,216)	1:154:A:MET:HA	1:157:A:LEU:HD13	4	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,564)	1:82:A:VAL:HG22	1:9:A:VAL:HA	8	1.59
(1,268)	1:22:A:ALA:HB2	1:20:A:PHE:HD2	4	1.59
(1,107)	1:153:A:MET:HE3	1:23:A:ALA:HA	6	1.56
(1,262)	1:151:A:ASP:HB2	1:148:A:ILE:HG22	1	1.55
(1,262)	1:151:A:ASP:HB2	1:148:A:ILE:HG22	6	1.55
(1,191)	1:64:A:VAL:HG13	1:63:A:GLU:HG2	8	1.55
(1,284)	1:160:A:ALA:HB2	1:163:A:LYS:HE3	4	1.53
(1,116)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	4	1.53
(1,10)	1:141:A:PRO:HA	1:143:A:LEU:HB2	5	1.53
(1,262)	1:151:A:ASP:HB2	1:148:A:ILE:HG22	4	1.52
(1,10)	1:141:A:PRO:HA	1:143:A:LEU:HB2	2	1.52
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD23	4	1.52
(1,284)	1:160:A:ALA:HB1	1:163:A:LYS:HE3	2	1.51
(1,166)	1:158:A:LEU:HD12	1:78:A:LEU:HD13	7	1.51
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD21	8	1.51
(2,596)	1:157:A:LEU:HD22	1:157:A:LEU:HA	8	1.5
(2,137)	1:83:A:ARG:HA	1:82:A:VAL:HG13	4	1.5
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG12	1	1.5
(1,169)	1:157:A:LEU:HD13	1:153:A:MET:HE3	8	1.5
(1,265)	1:27:A:PHE:HB3	1:26:A:ILE:HG21	1	1.48
(1,153)	1:41:A:LEU:HD13	1:72:A:VAL:HB	2	1.48
(1,153)	1:41:A:LEU:HD12	1:52:A:PRO:HB3	3	1.48
(2,443)	1:85:A:MET:HE3	1:86:A:LYS:HE2	7	1.47
(1,286)	1:36:A:ILE:HG22	1:71:A:THR:HB	8	1.47
(1,268)	1:22:A:ALA:HB1	1:20:A:PHE:HD1	3	1.46
(2,1501)	1:11:A:GLN:H	1:11:A:GLN:HG2	8	1.45
(2,1111)	1:153:A:MET:HE1	1:44:A:VAL:HG21	1	1.45
(2,1104)	1:143:A:LEU:HD11	1:63:A:GLU:HG3	7	1.45
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD1	6	1.45
(1,107)	1:153:A:MET:HE2	1:23:A:ALA:HA	7	1.45
(1,136)	1:146:A:VAL:HG11	1:145:A:ARG:HA	7	1.44
(1,297)	1:4:A:ILE:HD12	1:2:A:ASP:HB2	3	1.43
(1,286)	1:36:A:ILE:HG22	1:71:A:THR:HB	6	1.43
(2,487)	1:152:A:ALA:HB1	1:148:A:ILE:HA	8	1.42
(1,39)	1:63:A:GLU:HA	1:64:A:VAL:HG21	4	1.42
(2,434)	1:85:A:MET:HE3	1:12:A:LEU:HD22	8	1.41
(1,181)	1:152:A:ALA:HB1	1:155:A:GLN:HB2	1	1.41
(1,29)	1:59:A:GLU:HA	1:143:A:LEU:HG	8	1.41
(2,481)	1:4:A:ILE:HG22	1:7:A:ALA:HB2	5	1.4
(2,597)	1:27:A:PHE:HA	1:157:A:LEU:HD23	1	1.39
(1,268)	1:22:A:ALA:HB2	1:20:A:PHE:HD2	2	1.39
(2,785)	1:60:A:MET:HG3	1:41:A:LEU:HD22	7	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,487)	1:152:A:ALA:HB2	1:148:A:ILE:HA	7	1.38
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB3	3	1.38
(1,268)	1:22:A:ALA:HB2	1:20:A:PHE:HD2	5	1.38
(1,138)	1:13:A:THR:HG23	1:15:A:GLU:HB2	7	1.38
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE3	7	1.37
(2,481)	1:4:A:ILE:HG23	1:7:A:ALA:HB2	1	1.37
(2,481)	1:4:A:ILE:HG21	1:7:A:ALA:HB1	8	1.37
(1,116)	1:8:A:ALA:HB2	1:11:A:GLN:HG2	5	1.37
(1,101)	1:85:A:MET:HE2	1:84:A:SER:HB3	1	1.37
(2,1073)	1:157:A:LEU:HD22	1:27:A:PHE:HB3	2	1.36
(2,597)	1:27:A:PHE:HA	1:157:A:LEU:HD22	4	1.36
(1,265)	1:148:A:ILE:HG21	1:147:A:ARG:HD3	4	1.35
(1,110)	1:154:A:MET:HE1	1:155:A:GLN:HA	2	1.35
(1,265)	1:27:A:PHE:HB3	1:26:A:ILE:HG23	6	1.33
(1,110)	1:154:A:MET:HE3	1:155:A:GLN:HA	8	1.33
(2,806)	1:80:A:MET:HG3	1:84:A:SER:HB2	7	1.32
(2,596)	1:157:A:LEU:HD21	1:157:A:LEU:HA	6	1.32
(1,142)	1:38:A:THR:HG22	1:60:A:MET:HE3	4	1.32
(1,116)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	3	1.32
(1,101)	1:85:A:MET:HE2	1:17:A:LYS:HA	2	1.32
(1,166)	1:158:A:LEU:HD11	1:78:A:LEU:HD12	8	1.31
(1,152)	1:41:A:LEU:HD13	1:153:A:MET:HE3	3	1.31
(2,1177)	1:89:A:SER:HA	1:139:A:LYS:HE2	7	1.3
(2,438)	1:1:A:MET:HE2	1:78:A:LEU:HB2	7	1.3
(1,268)	1:22:A:ALA:HB2	1:20:A:PHE:HD2	1	1.3
(1,181)	1:152:A:ALA:HB2	1:155:A:GLN:HB2	3	1.3
(1,153)	1:41:A:LEU:HD11	1:72:A:VAL:HB	5	1.3
(1,138)	1:13:A:THR:HG22	1:15:A:GLU:HB3	6	1.3
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG11	7	1.29
(2,1041)	1:78:A:LEU:HD13	1:75:A:ASP:HB3	7	1.28
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	8	1.28
(2,481)	1:4:A:ILE:HG22	1:7:A:ALA:HB1	3	1.28
(2,481)	1:4:A:ILE:HG22	1:7:A:ALA:HB2	4	1.28
(2,443)	1:85:A:MET:HE2	1:86:A:LYS:HE3	5	1.28
(1,361)	1:57:A:LEU:H	1:56:A:GLU:HB2	8	1.28
(1,39)	1:63:A:GLU:HA	1:64:A:VAL:HG23	5	1.28
(1,181)	1:156:A:ALA:HB3	1:155:A:GLN:HB2	8	1.27
(1,116)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	6	1.27
(1,110)	1:154:A:MET:HE3	1:155:A:GLN:HA	6	1.27
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE3	1	1.26
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	3	1.26
(2,481)	1:4:A:ILE:HG21	1:7:A:ALA:HB3	6	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB2	1	1.26
(1,110)	1:154:A:MET:HE2	1:155:A:GLN:HA	5	1.26
(2,1154)	1:10:A:GLU:HG3	1:9:A:VAL:HG13	7	1.25
(2,1059)	1:137:A:LYS:HB2	1:138:A:PHE:HD2	5	1.25
(2,922)	1:4:A:ILE:HG13	1:5:A:TYR:HE2	4	1.25
(2,1115)	1:162:A:ALA:HB1	1:163:A:LYS:HE3	4	1.24
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD23	6	1.24
(1,284)	1:160:A:ALA:HB2	1:163:A:LYS:HE2	5	1.24
(1,265)	1:27:A:PHE:HB3	1:26:A:ILE:HG22	3	1.24
(1,21)	1:14:A:GLU:HA	1:18:A:ASN:HB2	6	1.24
(1,21)	1:14:A:GLU:HA	1:18:A:ASN:HB2	8	1.24
(2,1076)	1:157:A:LEU:HD12	1:27:A:PHE:HB3	8	1.23
(2,1008)	1:64:A:VAL:HG21	1:65:A:ASP:HA	8	1.23
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB2	4	1.23
(1,248)	1:61:A:ILE:HD12	1:57:A:LEU:HA	2	1.23
(1,138)	1:13:A:THR:HG21	1:15:A:GLU:HB2	8	1.23
(2,1501)	1:11:A:GLN:H	1:11:A:GLN:HG2	7	1.22
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD23	2	1.22
(2,481)	1:4:A:ILE:HG22	1:7:A:ALA:HB1	2	1.22
(2,453)	1:2:A:ASP:HB2	1:4:A:ILE:HG21	8	1.22
(1,297)	1:4:A:ILE:HD12	1:2:A:ASP:HB2	5	1.22
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB2	2	1.22
(1,268)	1:22:A:ALA:HB1	1:20:A:PHE:HD1	6	1.22
(2,1115)	1:162:A:ALA:HB1	1:163:A:LYS:HE3	7	1.21
(2,564)	1:82:A:VAL:HG22	1:9:A:VAL:HA	7	1.21
(2,481)	1:4:A:ILE:HG23	1:7:A:ALA:HB2	7	1.21
(1,286)	1:36:A:ILE:HG21	1:71:A:THR:HB	7	1.21
(1,110)	1:154:A:MET:HE3	1:155:A:GLN:HA	1	1.21
(1,7)	1:44:A:VAL:HA	1:26:A:ILE:HG23	2	1.21
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD23	7	1.2
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD13	4	1.2
(1,289)	1:146:A:VAL:HG22	1:145:A:ARG:HD2	4	1.2
(1,107)	1:153:A:MET:HE2	1:23:A:ALA:HA	1	1.2
(1,297)	1:4:A:ILE:HD11	1:2:A:ASP:HB2	1	1.19
(1,297)	1:4:A:ILE:HD12	1:2:A:ASP:HB2	4	1.19
(1,281)	1:154:A:MET:HG3	1:152:A:ALA:HB1	5	1.19
(1,104)	1:4:A:ILE:HG22	1:80:A:MET:HB2	3	1.19
(1,93)	1:61:A:ILE:HD11	1:38:A:THR:HB	5	1.19
(1,29)	1:59:A:GLU:HA	1:143:A:LEU:HG	6	1.19
(1,361)	1:57:A:LEU:H	1:56:A:GLU:HB2	6	1.18
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG11	1	1.18
(1,197)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	6	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:48:A:LEU:HD22	1:156:A:ALA:HA	6	1.18
(1,39)	1:63:A:GLU:HA	1:143:A:LEU:HD13	1	1.18
(2,1157)	1:28:A:VAL:HG22	1:24:A:PHE:HD2	3	1.17
(2,1152)	1:4:A:ILE:HD13	1:86:A:LYS:HE3	5	1.17
(2,910)	1:41:A:LEU:HD12	1:77:A:PHE:HD1	7	1.17
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD23	5	1.17
(2,487)	1:152:A:ALA:HB2	1:148:A:ILE:HA	6	1.17
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG11	3	1.17
(1,182)	1:26:A:ILE:HG12	1:157:A:LEU:HB3	7	1.17
(1,110)	1:154:A:MET:HE3	1:155:A:GLN:HA	7	1.17
(2,441)	1:47:A:MET:HE1	1:157:A:LEU:HD21	4	1.16
(1,217)	1:12:A:LEU:HD22	1:16:A:GLN:HB2	6	1.16
(1,116)	1:8:A:ALA:HB3	1:11:A:GLN:HG2	1	1.16
(1,54)	1:87:A:ASP:HA	1:90:A:LYS:HD2	4	1.16
(2,1501)	1:11:A:GLN:H	1:11:A:GLN:HG2	6	1.15
(2,597)	1:27:A:PHE:HA	1:157:A:LEU:HD22	2	1.15
(1,297)	1:4:A:ILE:HD13	1:2:A:ASP:HB2	2	1.15
(1,154)	1:47:A:MET:HE1	1:157:A:LEU:HD23	3	1.15
(1,70)	1:12:A:LEU:HB2	1:16:A:GLN:HB2	3	1.15
(2,922)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	5	1.14
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	4	1.14
(2,443)	1:85:A:MET:HE3	1:86:A:LYS:HE2	8	1.14
(1,296)	1:145:A:ARG:HD3	1:146:A:VAL:HG13	6	1.14
(2,1585)	1:162:A:ALA:HA	1:158:A:LEU:HD11	3	1.13
(2,596)	1:157:A:LEU:HD21	1:157:A:LEU:HA	2	1.13
(2,438)	1:1:A:MET:HE3	1:78:A:LEU:HB2	1	1.13
(1,214)	1:19:A:GLU:HB3	1:158:A:LEU:HD13	6	1.13
(1,21)	1:14:A:GLU:HA	1:18:A:ASN:HB2	7	1.13
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	4	1.12
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	1	1.11
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	7	1.11
(1,279)	1:60:A:MET:HE3	1:145:A:ARG:HD2	5	1.11
(2,1141)	1:57:A:LEU:HA	1:41:A:LEU:HD22	7	1.1
(2,912)	1:82:A:VAL:HG22	1:20:A:PHE:HE1	8	1.1
(2,596)	1:157:A:LEU:HD22	1:157:A:LEU:HA	1	1.1
(2,502)	1:28:A:VAL:HG23	1:36:A:ILE:HD11	7	1.1
(1,181)	1:152:A:ALA:HB1	1:155:A:GLN:HB2	7	1.1
(2,1111)	1:153:A:MET:HE3	1:44:A:VAL:HG21	2	1.09
(2,1083)	1:148:A:ILE:HG22	1:154:A:MET:HG3	5	1.09
(1,181)	1:152:A:ALA:HB1	1:155:A:GLN:HB2	4	1.09
(1,123)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	5	1.09
(1,123)	1:28:A:VAL:HG21	1:26:A:ILE:HG13	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:148:A:ILE:HG22	1:149:A:SER:HB3	6	1.09
(2,829)	1:76:A:GLU:HB3	1:64:A:VAL:HG23	6	1.08
(1,268)	1:22:A:ALA:HB1	1:20:A:PHE:HD2	8	1.08
(1,142)	1:38:A:THR:HG21	1:60:A:MET:HE3	2	1.08
(2,1152)	1:4:A:ILE:HD12	1:86:A:LYS:HE3	6	1.07
(2,1083)	1:148:A:ILE:HG21	1:154:A:MET:HG3	7	1.07
(2,922)	1:4:A:ILE:HG13	1:5:A:TYR:HE2	1	1.07
(2,851)	1:161:A:ARG:HB2	1:161:A:ARG:HD2	6	1.07
(2,502)	1:28:A:VAL:HG23	1:36:A:ILE:HD12	5	1.07
(2,495)	1:156:A:ALA:HB1	1:157:A:LEU:HD23	6	1.07
(1,296)	1:145:A:ARG:HD3	1:146:A:VAL:HG12	2	1.07
(1,268)	1:22:A:ALA:HB1	1:20:A:PHE:HD2	7	1.07
(1,181)	1:152:A:ALA:HB1	1:155:A:GLN:HB2	2	1.07
(1,123)	1:28:A:VAL:HG22	1:29:A:LEU:HB2	2	1.07
(2,1111)	1:153:A:MET:HE2	1:44:A:VAL:HG22	6	1.06
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD13	8	1.06
(2,922)	1:4:A:ILE:HG13	1:5:A:TYR:HE1	6	1.06
(2,851)	1:161:A:ARG:HB2	1:161:A:ARG:HD2	8	1.06
(1,313)	1:27:A:PHE:HE2	1:36:A:ILE:HG22	2	1.06
(1,248)	1:61:A:ILE:HD12	1:57:A:LEU:HA	6	1.06
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG12	8	1.06
(1,136)	1:146:A:VAL:HG11	1:144:A:ARG:HA	4	1.06
(1,93)	1:61:A:ILE:HD12	1:38:A:THR:HB	4	1.06
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD2	8	1.05
(1,361)	1:57:A:LEU:H	1:56:A:GLU:HB2	7	1.05
(1,222)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	7	1.05
(1,54)	1:2:A:ASP:HA	1:6:A:LYS:HD2	6	1.05
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE3	3	1.04
(2,1082)	1:26:A:ILE:HD12	1:161:A:ARG:HD3	7	1.04
(2,502)	1:28:A:VAL:HG22	1:36:A:ILE:HD12	3	1.04
(2,414)	1:61:A:ILE:HD11	1:61:A:ILE:HA	1	1.04
(2,151)	1:11:A:GLN:HA	1:11:A:GLN:HG2	8	1.04
(1,198)	1:50:A:GLN:HG3	1:52:A:PRO:HD2	5	1.04
(1,153)	1:41:A:LEU:HD12	1:72:A:VAL:HB	4	1.04
(1,142)	1:38:A:THR:HG22	1:60:A:MET:HE3	5	1.04
(1,54)	1:87:A:ASP:HA	1:90:A:LYS:HD3	7	1.04
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD12	7	1.03
(1,202)	1:148:A:ILE:HD13	1:45:A:MET:HG2	8	1.03
(1,127)	1:156:A:ALA:HB2	1:47:A:MET:HG2	5	1.03
(2,1190)	1:4:A:ILE:HD12	1:5:A:TYR:HD1	7	1.02
(2,1111)	1:153:A:MET:HE1	1:44:A:VAL:HG23	4	1.02
(2,1062)	1:145:A:ARG:HD3	1:145:A:ARG:HA	2	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD1	6	1.02
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD11	5	1.02
(2,828)	1:63:A:GLU:HB3	1:64:A:VAL:HG21	3	1.02
(1,123)	1:28:A:VAL:HG22	1:26:A:ILE:HG13	1	1.02
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD21	7	1.02
(2,502)	1:28:A:VAL:HG22	1:36:A:ILE:HD11	1	1.01
(2,473)	1:154:A:MET:HE2	1:158:A:LEU:HD23	6	1.01
(2,414)	1:61:A:ILE:HD11	1:61:A:ILE:HA	3	1.01
(1,136)	1:146:A:VAL:HG12	1:144:A:ARG:HA	1	1.01
(1,70)	1:12:A:LEU:HB2	1:16:A:GLN:HB2	5	1.01
(2,1226)	1:20:A:PHE:HE2	1:78:A:LEU:HD23	6	1.0
(2,1226)	1:20:A:PHE:HE1	1:78:A:LEU:HD21	7	1.0
(2,1111)	1:153:A:MET:HE3	1:44:A:VAL:HG22	5	1.0
(2,1104)	1:143:A:LEU:HD12	1:63:A:GLU:HG3	6	1.0
(2,1083)	1:148:A:ILE:HG22	1:154:A:MET:HG3	8	1.0
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD22	6	1.0
(1,189)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	1	1.0
(1,168)	1:157:A:LEU:HD11	1:153:A:MET:HA	6	1.0
(1,126)	1:160:A:ALA:HB2	1:26:A:ILE:HD12	7	1.0
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	2	1.0
(2,1115)	1:162:A:ALA:HB1	1:163:A:LYS:HE2	3	0.99
(2,1073)	1:157:A:LEU:HD21	1:27:A:PHE:HB3	3	0.99
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	7	0.99
(2,749)	1:55:A:GLU:HA	1:55:A:GLU:HG2	4	0.99
(2,441)	1:47:A:MET:HE1	1:157:A:LEU:HD21	2	0.99
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB2	8	0.99
(1,123)	1:28:A:VAL:HG23	1:29:A:LEU:HB2	8	0.99
(1,107)	1:153:A:MET:HE3	1:23:A:ALA:HA	5	0.99
(1,70)	1:12:A:LEU:HB2	1:16:A:GLN:HG3	2	0.99
(2,1184)	1:5:A:TYR:HD1	1:85:A:MET:HG3	7	0.98
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE2	6	0.98
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	3	0.98
(2,1059)	1:137:A:LYS:HB2	1:138:A:PHE:HD2	8	0.98
(1,154)	1:157:A:LEU:HD23	1:26:A:ILE:HB	2	0.98
(1,110)	1:154:A:MET:HE3	1:155:A:GLN:HA	3	0.98
(1,54)	1:2:A:ASP:HA	1:4:A:ILE:HB	3	0.98
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	8	0.97
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD22	1	0.97
(1,248)	1:61:A:ILE:HD11	1:57:A:LEU:HA	5	0.97
(1,147)	1:2:A:ASP:HB2	1:79:A:VAL:HG22	6	0.97
(1,125)	1:160:A:ALA:HB1	1:26:A:ILE:HB	4	0.97
(1,123)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	4	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE3	4	0.96
(2,1501)	1:11:A:GLN:H	1:11:A:GLN:HG2	4	0.96
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD12	7	0.96
(2,443)	1:85:A:MET:HE3	1:86:A:LYS:HE2	6	0.96
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD22	2	0.96
(1,265)	1:27:A:PHE:HB3	1:26:A:ILE:HG21	8	0.96
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG11	5	0.96
(1,123)	1:28:A:VAL:HG22	1:26:A:ILE:HG13	3	0.96
(2,1592)	2:201:A:9XG:HAF	1:61:A:ILE:HD11	3	0.95
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD13	7	0.95
(2,1019)	1:72:A:VAL:HG22	1:36:A:ILE:HD13	3	0.95
(1,279)	1:60:A:MET:HE1	1:145:A:ARG:HD2	2	0.95
(1,181)	1:152:A:ALA:HB3	1:155:A:GLN:HB2	5	0.95
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD2	7	0.94
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	2	0.94
(2,1007)	1:64:A:VAL:HG23	1:72:A:VAL:HA	6	0.94
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	6	0.94
(2,539)	1:79:A:VAL:HA	1:82:A:VAL:HG11	4	0.94
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD11	3	0.94
(1,235)	1:28:A:VAL:HG13	1:43:A:LYS:HD3	6	0.94
(1,193)	1:76:A:GLU:HG3	1:66:A:GLU:HB3	2	0.94
(1,181)	1:152:A:ALA:HB1	1:155:A:GLN:HB2	6	0.94
(1,110)	1:154:A:MET:HE3	1:155:A:GLN:HA	4	0.94
(1,82)	1:17:A:LYS:HE3	1:12:A:LEU:HD12	6	0.94
(1,289)	1:146:A:VAL:HG22	1:145:A:ARG:HD3	8	0.93
(1,265)	1:147:A:ARG:HD2	1:148:A:ILE:HG21	7	0.93
(1,235)	1:28:A:VAL:HG12	1:43:A:LYS:HD3	8	0.93
(1,222)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	2	0.93
(1,101)	1:85:A:MET:HE1	1:84:A:SER:HB3	4	0.93
(2,1152)	1:4:A:ILE:HD13	1:86:A:LYS:HE2	4	0.92
(2,1111)	1:153:A:MET:HE1	1:44:A:VAL:HG21	7	0.92
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE2	8	0.92
(2,1083)	1:148:A:ILE:HG22	1:154:A:MET:HG3	6	0.92
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD12	2	0.92
(1,248)	1:61:A:ILE:HD12	1:57:A:LEU:HA	8	0.92
(1,222)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	6	0.92
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD23	7	0.92
(2,1184)	1:5:A:TYR:HD2	1:85:A:MET:HG3	5	0.91
(2,1157)	1:28:A:VAL:HG23	1:24:A:PHE:HD2	1	0.91
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD13	4	0.91
(2,1069)	1:148:A:ILE:HD12	1:147:A:ARG:HD2	4	0.91
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE2	2	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,432)	1:61:A:ILE:HG21	1:38:A:THR:HG23	8	0.91
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD12	2	0.91
(1,222)	1:6:A:LYS:HB3	1:6:A:LYS:HE2	1	0.91
(1,198)	1:50:A:GLN:HG3	1:52:A:PRO:HD2	6	0.91
(1,150)	1:48:A:LEU:HD23	1:156:A:ALA:HA	7	0.91
(1,105)	1:148:A:ILE:HG22	1:152:A:ALA:HA	4	0.91
(1,93)	1:61:A:ILE:HD12	1:38:A:THR:HB	6	0.91
(2,912)	1:82:A:VAL:HG23	1:20:A:PHE:HE1	7	0.9
(2,469)	1:154:A:MET:HE3	1:154:A:MET:HA	7	0.9
(2,435)	1:1:A:MET:HE3	1:6:A:LYS:HG2	7	0.9
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD1	7	0.9
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB3	7	0.9
(1,82)	1:17:A:LYS:HE3	1:12:A:LEU:HD13	8	0.9
(2,1152)	1:4:A:ILE:HD11	1:86:A:LYS:HE3	7	0.89
(2,1083)	1:148:A:ILE:HG23	1:154:A:MET:HG3	3	0.89
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD11	1	0.89
(2,922)	1:4:A:ILE:HG13	1:5:A:TYR:HE2	3	0.89
(2,502)	1:28:A:VAL:HG23	1:36:A:ILE:HD13	2	0.89
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD13	7	0.89
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB3	3	0.89
(1,142)	1:38:A:THR:HG22	1:60:A:MET:HE2	1	0.89
(2,1157)	1:28:A:VAL:HG21	1:24:A:PHE:HD2	4	0.88
(2,1157)	1:28:A:VAL:HG21	1:24:A:PHE:HD2	7	0.88
(2,1152)	1:4:A:ILE:HD12	1:86:A:LYS:HE3	1	0.88
(2,1152)	1:4:A:ILE:HD12	1:86:A:LYS:HE3	2	0.88
(2,1104)	1:143:A:LEU:HD12	1:63:A:GLU:HG3	5	0.88
(2,1100)	1:142:A:THR:HB	1:143:A:LEU:HD23	3	0.88
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD12	4	0.88
(2,568)	1:82:A:VAL:HG22	1:86:A:LYS:HD3	1	0.88
(2,432)	1:61:A:ILE:HG21	1:38:A:THR:HG21	7	0.88
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD23	6	0.88
(1,248)	1:61:A:ILE:HD11	1:57:A:LEU:HA	7	0.88
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG13	4	0.88
(1,198)	1:50:A:GLN:HG3	1:52:A:PRO:HD2	4	0.88
(1,189)	1:59:A:GLU:HG3	1:61:A:ILE:HG13	3	0.88
(1,152)	1:41:A:LEU:HD12	1:153:A:MET:HE2	8	0.88
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	6	0.88
(2,1529)	1:64:A:VAL:H	1:64:A:VAL:HG22	6	0.87
(2,1152)	1:4:A:ILE:HD11	1:86:A:LYS:HE3	3	0.87
(2,1047)	1:79:A:VAL:HG11	1:5:A:TYR:HE2	1	0.87
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD1	8	0.87
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB2	1	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:160:A:ALA:HB3	1:26:A:ILE:HB	2	0.87
(1,125)	1:160:A:ALA:HB3	1:26:A:ILE:HB	5	0.87
(1,93)	1:61:A:ILE:HD11	1:38:A:THR:HB	2	0.87
(2,1529)	1:64:A:VAL:H	1:64:A:VAL:HG22	7	0.86
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD11	8	0.86
(2,507)	1:162:A:ALA:HB3	1:19:A:GLU:HG3	1	0.86
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD1	6	0.86
(1,289)	1:146:A:VAL:HG22	1:145:A:ARG:HD3	7	0.86
(1,143)	1:71:A:THR:HG23	1:33:A:ASP:HB3	5	0.86
(1,123)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	7	0.86
(1,93)	1:61:A:ILE:HD12	1:38:A:THR:HB	3	0.86
(1,77)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	8	0.86
(2,1083)	1:148:A:ILE:HG22	1:154:A:MET:HG3	1	0.85
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD12	8	0.85
(2,448)	1:1:A:MET:HE2	1:5:A:TYR:HB2	6	0.85
(1,198)	1:72:A:VAL:HB	1:77:A:PHE:HB3	1	0.85
(1,138)	1:13:A:THR:HG21	1:15:A:GLU:HB3	1	0.85
(1,107)	1:153:A:MET:HE3	1:23:A:ALA:HA	2	0.85
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD12	8	0.84
(2,1115)	1:162:A:ALA:HB3	1:163:A:LYS:HE3	2	0.84
(2,547)	1:45:A:MET:HE2	1:146:A:VAL:HG13	4	0.84
(2,441)	1:47:A:MET:HE1	1:157:A:LEU:HD22	1	0.84
(2,414)	1:61:A:ILE:HD12	1:61:A:ILE:HA	7	0.84
(1,289)	1:146:A:VAL:HG22	1:147:A:ARG:HD2	1	0.84
(1,198)	1:50:A:GLN:HG3	1:52:A:PRO:HD2	7	0.84
(1,153)	1:41:A:LEU:HD13	1:52:A:PRO:HB3	7	0.84
(1,152)	1:41:A:LEU:HD13	1:153:A:MET:HE2	6	0.84
(1,142)	1:38:A:THR:HG22	1:60:A:MET:HE2	7	0.84
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	5	0.84
(2,1214)	1:138:A:PHE:HD1	1:139:A:LYS:HD3	5	0.83
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD12	8	0.83
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG22	8	0.83
(2,1069)	1:148:A:ILE:HD11	1:147:A:ARG:HD2	2	0.83
(2,749)	1:55:A:GLU:HA	1:55:A:GLU:HG2	6	0.83
(2,596)	1:157:A:LEU:HD21	1:157:A:LEU:HA	4	0.83
(2,414)	1:61:A:ILE:HD13	1:61:A:ILE:HA	8	0.83
(1,286)	1:36:A:ILE:HG23	1:71:A:THR:HB	4	0.83
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG12	6	0.83
(1,248)	1:61:A:ILE:HD13	1:57:A:LEU:HA	3	0.83
(1,116)	1:8:A:ALA:HB3	1:11:A:GLN:HG2	2	0.83
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	8	0.83
(2,615)	1:143:A:LEU:HD13	1:59:A:GLU:HB3	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:50:A:GLN:HG3	1:52:A:PRO:HD2	8	0.82
(1,105)	1:23:A:ALA:HA	1:26:A:ILE:HG22	8	0.82
(1,93)	1:61:A:ILE:HD13	1:38:A:THR:HB	7	0.82
(1,65)	1:52:A:PRO:HD3	1:57:A:LEU:HD11	6	0.82
(1,46)	1:85:A:MET:HA	1:150:A:ALA:HB2	6	0.82
(2,1103)	1:143:A:LEU:HD13	1:143:A:LEU:HA	6	0.81
(2,1083)	1:148:A:ILE:HG21	1:154:A:MET:HG3	2	0.81
(2,1083)	1:148:A:ILE:HG22	1:154:A:MET:HG3	4	0.81
(2,1047)	1:79:A:VAL:HG11	1:5:A:TYR:HE1	6	0.81
(2,547)	1:45:A:MET:HE1	1:146:A:VAL:HG11	3	0.81
(2,502)	1:28:A:VAL:HG23	1:36:A:ILE:HD13	4	0.81
(2,469)	1:154:A:MET:HE3	1:154:A:MET:HA	6	0.81
(2,469)	1:154:A:MET:HE3	1:154:A:MET:HA	8	0.81
(2,455)	1:148:A:ILE:HG21	1:153:A:MET:HG2	3	0.81
(1,275)	1:13:A:THR:HB	1:16:A:GLN:HB2	7	0.81
(1,202)	1:148:A:ILE:HD13	1:45:A:MET:HG2	6	0.81
(1,197)	1:155:A:GLN:HG3	1:158:A:LEU:HB2	5	0.81
(1,126)	1:160:A:ALA:HB3	1:26:A:ILE:HD11	6	0.81
(2,1047)	1:79:A:VAL:HG13	1:5:A:TYR:HE1	2	0.8
(2,1019)	1:72:A:VAL:HG21	1:36:A:ILE:HD11	5	0.8
(2,596)	1:157:A:LEU:HD21	1:157:A:LEU:HA	7	0.8
(2,438)	1:1:A:MET:HE2	1:78:A:LEU:HB2	4	0.8
(2,414)	1:61:A:ILE:HD13	1:61:A:ILE:HA	2	0.8
(2,105)	1:84:A:SER:HA	1:88:A:ASP:HB2	8	0.8
(1,321)	1:39:A:LYS:H	1:38:A:THR:HB	4	0.8
(1,286)	1:36:A:ILE:HG23	1:71:A:THR:HB	2	0.8
(1,198)	1:50:A:GLN:HG3	1:52:A:PRO:HD2	2	0.8
(1,95)	1:26:A:ILE:HD13	1:157:A:LEU:HB3	7	0.8
(2,1184)	1:5:A:TYR:HD2	1:85:A:MET:HG3	6	0.79
(2,864)	1:81:A:MET:HE2	1:84:A:SER:HB3	8	0.79
(1,313)	1:27:A:PHE:HE2	1:36:A:ILE:HG23	1	0.79
(1,296)	1:147:A:ARG:HD2	1:146:A:VAL:HG12	4	0.79
(1,198)	1:72:A:VAL:HB	1:77:A:PHE:HB3	3	0.79
(1,189)	1:59:A:GLU:HG3	1:61:A:ILE:HG13	6	0.79
(1,142)	1:38:A:THR:HG21	1:60:A:MET:HE2	6	0.79
(1,105)	1:148:A:ILE:HG21	1:149:A:SER:HB3	7	0.79
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD11	6	0.78
(2,1154)	1:10:A:GLU:HG3	1:9:A:VAL:HG12	6	0.78
(2,1113)	1:22:A:ALA:HB3	1:25:A:ASP:HB2	8	0.78
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG23	4	0.78
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG21	7	0.78
(2,502)	1:28:A:VAL:HG21	1:36:A:ILE:HD12	8	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,455)	1:148:A:ILE:HG22	1:153:A:MET:HG3	7	0.78
(2,414)	1:61:A:ILE:HD13	1:61:A:ILE:HA	6	0.78
(1,313)	1:27:A:PHE:HE2	1:36:A:ILE:HG23	6	0.78
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD22	3	0.78
(1,202)	1:48:A:LEU:HD13	1:45:A:MET:HG2	4	0.78
(1,116)	1:8:A:ALA:HB2	1:11:A:GLN:HG2	7	0.78
(1,16)	1:52:A:PRO:HA	1:56:A:GLU:HB2	7	0.78
(2,1408)	1:86:A:LYS:H	1:86:A:LYS:HG3	5	0.77
(2,1103)	1:143:A:LEU:HD12	1:143:A:LEU:HA	7	0.77
(2,1063)	1:145:A:ARG:HD2	1:142:A:THR:HA	2	0.77
(2,910)	1:41:A:LEU:HD13	1:77:A:PHE:HD2	3	0.77
(2,640)	1:157:A:LEU:HD11	1:153:A:MET:HG2	2	0.77
(2,630)	1:158:A:LEU:HD11	1:158:A:LEU:HA	6	0.77
(2,572)	1:158:A:LEU:HB2	1:158:A:LEU:HD21	1	0.77
(2,473)	1:154:A:MET:HE2	1:158:A:LEU:HD23	7	0.77
(2,455)	1:148:A:ILE:HG23	1:153:A:MET:HG2	1	0.77
(2,438)	1:1:A:MET:HE1	1:78:A:LEU:HB2	8	0.77
(2,179)	1:63:A:GLU:HA	1:63:A:GLU:HG3	4	0.77
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD23	5	0.77
(1,107)	1:153:A:MET:HE1	1:23:A:ALA:HA	4	0.77
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD22	4	0.77
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE1	8	0.76
(2,1592)	2:201:A:9XG:HAE	1:61:A:ILE:HD13	2	0.76
(2,1115)	1:162:A:ALA:HB2	1:163:A:LYS:HE2	6	0.76
(2,1104)	1:143:A:LEU:HD13	1:63:A:GLU:HG3	8	0.76
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD13	1	0.76
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD11	3	0.76
(2,448)	1:1:A:MET:HE2	1:5:A:TYR:HB2	8	0.76
(2,441)	1:47:A:MET:HE1	1:157:A:LEU:HD23	3	0.76
(1,222)	1:6:A:LYS:HB3	1:6:A:LYS:HE2	4	0.76
(1,177)	1:41:A:LEU:HD21	1:61:A:ILE:HB	8	0.76
(1,14)	1:146:A:VAL:HA	1:147:A:ARG:HB3	2	0.76
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD13	7	0.75
(2,1226)	1:20:A:PHE:HE1	1:78:A:LEU:HD22	4	0.75
(2,1157)	1:28:A:VAL:HG21	1:24:A:PHE:HD1	5	0.75
(2,1115)	1:162:A:ALA:HB3	1:163:A:LYS:HE2	5	0.75
(2,1019)	1:72:A:VAL:HG23	1:36:A:ILE:HD13	1	0.75
(2,922)	1:4:A:ILE:HG13	1:5:A:TYR:HE1	2	0.75
(2,642)	1:157:A:LEU:HD11	1:157:A:LEU:HB2	1	0.75
(2,365)	1:2:A:ASP:HB2	1:79:A:VAL:HG22	6	0.75
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE1	8	0.75
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD11	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:157:A:LEU:HD12	1:27:A:PHE:HB2	8	0.75
(1,209)	1:150:A:ALA:HB1	1:85:A:MET:HG2	5	0.75
(1,197)	1:8:A:ALA:HB3	1:11:A:GLN:HG2	2	0.75
(1,98)	1:85:A:MET:HE3	1:150:A:ALA:HB2	5	0.75
(1,93)	1:61:A:ILE:HD12	1:38:A:THR:HB	8	0.75
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD12	6	0.74
(2,1076)	1:157:A:LEU:HD11	1:27:A:PHE:HB3	2	0.74
(2,1047)	1:79:A:VAL:HG12	1:5:A:TYR:HE1	5	0.74
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD23	8	0.74
(2,635)	1:78:A:LEU:HD13	1:78:A:LEU:HA	5	0.74
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE2	4	0.74
(1,248)	1:61:A:ILE:HD12	1:57:A:LEU:HA	4	0.74
(2,1226)	1:20:A:PHE:HE1	1:78:A:LEU:HD21	8	0.73
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE2	4	0.73
(2,1019)	1:72:A:VAL:HG22	1:36:A:ILE:HD12	2	0.73
(2,1007)	1:64:A:VAL:HG22	1:72:A:VAL:HA	7	0.73
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD11	6	0.73
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	2	0.73
(2,642)	1:157:A:LEU:HD11	1:157:A:LEU:HB2	4	0.73
(2,616)	1:143:A:LEU:HD12	1:59:A:GLU:HB2	7	0.73
(2,580)	1:72:A:VAL:HG21	1:76:A:GLU:HA	2	0.73
(2,453)	1:2:A:ASP:HB2	1:4:A:ILE:HG22	6	0.73
(1,246)	1:85:A:MET:HG3	1:84:A:SER:HB3	5	0.73
(1,142)	1:38:A:THR:HG21	1:60:A:MET:HE3	3	0.73
(1,142)	1:38:A:THR:HG21	1:60:A:MET:HE2	8	0.73
(1,138)	1:13:A:THR:HG22	1:15:A:GLU:HB2	5	0.73
(2,1189)	1:82:A:VAL:HG11	1:5:A:TYR:HD2	4	0.72
(2,1115)	1:162:A:ALA:HB1	1:163:A:LYS:HE2	8	0.72
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG23	6	0.72
(2,580)	1:72:A:VAL:HG21	1:76:A:GLU:HA	3	0.72
(2,513)	1:31:A:ALA:HB1	1:36:A:ILE:HG23	7	0.72
(2,432)	1:61:A:ILE:HG22	1:38:A:THR:HG23	6	0.72
(1,304)	1:155:A:GLN:HG3	1:158:A:LEU:HD12	6	0.72
(1,214)	1:19:A:GLU:HB3	1:158:A:LEU:HD12	7	0.72
(1,154)	1:157:A:LEU:HD21	1:26:A:ILE:HB	1	0.72
(1,54)	1:87:A:ASP:HA	1:90:A:LYS:HD3	8	0.72
(1,47)	1:151:A:ASP:HA	1:81:A:MET:HE2	8	0.72
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD21	4	0.72
(2,1139)	1:41:A:LEU:HD21	1:45:A:MET:HG3	7	0.71
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE2	1	0.71
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG21	1	0.71
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,727)	1:11:A:GLN:HB2	1:11:A:GLN:HG2	6	0.71
(2,727)	1:11:A:GLN:HB2	1:11:A:GLN:HG2	7	0.71
(2,635)	1:78:A:LEU:HD13	1:78:A:LEU:HA	2	0.71
(2,432)	1:61:A:ILE:HG21	1:38:A:THR:HG21	1	0.71
(1,275)	1:13:A:THR:HB	1:16:A:GLN:HB2	8	0.71
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB2	4	0.71
(1,235)	1:28:A:VAL:HG11	1:43:A:LYS:HD3	4	0.71
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	8	0.71
(1,105)	1:148:A:ILE:HG22	1:152:A:ALA:HA	5	0.71
(2,1154)	1:10:A:GLU:HG3	1:9:A:VAL:HG12	8	0.7
(2,1073)	1:157:A:LEU:HD22	1:27:A:PHE:HB3	7	0.7
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD21	1	0.7
(2,882)	1:83:A:ARG:HA	1:86:A:LYS:HB3	7	0.7
(2,727)	1:11:A:GLN:HB2	1:11:A:GLN:HG2	3	0.7
(2,594)	1:41:A:LEU:HD11	1:41:A:LEU:HB3	6	0.7
(2,479)	1:45:A:MET:HE2	1:45:A:MET:HG2	7	0.7
(2,432)	1:61:A:ILE:HG22	1:38:A:THR:HG23	2	0.7
(2,183)	1:63:A:GLU:HA	1:64:A:VAL:HG13	6	0.7
(2,179)	1:63:A:GLU:HA	1:63:A:GLU:HG3	2	0.7
(1,197)	1:8:A:ALA:HB2	1:11:A:GLN:HG2	7	0.7
(1,118)	1:150:A:ALA:HB3	1:85:A:MET:HB2	1	0.7
(1,101)	1:85:A:MET:HE1	1:84:A:SER:HB3	3	0.7
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	1	0.7
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD23	3	0.7
(2,1063)	1:145:A:ARG:HD2	1:142:A:THR:HA	5	0.69
(2,1059)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	7	0.69
(2,1044)	1:78:A:LEU:HG	1:74:A:PHE:HE1	1	0.69
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	6	0.69
(2,745)	1:4:A:ILE:HD11	1:4:A:ILE:HB	6	0.69
(2,643)	1:48:A:LEU:HD11	1:48:A:LEU:HA	3	0.69
(2,432)	1:61:A:ILE:HG21	1:38:A:THR:HG21	5	0.69
(1,286)	1:36:A:ILE:HG23	1:71:A:THR:HB	3	0.69
(1,214)	1:19:A:GLU:HB3	1:158:A:LEU:HD11	8	0.69
(1,193)	1:76:A:GLU:HG3	1:66:A:GLU:HB3	5	0.69
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG13	8	0.69
(1,6)	1:38:A:THR:HA	1:57:A:LEU:HD13	7	0.69
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE2	5	0.68
(2,1189)	1:82:A:VAL:HG12	1:5:A:TYR:HD2	8	0.68
(2,1001)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	6	0.68
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD11	3	0.68
(2,845)	1:76:A:GLU:HB2	1:64:A:VAL:HG23	6	0.68
(2,727)	1:11:A:GLN:HB2	1:11:A:GLN:HG2	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,643)	1:48:A:LEU:HD13	1:48:A:LEU:HA	5	0.68
(2,568)	1:82:A:VAL:HG22	1:86:A:LYS:HD2	2	0.68
(2,479)	1:45:A:MET:HE3	1:45:A:MET:HG2	6	0.68
(2,125)	1:19:A:GLU:HA	1:161:A:ARG:HG3	4	0.68
(1,217)	1:12:A:LEU:HD23	1:16:A:GLN:HB2	2	0.68
(1,192)	1:63:A:GLU:HG2	1:143:A:LEU:HD13	4	0.68
(1,105)	1:23:A:ALA:HA	1:26:A:ILE:HG22	1	0.68
(1,98)	1:85:A:MET:HE3	1:86:A:LYS:HG2	4	0.68
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG23	3	0.68
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HD2	2	0.68
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE2	8	0.67
(2,1157)	1:28:A:VAL:HG21	1:24:A:PHE:HD1	2	0.67
(2,1113)	1:22:A:ALA:HB3	1:25:A:ASP:HB2	6	0.67
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE3	5	0.67
(2,745)	1:4:A:ILE:HD12	1:4:A:ILE:HB	4	0.67
(2,643)	1:48:A:LEU:HD12	1:48:A:LEU:HA	4	0.67
(2,642)	1:157:A:LEU:HD11	1:157:A:LEU:HB2	3	0.67
(2,567)	1:82:A:VAL:HG21	1:86:A:LYS:HB3	3	0.67
(1,279)	1:60:A:MET:HE1	1:147:A:ARG:HD3	1	0.67
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	6	0.67
(1,152)	1:41:A:LEU:HD11	1:153:A:MET:HE1	7	0.67
(1,97)	1:148:A:ILE:HD13	1:146:A:VAL:HB	4	0.67
(1,46)	1:151:A:ASP:HA	1:150:A:ALA:HB2	7	0.67
(1,14)	1:146:A:VAL:HA	1:147:A:ARG:HB3	5	0.67
(2,1585)	1:162:A:ALA:HA	1:158:A:LEU:HD12	2	0.66
(2,1049)	1:78:A:LEU:HD13	1:81:A:MET:HE1	8	0.66
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	2	0.66
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG13	8	0.66
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	5	0.66
(2,643)	1:48:A:LEU:HD11	1:48:A:LEU:HA	1	0.66
(2,594)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	2	0.66
(2,548)	1:79:A:VAL:HG11	1:5:A:TYR:HD2	1	0.66
(2,537)	1:9:A:VAL:HG13	1:6:A:LYS:HA	6	0.66
(2,479)	1:45:A:MET:HE2	1:45:A:MET:HG2	8	0.66
(1,217)	1:12:A:LEU:HD22	1:16:A:GLN:HB2	5	0.66
(1,165)	1:78:A:LEU:HD23	1:17:A:LYS:HG3	2	0.66
(1,154)	1:157:A:LEU:HD23	1:26:A:ILE:HB	4	0.66
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG12	5	0.66
(1,125)	1:160:A:ALA:HB1	1:26:A:ILE:HB	3	0.66
(1,15)	1:52:A:PRO:HA	1:146:A:VAL:HG21	1	0.66
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD22	7	0.66
(2,1197)	1:4:A:ILE:HD12	1:5:A:TYR:HE2	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE1	7	0.65
(2,1157)	1:28:A:VAL:HG21	1:24:A:PHE:HD1	8	0.65
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG22	1	0.65
(2,1074)	1:158:A:LEU:HD23	1:154:A:MET:HG2	4	0.65
(2,745)	1:4:A:ILE:HD13	1:4:A:ILE:HB	2	0.65
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD13	7	0.65
(2,617)	1:78:A:LEU:HD23	1:20:A:PHE:HB2	7	0.65
(2,537)	1:9:A:VAL:HG13	1:6:A:LYS:HA	8	0.65
(2,509)	1:162:A:ALA:HB2	1:158:A:LEU:HD22	8	0.65
(2,480)	1:26:A:ILE:HD13	1:22:A:ALA:HB3	8	0.65
(2,432)	1:61:A:ILE:HG22	1:38:A:THR:HG23	3	0.65
(2,432)	1:61:A:ILE:HG22	1:38:A:THR:HG21	4	0.65
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG13	7	0.65
(1,235)	1:28:A:VAL:HG13	1:43:A:LYS:HD3	7	0.65
(1,202)	1:148:A:ILE:HD13	1:45:A:MET:HG2	7	0.65
(1,186)	1:18:A:ASN:HB3	1:19:A:GLU:HB3	3	0.65
(1,106)	1:36:A:ILE:HG23	1:27:A:PHE:HB2	8	0.65
(2,1421)	1:10:A:GLU:H	1:9:A:VAL:HG23	8	0.64
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE2	6	0.64
(2,1153)	1:12:A:LEU:HB3	1:17:A:LYS:HD2	6	0.64
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD13	3	0.64
(2,1044)	1:78:A:LEU:HG	1:74:A:PHE:HE2	4	0.64
(2,912)	1:82:A:VAL:HG22	1:20:A:PHE:HE1	5	0.64
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE1	1	0.64
(1,256)	1:78:A:LEU:HD23	1:24:A:PHE:HB2	3	0.64
(1,202)	1:48:A:LEU:HD11	1:45:A:MET:HG2	5	0.64
(1,169)	1:157:A:LEU:HD12	1:26:A:ILE:HB	4	0.64
(1,138)	1:13:A:THR:HG22	1:15:A:GLU:HB2	4	0.64
(1,109)	1:154:A:MET:HE2	1:19:A:GLU:HA	4	0.64
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	4	0.64
(1,42)	1:16:A:GLN:HA	1:19:A:GLU:HB2	2	0.64
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE1	3	0.63
(2,1130)	1:50:A:GLN:HG3	1:148:A:ILE:HG13	8	0.63
(2,1001)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	7	0.63
(2,999)	1:37:A:SER:HB3	1:61:A:ILE:HD12	6	0.63
(2,594)	1:41:A:LEU:HD11	1:41:A:LEU:HB3	5	0.63
(2,516)	1:64:A:VAL:HA	1:64:A:VAL:HG23	2	0.63
(2,516)	1:64:A:VAL:HA	1:64:A:VAL:HG22	5	0.63
(2,515)	1:31:A:ALA:HB1	1:28:A:VAL:HG13	7	0.63
(2,514)	1:31:A:ALA:HB3	1:28:A:VAL:HG22	2	0.63
(2,480)	1:26:A:ILE:HD13	1:22:A:ALA:HB3	6	0.63
(2,414)	1:61:A:ILE:HD12	1:61:A:ILE:HA	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:78:A:LEU:HB2	1:78:A:LEU:HD22	2	0.63
(2,358)	1:137:A:LYS:HE2	1:137:A:LYS:HG2	6	0.63
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE1	7	0.63
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD13	6	0.63
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB2	6	0.63
(1,286)	1:36:A:ILE:HG22	1:71:A:THR:HB	1	0.63
(1,139)	1:38:A:THR:HG21	1:57:A:LEU:HA	2	0.63
(1,101)	1:85:A:MET:HE1	1:84:A:SER:HB3	6	0.63
(2,1421)	1:10:A:GLU:H	1:9:A:VAL:HG21	7	0.62
(2,1150)	1:148:A:ILE:HD11	1:148:A:ILE:HA	2	0.62
(2,1123)	1:157:A:LEU:HD23	1:44:A:VAL:HG21	1	0.62
(2,912)	1:82:A:VAL:HG22	1:20:A:PHE:HE2	6	0.62
(2,745)	1:4:A:ILE:HD11	1:4:A:ILE:HB	1	0.62
(2,745)	1:4:A:ILE:HD12	1:4:A:ILE:HB	5	0.62
(2,643)	1:48:A:LEU:HD11	1:48:A:LEU:HA	2	0.62
(2,635)	1:78:A:LEU:HD11	1:78:A:LEU:HA	3	0.62
(2,566)	1:82:A:VAL:HG23	1:5:A:TYR:HB3	6	0.62
(2,537)	1:9:A:VAL:HG11	1:6:A:LYS:HA	7	0.62
(2,533)	1:72:A:VAL:HG11	1:73:A:ASP:HB3	6	0.62
(2,517)	1:146:A:VAL:HG22	1:146:A:VAL:HA	7	0.62
(2,479)	1:45:A:MET:HE3	1:45:A:MET:HG2	1	0.62
(2,479)	1:45:A:MET:HE2	1:45:A:MET:HG2	4	0.62
(2,381)	1:78:A:LEU:HB2	1:78:A:LEU:HD21	5	0.62
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG22	5	0.62
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG12	6	0.62
(1,157)	1:29:A:LEU:HD21	1:26:A:ILE:HB	8	0.62
(1,138)	1:13:A:THR:HG22	1:15:A:GLU:HB2	3	0.62
(1,6)	1:38:A:THR:HA	1:57:A:LEU:HD12	1	0.62
(1,6)	1:38:A:THR:HA	1:57:A:LEU:HD13	8	0.62
(2,1152)	1:4:A:ILE:HD12	1:86:A:LYS:HE3	8	0.61
(2,1081)	1:26:A:ILE:HD11	1:25:A:ASP:HB2	5	0.61
(2,912)	1:82:A:VAL:HG23	1:20:A:PHE:HE2	3	0.61
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	8	0.61
(2,517)	1:146:A:VAL:HG22	1:146:A:VAL:HA	8	0.61
(2,515)	1:31:A:ALA:HB3	1:28:A:VAL:HG12	5	0.61
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG23	2	0.61
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG23	7	0.61
(2,479)	1:45:A:MET:HE3	1:45:A:MET:HG2	2	0.61
(2,453)	1:2:A:ASP:HB2	1:4:A:ILE:HG21	7	0.61
(2,414)	1:61:A:ILE:HD13	1:61:A:ILE:HA	4	0.61
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD23	8	0.61
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD22	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	4	0.61
(1,150)	1:48:A:LEU:HD23	1:156:A:ALA:HA	1	0.61
(1,150)	1:48:A:LEU:HD21	1:156:A:ALA:HA	4	0.61
(1,97)	1:148:A:ILE:HD12	1:146:A:VAL:HB	6	0.61
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	3	0.61
(1,9)	1:141:A:PRO:HA	1:140:A:ARG:HD2	5	0.61
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE1	6	0.6
(2,1226)	1:20:A:PHE:HE1	1:78:A:LEU:HD22	1	0.6
(2,1189)	1:82:A:VAL:HG12	1:5:A:TYR:HD1	7	0.6
(2,1115)	1:162:A:ALA:HB2	1:163:A:LYS:HE2	1	0.6
(2,1103)	1:143:A:LEU:HD12	1:143:A:LEU:HA	4	0.6
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG23	2	0.6
(2,1088)	1:78:A:LEU:HD11	1:74:A:PHE:HD1	6	0.6
(2,1088)	1:78:A:LEU:HD12	1:74:A:PHE:HD2	8	0.6
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG21	4	0.6
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	6	0.6
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG22	5	0.6
(2,479)	1:45:A:MET:HE2	1:45:A:MET:HG2	3	0.6
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE2	6	0.6
(1,248)	1:61:A:ILE:HD12	1:57:A:LEU:HA	1	0.6
(1,235)	1:28:A:VAL:HG12	1:43:A:LYS:HD2	2	0.6
(1,202)	1:48:A:LEU:HD11	1:45:A:MET:HG2	2	0.6
(1,157)	1:29:A:LEU:HD23	1:26:A:ILE:HB	5	0.6
(1,46)	1:85:A:MET:HA	1:150:A:ALA:HB1	8	0.6
(2,1224)	1:20:A:PHE:HE1	1:20:A:PHE:HB2	5	0.59
(2,1197)	1:4:A:ILE:HD12	1:5:A:TYR:HE1	5	0.59
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE1	1	0.59
(2,1192)	1:5:A:TYR:HB3	1:5:A:TYR:HE2	2	0.59
(2,1042)	1:20:A:PHE:HA	1:78:A:LEU:HD21	4	0.59
(2,1023)	1:35:A:SER:HB2	1:73:A:ASP:HB3	2	0.59
(2,1019)	1:72:A:VAL:HG21	1:36:A:ILE:HD13	6	0.59
(2,745)	1:4:A:ILE:HD12	1:4:A:ILE:HB	3	0.59
(2,643)	1:48:A:LEU:HD12	1:48:A:LEU:HA	7	0.59
(2,608)	1:21:A:LYS:HE2	1:21:A:LYS:HG2	1	0.59
(2,590)	1:12:A:LEU:HD22	1:16:A:GLN:HB3	6	0.59
(2,548)	1:79:A:VAL:HG13	1:5:A:TYR:HD1	2	0.59
(2,515)	1:31:A:ALA:HB1	1:28:A:VAL:HG12	2	0.59
(2,506)	1:23:A:ALA:HB2	1:157:A:LEU:HD21	5	0.59
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG21	1	0.59
(2,479)	1:45:A:MET:HE1	1:45:A:MET:HG2	5	0.59
(2,381)	1:78:A:LEU:HB2	1:78:A:LEU:HD21	3	0.59
(1,313)	1:27:A:PHE:HE1	1:36:A:ILE:HG21	5	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:48:A:LEU:HD12	1:45:A:MET:HG2	3	0.59
(1,150)	1:48:A:LEU:HD21	1:156:A:ALA:HA	3	0.59
(1,138)	1:13:A:THR:HG22	1:15:A:GLU:HB2	2	0.59
(1,132)	1:142:A:THR:HG21	1:140:A:ARG:HD2	3	0.59
(1,126)	1:160:A:ALA:HB2	1:26:A:ILE:HD11	8	0.59
(1,96)	1:148:A:ILE:HD13	1:153:A:MET:HG3	8	0.59
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG22	5	0.59
(1,73)	1:57:A:LEU:HB2	1:52:A:PRO:HB2	7	0.59
(2,1600)	2:201:A:9XG:HAG	1:150:A:ALA:HB1	1	0.58
(2,1421)	1:10:A:GLU:H	1:9:A:VAL:HG21	6	0.58
(2,1224)	1:20:A:PHE:HE1	1:20:A:PHE:HB2	1	0.58
(2,1224)	1:20:A:PHE:HE2	1:20:A:PHE:HB2	3	0.58
(2,1047)	1:79:A:VAL:HG11	1:5:A:TYR:HE2	3	0.58
(2,851)	1:161:A:ARG:HB2	1:161:A:ARG:HD2	2	0.58
(2,648)	1:48:A:LEU:HD12	1:156:A:ALA:HB2	2	0.58
(2,615)	1:143:A:LEU:HD11	1:59:A:GLU:HB3	8	0.58
(2,547)	1:45:A:MET:HE1	1:146:A:VAL:HG13	7	0.58
(2,509)	1:162:A:ALA:HB2	1:158:A:LEU:HD22	7	0.58
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG12	6	0.58
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD11	3	0.58
(1,246)	1:85:A:MET:HG3	1:84:A:SER:HB3	3	0.58
(1,189)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	8	0.58
(1,125)	1:160:A:ALA:HB1	1:26:A:ILE:HB	1	0.58
(1,59)	1:160:A:ALA:HA	1:163:A:LYS:HD2	3	0.58
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD22	1	0.58
(2,1224)	1:20:A:PHE:HE1	1:20:A:PHE:HB2	4	0.57
(2,1224)	1:20:A:PHE:HE1	1:20:A:PHE:HB2	8	0.57
(2,1044)	1:78:A:LEU:HG	1:74:A:PHE:HE2	8	0.57
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE1	8	0.57
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	7	0.57
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD11	1	0.57
(2,608)	1:21:A:LYS:HE2	1:21:A:LYS:HG2	6	0.57
(2,596)	1:157:A:LEU:HD23	1:157:A:LEU:HA	3	0.57
(2,594)	1:41:A:LEU:HD12	1:41:A:LEU:HB3	4	0.57
(2,549)	1:79:A:VAL:HG13	1:5:A:TYR:HB3	4	0.57
(2,533)	1:72:A:VAL:HG11	1:73:A:ASP:HB3	3	0.57
(2,517)	1:146:A:VAL:HG23	1:146:A:VAL:HA	1	0.57
(2,517)	1:146:A:VAL:HG23	1:146:A:VAL:HA	3	0.57
(2,516)	1:64:A:VAL:HA	1:64:A:VAL:HG22	1	0.57
(2,516)	1:64:A:VAL:HA	1:64:A:VAL:HG23	4	0.57
(2,507)	1:162:A:ALA:HB2	1:19:A:GLU:HG3	3	0.57
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG23	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,455)	1:148:A:ILE:HG23	1:153:A:MET:HG3	6	0.57
(2,424)	1:148:A:ILE:HD12	1:45:A:MET:HB3	2	0.57
(2,420)	1:157:A:LEU:HB2	1:26:A:ILE:HD12	8	0.57
(2,189)	1:10:A:GLU:HA	1:10:A:GLU:HG3	7	0.57
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD13	5	0.57
(1,269)	1:56:A:GLU:HG3	1:57:A:LEU:HD12	2	0.57
(1,244)	1:155:A:GLN:HB2	1:48:A:LEU:HD23	8	0.57
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	1	0.57
(1,236)	1:50:A:GLN:HB2	1:146:A:VAL:HG11	2	0.57
(1,225)	1:12:A:LEU:HD22	1:16:A:GLN:HB3	6	0.57
(1,189)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	2	0.57
(1,162)	1:29:A:LEU:HD13	1:26:A:ILE:HB	7	0.57
(1,157)	1:29:A:LEU:HD22	1:26:A:ILE:HB	2	0.57
(1,132)	1:142:A:THR:HG21	1:140:A:ARG:HD3	5	0.57
(1,65)	1:52:A:PRO:HD3	1:57:A:LEU:HD11	1	0.57
(1,35)	1:12:A:LEU:HA	1:16:A:GLN:HB2	3	0.57
(1,16)	1:52:A:PRO:HA	1:56:A:GLU:HB2	6	0.57
(2,1592)	2:201:A:9XG:HAE	1:61:A:ILE:HD11	7	0.56
(2,1582)	1:146:A:VAL:HG22	1:52:A:PRO:HA	2	0.56
(2,1140)	1:41:A:LEU:HD23	1:41:A:LEU:HA	4	0.56
(2,1103)	1:143:A:LEU:HD11	1:143:A:LEU:HA	8	0.56
(2,1079)	1:164:A:GLY:HA3	1:163:A:LYS:HE2	4	0.56
(2,1063)	1:145:A:ARG:HD2	1:142:A:THR:HA	3	0.56
(2,1044)	1:78:A:LEU:HG	1:74:A:PHE:HE2	7	0.56
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD12	4	0.56
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	3	0.56
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	7	0.56
(2,695)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	7	0.56
(2,648)	1:48:A:LEU:HD11	1:156:A:ALA:HB3	4	0.56
(2,642)	1:157:A:LEU:HD12	1:157:A:LEU:HB2	2	0.56
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD12	6	0.56
(2,615)	1:143:A:LEU:HD12	1:59:A:GLU:HB3	7	0.56
(2,608)	1:21:A:LYS:HE2	1:21:A:LYS:HG2	3	0.56
(2,573)	1:64:A:VAL:HA	1:64:A:VAL:HG11	7	0.56
(2,506)	1:23:A:ALA:HB3	1:157:A:LEU:HD23	7	0.56
(2,441)	1:47:A:MET:HE2	1:157:A:LEU:HD21	8	0.56
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG21	2	0.56
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD12	2	0.56
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB2	5	0.56
(1,209)	1:150:A:ALA:HB1	1:85:A:MET:HG2	3	0.56
(1,157)	1:29:A:LEU:HD23	1:26:A:ILE:HB	3	0.56
(1,150)	1:48:A:LEU:HD22	1:156:A:ALA:HA	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	8	0.56
(1,82)	1:17:A:LYS:HE3	1:12:A:LEU:HD11	7	0.56
(1,59)	1:160:A:ALA:HA	1:163:A:LYS:HD3	5	0.56
(1,54)	1:87:A:ASP:HA	1:86:A:LYS:HD3	2	0.56
(1,42)	1:16:A:GLN:HA	1:19:A:GLU:HB2	4	0.56
(2,1224)	1:20:A:PHE:HE2	1:20:A:PHE:HB2	6	0.55
(2,1224)	1:20:A:PHE:HE1	1:20:A:PHE:HB2	7	0.55
(2,1139)	1:41:A:LEU:HD21	1:45:A:MET:HG3	6	0.55
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD13	1	0.55
(2,1113)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	5	0.55
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE1	7	0.55
(2,1088)	1:78:A:LEU:HD13	1:74:A:PHE:HD1	1	0.55
(2,1075)	1:158:A:LEU:HD13	1:161:A:ARG:HD3	7	0.55
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG23	7	0.55
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD12	7	0.55
(2,884)	1:163:A:LYS:HB3	1:163:A:LYS:HE3	6	0.55
(2,884)	1:163:A:LYS:HB3	1:163:A:LYS:HE3	8	0.55
(2,883)	1:80:A:MET:HA	1:6:A:LYS:HB2	1	0.55
(2,649)	1:48:A:LEU:HD13	1:44:A:VAL:HG21	8	0.55
(2,605)	1:57:A:LEU:HD23	1:45:A:MET:HG2	1	0.55
(2,549)	1:79:A:VAL:HG11	1:5:A:TYR:HB3	3	0.55
(2,509)	1:162:A:ALA:HB3	1:158:A:LEU:HD22	1	0.55
(2,507)	1:162:A:ALA:HB2	1:19:A:GLU:HG3	8	0.55
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG22	3	0.55
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG21	6	0.55
(2,485)	1:150:A:ALA:HB1	1:20:A:PHE:HE2	2	0.55
(2,482)	1:81:A:MET:HE2	1:20:A:PHE:HD1	3	0.55
(2,469)	1:154:A:MET:HE2	1:154:A:MET:HA	3	0.55
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG23	3	0.55
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG22	6	0.55
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG13	4	0.55
(1,313)	1:27:A:PHE:HE2	1:41:A:LEU:HD21	3	0.55
(1,256)	1:78:A:LEU:HD23	1:24:A:PHE:HB2	5	0.55
(1,191)	1:64:A:VAL:HG13	1:63:A:GLU:HG2	5	0.55
(1,15)	1:52:A:PRO:HA	1:146:A:VAL:HG21	6	0.55
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG21	5	0.54
(2,1081)	1:26:A:ILE:HD12	1:25:A:ASP:HB2	4	0.54
(2,1001)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	8	0.54
(2,829)	1:76:A:GLU:HB3	1:64:A:VAL:HG22	7	0.54
(2,648)	1:48:A:LEU:HD13	1:156:A:ALA:HB1	1	0.54
(2,600)	1:157:A:LEU:HB2	1:157:A:LEU:HD22	7	0.54
(2,549)	1:79:A:VAL:HG12	1:5:A:TYR:HB3	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,548)	1:79:A:VAL:HG11	1:5:A:TYR:HD1	6	0.54
(2,533)	1:72:A:VAL:HG11	1:73:A:ASP:HB3	8	0.54
(2,475)	1:45:A:MET:HE2	1:45:A:MET:HA	1	0.54
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG22	2	0.54
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG23	4	0.54
(2,448)	1:1:A:MET:HE1	1:5:A:TYR:HB2	1	0.54
(2,424)	1:148:A:ILE:HD11	1:45:A:MET:HB3	3	0.54
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG11	8	0.54
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE1	2	0.54
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD11	7	0.54
(1,313)	1:27:A:PHE:HE1	1:36:A:ILE:HG21	4	0.54
(1,284)	1:160:A:ALA:HB2	1:163:A:LYS:HE2	1	0.54
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	8	0.54
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD21	3	0.54
(1,157)	1:29:A:LEU:HD21	1:26:A:ILE:HB	6	0.54
(1,132)	1:142:A:THR:HG23	1:140:A:ARG:HD2	2	0.54
(1,131)	1:72:A:VAL:HG11	1:24:A:PHE:HD1	8	0.54
(1,122)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	6	0.54
(1,16)	1:52:A:PRO:HA	1:56:A:GLU:HB2	8	0.54
(2,1585)	1:162:A:ALA:HA	1:158:A:LEU:HD13	5	0.53
(2,1224)	1:20:A:PHE:HE1	1:20:A:PHE:HB2	2	0.53
(2,1142)	1:45:A:MET:HE2	1:147:A:ARG:HA	2	0.53
(2,580)	1:72:A:VAL:HG23	1:76:A:GLU:HA	4	0.53
(2,580)	1:72:A:VAL:HG21	1:76:A:GLU:HA	7	0.53
(2,568)	1:82:A:VAL:HG23	1:86:A:LYS:HD3	8	0.53
(2,513)	1:31:A:ALA:HB1	1:36:A:ILE:HG22	2	0.53
(2,500)	1:28:A:VAL:HA	1:28:A:VAL:HG23	8	0.53
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB1	1	0.53
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB2	2	0.53
(1,321)	1:39:A:LYS:H	1:38:A:THR:HB	7	0.53
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD22	4	0.53
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG12	2	0.53
(1,265)	1:147:A:ARG:HD2	1:148:A:ILE:HG22	5	0.53
(1,256)	1:78:A:LEU:HD21	1:24:A:PHE:HB2	2	0.53
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	6	0.53
(1,189)	1:8:A:ALA:HB1	1:10:A:GLU:HG3	5	0.53
(1,147)	1:2:A:ASP:HB2	1:79:A:VAL:HG23	7	0.53
(1,132)	1:142:A:THR:HG23	1:140:A:ARG:HD2	6	0.53
(1,118)	1:150:A:ALA:HB2	1:85:A:MET:HB2	2	0.53
(1,118)	1:85:A:MET:HE1	1:150:A:ALA:HB2	3	0.53
(1,93)	1:61:A:ILE:HD12	1:38:A:THR:HB	1	0.53
(1,46)	1:85:A:MET:HA	1:150:A:ALA:HB3	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG21	1	0.53
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	1	0.53
(2,1214)	1:138:A:PHE:HD2	1:139:A:LYS:HD3	3	0.52
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD13	3	0.52
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG22	3	0.52
(2,1103)	1:143:A:LEU:HD12	1:143:A:LEU:HA	3	0.52
(2,1095)	1:71:A:THR:HB	1:61:A:ILE:HG23	3	0.52
(2,882)	1:83:A:ARG:HA	1:86:A:LYS:HB3	8	0.52
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD13	8	0.52
(2,603)	1:57:A:LEU:HD23	1:38:A:THR:HA	2	0.52
(2,580)	1:72:A:VAL:HG22	1:76:A:GLU:HA	1	0.52
(2,580)	1:72:A:VAL:HG23	1:76:A:GLU:HA	6	0.52
(2,574)	1:64:A:VAL:HG11	1:76:A:GLU:HA	3	0.52
(2,517)	1:146:A:VAL:HG23	1:146:A:VAL:HA	5	0.52
(2,485)	1:150:A:ALA:HB2	1:20:A:PHE:HE2	5	0.52
(2,484)	1:81:A:MET:HE1	1:81:A:MET:HB3	8	0.52
(2,473)	1:154:A:MET:HE2	1:158:A:LEU:HD23	8	0.52
(2,469)	1:154:A:MET:HE2	1:154:A:MET:HA	4	0.52
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG23	5	0.52
(2,448)	1:1:A:MET:HE2	1:5:A:TYR:HB2	5	0.52
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE3	5	0.52
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD11	5	0.52
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	4	0.52
(1,169)	1:157:A:LEU:HD12	1:26:A:ILE:HB	1	0.52
(1,157)	1:29:A:LEU:HD21	1:26:A:ILE:HB	7	0.52
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG12	3	0.52
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG13	7	0.52
(1,106)	1:36:A:ILE:HG21	1:27:A:PHE:HB2	4	0.52
(1,101)	1:85:A:MET:HE1	1:84:A:SER:HB3	8	0.52
(1,97)	1:148:A:ILE:HD11	1:146:A:VAL:HB	3	0.52
(1,96)	1:148:A:ILE:HD13	1:45:A:MET:HG2	6	0.52
(1,77)	1:157:A:LEU:HB2	1:26:A:ILE:HD11	3	0.52
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB3	3	0.51
(2,1190)	1:4:A:ILE:HD11	1:5:A:TYR:HD1	3	0.51
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG22	1	0.51
(2,1081)	1:26:A:ILE:HD12	1:25:A:ASP:HB2	3	0.51
(2,1001)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	4	0.51
(2,909)	1:78:A:LEU:HD22	1:77:A:PHE:HD2	6	0.51
(2,785)	1:60:A:MET:HG3	1:41:A:LEU:HD22	1	0.51
(2,747)	1:55:A:GLU:HG3	1:55:A:GLU:HB2	6	0.51
(2,636)	1:78:A:LEU:HB3	1:78:A:LEU:HD13	4	0.51
(2,533)	1:72:A:VAL:HG11	1:73:A:ASP:HB3	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:146:A:VAL:HG23	1:146:A:VAL:HA	4	0.51
(2,502)	1:28:A:VAL:HG22	1:36:A:ILE:HD11	6	0.51
(2,477)	1:45:A:MET:HE3	1:60:A:MET:HG3	3	0.51
(2,330)	1:145:A:ARG:HD3	1:145:A:ARG:HG2	1	0.51
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD13	1	0.51
(2,183)	1:63:A:GLU:HA	1:64:A:VAL:HG11	7	0.51
(1,280)	1:22:A:ALA:HB3	1:25:A:ASP:HB3	6	0.51
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	5	0.51
(1,98)	1:85:A:MET:HE3	1:86:A:LYS:HG2	2	0.51
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG21	2	0.51
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE3	3	0.51
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD2	5	0.51
(1,6)	1:38:A:THR:HA	1:57:A:LEU:HD11	3	0.51
(2,1197)	1:4:A:ILE:HD11	1:5:A:TYR:HE2	6	0.5
(2,1190)	1:4:A:ILE:HD13	1:5:A:TYR:HD1	2	0.5
(2,1103)	1:143:A:LEU:HD11	1:143:A:LEU:HA	2	0.5
(2,1081)	1:26:A:ILE:HD11	1:25:A:ASP:HB2	2	0.5
(2,1076)	1:157:A:LEU:HD12	1:27:A:PHE:HB3	1	0.5
(2,1064)	1:142:A:THR:HA	1:141:A:PRO:HD2	2	0.5
(2,1001)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	3	0.5
(2,909)	1:78:A:LEU:HD23	1:77:A:PHE:HD2	7	0.5
(2,819)	1:7:A:ALA:HB3	1:10:A:GLU:HB2	3	0.5
(2,643)	1:48:A:LEU:HD11	1:48:A:LEU:HA	6	0.5
(2,634)	1:78:A:LEU:HD11	1:74:A:PHE:HZ	6	0.5
(2,630)	1:158:A:LEU:HD12	1:158:A:LEU:HA	8	0.5
(2,594)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	8	0.5
(2,548)	1:79:A:VAL:HG12	1:5:A:TYR:HD1	5	0.5
(2,507)	1:162:A:ALA:HB2	1:19:A:GLU:HG3	7	0.5
(2,469)	1:154:A:MET:HE3	1:154:A:MET:HA	1	0.5
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG21	1	0.5
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG21	7	0.5
(2,448)	1:1:A:MET:HE1	1:5:A:TYR:HB2	3	0.5
(2,254)	1:50:A:GLN:HA	1:52:A:PRO:HD2	1	0.5
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD11	1	0.5
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD22	3	0.5
(1,290)	1:64:A:VAL:HG21	1:65:A:ASP:HB3	2	0.5
(1,286)	1:36:A:ILE:HG23	1:71:A:THR:HB	5	0.5
(1,182)	1:26:A:ILE:HG12	1:157:A:LEU:HB3	6	0.5
(1,167)	1:78:A:LEU:HD12	1:17:A:LYS:HG3	1	0.5
(1,139)	1:38:A:THR:HG21	1:57:A:LEU:HA	8	0.5
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG12	2	0.5
(1,132)	1:142:A:THR:HG21	1:140:A:ARG:HD3	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:36:A:ILE:HG21	1:27:A:PHE:HB2	5	0.5
(1,97)	1:148:A:ILE:HD13	1:146:A:VAL:HB	5	0.5
(1,95)	1:26:A:ILE:HD12	1:157:A:LEU:HB3	6	0.5
(1,42)	1:16:A:GLN:HA	1:15:A:GLU:HB2	8	0.5
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG21	4	0.5
(2,1230)	1:74:A:PHE:HE1	1:78:A:LEU:HD21	2	0.49
(2,1157)	1:28:A:VAL:HG22	1:24:A:PHE:HD1	6	0.49
(2,1123)	1:157:A:LEU:HD22	1:44:A:VAL:HG23	4	0.49
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG23	7	0.49
(2,1065)	1:151:A:ASP:HB3	1:152:A:ALA:HA	6	0.49
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE3	4	0.49
(2,864)	1:81:A:MET:HE2	1:84:A:SER:HB3	1	0.49
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	8	0.49
(2,573)	1:64:A:VAL:HA	1:64:A:VAL:HG12	6	0.49
(2,538)	1:9:A:VAL:HG13	1:9:A:VAL:HA	3	0.49
(2,330)	1:145:A:ARG:HD2	1:145:A:ARG:HG3	7	0.49
(2,165)	1:23:A:ALA:HA	1:157:A:LEU:HD22	7	0.49
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	0.49
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	7	0.49
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD21	1	0.49
(1,218)	1:79:A:VAL:HB	1:76:A:GLU:HA	1	0.49
(1,192)	1:63:A:GLU:HG2	1:143:A:LEU:HD11	7	0.49
(1,145)	1:158:A:LEU:HB3	1:158:A:LEU:HD22	7	0.49
(1,131)	1:72:A:VAL:HG11	1:24:A:PHE:HD2	3	0.49
(1,106)	1:36:A:ILE:HG23	1:27:A:PHE:HB2	1	0.49
(1,97)	1:148:A:ILE:HD12	1:146:A:VAL:HB	1	0.49
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG23	1	0.49
(1,61)	1:51:A:ASN:HA	1:46:A:ARG:HG2	4	0.49
(1,35)	1:12:A:LEU:HA	1:16:A:GLN:HB2	2	0.49
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	2	0.49
(2,1582)	1:146:A:VAL:HG21	1:52:A:PRO:HA	5	0.48
(2,1582)	1:146:A:VAL:HG23	1:52:A:PRO:HA	8	0.48
(2,1190)	1:4:A:ILE:HD13	1:5:A:TYR:HD1	1	0.48
(2,1171)	1:13:A:THR:HG23	1:16:A:GLN:HG3	5	0.48
(2,1151)	1:4:A:ILE:HA	1:4:A:ILE:HD13	7	0.48
(2,1070)	1:148:A:ILE:HD13	1:27:A:PHE:HZ	2	0.48
(2,1063)	1:145:A:ARG:HD3	1:142:A:THR:HA	1	0.48
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE2	7	0.48
(2,648)	1:48:A:LEU:HD13	1:156:A:ALA:HB2	3	0.48
(2,594)	1:41:A:LEU:HD12	1:41:A:LEU:HB3	1	0.48
(2,515)	1:31:A:ALA:HB2	1:28:A:VAL:HG13	1	0.48
(2,513)	1:31:A:ALA:HB1	1:36:A:ILE:HG22	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,507)	1:162:A:ALA:HB3	1:19:A:GLU:HG3	6	0.48
(2,487)	1:152:A:ALA:HB3	1:148:A:ILE:HA	3	0.48
(2,485)	1:150:A:ALA:HB3	1:20:A:PHE:HE2	4	0.48
(2,458)	1:148:A:ILE:HG22	1:152:A:ALA:HB1	8	0.48
(2,446)	1:1:A:MET:HE1	1:1:A:MET:HA	2	0.48
(2,330)	1:145:A:ARG:HD3	1:145:A:ARG:HG3	2	0.48
(2,187)	1:16:A:GLN:HA	1:12:A:LEU:HD22	6	0.48
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD12	4	0.48
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD21	4	0.48
(1,167)	1:78:A:LEU:HD11	1:17:A:LYS:HG3	4	0.48
(1,157)	1:29:A:LEU:HD23	1:26:A:ILE:HB	1	0.48
(1,137)	1:146:A:VAL:HG11	1:52:A:PRO:HB3	3	0.48
(1,122)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	7	0.48
(1,113)	1:7:A:ALA:HB1	1:4:A:ILE:HG12	3	0.48
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD1	2	0.48
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	5	0.48
(2,1583)	1:154:A:MET:HE2	1:20:A:PHE:HB3	6	0.47
(2,1408)	1:86:A:LYS:H	1:86:A:LYS:HG3	3	0.47
(2,1174)	1:145:A:ARG:HG3	1:145:A:ARG:HA	2	0.47
(2,1063)	1:145:A:ARG:HD3	1:142:A:THR:HA	4	0.47
(2,580)	1:72:A:VAL:HG22	1:76:A:GLU:HA	8	0.47
(2,549)	1:79:A:VAL:HG11	1:5:A:TYR:HB3	1	0.47
(2,540)	1:9:A:VAL:HG13	1:79:A:VAL:HA	8	0.47
(2,482)	1:81:A:MET:HE3	1:20:A:PHE:HD2	1	0.47
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD11	1	0.47
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD12	5	0.47
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD11	2	0.47
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD13	8	0.47
(2,98)	1:40:A:GLU:HA	1:43:A:LYS:HD2	7	0.47
(1,291)	1:158:A:LEU:HD12	1:155:A:GLN:HA	6	0.47
(1,276)	1:142:A:THR:HA	1:143:A:LEU:HG	8	0.47
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG11	4	0.47
(1,266)	1:157:A:LEU:HD11	1:27:A:PHE:HB2	2	0.47
(1,212)	1:90:A:LYS:HG3	1:90:A:LYS:HB3	4	0.47
(1,202)	1:148:A:ILE:HD11	1:45:A:MET:HG2	1	0.47
(1,197)	1:8:A:ALA:HB1	1:11:A:GLN:HG2	8	0.47
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG13	1	0.47
(1,82)	1:17:A:LYS:HE3	1:9:A:VAL:HG21	4	0.47
(1,75)	1:143:A:LEU:HB2	1:144:A:ARG:HA	5	0.47
(1,65)	1:52:A:PRO:HD3	1:146:A:VAL:HG13	8	0.47
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG21	2	0.46
(2,1103)	1:143:A:LEU:HD11	1:143:A:LEU:HA	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1065)	1:151:A:ASP:HB2	1:152:A:ALA:HA	5	0.46
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG23	8	0.46
(2,1047)	1:79:A:VAL:HG13	1:5:A:TYR:HE1	4	0.46
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE3	1	0.46
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD11	6	0.46
(2,640)	1:157:A:LEU:HD13	1:153:A:MET:HG2	4	0.46
(2,565)	1:35:A:SER:HB2	1:71:A:THR:HG23	5	0.46
(2,564)	1:82:A:VAL:HG22	1:9:A:VAL:HA	4	0.46
(2,487)	1:152:A:ALA:HB2	1:148:A:ILE:HA	1	0.46
(2,485)	1:150:A:ALA:HB3	1:20:A:PHE:HE1	6	0.46
(2,462)	1:36:A:ILE:HG23	1:72:A:VAL:HB	3	0.46
(2,451)	1:4:A:ILE:HA	1:4:A:ILE:HG22	8	0.46
(2,448)	1:1:A:MET:HE1	1:5:A:TYR:HB2	2	0.46
(2,424)	1:148:A:ILE:HD13	1:45:A:MET:HB3	1	0.46
(2,424)	1:148:A:ILE:HD12	1:45:A:MET:HB3	8	0.46
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE3	5	0.46
(2,330)	1:145:A:ARG:HD2	1:145:A:ARG:HG3	6	0.46
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG22	1	0.46
(1,280)	1:22:A:ALA:HB3	1:25:A:ASP:HB3	8	0.46
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB2	2	0.46
(1,235)	1:28:A:VAL:HG13	1:43:A:LYS:HD2	1	0.46
(1,218)	1:79:A:VAL:HB	1:6:A:LYS:HA	4	0.46
(1,214)	1:19:A:GLU:HB3	1:158:A:LEU:HD12	2	0.46
(1,212)	1:6:A:LYS:HB3	1:6:A:LYS:HG2	1	0.46
(1,212)	1:6:A:LYS:HB3	1:6:A:LYS:HG2	2	0.46
(1,191)	1:64:A:VAL:HG13	1:63:A:GLU:HG2	3	0.46
(1,131)	1:72:A:VAL:HG11	1:24:A:PHE:HD1	6	0.46
(1,53)	1:2:A:ASP:HA	1:6:A:LYS:HB2	8	0.46
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD21	6	0.46
(2,1606)	2:201:A:9XG:HAA	1:45:A:MET:HE1	6	0.45
(2,1602)	2:201:A:9XG:HAG	1:153:A:MET:HE1	5	0.45
(2,1416)	1:82:A:VAL:H	1:81:A:MET:HB3	6	0.45
(2,1416)	1:82:A:VAL:H	1:81:A:MET:HB3	7	0.45
(2,1196)	1:4:A:ILE:HG22	1:5:A:TYR:HE1	5	0.45
(2,1177)	1:89:A:SER:HA	1:139:A:LYS:HE2	6	0.45
(2,1113)	1:22:A:ALA:HB3	1:25:A:ASP:HB2	3	0.45
(2,1088)	1:78:A:LEU:HD12	1:74:A:PHE:HD1	4	0.45
(2,1079)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	7	0.45
(2,1065)	1:151:A:ASP:HB2	1:152:A:ALA:HA	8	0.45
(2,1004)	1:72:A:VAL:HG22	1:65:A:ASP:HB3	6	0.45
(2,769)	1:11:A:GLN:HG3	1:11:A:GLN:HB3	3	0.45
(2,747)	1:55:A:GLU:HG3	1:55:A:GLU:HB2	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,649)	1:48:A:LEU:HD12	1:44:A:VAL:HG23	2	0.45
(2,517)	1:146:A:VAL:HG21	1:146:A:VAL:HA	2	0.45
(2,455)	1:148:A:ILE:HG23	1:153:A:MET:HG3	4	0.45
(2,455)	1:148:A:ILE:HG23	1:153:A:MET:HG3	5	0.45
(2,429)	1:61:A:ILE:HG22	1:58:A:GLN:HA	3	0.45
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD12	3	0.45
(2,115)	1:19:A:GLU:HA	1:19:A:GLU:HG2	5	0.45
(1,321)	1:39:A:LYS:H	1:38:A:THR:HB	6	0.45
(1,321)	1:39:A:LYS:H	1:38:A:THR:HB	8	0.45
(1,218)	1:79:A:VAL:HB	1:76:A:GLU:HA	5	0.45
(1,217)	1:12:A:LEU:HD21	1:16:A:GLN:HB2	8	0.45
(1,143)	1:82:A:VAL:HG21	1:5:A:TYR:HB2	7	0.45
(1,97)	1:148:A:ILE:HD11	1:146:A:VAL:HB	8	0.45
(1,89)	1:6:A:LYS:HE2	1:6:A:LYS:HD3	1	0.45
(1,61)	1:51:A:ASN:HA	1:46:A:ARG:HG2	1	0.45
(1,35)	1:12:A:LEU:HA	1:16:A:GLN:HB2	5	0.45
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD2	4	0.45
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB1	4	0.44
(2,1174)	1:145:A:ARG:HG2	1:145:A:ARG:HA	4	0.44
(2,1140)	1:41:A:LEU:HD22	1:41:A:LEU:HA	5	0.44
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD12	5	0.44
(2,1100)	1:142:A:THR:HB	1:143:A:LEU:HD22	2	0.44
(2,1081)	1:26:A:ILE:HD11	1:25:A:ASP:HB2	7	0.44
(2,819)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	7	0.44
(2,769)	1:11:A:GLN:HG3	1:11:A:GLN:HB3	4	0.44
(2,675)	1:157:A:LEU:HG	1:157:A:LEU:HA	4	0.44
(2,533)	1:72:A:VAL:HG13	1:73:A:ASP:HB3	4	0.44
(2,533)	1:72:A:VAL:HG11	1:73:A:ASP:HB3	5	0.44
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB3	8	0.44
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE3	4	0.44
(2,125)	1:19:A:GLU:HA	1:161:A:ARG:HG2	5	0.44
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB2	4	0.44
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE2	1	0.44
(1,253)	1:71:A:THR:HB	1:37:A:SER:HB2	5	0.44
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	2	0.44
(1,235)	1:28:A:VAL:HG12	1:43:A:LYS:HD2	5	0.44
(1,221)	1:57:A:LEU:HA	1:60:A:MET:HB2	3	0.44
(1,218)	1:79:A:VAL:HB	1:76:A:GLU:HA	3	0.44
(1,143)	1:82:A:VAL:HG21	1:5:A:TYR:HB2	8	0.44
(1,98)	1:85:A:MET:HE1	1:86:A:LYS:HG2	1	0.44
(1,69)	1:46:A:ARG:HD3	1:46:A:ARG:HG2	2	0.44
(1,69)	1:46:A:ARG:HD3	1:46:A:ARG:HG2	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:46:A:ARG:HD3	1:46:A:ARG:HG2	5	0.44
(1,69)	1:46:A:ARG:HD3	1:46:A:ARG:HG2	7	0.44
(1,61)	1:51:A:ASN:HA	1:46:A:ARG:HG2	6	0.44
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB3	2	0.43
(2,1408)	1:86:A:LYS:H	1:86:A:LYS:HG3	6	0.43
(2,1230)	1:74:A:PHE:HE1	1:78:A:LEU:HD23	5	0.43
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE3	2	0.43
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE3	2	0.43
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE2	5	0.43
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE2	3	0.43
(2,910)	1:41:A:LEU:HD11	1:77:A:PHE:HD1	1	0.43
(2,819)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	1	0.43
(2,819)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	5	0.43
(2,794)	1:148:A:ILE:HD12	1:50:A:GLN:HG3	8	0.43
(2,785)	1:60:A:MET:HG3	1:41:A:LEU:HD23	8	0.43
(2,769)	1:11:A:GLN:HG3	1:11:A:GLN:HB3	7	0.43
(2,660)	1:140:A:ARG:HG2	1:141:A:PRO:HD2	5	0.43
(2,648)	1:48:A:LEU:HD12	1:156:A:ALA:HB1	5	0.43
(2,567)	1:82:A:VAL:HG23	1:86:A:LYS:HB3	6	0.43
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB1	1	0.43
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB1	7	0.43
(2,472)	1:154:A:MET:HE3	1:151:A:ASP:HB3	1	0.43
(2,469)	1:154:A:MET:HE1	1:154:A:MET:HA	2	0.43
(2,469)	1:154:A:MET:HE2	1:154:A:MET:HA	5	0.43
(2,462)	1:36:A:ILE:HG22	1:72:A:VAL:HB	7	0.43
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD13	2	0.43
(2,285)	1:54:A:PRO:HD3	1:53:A:THR:HG21	6	0.43
(2,262)	1:162:A:ALA:HA	1:161:A:ARG:HG3	8	0.43
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG22	6	0.43
(2,98)	1:40:A:GLU:HA	1:43:A:LYS:HD3	8	0.43
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG11	3	0.43
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG12	5	0.43
(1,263)	1:149:A:SER:HB2	1:151:A:ASP:HB2	6	0.43
(1,212)	1:6:A:LYS:HB3	1:6:A:LYS:HG2	8	0.43
(1,186)	1:18:A:ASN:HB3	1:19:A:GLU:HB3	1	0.43
(1,186)	1:18:A:ASN:HB3	1:21:A:LYS:HB3	4	0.43
(1,186)	1:18:A:ASN:HB3	1:21:A:LYS:HB3	5	0.43
(1,161)	1:90:A:LYS:HG2	1:90:A:LYS:HB3	6	0.43
(1,161)	1:90:A:LYS:HG3	1:90:A:LYS:HB3	8	0.43
(1,150)	1:48:A:LEU:HD23	1:156:A:ALA:HA	5	0.43
(1,139)	1:38:A:THR:HG22	1:57:A:LEU:HA	7	0.43
(1,127)	1:150:A:ALA:HB2	1:85:A:MET:HG2	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:154:A:MET:HE3	1:19:A:GLU:HA	2	0.43
(1,106)	1:36:A:ILE:HG22	1:27:A:PHE:HB2	3	0.43
(1,53)	1:2:A:ASP:HA	1:6:A:LYS:HB2	7	0.43
(1,36)	1:23:A:ALA:HA	1:26:A:ILE:HG13	4	0.43
(1,14)	1:146:A:VAL:HA	1:45:A:MET:HE1	6	0.43
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB3	8	0.42
(2,1191)	1:83:A:ARG:HA	1:5:A:TYR:HE2	7	0.42
(2,1081)	1:26:A:ILE:HD11	1:25:A:ASP:HB2	1	0.42
(2,1079)	1:164:A:GLY:HA3	1:163:A:LYS:HE2	2	0.42
(2,1070)	1:148:A:ILE:HD12	1:27:A:PHE:HZ	5	0.42
(2,1065)	1:151:A:ASP:HB2	1:152:A:ALA:HA	4	0.42
(2,769)	1:11:A:GLN:HG3	1:11:A:GLN:HB3	6	0.42
(2,660)	1:140:A:ARG:HG2	1:141:A:PRO:HD2	1	0.42
(2,643)	1:48:A:LEU:HD11	1:48:A:LEU:HA	8	0.42
(2,561)	1:37:A:SER:HB2	1:71:A:THR:HG22	2	0.42
(2,538)	1:9:A:VAL:HG12	1:9:A:VAL:HA	1	0.42
(2,507)	1:162:A:ALA:HB2	1:19:A:GLU:HG3	4	0.42
(2,492)	1:79:A:VAL:HA	1:8:A:ALA:HB3	7	0.42
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB2	3	0.42
(2,483)	1:81:A:MET:HE1	1:154:A:MET:HG3	1	0.42
(2,480)	1:26:A:ILE:HD11	1:22:A:ALA:HB3	7	0.42
(2,424)	1:148:A:ILE:HD11	1:45:A:MET:HB3	5	0.42
(2,330)	1:145:A:ARG:HD2	1:145:A:ARG:HG3	8	0.42
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG12	7	0.42
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	8	0.42
(2,125)	1:19:A:GLU:HA	1:161:A:ARG:HG3	2	0.42
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD21	2	0.42
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD21	1	0.42
(1,217)	1:12:A:LEU:HD23	1:16:A:GLN:HB2	7	0.42
(1,89)	1:6:A:LYS:HE2	1:6:A:LYS:HD3	6	0.42
(1,89)	1:6:A:LYS:HE3	1:6:A:LYS:HD2	8	0.42
(1,84)	1:2:A:ASP:HB3	1:79:A:VAL:HG21	2	0.42
(1,17)	1:55:A:GLU:HA	1:55:A:GLU:HG2	2	0.42
(1,12)	1:24:A:PHE:HA	1:77:A:PHE:HZ	8	0.42
(2,1602)	2:201:A:9XG:HAG	1:153:A:MET:HE1	2	0.41
(2,1602)	2:201:A:9XG:HAG	1:153:A:MET:HE2	4	0.41
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB1	1	0.41
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE2	7	0.41
(2,1191)	1:83:A:ARG:HA	1:5:A:TYR:HE1	8	0.41
(2,1190)	1:4:A:ILE:HD13	1:5:A:TYR:HD2	6	0.41
(2,1150)	1:148:A:ILE:HD12	1:148:A:ILE:HA	4	0.41
(2,1090)	1:21:A:LYS:HB3	1:74:A:PHE:HZ	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1069)	1:148:A:ILE:HD11	1:147:A:ARG:HD2	8	0.41
(2,1065)	1:151:A:ASP:HB2	1:152:A:ALA:HA	2	0.41
(2,1052)	1:82:A:VAL:HG12	1:5:A:TYR:HE2	8	0.41
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE2	1	0.41
(2,923)	1:157:A:LEU:HD13	1:27:A:PHE:HD1	1	0.41
(2,860)	1:47:A:MET:HE3	1:47:A:MET:HG3	2	0.41
(2,860)	1:47:A:MET:HE1	1:47:A:MET:HG3	6	0.41
(2,549)	1:79:A:VAL:HG13	1:5:A:TYR:HB3	2	0.41
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB1	4	0.41
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB2	5	0.41
(2,462)	1:36:A:ILE:HG22	1:72:A:VAL:HB	6	0.41
(2,448)	1:1:A:MET:HE3	1:5:A:TYR:HB2	4	0.41
(2,446)	1:1:A:MET:HE2	1:1:A:MET:HA	4	0.41
(2,446)	1:1:A:MET:HE1	1:1:A:MET:HA	5	0.41
(2,429)	1:61:A:ILE:HG22	1:58:A:GLN:HA	6	0.41
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD12	3	0.41
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	7	0.41
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG13	4	0.41
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE1	8	0.41
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE1	4	0.41
(1,287)	1:44:A:VAL:HG23	1:156:A:ALA:HB2	8	0.41
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	3	0.41
(1,243)	1:53:A:THR:HB	1:54:A:PRO:HB3	5	0.41
(1,215)	1:10:A:GLU:HB3	1:9:A:VAL:HG12	8	0.41
(1,212)	1:6:A:LYS:HB3	1:6:A:LYS:HG2	6	0.41
(1,204)	1:154:A:MET:HG3	1:152:A:ALA:HB2	1	0.41
(1,136)	1:146:A:VAL:HG12	1:145:A:ARG:HA	3	0.41
(1,113)	1:7:A:ALA:HB1	1:4:A:ILE:HG12	2	0.41
(1,105)	1:23:A:ALA:HA	1:26:A:ILE:HG21	2	0.41
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE2	5	0.41
(1,42)	1:16:A:GLN:HA	1:19:A:GLU:HB2	7	0.41
(2,1171)	1:13:A:THR:HG23	1:16:A:GLN:HG3	6	0.4
(2,1088)	1:78:A:LEU:HD13	1:74:A:PHE:HD2	7	0.4
(2,1081)	1:26:A:ILE:HD13	1:25:A:ASP:HB2	6	0.4
(2,1076)	1:157:A:LEU:HD12	1:27:A:PHE:HB3	4	0.4
(2,1004)	1:72:A:VAL:HG21	1:65:A:ASP:HB3	1	0.4
(2,1004)	1:72:A:VAL:HG23	1:65:A:ASP:HB3	2	0.4
(2,974)	1:51:A:ASN:HB3	1:46:A:ARG:HG2	2	0.4
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG11	7	0.4
(2,860)	1:47:A:MET:HE1	1:47:A:MET:HG3	3	0.4
(2,819)	1:7:A:ALA:HB3	1:10:A:GLU:HB2	2	0.4
(2,613)	1:29:A:LEU:HD12	1:157:A:LEU:HB3	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,580)	1:72:A:VAL:HG23	1:76:A:GLU:HA	5	0.4
(2,533)	1:72:A:VAL:HG12	1:73:A:ASP:HB3	1	0.4
(2,482)	1:81:A:MET:HE2	1:20:A:PHE:HD2	4	0.4
(2,424)	1:148:A:ILE:HD13	1:45:A:MET:HB3	4	0.4
(2,330)	1:145:A:ARG:HD2	1:145:A:ARG:HG3	3	0.4
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB2	3	0.4
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB2	5	0.4
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG23	2	0.4
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG11	1	0.4
(1,264)	1:26:A:ILE:HG23	1:29:A:LEU:H	2	0.4
(1,251)	1:9:A:VAL:HG22	1:75:A:ASP:HB3	3	0.4
(1,217)	1:12:A:LEU:HD22	1:16:A:GLN:HB2	1	0.4
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	7	0.4
(1,166)	1:158:A:LEU:HD12	1:44:A:VAL:HG13	6	0.4
(1,147)	1:2:A:ASP:HB2	1:79:A:VAL:HG21	8	0.4
(1,146)	1:12:A:LEU:HD21	1:82:A:VAL:HA	7	0.4
(1,113)	1:7:A:ALA:HB2	1:4:A:ILE:HG12	5	0.4
(1,89)	1:86:A:LYS:HE3	1:86:A:LYS:HD2	2	0.4
(1,89)	1:86:A:LYS:HE2	1:86:A:LYS:HD2	5	0.4
(1,89)	1:6:A:LYS:HE3	1:6:A:LYS:HD2	7	0.4
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE1	2	0.4
(1,41)	1:16:A:GLN:HA	1:16:A:GLN:HB2	7	0.4
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	3	0.4
(1,23)	1:60:A:MET:HA	1:60:A:MET:HG2	5	0.4
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG2	4	0.4
(2,1214)	1:138:A:PHE:HD1	1:139:A:LYS:HD3	6	0.39
(2,1179)	1:140:A:ARG:HA	1:141:A:PRO:HG3	2	0.39
(2,1171)	1:13:A:THR:HG23	1:16:A:GLN:HG3	2	0.39
(2,1139)	1:41:A:LEU:HD22	1:45:A:MET:HG3	2	0.39
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG23	8	0.39
(2,1087)	1:78:A:LEU:HD12	1:74:A:PHE:HE2	8	0.39
(2,1076)	1:157:A:LEU:HD12	1:27:A:PHE:HB3	5	0.39
(2,1070)	1:148:A:ILE:HD12	1:27:A:PHE:HZ	3	0.39
(2,860)	1:47:A:MET:HE2	1:47:A:MET:HG3	4	0.39
(2,832)	1:141:A:PRO:HD2	1:140:A:ARG:HB3	4	0.39
(2,819)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	4	0.39
(2,630)	1:158:A:LEU:HD12	1:158:A:LEU:HA	4	0.39
(2,597)	1:27:A:PHE:HA	1:157:A:LEU:HD21	3	0.39
(2,560)	1:37:A:SER:HB3	1:71:A:THR:HG21	6	0.39
(2,493)	1:151:A:ASP:HB3	1:152:A:ALA:HB1	3	0.39
(2,485)	1:150:A:ALA:HB2	1:20:A:PHE:HE2	7	0.39
(2,422)	1:153:A:MET:HA	1:148:A:ILE:HD11	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,262)	1:162:A:ALA:HA	1:161:A:ARG:HG3	6	0.39
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE1	5	0.39
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG11	6	0.39
(1,289)	1:146:A:VAL:HG23	1:145:A:ARG:HD2	5	0.39
(1,275)	1:13:A:THR:HB	1:16:A:GLN:HB2	1	0.39
(1,266)	1:157:A:LEU:HD12	1:27:A:PHE:HB2	1	0.39
(1,253)	1:71:A:THR:HB	1:69:A:SER:HB3	8	0.39
(1,218)	1:79:A:VAL:HB	1:6:A:LYS:HA	6	0.39
(1,215)	1:10:A:GLU:HB3	1:9:A:VAL:HG12	6	0.39
(1,193)	1:76:A:GLU:HG3	1:66:A:GLU:HB3	4	0.39
(1,137)	1:146:A:VAL:HG11	1:50:A:GLN:HG3	5	0.39
(1,122)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	8	0.39
(1,106)	1:36:A:ILE:HG23	1:27:A:PHE:HB2	7	0.39
(1,94)	1:27:A:PHE:HA	1:26:A:ILE:HD13	6	0.39
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE2	7	0.39
(1,42)	1:16:A:GLN:HA	1:15:A:GLU:HB2	5	0.39
(1,41)	1:16:A:GLN:HA	1:16:A:GLN:HB2	8	0.39
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	3	0.39
(2,1197)	1:4:A:ILE:HD11	1:5:A:TYR:HE2	1	0.38
(2,1139)	1:41:A:LEU:HD22	1:45:A:MET:HG3	3	0.38
(2,1113)	1:22:A:ALA:HB3	1:25:A:ASP:HB2	7	0.38
(2,1079)	1:164:A:GLY:HA3	1:163:A:LYS:HE2	3	0.38
(2,1064)	1:142:A:THR:HA	1:141:A:PRO:HD2	5	0.38
(2,1019)	1:72:A:VAL:HG21	1:36:A:ILE:HD12	4	0.38
(2,906)	1:12:A:LEU:HD22	1:20:A:PHE:HE1	1	0.38
(2,864)	1:81:A:MET:HE2	1:84:A:SER:HB3	2	0.38
(2,860)	1:47:A:MET:HE3	1:47:A:MET:HG3	8	0.38
(2,675)	1:157:A:LEU:HG	1:157:A:LEU:HA	1	0.38
(2,649)	1:48:A:LEU:HD13	1:44:A:VAL:HG22	3	0.38
(2,649)	1:48:A:LEU:HD13	1:44:A:VAL:HG21	6	0.38
(2,640)	1:157:A:LEU:HD13	1:153:A:MET:HG2	1	0.38
(2,562)	1:82:A:VAL:HG21	1:5:A:TYR:HA	6	0.38
(2,561)	1:37:A:SER:HB2	1:71:A:THR:HG23	7	0.38
(2,549)	1:79:A:VAL:HG11	1:5:A:TYR:HB3	6	0.38
(2,540)	1:9:A:VAL:HG13	1:79:A:VAL:HA	6	0.38
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB3	2	0.38
(2,485)	1:150:A:ALA:HB3	1:20:A:PHE:HE2	8	0.38
(2,424)	1:148:A:ILE:HD12	1:45:A:MET:HB3	6	0.38
(2,364)	1:43:A:LYS:HE3	1:29:A:LEU:HD12	5	0.38
(2,127)	1:39:A:LYS:HA	1:39:A:LYS:HG3	2	0.38
(2,127)	1:39:A:LYS:HA	1:39:A:LYS:HG3	6	0.38
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB2	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE2	2	0.38
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD21	7	0.38
(1,335)	1:12:A:LEU:H	1:12:A:LEU:HD23	4	0.38
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD22	7	0.38
(1,204)	1:154:A:MET:HG3	1:152:A:ALA:HB2	4	0.38
(1,132)	1:142:A:THR:HG23	1:140:A:ARG:HD2	7	0.38
(1,124)	1:23:A:ALA:HB2	1:158:A:LEU:HD23	7	0.38
(1,113)	1:7:A:ALA:HB1	1:4:A:ILE:HG13	8	0.38
(1,109)	1:154:A:MET:HE1	1:19:A:GLU:HA	5	0.38
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE3	1	0.38
(1,58)	1:50:A:GLN:HA	1:46:A:ARG:HG3	6	0.38
(1,41)	1:16:A:GLN:HA	1:16:A:GLN:HB2	1	0.38
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG2	5	0.38
(1,15)	1:52:A:PRO:HA	1:146:A:VAL:HG13	8	0.38
(1,7)	1:44:A:VAL:HA	1:48:A:LEU:HD21	8	0.38
(2,1408)	1:86:A:LYS:H	1:86:A:LYS:HG2	2	0.37
(2,1153)	1:12:A:LEU:HB3	1:17:A:LYS:HD2	8	0.37
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE2	4	0.37
(2,1065)	1:151:A:ASP:HB2	1:152:A:ALA:HA	1	0.37
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE1	7	0.37
(2,1014)	1:71:A:THR:HA	1:38:A:THR:HG23	6	0.37
(2,1001)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	1	0.37
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	8	0.37
(2,860)	1:47:A:MET:HE3	1:47:A:MET:HG3	7	0.37
(2,772)	1:7:A:ALA:HB3	1:11:A:GLN:HG2	3	0.37
(2,694)	1:41:A:LEU:HD23	1:60:A:MET:HB3	5	0.37
(2,618)	1:78:A:LEU:HD22	1:17:A:LYS:HB3	5	0.37
(2,617)	1:78:A:LEU:HD22	1:20:A:PHE:HB2	6	0.37
(2,507)	1:162:A:ALA:HB1	1:19:A:GLU:HG3	5	0.37
(2,493)	1:151:A:ASP:HB2	1:152:A:ALA:HB2	5	0.37
(2,487)	1:152:A:ALA:HB2	1:148:A:ILE:HA	4	0.37
(2,475)	1:45:A:MET:HE1	1:45:A:MET:HA	5	0.37
(2,445)	1:85:A:MET:HE1	1:85:A:MET:HG2	8	0.37
(2,415)	1:61:A:ILE:HD13	1:72:A:VAL:HB	6	0.37
(2,330)	1:145:A:ARG:HD2	1:145:A:ARG:HG3	5	0.37
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG22	5	0.37
(2,160)	1:22:A:ALA:HA	1:26:A:ILE:HD12	4	0.37
(2,98)	1:40:A:GLU:HA	1:43:A:LYS:HD2	6	0.37
(2,22)	1:82:A:VAL:HA	1:82:A:VAL:HG22	4	0.37
(2,13)	1:79:A:VAL:HA	1:79:A:VAL:HG13	2	0.37
(1,343)	1:59:A:GLU:H	1:58:A:GLN:HB3	5	0.37
(1,343)	1:59:A:GLU:H	1:58:A:GLN:HB3	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:160:A:ALA:HB1	1:163:A:LYS:HE3	7	0.37
(1,167)	1:78:A:LEU:HD11	1:17:A:LYS:HG3	8	0.37
(1,161)	1:39:A:LYS:HG3	1:39:A:LYS:HB3	2	0.37
(1,115)	1:156:A:ALA:HB2	1:153:A:MET:HG2	8	0.37
(1,89)	1:86:A:LYS:HE2	1:86:A:LYS:HD2	4	0.37
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG23	6	0.37
(2,1585)	1:162:A:ALA:HA	1:158:A:LEU:HD12	4	0.36
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	3	0.36
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD13	2	0.36
(2,594)	1:41:A:LEU:HD11	1:41:A:LEU:HB3	3	0.36
(2,538)	1:9:A:VAL:HG13	1:9:A:VAL:HA	2	0.36
(2,533)	1:72:A:VAL:HG12	1:73:A:ASP:HB3	7	0.36
(2,493)	1:151:A:ASP:HB2	1:152:A:ALA:HB3	2	0.36
(2,475)	1:45:A:MET:HE2	1:45:A:MET:HA	6	0.36
(2,135)	1:19:A:GLU:HA	1:158:A:LEU:HD11	3	0.36
(2,127)	1:39:A:LYS:HA	1:39:A:LYS:HG3	8	0.36
(1,280)	1:22:A:ALA:HB1	1:25:A:ASP:HB3	1	0.36
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB3	2	0.36
(1,194)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	5	0.36
(1,145)	1:158:A:LEU:HB3	1:158:A:LEU:HD22	4	0.36
(1,122)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	4	0.36
(1,113)	1:7:A:ALA:HB2	1:4:A:ILE:HG12	1	0.36
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE3	6	0.36
(1,42)	1:16:A:GLN:HA	1:19:A:GLU:HB2	3	0.36
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	6	0.36
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG23	7	0.36
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD1	3	0.36
(2,1583)	1:154:A:MET:HE2	1:20:A:PHE:HB3	4	0.35
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB3	6	0.35
(2,1230)	1:74:A:PHE:HE2	1:78:A:LEU:HD23	3	0.35
(2,1196)	1:4:A:ILE:HG22	1:5:A:TYR:HE1	4	0.35
(2,1150)	1:148:A:ILE:HD13	1:148:A:ILE:HA	5	0.35
(2,1113)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	4	0.35
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG22	5	0.35
(2,1090)	1:21:A:LYS:HB3	1:74:A:PHE:HZ	2	0.35
(2,1019)	1:72:A:VAL:HG22	1:36:A:ILE:HD13	7	0.35
(2,1002)	1:75:A:ASP:HB2	1:1:A:MET:HE2	3	0.35
(2,910)	1:41:A:LEU:HD12	1:77:A:PHE:HD2	8	0.35
(2,864)	1:81:A:MET:HE1	1:84:A:SER:HB3	5	0.35
(2,860)	1:47:A:MET:HE3	1:47:A:MET:HG3	1	0.35
(2,818)	1:43:A:LYS:HD3	1:43:A:LYS:HG3	5	0.35
(2,660)	1:140:A:ARG:HG2	1:141:A:PRO:HD2	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,618)	1:78:A:LEU:HD23	1:17:A:LYS:HB3	2	0.35
(2,618)	1:78:A:LEU:HD22	1:17:A:LYS:HB3	3	0.35
(2,548)	1:79:A:VAL:HG11	1:5:A:TYR:HD2	3	0.35
(2,547)	1:45:A:MET:HE1	1:146:A:VAL:HG11	1	0.35
(2,514)	1:31:A:ALA:HB2	1:28:A:VAL:HG22	4	0.35
(2,514)	1:31:A:ALA:HB1	1:28:A:VAL:HG22	8	0.35
(2,488)	1:152:A:ALA:HA	1:152:A:ALA:HB1	6	0.35
(2,485)	1:150:A:ALA:HB2	1:20:A:PHE:HE1	3	0.35
(2,446)	1:1:A:MET:HE2	1:1:A:MET:HA	6	0.35
(2,424)	1:148:A:ILE:HD12	1:45:A:MET:HB3	7	0.35
(2,351)	1:158:A:LEU:HB2	1:158:A:LEU:HD12	1	0.35
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	6	0.35
(2,152)	1:11:A:GLN:HA	1:11:A:GLN:HB3	6	0.35
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB3	1	0.35
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB3	5	0.35
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD22	6	0.35
(1,315)	1:20:A:PHE:HE2	1:19:A:GLU:HB3	4	0.35
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	5	0.35
(1,235)	1:28:A:VAL:HG11	1:43:A:LYS:HD2	3	0.35
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	2	0.35
(1,212)	1:90:A:LYS:HG3	1:90:A:LYS:HB3	7	0.35
(1,206)	1:85:A:MET:HA	1:85:A:MET:HG2	3	0.35
(1,194)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	6	0.35
(1,122)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	3	0.35
(1,41)	1:16:A:GLN:HA	1:16:A:GLN:HB2	4	0.35
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	5	0.35
(1,29)	1:59:A:GLU:HA	1:143:A:LEU:HG	5	0.35
(1,3)	1:79:A:VAL:HA	1:8:A:ALA:HB3	7	0.35
(2,1130)	1:50:A:GLN:HG3	1:148:A:ILE:HG13	6	0.34
(2,1113)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	2	0.34
(2,1079)	1:164:A:GLY:HA3	1:163:A:LYS:HE3	6	0.34
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG23	2	0.34
(2,1052)	1:82:A:VAL:HG12	1:5:A:TYR:HE1	7	0.34
(2,1001)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	2	0.34
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	6	0.34
(2,955)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	8	0.34
(2,882)	1:83:A:ARG:HA	1:86:A:LYS:HB3	6	0.34
(2,862)	1:47:A:MET:HE3	1:47:A:MET:HG2	5	0.34
(2,564)	1:82:A:VAL:HG21	1:9:A:VAL:HA	5	0.34
(2,482)	1:81:A:MET:HE3	1:20:A:PHE:HD2	2	0.34
(2,438)	1:1:A:MET:HE3	1:78:A:LEU:HB2	3	0.34
(2,408)	1:138:A:PHE:HB3	1:137:A:LYS:HB2	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,285)	1:54:A:PRO:HD2	1:53:A:THR:HG22	1	0.34
(2,220)	1:85:A:MET:HA	1:85:A:MET:HB3	8	0.34
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG21	1	0.34
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG22	4	0.34
(2,152)	1:11:A:GLN:HA	1:11:A:GLN:HB3	8	0.34
(1,304)	1:155:A:GLN:HG3	1:158:A:LEU:HD11	7	0.34
(1,294)	1:45:A:MET:HG2	1:41:A:LEU:HD21	7	0.34
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD23	2	0.34
(1,218)	1:79:A:VAL:HB	1:76:A:GLU:HA	2	0.34
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	4	0.34
(1,204)	1:154:A:MET:HG3	1:152:A:ALA:HB1	5	0.34
(1,194)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	2	0.34
(1,192)	1:59:A:GLU:HG2	1:143:A:LEU:HD12	5	0.34
(1,192)	1:59:A:GLU:HG2	1:143:A:LEU:HD13	6	0.34
(1,146)	1:12:A:LEU:HD23	1:82:A:VAL:HA	6	0.34
(1,127)	1:150:A:ALA:HB3	1:151:A:ASP:HB2	3	0.34
(1,115)	1:156:A:ALA:HB1	1:47:A:MET:HB2	7	0.34
(1,61)	1:51:A:ASN:HA	1:46:A:ARG:HG2	8	0.34
(1,57)	1:140:A:ARG:HA	1:141:A:PRO:HG3	2	0.34
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE3	1	0.33
(2,1293)	1:39:A:LYS:H	1:39:A:LYS:HB3	2	0.33
(2,1177)	1:89:A:SER:HA	1:139:A:LYS:HE2	3	0.33
(2,1173)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	8	0.33
(2,1151)	1:4:A:ILE:HA	1:4:A:ILE:HD11	8	0.33
(2,1103)	1:143:A:LEU:HD12	1:143:A:LEU:HA	1	0.33
(2,884)	1:163:A:LYS:HB3	1:163:A:LYS:HE3	1	0.33
(2,695)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	3	0.33
(2,649)	1:48:A:LEU:HD12	1:44:A:VAL:HG22	5	0.33
(2,634)	1:78:A:LEU:HD12	1:74:A:PHE:HZ	8	0.33
(2,515)	1:31:A:ALA:HB1	1:28:A:VAL:HG11	3	0.33
(2,514)	1:31:A:ALA:HB3	1:28:A:VAL:HG21	3	0.33
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB2	5	0.33
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD1	1	0.33
(2,152)	1:11:A:GLN:HA	1:11:A:GLN:HB3	7	0.33
(2,151)	1:11:A:GLN:HA	1:11:A:GLN:HG2	7	0.33
(2,135)	1:19:A:GLU:HA	1:158:A:LEU:HD12	2	0.33
(1,296)	1:145:A:ARG:HD2	1:146:A:VAL:HG11	8	0.33
(1,271)	1:61:A:ILE:HD11	1:58:A:GLN:HG3	1	0.33
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG12	3	0.33
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	3	0.33
(1,253)	1:71:A:THR:HB	1:69:A:SER:HB3	3	0.33
(1,221)	1:57:A:LEU:HA	1:60:A:MET:HB2	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB3	8	0.33
(1,212)	1:90:A:LYS:HG2	1:90:A:LYS:HB3	5	0.33
(1,206)	1:85:A:MET:HA	1:85:A:MET:HG2	2	0.33
(1,194)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	8	0.33
(1,161)	1:39:A:LYS:HG3	1:39:A:LYS:HB3	4	0.33
(1,139)	1:38:A:THR:HG22	1:57:A:LEU:HA	1	0.33
(1,113)	1:7:A:ALA:HB2	1:4:A:ILE:HG12	4	0.33
(1,101)	1:85:A:MET:HE3	1:84:A:SER:HB3	5	0.33
(1,98)	1:85:A:MET:HE1	1:150:A:ALA:HB2	3	0.33
(1,89)	1:6:A:LYS:HE3	1:6:A:LYS:HD2	3	0.33
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE3	8	0.33
(1,63)	1:52:A:PRO:HD3	1:45:A:MET:HG3	3	0.33
(1,53)	1:87:A:ASP:HA	1:86:A:LYS:HB3	1	0.33
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	2	0.33
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	4	0.33
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HB2	1	0.33
(2,1522)	1:35:A:SER:H	1:31:A:ALA:HB2	7	0.32
(2,1139)	1:41:A:LEU:HD22	1:45:A:MET:HG3	1	0.32
(2,1070)	1:148:A:ILE:HD11	1:27:A:PHE:HZ	1	0.32
(2,1070)	1:148:A:ILE:HD11	1:27:A:PHE:HZ	4	0.32
(2,1065)	1:151:A:ASP:HB3	1:152:A:ALA:HA	3	0.32
(2,1060)	1:141:A:PRO:HA	1:142:A:THR:HG23	6	0.32
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	4	0.32
(2,955)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	2	0.32
(2,955)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	6	0.32
(2,680)	1:157:A:LEU:HG	1:157:A:LEU:HB2	8	0.32
(2,649)	1:48:A:LEU:HD11	1:44:A:VAL:HG21	7	0.32
(2,613)	1:29:A:LEU:HD12	1:157:A:LEU:HB3	2	0.32
(2,462)	1:36:A:ILE:HG22	1:72:A:VAL:HB	8	0.32
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	8	0.32
(2,365)	1:2:A:ASP:HB2	1:79:A:VAL:HG23	7	0.32
(2,293)	1:52:A:PRO:HD2	1:46:A:ARG:HD2	8	0.32
(2,276)	1:141:A:PRO:HD3	1:140:A:ARG:HD3	3	0.32
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD2	5	0.32
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG23	5	0.32
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	5	0.32
(2,175)	1:47:A:MET:HA	1:47:A:MET:HE1	3	0.32
(2,106)	1:84:A:SER:HA	1:80:A:MET:HE1	5	0.32
(1,343)	1:59:A:GLU:H	1:58:A:GLN:HB3	7	0.32
(1,291)	1:158:A:LEU:HD12	1:155:A:GLN:HA	1	0.32
(1,280)	1:22:A:ALA:HB3	1:25:A:ASP:HB3	3	0.32
(1,271)	1:61:A:ILE:HD12	1:58:A:GLN:HG3	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:56:A:GLU:HB2	1:146:A:VAL:HG21	4	0.32
(1,212)	1:90:A:LYS:HG2	1:90:A:LYS:HB3	3	0.32
(1,194)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	4	0.32
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD12	7	0.32
(1,161)	1:39:A:LYS:HG3	1:39:A:LYS:HB3	1	0.32
(1,161)	1:90:A:LYS:HG3	1:90:A:LYS:HB3	7	0.32
(1,145)	1:23:A:ALA:HB2	1:158:A:LEU:HD23	2	0.32
(1,139)	1:38:A:THR:HG21	1:57:A:LEU:HA	3	0.32
(1,113)	1:7:A:ALA:HB3	1:4:A:ILE:HG12	6	0.32
(1,58)	1:50:A:GLN:HA	1:45:A:MET:HE2	8	0.32
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD23	5	0.32
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HD2	3	0.32
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HD2	8	0.32
(2,1589)	2:201:A:9XG:HAD	1:36:A:ILE:HD12	1	0.31
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE1	5	0.31
(2,1407)	1:16:A:GLN:H	1:16:A:GLN:HB3	7	0.31
(2,1197)	1:4:A:ILE:HD12	1:5:A:TYR:HE2	3	0.31
(2,1142)	1:45:A:MET:HE3	1:147:A:ARG:HA	5	0.31
(2,1139)	1:41:A:LEU:HD23	1:45:A:MET:HG3	8	0.31
(2,1123)	1:157:A:LEU:HD22	1:44:A:VAL:HG21	2	0.31
(2,1113)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	1	0.31
(2,1111)	1:153:A:MET:HE2	1:44:A:VAL:HG21	8	0.31
(2,1081)	1:26:A:ILE:HD13	1:25:A:ASP:HB2	8	0.31
(2,1049)	1:78:A:LEU:HD12	1:81:A:MET:HE3	6	0.31
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	5	0.31
(2,692)	1:38:A:THR:HA	1:41:A:LEU:HD23	7	0.31
(2,570)	1:158:A:LEU:HD22	1:161:A:ARG:HD3	7	0.31
(2,562)	1:82:A:VAL:HG22	1:5:A:TYR:HA	2	0.31
(2,538)	1:9:A:VAL:HG11	1:9:A:VAL:HA	5	0.31
(2,438)	1:1:A:MET:HE1	1:78:A:LEU:HB2	5	0.31
(2,438)	1:1:A:MET:HE1	1:78:A:LEU:HB2	6	0.31
(2,429)	1:61:A:ILE:HG22	1:58:A:GLN:HA	4	0.31
(2,331)	1:46:A:ARG:HA	1:46:A:ARG:HD2	5	0.31
(2,285)	1:54:A:PRO:HD2	1:53:A:THR:HG23	5	0.31
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB3	1	0.31
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB3	5	0.31
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG21	8	0.31
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD12	2	0.31
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD12	8	0.31
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	6	0.31
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	7	0.31
(2,56)	1:26:A:ILE:HA	1:26:A:ILE:HG23	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:57:A:LEU:HA	1:60:A:MET:HB2	8	0.31
(1,206)	1:85:A:MET:HA	1:85:A:MET:HG2	4	0.31
(1,194)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	3	0.31
(1,139)	1:38:A:THR:HG21	1:57:A:LEU:HA	6	0.31
(1,133)	1:83:A:ARG:HA	1:82:A:VAL:HG13	6	0.31
(1,127)	1:150:A:ALA:HB1	1:85:A:MET:HG2	8	0.31
(1,118)	1:85:A:MET:HE2	1:150:A:ALA:HB3	8	0.31
(1,94)	1:27:A:PHE:HA	1:26:A:ILE:HD13	7	0.31
(1,78)	1:41:A:LEU:HB2	1:45:A:MET:HE3	4	0.31
(1,58)	1:50:A:GLN:HA	1:46:A:ARG:HG3	2	0.31
(1,39)	1:63:A:GLU:HA	1:143:A:LEU:HD11	7	0.31
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG2	3	0.31
(1,14)	1:146:A:VAL:HA	1:45:A:MET:HE1	1	0.31
(1,6)	1:38:A:THR:HA	1:41:A:LEU:HD23	2	0.31
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE2	5	0.3
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD11	5	0.3
(2,1175)	1:39:A:LYS:HG2	1:39:A:LYS:HE2	5	0.3
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE1	5	0.3
(2,1090)	1:21:A:LYS:HB3	1:74:A:PHE:HZ	4	0.3
(2,1062)	1:145:A:ARG:HD3	1:145:A:ARG:HA	5	0.3
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	5	0.3
(2,923)	1:157:A:LEU:HD11	1:27:A:PHE:HD1	2	0.3
(2,880)	1:163:A:LYS:HA	1:163:A:LYS:HB3	7	0.3
(2,864)	1:81:A:MET:HE1	1:84:A:SER:HB3	4	0.3
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	4	0.3
(2,832)	1:141:A:PRO:HD2	1:140:A:ARG:HB3	1	0.3
(2,794)	1:148:A:ILE:HD12	1:50:A:GLN:HG3	6	0.3
(2,680)	1:157:A:LEU:HG	1:157:A:LEU:HB2	6	0.3
(2,613)	1:29:A:LEU:HD12	1:157:A:LEU:HB3	3	0.3
(2,568)	1:82:A:VAL:HG23	1:86:A:LYS:HD3	7	0.3
(2,553)	1:34:A:GLY:HA2	1:28:A:VAL:HG13	5	0.3
(2,492)	1:79:A:VAL:HA	1:8:A:ALA:HB2	8	0.3
(2,487)	1:152:A:ALA:HB1	1:148:A:ILE:HA	5	0.3
(2,485)	1:150:A:ALA:HB2	1:20:A:PHE:HE2	1	0.3
(2,475)	1:45:A:MET:HE1	1:45:A:MET:HA	7	0.3
(2,446)	1:1:A:MET:HE3	1:1:A:MET:HA	3	0.3
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	6	0.3
(2,285)	1:54:A:PRO:HD3	1:53:A:THR:HG23	3	0.3
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD2	2	0.3
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB2	2	0.3
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB1	6	0.3
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB3	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	4	0.3
(2,145)	1:12:A:LEU:HA	1:12:A:LEU:HG	6	0.3
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	1	0.3
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	8	0.3
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD22	8	0.3
(1,293)	1:36:A:ILE:HD11	1:36:A:ILE:HA	3	0.3
(1,271)	1:61:A:ILE:HD11	1:58:A:GLN:HG3	6	0.3
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	1	0.3
(1,251)	1:9:A:VAL:HG22	1:75:A:ASP:HB3	8	0.3
(1,222)	1:90:A:LYS:HB3	1:90:A:LYS:HE3	3	0.3
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB3	5	0.3
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	1	0.3
(1,194)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	7	0.3
(1,184)	1:163:A:LYS:HD3	1:163:A:LYS:HE2	1	0.3
(1,177)	1:41:A:LEU:HD23	1:61:A:ILE:HB	1	0.3
(1,177)	1:57:A:LEU:HB2	1:41:A:LEU:HD23	4	0.3
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG3	2	0.3
(1,83)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	5	0.3
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD1	1	0.3
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	6	0.3
(1,8)	1:9:A:VAL:HA	1:17:A:LYS:HG2	3	0.3
(2,1583)	1:154:A:MET:HE2	1:20:A:PHE:HB3	1	0.29
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE1	2	0.29
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE2	4	0.29
(2,1185)	1:2:A:ASP:HB2	1:5:A:TYR:HD1	6	0.29
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	4	0.29
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD1	2	0.29
(2,1074)	1:158:A:LEU:HD23	1:154:A:MET:HG2	7	0.29
(2,1069)	1:148:A:ILE:HD12	1:147:A:ARG:HD2	1	0.29
(2,1026)	1:73:A:ASP:HB2	1:24:A:PHE:HE1	6	0.29
(2,1014)	1:71:A:THR:HA	1:38:A:THR:HG21	7	0.29
(2,1008)	1:64:A:VAL:HG23	1:65:A:ASP:HA	6	0.29
(2,1001)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	5	0.29
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	3	0.29
(2,880)	1:163:A:LYS:HA	1:163:A:LYS:HB3	2	0.29
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	2	0.29
(2,605)	1:57:A:LEU:HD23	1:45:A:MET:HG2	5	0.29
(2,596)	1:157:A:LEU:HD23	1:157:A:LEU:HA	5	0.29
(2,564)	1:82:A:VAL:HG22	1:9:A:VAL:HA	3	0.29
(2,561)	1:37:A:SER:HB2	1:71:A:THR:HG21	3	0.29
(2,538)	1:9:A:VAL:HG12	1:9:A:VAL:HA	4	0.29
(2,482)	1:81:A:MET:HE2	1:20:A:PHE:HD2	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,476)	1:45:A:MET:HE3	1:57:A:LEU:HA	1	0.29
(2,473)	1:154:A:MET:HE2	1:158:A:LEU:HD23	4	0.29
(2,458)	1:148:A:ILE:HG22	1:152:A:ALA:HB2	6	0.29
(2,360)	1:2:A:ASP:HB3	1:2:A:ASP:HA	6	0.29
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	7	0.29
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD1	4	0.29
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG21	4	0.29
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG23	4	0.29
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB2	8	0.29
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB2	3	0.29
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB3	7	0.29
(2,147)	1:12:A:LEU:HA	1:17:A:LYS:HD2	8	0.29
(2,100)	1:15:A:GLU:HA	1:18:A:ASN:HB2	3	0.29
(1,291)	1:158:A:LEU:HD11	1:155:A:GLN:HA	7	0.29
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB3	7	0.29
(1,191)	1:64:A:VAL:HG12	1:63:A:GLU:HG2	1	0.29
(1,186)	1:18:A:ASN:HB3	1:21:A:LYS:HB3	2	0.29
(1,182)	1:26:A:ILE:HG12	1:157:A:LEU:HB3	4	0.29
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD11	5	0.29
(1,134)	1:9:A:VAL:HA	1:82:A:VAL:HG12	6	0.29
(1,130)	1:13:A:THR:HG22	1:16:A:GLN:HG3	8	0.29
(1,59)	1:160:A:ALA:HA	1:163:A:LYS:HD2	4	0.29
(1,31)	1:39:A:LYS:HA	1:57:A:LEU:HD12	4	0.29
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE3	3	0.28
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE1	8	0.28
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD1	8	0.28
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE1	1	0.28
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE1	5	0.28
(2,1196)	1:4:A:ILE:HG23	1:5:A:TYR:HE2	1	0.28
(2,1141)	1:57:A:LEU:HA	1:41:A:LEU:HD22	3	0.28
(2,1140)	1:41:A:LEU:HD21	1:41:A:LEU:HA	2	0.28
(2,1130)	1:50:A:GLN:HG3	1:148:A:ILE:HG13	7	0.28
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	4	0.28
(2,880)	1:163:A:LYS:HA	1:163:A:LYS:HB3	3	0.28
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	7	0.28
(2,822)	1:12:A:LEU:HB3	1:16:A:GLN:HB2	3	0.28
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	4	0.28
(2,630)	1:158:A:LEU:HD11	1:158:A:LEU:HA	3	0.28
(2,560)	1:37:A:SER:HB3	1:71:A:THR:HG22	4	0.28
(2,548)	1:79:A:VAL:HG13	1:5:A:TYR:HD1	4	0.28
(2,476)	1:45:A:MET:HE2	1:57:A:LEU:HA	7	0.28
(2,408)	1:138:A:PHE:HB3	1:137:A:LYS:HB3	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,331)	1:46:A:ARG:HA	1:46:A:ARG:HD2	3	0.28
(2,330)	1:145:A:ARG:HD3	1:145:A:ARG:HG2	4	0.28
(2,298)	1:51:A:ASN:HA	1:52:A:PRO:HD3	7	0.28
(2,285)	1:54:A:PRO:HD2	1:53:A:THR:HG22	7	0.28
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	8	0.28
(2,220)	1:85:A:MET:HA	1:85:A:MET:HB3	5	0.28
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB2	6	0.28
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG23	3	0.28
(2,145)	1:12:A:LEU:HA	1:12:A:LEU:HG	8	0.28
(2,58)	1:4:A:ILE:HA	1:7:A:ALA:HB1	3	0.28
(2,20)	1:54:A:PRO:HA	1:57:A:LEU:HD22	5	0.28
(1,331)	1:83:A:ARG:H	1:82:A:VAL:HB	8	0.28
(1,321)	1:39:A:LYS:H	1:37:A:SER:HB2	2	0.28
(1,321)	1:39:A:LYS:H	1:37:A:SER:HB2	5	0.28
(1,267)	1:159:A:GLY:HA3	1:160:A:ALA:HB1	6	0.28
(1,266)	1:157:A:LEU:HD12	1:27:A:PHE:HB2	4	0.28
(1,253)	1:71:A:THR:HB	1:69:A:SER:HB3	7	0.28
(1,206)	1:85:A:MET:HA	1:85:A:MET:HG2	1	0.28
(1,184)	1:86:A:LYS:HE2	1:86:A:LYS:HD2	5	0.28
(1,177)	1:41:A:LEU:HD23	1:61:A:ILE:HB	3	0.28
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD12	8	0.28
(1,161)	1:39:A:LYS:HG3	1:39:A:LYS:HB3	5	0.28
(1,146)	1:16:A:GLN:HA	1:12:A:LEU:HD21	8	0.28
(1,132)	1:142:A:THR:HG21	1:140:A:ARG:HD2	4	0.28
(1,128)	1:153:A:MET:HA	1:44:A:VAL:HG12	8	0.28
(1,58)	1:50:A:GLN:HA	1:45:A:MET:HE2	4	0.28
(1,53)	1:87:A:ASP:HA	1:86:A:LYS:HB3	3	0.28
(1,53)	1:2:A:ASP:HA	1:6:A:LYS:HB2	6	0.28
(1,39)	1:63:A:GLU:HA	1:143:A:LEU:HD13	8	0.28
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	8	0.28
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HB2	7	0.28
(1,8)	1:9:A:VAL:HA	1:17:A:LYS:HG2	5	0.28
(1,2)	1:38:A:THR:HB	1:41:A:LEU:HB3	8	0.28
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD13	4	0.27
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE1	3	0.27
(2,1156)	1:35:A:SER:HA	1:28:A:VAL:HG22	8	0.27
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG21	3	0.27
(2,1087)	1:78:A:LEU:HD11	1:74:A:PHE:HE1	6	0.27
(2,1019)	1:72:A:VAL:HG23	1:36:A:ILE:HD11	8	0.27
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	1	0.27
(2,864)	1:81:A:MET:HE1	1:84:A:SER:HB3	3	0.27
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,820)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	6	0.27
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	1	0.27
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	8	0.27
(2,748)	1:55:A:GLU:HB3	1:55:A:GLU:HG3	5	0.27
(2,507)	1:162:A:ALA:HB1	1:19:A:GLU:HG3	2	0.27
(2,494)	1:8:A:ALA:HB2	1:82:A:VAL:HG11	2	0.27
(2,446)	1:1:A:MET:HE1	1:1:A:MET:HA	8	0.27
(2,415)	1:61:A:ILE:HD13	1:72:A:VAL:HB	8	0.27
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB1	1	0.27
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB3	4	0.27
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB3	8	0.27
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG23	7	0.27
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	1	0.27
(2,151)	1:11:A:GLN:HA	1:11:A:GLN:HG2	6	0.27
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	2	0.27
(2,56)	1:26:A:ILE:HA	1:26:A:ILE:HG21	3	0.27
(1,321)	1:39:A:LYS:H	1:37:A:SER:HB2	3	0.27
(1,279)	1:60:A:MET:HE1	1:147:A:ARG:HD3	3	0.27
(1,184)	1:163:A:LYS:HD2	1:163:A:LYS:HE3	2	0.27
(1,184)	1:163:A:LYS:HD3	1:163:A:LYS:HE2	8	0.27
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD11	6	0.27
(1,134)	1:9:A:VAL:HA	1:82:A:VAL:HG11	8	0.27
(1,63)	1:52:A:PRO:HD3	1:45:A:MET:HG3	1	0.27
(1,42)	1:16:A:GLN:HA	1:15:A:GLU:HB3	1	0.27
(1,31)	1:39:A:LYS:HA	1:57:A:LEU:HD12	1	0.27
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	1	0.27
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG22	3	0.27
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB2	1	0.27
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG3	8	0.27
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD1	6	0.27
(1,2)	1:38:A:THR:HB	1:57:A:LEU:HG	3	0.27
(2,1407)	1:16:A:GLN:H	1:16:A:GLN:HB3	8	0.26
(2,1385)	1:17:A:LYS:H	1:16:A:GLN:HB2	6	0.26
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE1	6	0.26
(2,1197)	1:4:A:ILE:HD13	1:5:A:TYR:HE2	8	0.26
(2,1196)	1:4:A:ILE:HG21	1:5:A:TYR:HE1	2	0.26
(2,1190)	1:4:A:ILE:HD11	1:5:A:TYR:HD2	5	0.26
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	5	0.26
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE2	6	0.26
(2,1125)	1:44:A:VAL:HG11	1:47:A:MET:HG3	7	0.26
(2,1065)	1:151:A:ASP:HB3	1:152:A:ALA:HA	7	0.26
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE1	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD12	5	0.26
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	2	0.26
(2,991)	1:53:A:THR:HA	1:54:A:PRO:HB3	7	0.26
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	1	0.26
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG11	6	0.26
(2,822)	1:12:A:LEU:HB3	1:16:A:GLN:HB2	2	0.26
(2,822)	1:12:A:LEU:HB3	1:16:A:GLN:HB2	6	0.26
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	5	0.26
(2,702)	1:155:A:GLN:HA	1:155:A:GLN:HB2	3	0.26
(2,600)	1:157:A:LEU:HB2	1:157:A:LEU:HD21	5	0.26
(2,540)	1:9:A:VAL:HG11	1:79:A:VAL:HA	7	0.26
(2,513)	1:31:A:ALA:HB2	1:36:A:ILE:HG21	1	0.26
(2,458)	1:148:A:ILE:HG21	1:152:A:ALA:HB2	7	0.26
(2,444)	1:85:A:MET:HE1	1:85:A:MET:HG3	3	0.26
(2,323)	1:83:A:ARG:HD3	1:79:A:VAL:HG11	3	0.26
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	2	0.26
(2,251)	1:7:A:ALA:HA	1:7:A:ALA:HB2	3	0.26
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB3	6	0.26
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB2	7	0.26
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB3	1	0.26
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB3	2	0.26
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB1	5	0.26
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB3	7	0.26
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB3	8	0.26
(2,100)	1:15:A:GLU:HA	1:18:A:ASN:HB2	5	0.26
(1,344)	1:82:A:VAL:H	1:85:A:MET:HE1	4	0.26
(1,344)	1:82:A:VAL:H	1:82:A:VAL:HB	8	0.26
(1,296)	1:145:A:ARG:HD3	1:146:A:VAL:HG12	5	0.26
(1,293)	1:36:A:ILE:HD13	1:77:A:PHE:HA	1	0.26
(1,280)	1:22:A:ALA:HB1	1:25:A:ASP:HB3	5	0.26
(1,276)	1:142:A:THR:HA	1:143:A:LEU:HG	6	0.26
(1,270)	1:56:A:GLU:HG2	1:146:A:VAL:HG12	5	0.26
(1,267)	1:159:A:GLY:HA3	1:160:A:ALA:HB3	7	0.26
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	2	0.26
(1,211)	1:9:A:VAL:HG23	1:9:A:VAL:HB	1	0.26
(1,194)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	1	0.26
(1,167)	1:78:A:LEU:HD13	1:17:A:LYS:HG3	6	0.26
(1,130)	1:13:A:THR:HG23	1:16:A:GLN:HG3	4	0.26
(1,106)	1:36:A:ILE:HG22	1:27:A:PHE:HB2	2	0.26
(1,85)	1:17:A:LYS:HE2	1:17:A:LYS:HB2	2	0.26
(1,85)	1:17:A:LYS:HE2	1:17:A:LYS:HB2	4	0.26
(1,65)	1:52:A:PRO:HD3	1:146:A:VAL:HG11	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:50:A:GLN:HA	1:45:A:MET:HE1	7	0.26
(1,49)	1:35:A:SER:HA	1:34:A:GLY:HA2	7	0.26
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG3	6	0.26
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	4	0.26
(1,11)	1:4:A:ILE:HA	1:3:A:ASP:HB2	7	0.26
(1,10)	1:141:A:PRO:HA	1:145:A:ARG:HG3	3	0.26
(1,2)	1:38:A:THR:HB	1:41:A:LEU:HB3	6	0.26
(2,1606)	2:201:A:9XG:HAB	1:45:A:MET:HE1	8	0.25
(2,1407)	1:16:A:GLN:H	1:16:A:GLN:HB3	1	0.25
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE1	8	0.25
(2,1190)	1:4:A:ILE:HD11	1:5:A:TYR:HD2	4	0.25
(2,1171)	1:13:A:THR:HG23	1:16:A:GLN:HG3	3	0.25
(2,1150)	1:148:A:ILE:HD11	1:148:A:ILE:HA	7	0.25
(2,1129)	1:154:A:MET:HG2	1:158:A:LEU:HD11	2	0.25
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD2	3	0.25
(2,1064)	1:142:A:THR:HA	1:141:A:PRO:HD2	6	0.25
(2,1004)	1:72:A:VAL:HG21	1:65:A:ASP:HB3	8	0.25
(2,963)	1:43:A:LYS:HG2	1:40:A:GLU:HA	5	0.25
(2,954)	1:61:A:ILE:HD11	1:37:A:SER:HB2	4	0.25
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG11	1	0.25
(2,943)	1:28:A:VAL:HG23	1:40:A:GLU:HG2	6	0.25
(2,941)	1:28:A:VAL:HA	1:41:A:LEU:HD11	5	0.25
(2,748)	1:55:A:GLU:HB3	1:55:A:GLU:HG3	7	0.25
(2,566)	1:82:A:VAL:HG22	1:5:A:TYR:HB3	2	0.25
(2,552)	1:28:A:VAL:HG13	1:24:A:PHE:HD1	4	0.25
(2,509)	1:162:A:ALA:HB3	1:158:A:LEU:HD23	6	0.25
(2,453)	1:2:A:ASP:HB2	1:4:A:ILE:HG23	1	0.25
(2,433)	1:85:A:MET:HE2	1:81:A:MET:HG3	1	0.25
(2,388)	1:65:A:ASP:HB3	1:61:A:ILE:HG23	8	0.25
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB1	6	0.25
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	7	0.25
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	2	0.25
(2,189)	1:10:A:GLU:HA	1:10:A:GLU:HG3	4	0.25
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD11	6	0.25
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB3	4	0.25
(2,147)	1:12:A:LEU:HA	1:17:A:LYS:HD2	6	0.25
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	4	0.25
(2,114)	1:6:A:LYS:HA	1:1:A:MET:HG3	3	0.25
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB3	3	0.25
(1,356)	1:155:A:GLN:H	1:155:A:GLN:HA	3	0.25
(1,343)	1:59:A:GLU:H	1:59:A:GLU:HB3	3	0.25
(1,293)	1:36:A:ILE:HD12	1:77:A:PHE:HA	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:19:A:GLU:HA	1:158:A:LEU:HD11	4	0.25
(1,211)	1:9:A:VAL:HG11	1:9:A:VAL:HB	2	0.25
(1,211)	1:9:A:VAL:HG13	1:9:A:VAL:HB	4	0.25
(1,211)	1:9:A:VAL:HG12	1:9:A:VAL:HB	5	0.25
(1,184)	1:163:A:LYS:HD2	1:163:A:LYS:HE3	3	0.25
(1,184)	1:163:A:LYS:HD2	1:163:A:LYS:HE3	7	0.25
(1,161)	1:39:A:LYS:HG3	1:39:A:LYS:HB3	3	0.25
(1,113)	1:7:A:ALA:HB2	1:4:A:ILE:HG13	7	0.25
(1,106)	1:36:A:ILE:HG23	1:27:A:PHE:HB2	6	0.25
(1,100)	1:47:A:MET:HE2	1:26:A:ILE:HG23	7	0.25
(1,56)	1:8:A:ALA:HA	1:11:A:GLN:HB3	5	0.25
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD12	1	0.24
(2,1237)	1:78:A:LEU:HD23	1:20:A:PHE:HD2	6	0.24
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD2	6	0.24
(2,1199)	1:27:A:PHE:HZ	1:27:A:PHE:HE2	7	0.24
(2,1109)	1:52:A:PRO:HD2	1:45:A:MET:HE2	3	0.24
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG23	4	0.24
(2,1106)	1:5:A:TYR:HA	1:79:A:VAL:HG22	6	0.24
(2,1044)	1:78:A:LEU:HG	1:74:A:PHE:HE1	6	0.24
(2,1004)	1:72:A:VAL:HG23	1:65:A:ASP:HB3	7	0.24
(2,923)	1:157:A:LEU:HD13	1:27:A:PHE:HD1	3	0.24
(2,912)	1:82:A:VAL:HG22	1:20:A:PHE:HE1	1	0.24
(2,912)	1:82:A:VAL:HG21	1:20:A:PHE:HE1	2	0.24
(2,879)	1:86:A:LYS:HB3	1:86:A:LYS:HA	5	0.24
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	1	0.24
(2,845)	1:76:A:GLU:HB2	1:64:A:VAL:HG22	7	0.24
(2,748)	1:55:A:GLU:HB3	1:55:A:GLU:HG3	8	0.24
(2,630)	1:158:A:LEU:HD12	1:158:A:LEU:HA	2	0.24
(2,531)	1:77:A:PHE:HB3	1:72:A:VAL:HG11	6	0.24
(2,476)	1:45:A:MET:HE3	1:57:A:LEU:HA	3	0.24
(2,455)	1:148:A:ILE:HG23	1:153:A:MET:HG3	8	0.24
(2,356)	1:21:A:LYS:HE3	1:21:A:LYS:HG3	7	0.24
(2,331)	1:46:A:ARG:HA	1:46:A:ARG:HD2	2	0.24
(2,327)	1:147:A:ARG:HD2	1:147:A:ARG:HA	4	0.24
(2,323)	1:83:A:ARG:HD3	1:79:A:VAL:HG13	8	0.24
(2,293)	1:52:A:PRO:HD2	1:46:A:ARG:HD2	4	0.24
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG23	8	0.24
(2,235)	1:25:A:ASP:HA	1:28:A:VAL:HG13	3	0.24
(2,210)	1:58:A:GLN:HA	1:61:A:ILE:HD12	1	0.24
(2,189)	1:10:A:GLU:HA	1:10:A:GLU:HG3	2	0.24
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD12	5	0.24
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB3	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:60:A:MET:HA	1:143:A:LEU:HB2	5	0.24
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	5	0.24
(2,56)	1:26:A:ILE:HA	1:26:A:ILE:HG23	1	0.24
(1,356)	1:155:A:GLN:H	1:155:A:GLN:HA	6	0.24
(1,356)	1:155:A:GLN:H	1:155:A:GLN:HA	8	0.24
(1,343)	1:59:A:GLU:H	1:58:A:GLN:HB3	2	0.24
(1,321)	1:39:A:LYS:H	1:37:A:SER:HB2	1	0.24
(1,308)	1:5:A:TYR:HE2	1:86:A:LYS:HD2	8	0.24
(1,284)	1:160:A:ALA:HB1	1:163:A:LYS:HE2	8	0.24
(1,276)	1:142:A:THR:HA	1:143:A:LEU:HG	7	0.24
(1,267)	1:159:A:GLY:HA3	1:160:A:ALA:HB3	8	0.24
(1,250)	1:62:A:ASP:HB2	1:61:A:ILE:HB	1	0.24
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD22	6	0.24
(1,216)	1:59:A:GLU:HA	1:59:A:GLU:HB2	3	0.24
(1,211)	1:9:A:VAL:HG22	1:9:A:VAL:HB	3	0.24
(1,191)	1:64:A:VAL:HG11	1:63:A:GLU:HG2	2	0.24
(1,184)	1:86:A:LYS:HE2	1:86:A:LYS:HD2	4	0.24
(1,184)	1:163:A:LYS:HD3	1:163:A:LYS:HE2	6	0.24
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG2	3	0.24
(1,61)	1:51:A:ASN:HA	1:46:A:ARG:HG2	7	0.24
(1,3)	1:79:A:VAL:HA	1:8:A:ALA:HB2	8	0.24
(1,2)	1:38:A:THR:HB	1:41:A:LEU:HB3	4	0.24
(2,1591)	2:201:A:9XG:HAD	1:61:A:ILE:HD13	6	0.23
(2,1578)	1:35:A:SER:H	1:28:A:VAL:HG13	8	0.23
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD11	5	0.23
(2,1385)	1:17:A:LYS:H	1:16:A:GLN:HB2	2	0.23
(2,1209)	1:27:A:PHE:HA	1:27:A:PHE:HD2	4	0.23
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	8	0.23
(2,1124)	1:61:A:ILE:HA	1:64:A:VAL:HG21	4	0.23
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD1	1	0.23
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD1	5	0.23
(2,1072)	1:157:A:LEU:HD23	1:27:A:PHE:HB2	4	0.23
(2,1064)	1:142:A:THR:HA	1:141:A:PRO:HD2	7	0.23
(2,1032)	1:77:A:PHE:HB2	1:74:A:PHE:HD2	7	0.23
(2,1023)	1:35:A:SER:HB2	1:73:A:ASP:HB3	6	0.23
(2,1014)	1:71:A:THR:HA	1:38:A:THR:HG21	4	0.23
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE2	8	0.23
(2,851)	1:161:A:ARG:HB2	1:161:A:ARG:HD2	1	0.23
(2,770)	1:11:A:GLN:HG3	1:11:A:GLN:HB2	8	0.23
(2,748)	1:55:A:GLU:HB3	1:55:A:GLU:HG3	1	0.23
(2,727)	1:11:A:GLN:HB2	1:11:A:GLN:HG2	5	0.23
(2,630)	1:158:A:LEU:HD13	1:158:A:LEU:HA	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,549)	1:79:A:VAL:HG13	1:5:A:TYR:HB3	7	0.23
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG11	1	0.23
(2,492)	1:79:A:VAL:HA	1:8:A:ALA:HB2	3	0.23
(2,489)	1:156:A:ALA:HB1	1:156:A:ALA:HA	8	0.23
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	5	0.23
(2,366)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	4	0.23
(2,310)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	2	0.23
(2,270)	1:31:A:ALA:HA	1:32:A:GLU:HB2	4	0.23
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG21	3	0.23
(2,189)	1:10:A:GLU:HA	1:10:A:GLU:HG3	5	0.23
(2,187)	1:16:A:GLN:HA	1:12:A:LEU:HD21	3	0.23
(2,158)	1:22:A:ALA:HA	1:22:A:ALA:HB2	6	0.23
(2,125)	1:19:A:GLU:HA	1:161:A:ARG:HG2	1	0.23
(2,121)	1:6:A:LYS:HA	1:6:A:LYS:HB2	3	0.23
(2,100)	1:15:A:GLU:HA	1:18:A:ASN:HB2	2	0.23
(1,356)	1:155:A:GLN:H	1:155:A:GLN:HA	7	0.23
(1,304)	1:155:A:GLN:HG3	1:158:A:LEU:HD11	5	0.23
(1,253)	1:71:A:THR:HB	1:37:A:SER:HB2	4	0.23
(1,249)	1:75:A:ASP:HB2	1:9:A:VAL:HG22	3	0.23
(1,244)	1:155:A:GLN:HB2	1:48:A:LEU:HD23	6	0.23
(1,233)	1:28:A:VAL:HA	1:29:A:LEU:HD22	8	0.23
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	2	0.23
(1,218)	1:79:A:VAL:HB	1:76:A:GLU:HA	7	0.23
(1,186)	1:18:A:ASN:HB3	1:19:A:GLU:HB3	7	0.23
(1,169)	1:157:A:LEU:HD12	1:26:A:ILE:HB	6	0.23
(1,137)	1:146:A:VAL:HG11	1:50:A:GLN:HG3	1	0.23
(1,131)	1:72:A:VAL:HG12	1:24:A:PHE:HD1	7	0.23
(1,96)	1:148:A:ILE:HD13	1:153:A:MET:HG3	2	0.23
(1,96)	1:148:A:ILE:HD12	1:153:A:MET:HG3	3	0.23
(1,94)	1:26:A:ILE:HD13	1:159:A:GLY:HA2	2	0.23
(1,84)	1:2:A:ASP:HB3	1:79:A:VAL:HG22	1	0.23
(1,58)	1:50:A:GLN:HA	1:45:A:MET:HE1	5	0.23
(1,19)	1:27:A:PHE:HA	1:26:A:ILE:HG21	5	0.23
(2,1480)	1:48:A:LEU:H	1:48:A:LEU:HD12	3	0.22
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE3	2	0.22
(2,1391)	1:59:A:GLU:H	1:59:A:GLU:HG3	7	0.22
(2,1237)	1:78:A:LEU:HD21	1:20:A:PHE:HD1	7	0.22
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	6	0.22
(2,1176)	1:163:A:LYS:HG2	1:163:A:LYS:HA	6	0.22
(2,1174)	1:145:A:ARG:HG3	1:145:A:ARG:HA	1	0.22
(2,1061)	1:147:A:ARG:HD3	1:147:A:ARG:HA	4	0.22
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE2	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1004)	1:72:A:VAL:HG22	1:65:A:ASP:HB3	4	0.22
(2,923)	1:157:A:LEU:HD12	1:27:A:PHE:HD1	8	0.22
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	8	0.22
(2,863)	1:29:A:LEU:HB3	1:26:A:ILE:HA	3	0.22
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	6	0.22
(2,749)	1:55:A:GLU:HA	1:55:A:GLU:HG2	8	0.22
(2,748)	1:55:A:GLU:HB3	1:55:A:GLU:HG3	2	0.22
(2,748)	1:55:A:GLU:HB3	1:55:A:GLU:HG3	3	0.22
(2,630)	1:158:A:LEU:HD13	1:158:A:LEU:HA	5	0.22
(2,493)	1:151:A:ASP:HB2	1:152:A:ALA:HB3	1	0.22
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	2	0.22
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE2	8	0.22
(2,343)	1:158:A:LEU:HB3	1:158:A:LEU:HD22	1	0.22
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	4	0.22
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG22	1	0.22
(2,237)	1:86:A:LYS:HA	1:86:A:LYS:HD2	6	0.22
(2,236)	1:86:A:LYS:HA	1:86:A:LYS:HG2	7	0.22
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	7	0.22
(2,145)	1:12:A:LEU:HA	1:12:A:LEU:HG	7	0.22
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB3	8	0.22
(2,100)	1:15:A:GLU:HA	1:18:A:ASN:HB2	4	0.22
(2,63)	1:84:A:SER:HB2	1:150:A:ALA:HB1	7	0.22
(1,356)	1:155:A:GLN:H	1:155:A:GLN:HA	2	0.22
(1,308)	1:5:A:TYR:HE1	1:86:A:LYS:HD2	1	0.22
(1,308)	1:5:A:TYR:HE2	1:86:A:LYS:HD2	2	0.22
(1,276)	1:142:A:THR:HA	1:143:A:LEU:HG	1	0.22
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB3	4	0.22
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB3	6	0.22
(1,122)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	1	0.22
(1,63)	1:52:A:PRO:HD3	1:45:A:MET:HG3	4	0.22
(1,63)	1:52:A:PRO:HD3	1:45:A:MET:HG3	5	0.22
(1,61)	1:51:A:ASN:HA	1:46:A:ARG:HG2	3	0.22
(1,46)	1:85:A:MET:HA	1:150:A:ALA:HB1	1	0.22
(1,33)	1:153:A:MET:HA	1:157:A:LEU:HD21	2	0.22
(1,2)	1:38:A:THR:HB	1:57:A:LEU:HG	2	0.22
(2,1176)	1:163:A:LYS:HG2	1:163:A:LYS:HA	1	0.21
(2,1120)	1:44:A:VAL:HG21	1:47:A:MET:HB2	5	0.21
(2,1114)	1:152:A:ALA:HB2	1:149:A:SER:HA	6	0.21
(2,1062)	1:145:A:ARG:HD3	1:145:A:ARG:HA	7	0.21
(2,1062)	1:145:A:ARG:HD3	1:145:A:ARG:HA	8	0.21
(2,1061)	1:147:A:ARG:HD3	1:147:A:ARG:HA	7	0.21
(2,1058)	1:149:A:SER:HB2	1:151:A:ASP:HB2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1014)	1:71:A:THR:HA	1:38:A:THR:HG23	8	0.21
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	6	0.21
(2,832)	1:141:A:PRO:HD2	1:140:A:ARG:HB3	6	0.21
(2,806)	1:80:A:MET:HG3	1:84:A:SER:HB2	2	0.21
(2,785)	1:60:A:MET:HG3	1:41:A:LEU:HD22	3	0.21
(2,785)	1:60:A:MET:HG3	1:41:A:LEU:HD23	6	0.21
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	4	0.21
(2,695)	1:41:A:LEU:HB3	1:41:A:LEU:HD23	1	0.21
(2,617)	1:78:A:LEU:HD21	1:20:A:PHE:HB2	1	0.21
(2,613)	1:29:A:LEU:HD13	1:157:A:LEU:HB3	7	0.21
(2,605)	1:57:A:LEU:HD23	1:45:A:MET:HG2	3	0.21
(2,566)	1:82:A:VAL:HG23	1:5:A:TYR:HB3	1	0.21
(2,564)	1:82:A:VAL:HG21	1:9:A:VAL:HA	1	0.21
(2,549)	1:79:A:VAL:HG13	1:5:A:TYR:HB3	8	0.21
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG11	7	0.21
(2,525)	1:13:A:THR:HA	1:13:A:THR:HG21	3	0.21
(2,523)	1:47:A:MET:HE3	1:44:A:VAL:HG11	4	0.21
(2,523)	1:47:A:MET:HE1	1:44:A:VAL:HG12	8	0.21
(2,493)	1:151:A:ASP:HB2	1:152:A:ALA:HB3	4	0.21
(2,489)	1:156:A:ALA:HB3	1:156:A:ALA:HA	6	0.21
(2,489)	1:156:A:ALA:HB3	1:156:A:ALA:HA	7	0.21
(2,472)	1:154:A:MET:HE1	1:151:A:ASP:HB3	2	0.21
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	3	0.21
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE3	2	0.21
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB1	8	0.21
(2,293)	1:52:A:PRO:HD2	1:46:A:ARG:HD2	6	0.21
(2,197)	1:41:A:LEU:HA	1:44:A:VAL:HB	3	0.21
(2,185)	1:21:A:LYS:HA	1:78:A:LEU:HD13	3	0.21
(2,180)	1:155:A:GLN:HA	1:155:A:GLN:HG2	3	0.21
(2,107)	1:84:A:SER:HA	1:81:A:MET:HE1	3	0.21
(1,343)	1:59:A:GLU:H	1:58:A:GLN:HB3	1	0.21
(1,315)	1:20:A:PHE:HE2	1:19:A:GLU:HB3	5	0.21
(1,274)	1:74:A:PHE:HB3	1:74:A:PHE:HE2	6	0.21
(1,265)	1:148:A:ILE:HG21	1:147:A:ARG:HD3	2	0.21
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	8	0.21
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	3	0.21
(1,197)	1:155:A:GLN:HG3	1:158:A:LEU:HB2	4	0.21
(1,167)	1:78:A:LEU:HD12	1:17:A:LYS:HG3	7	0.21
(1,145)	1:23:A:ALA:HB1	1:158:A:LEU:HD21	3	0.21
(1,59)	1:160:A:ALA:HA	1:163:A:LYS:HD3	1	0.21
(1,45)	1:71:A:THR:HA	1:70:A:GLY:HA2	5	0.21
(1,30)	1:6:A:LYS:HA	1:6:A:LYS:HG2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB3	4	0.21
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG3	1	0.21
(1,2)	1:38:A:THR:HB	1:57:A:LEU:HG	7	0.21
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	7	0.2
(2,1229)	1:74:A:PHE:HE1	1:20:A:PHE:HB2	6	0.2
(2,1209)	1:27:A:PHE:HA	1:27:A:PHE:HD2	1	0.2
(2,1177)	1:89:A:SER:HA	1:139:A:LYS:HE3	4	0.2
(2,1175)	1:39:A:LYS:HG2	1:39:A:LYS:HE2	4	0.2
(2,1072)	1:157:A:LEU:HD23	1:27:A:PHE:HB2	1	0.2
(2,1004)	1:72:A:VAL:HG22	1:65:A:ASP:HB3	5	0.2
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG12	3	0.2
(2,923)	1:157:A:LEU:HD11	1:27:A:PHE:HD1	6	0.2
(2,918)	1:50:A:GLN:HG2	1:45:A:MET:HA	1	0.2
(2,794)	1:148:A:ILE:HD12	1:50:A:GLN:HG3	7	0.2
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	3	0.2
(2,774)	1:155:A:GLN:HG3	1:155:A:GLN:HB2	7	0.2
(2,660)	1:140:A:ARG:HG3	1:141:A:PRO:HD2	3	0.2
(2,617)	1:78:A:LEU:HD23	1:20:A:PHE:HB2	8	0.2
(2,586)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	3	0.2
(2,566)	1:82:A:VAL:HG21	1:5:A:TYR:HB3	3	0.2
(2,531)	1:77:A:PHE:HB3	1:72:A:VAL:HG13	4	0.2
(2,516)	1:64:A:VAL:HA	1:64:A:VAL:HG23	3	0.2
(2,514)	1:31:A:ALA:HB1	1:28:A:VAL:HG21	1	0.2
(2,461)	1:36:A:ILE:HG22	1:40:A:GLU:HB2	2	0.2
(2,415)	1:61:A:ILE:HD12	1:72:A:VAL:HB	7	0.2
(2,388)	1:65:A:ASP:HB3	1:61:A:ILE:HG23	7	0.2
(2,322)	1:83:A:ARG:HD2	1:79:A:VAL:HG12	5	0.2
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	2	0.2
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	5	0.2
(2,270)	1:31:A:ALA:HA	1:32:A:GLU:HB2	2	0.2
(2,197)	1:41:A:LEU:HA	1:44:A:VAL:HB	6	0.2
(2,197)	1:41:A:LEU:HA	1:44:A:VAL:HB	7	0.2
(2,189)	1:10:A:GLU:HA	1:10:A:GLU:HG3	1	0.2
(2,105)	1:84:A:SER:HA	1:88:A:ASP:HB2	5	0.2
(1,326)	1:87:A:ASP:H	1:86:A:LYS:HA	1	0.2
(1,326)	1:87:A:ASP:H	1:86:A:LYS:HA	3	0.2
(1,291)	1:158:A:LEU:HD11	1:155:A:GLN:HA	5	0.2
(1,290)	1:146:A:VAL:HG21	1:60:A:MET:HG3	8	0.2
(1,276)	1:142:A:THR:HA	1:143:A:LEU:HG	4	0.2
(1,274)	1:74:A:PHE:HB3	1:74:A:PHE:HE1	7	0.2
(1,274)	1:74:A:PHE:HB3	1:74:A:PHE:HE1	8	0.2
(1,253)	1:71:A:THR:HB	1:69:A:SER:HB3	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:90:A:LYS:HB3	1:90:A:LYS:HE3	5	0.2
(1,186)	1:18:A:ASN:HB3	1:21:A:LYS:HB3	8	0.2
(1,151)	1:48:A:LEU:HD21	1:48:A:LEU:HG	6	0.2
(1,146)	1:16:A:GLN:HA	1:12:A:LEU:HD21	4	0.2
(1,109)	1:154:A:MET:HE2	1:19:A:GLU:HA	1	0.2
(1,84)	1:2:A:ASP:HB3	1:79:A:VAL:HG23	5	0.2
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG3	1	0.2
(1,83)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	4	0.2
(1,56)	1:8:A:ALA:HA	1:11:A:GLN:HB3	3	0.2
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB3	2	0.2
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	8	0.2
(1,12)	1:24:A:PHE:HA	1:27:A:PHE:HD2	7	0.2
(1,6)	1:38:A:THR:HA	1:41:A:LEU:HD21	6	0.2
(2,1578)	1:35:A:SER:H	1:28:A:VAL:HG11	7	0.19
(2,1478)	1:79:A:VAL:H	1:1:A:MET:HE2	4	0.19
(2,1393)	1:10:A:GLU:H	1:10:A:GLU:HB2	8	0.19
(2,1308)	1:56:A:GLU:H	1:52:A:PRO:HA	7	0.19
(2,1293)	1:39:A:LYS:H	1:39:A:LYS:HB3	8	0.19
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD1	7	0.19
(2,1176)	1:163:A:LYS:HG2	1:163:A:LYS:HA	8	0.19
(2,1173)	1:16:A:GLN:HG2	1:12:A:LEU:HD23	7	0.19
(2,1097)	1:24:A:PHE:HA	1:74:A:PHE:HD1	4	0.19
(2,1090)	1:21:A:LYS:HB3	1:74:A:PHE:HZ	5	0.19
(2,1087)	1:78:A:LEU:HD12	1:74:A:PHE:HE1	4	0.19
(2,938)	1:28:A:VAL:HG22	1:25:A:ASP:HB3	6	0.19
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	7	0.19
(2,886)	1:163:A:LYS:HB2	1:163:A:LYS:HA	4	0.19
(2,879)	1:86:A:LYS:HB3	1:86:A:LYS:HA	2	0.19
(2,702)	1:155:A:GLN:HA	1:155:A:GLN:HB3	1	0.19
(2,697)	1:12:A:LEU:HD13	1:12:A:LEU:HA	5	0.19
(2,652)	1:48:A:LEU:HD11	1:48:A:LEU:HG	2	0.19
(2,652)	1:48:A:LEU:HD13	1:48:A:LEU:HG	4	0.19
(2,605)	1:57:A:LEU:HD22	1:45:A:MET:HG2	7	0.19
(2,581)	1:9:A:VAL:HA	1:9:A:VAL:HG22	5	0.19
(2,570)	1:158:A:LEU:HD22	1:161:A:ARG:HD2	1	0.19
(2,561)	1:37:A:SER:HB2	1:71:A:THR:HG22	8	0.19
(2,553)	1:34:A:GLY:HA2	1:28:A:VAL:HG11	1	0.19
(2,531)	1:77:A:PHE:HB3	1:72:A:VAL:HG11	8	0.19
(2,504)	1:23:A:ALA:HB3	1:77:A:PHE:HZ	4	0.19
(2,489)	1:156:A:ALA:HB2	1:156:A:ALA:HA	5	0.19
(2,476)	1:45:A:MET:HE3	1:57:A:LEU:HA	4	0.19
(2,472)	1:154:A:MET:HE3	1:151:A:ASP:HB2	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,434)	1:85:A:MET:HE2	1:12:A:LEU:HD21	3	0.19
(2,417)	1:61:A:ILE:HD12	1:41:A:LEU:HB3	1	0.19
(2,363)	1:17:A:LYS:HE3	1:17:A:LYS:HB3	6	0.19
(2,298)	1:51:A:ASN:HA	1:52:A:PRO:HD3	8	0.19
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	1	0.19
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	6	0.19
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB3	1	0.19
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB3	4	0.19
(2,127)	1:39:A:LYS:HA	1:39:A:LYS:HG3	3	0.19
(2,114)	1:6:A:LYS:HA	1:1:A:MET:HG3	4	0.19
(2,112)	1:89:A:SER:HA	1:88:A:ASP:HB3	7	0.19
(2,97)	1:40:A:GLU:HA	1:43:A:LYS:HE2	6	0.19
(1,291)	1:158:A:LEU:HD13	1:155:A:GLN:HA	8	0.19
(1,275)	1:13:A:THR:HB	1:16:A:GLN:HB2	4	0.19
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	6	0.19
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	1	0.19
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	4	0.19
(1,211)	1:9:A:VAL:HG12	1:9:A:VAL:HB	6	0.19
(1,211)	1:9:A:VAL:HG12	1:9:A:VAL:HB	8	0.19
(1,168)	1:157:A:LEU:HD12	1:27:A:PHE:HA	5	0.19
(1,165)	1:78:A:LEU:HD22	1:17:A:LYS:HG3	3	0.19
(1,148)	1:72:A:VAL:HG21	1:65:A:ASP:HB2	1	0.19
(1,124)	1:23:A:ALA:HB2	1:158:A:LEU:HD23	4	0.19
(1,122)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	2	0.19
(1,105)	1:23:A:ALA:HA	1:26:A:ILE:HG23	3	0.19
(1,101)	1:85:A:MET:HE3	1:84:A:SER:HB2	7	0.19
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG3	8	0.19
(1,44)	1:78:A:LEU:HA	1:78:A:LEU:HB2	3	0.19
(1,23)	1:60:A:MET:HA	1:60:A:MET:HG2	4	0.19
(1,22)	1:14:A:GLU:HA	1:14:A:GLU:HG3	4	0.19
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	4	0.19
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	6	0.19
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	7	0.19
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	2	0.18
(2,1393)	1:10:A:GLU:H	1:10:A:GLU:HB2	4	0.18
(2,1209)	1:27:A:PHE:HA	1:27:A:PHE:HD1	5	0.18
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD2	7	0.18
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD1	3	0.18
(2,1175)	1:39:A:LYS:HG2	1:39:A:LYS:HE2	7	0.18
(2,1174)	1:145:A:ARG:HG2	1:145:A:ARG:HA	7	0.18
(2,1150)	1:148:A:ILE:HD12	1:148:A:ILE:HA	1	0.18
(2,1117)	1:4:A:ILE:HG21	1:4:A:ILE:HG13	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1023)	1:35:A:SER:HB2	1:73:A:ASP:HB3	8	0.18
(2,949)	1:35:A:SER:HB3	1:28:A:VAL:HG13	2	0.18
(2,909)	1:78:A:LEU:HD21	1:77:A:PHE:HD1	4	0.18
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	4	0.18
(2,874)	1:86:A:LYS:HB2	1:86:A:LYS:HA	8	0.18
(2,818)	1:43:A:LYS:HD2	1:43:A:LYS:HG3	1	0.18
(2,806)	1:80:A:MET:HG3	1:84:A:SER:HB2	3	0.18
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	5	0.18
(2,751)	1:16:A:GLN:HA	1:16:A:GLN:HG3	7	0.18
(2,739)	1:56:A:GLU:HA	1:56:A:GLU:HG2	8	0.18
(2,705)	1:46:A:ARG:HA	1:46:A:ARG:HG2	4	0.18
(2,652)	1:48:A:LEU:HD12	1:48:A:LEU:HG	1	0.18
(2,652)	1:48:A:LEU:HD12	1:48:A:LEU:HG	3	0.18
(2,650)	1:158:A:LEU:HD11	1:19:A:GLU:HG3	6	0.18
(2,558)	1:57:A:LEU:HB2	1:38:A:THR:HG22	7	0.18
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG12	4	0.18
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG13	5	0.18
(2,510)	1:28:A:VAL:HA	1:31:A:ALA:HB1	7	0.18
(2,489)	1:156:A:ALA:HB3	1:156:A:ALA:HA	2	0.18
(2,476)	1:45:A:MET:HE1	1:57:A:LEU:HA	2	0.18
(2,408)	1:138:A:PHE:HB3	1:137:A:LYS:HB2	8	0.18
(2,365)	1:2:A:ASP:HB2	1:79:A:VAL:HG21	8	0.18
(2,331)	1:46:A:ARG:HA	1:46:A:ARG:HD2	7	0.18
(2,310)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	7	0.18
(2,298)	1:51:A:ASN:HA	1:52:A:PRO:HD3	4	0.18
(2,259)	1:65:A:ASP:HA	1:61:A:ILE:HG21	6	0.18
(2,258)	1:65:A:ASP:HA	1:72:A:VAL:HG21	2	0.18
(2,236)	1:86:A:LYS:HA	1:86:A:LYS:HG2	8	0.18
(2,215)	1:154:A:MET:HA	1:23:A:ALA:HB3	4	0.18
(2,161)	1:1:A:MET:HA	1:1:A:MET:HG2	1	0.18
(2,21)	1:82:A:VAL:HA	1:85:A:MET:HE3	6	0.18
(1,356)	1:57:A:LEU:H	1:57:A:LEU:HA	1	0.18
(1,344)	1:82:A:VAL:H	1:82:A:VAL:HB	7	0.18
(1,331)	1:83:A:ARG:H	1:82:A:VAL:HB	7	0.18
(1,326)	1:87:A:ASP:H	1:86:A:LYS:HA	4	0.18
(1,277)	1:62:A:ASP:HB3	1:143:A:LEU:HD12	5	0.18
(1,261)	1:82:A:VAL:HB	1:83:A:ARG:HA	7	0.18
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	5	0.18
(1,213)	1:43:A:LYS:HD3	1:27:A:PHE:HA	3	0.18
(1,211)	1:9:A:VAL:HG13	1:9:A:VAL:HB	7	0.18
(1,157)	1:29:A:LEU:HD21	1:26:A:ILE:HB	4	0.18
(1,151)	1:48:A:LEU:HD23	1:48:A:LEU:HG	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:48:A:LEU:HD22	1:48:A:LEU:HG	8	0.18
(1,146)	1:12:A:LEU:HD23	1:82:A:VAL:HA	5	0.18
(1,145)	1:158:A:LEU:HB3	1:158:A:LEU:HD22	8	0.18
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG23	3	0.18
(1,129)	1:13:A:THR:HB	1:13:A:THR:HG21	4	0.18
(1,115)	1:156:A:ALA:HB3	1:47:A:MET:HB2	6	0.18
(1,96)	1:148:A:ILE:HD11	1:45:A:MET:HG2	1	0.18
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG3	7	0.18
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HB2	2	0.18
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HB2	4	0.18
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HB2	6	0.18
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HB2	8	0.18
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD23	2	0.18
(1,37)	1:5:A:TYR:HA	1:82:A:VAL:HG11	4	0.18
(1,35)	1:12:A:LEU:HA	1:16:A:GLN:HB2	6	0.18
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	1	0.18
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	2	0.18
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	3	0.18
(1,13)	1:24:A:PHE:HA	1:24:A:PHE:HB3	5	0.18
(1,2)	1:38:A:THR:HB	1:41:A:LEU:HB3	1	0.18
(2,1432)	1:155:A:GLN:H	1:156:A:ALA:H	2	0.17
(2,1407)	1:16:A:GLN:H	1:16:A:GLN:HB3	4	0.17
(2,1393)	1:10:A:GLU:H	1:10:A:GLU:HB2	2	0.17
(2,1202)	1:27:A:PHE:HZ	1:157:A:LEU:HD11	2	0.17
(2,1178)	1:140:A:ARG:HA	1:141:A:PRO:HG2	2	0.17
(2,1175)	1:39:A:LYS:HG2	1:39:A:LYS:HE2	1	0.17
(2,1140)	1:41:A:LEU:HD22	1:41:A:LEU:HA	6	0.17
(2,1076)	1:157:A:LEU:HD13	1:27:A:PHE:HB3	3	0.17
(2,1018)	1:71:A:THR:HB	1:37:A:SER:HB3	6	0.17
(2,967)	1:44:A:VAL:HA	1:27:A:PHE:HZ	8	0.17
(2,908)	1:41:A:LEU:HD13	1:27:A:PHE:HZ	3	0.17
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	2	0.17
(2,874)	1:86:A:LYS:HB2	1:86:A:LYS:HA	7	0.17
(2,826)	1:63:A:GLU:HA	1:63:A:GLU:HB2	3	0.17
(2,822)	1:12:A:LEU:HB3	1:16:A:GLN:HB2	5	0.17
(2,652)	1:48:A:LEU:HD11	1:48:A:LEU:HG	5	0.17
(2,564)	1:82:A:VAL:HG23	1:9:A:VAL:HA	2	0.17
(2,514)	1:31:A:ALA:HB3	1:28:A:VAL:HG22	7	0.17
(2,489)	1:156:A:ALA:HB2	1:156:A:ALA:HA	1	0.17
(2,487)	1:152:A:ALA:HB2	1:148:A:ILE:HA	2	0.17
(2,462)	1:36:A:ILE:HG23	1:72:A:VAL:HB	4	0.17
(2,444)	1:85:A:MET:HE2	1:85:A:MET:HG3	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,433)	1:85:A:MET:HE1	1:81:A:MET:HG3	2	0.17
(2,408)	1:138:A:PHE:HB3	1:137:A:LYS:HB3	1	0.17
(2,270)	1:31:A:ALA:HA	1:32:A:GLU:HB2	6	0.17
(2,250)	1:7:A:ALA:HA	1:10:A:GLU:HB2	2	0.17
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB3	2	0.17
(2,243)	1:151:A:ASP:HA	1:151:A:ASP:HB3	5	0.17
(2,241)	1:3:A:ASP:HA	1:6:A:LYS:HG2	1	0.17
(2,197)	1:41:A:LEU:HA	1:44:A:VAL:HB	2	0.17
(2,180)	1:155:A:GLN:HA	1:155:A:GLN:HG2	2	0.17
(2,135)	1:19:A:GLU:HA	1:158:A:LEU:HD11	1	0.17
(2,56)	1:26:A:ILE:HA	1:26:A:ILE:HG23	4	0.17
(2,25)	1:71:A:THR:HB	1:35:A:SER:HB3	1	0.17
(1,298)	1:63:A:GLU:HB2	1:64:A:VAL:HG13	5	0.17
(1,280)	1:22:A:ALA:HB3	1:25:A:ASP:HB3	7	0.17
(1,222)	1:90:A:LYS:HB3	1:90:A:LYS:HE3	8	0.17
(1,216)	1:32:A:GLU:HA	1:32:A:GLU:HB2	1	0.17
(1,197)	1:155:A:GLN:HG3	1:158:A:LEU:HB2	1	0.17
(1,186)	1:18:A:ASN:HB3	1:21:A:LYS:HB3	6	0.17
(1,148)	1:72:A:VAL:HG22	1:65:A:ASP:HB2	6	0.17
(1,139)	1:38:A:THR:HG22	1:57:A:LEU:HA	5	0.17
(1,129)	1:13:A:THR:HB	1:13:A:THR:HG23	1	0.17
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG21	2	0.17
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG23	5	0.17
(1,129)	1:13:A:THR:HB	1:13:A:THR:HG22	6	0.17
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG22	7	0.17
(1,129)	1:53:A:THR:HB	1:53:A:THR:HG22	8	0.17
(1,85)	1:17:A:LYS:HE2	1:17:A:LYS:HB2	1	0.17
(1,62)	1:51:A:ASN:HA	1:50:A:GLN:HB2	1	0.17
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HB2	5	0.17
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HB2	7	0.17
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	3	0.16
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	5	0.16
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	8	0.16
(2,1345)	1:156:A:ALA:H	1:155:A:GLN:HB2	1	0.16
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD1	5	0.16
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE2	8	0.16
(2,1084)	1:52:A:PRO:HA	1:146:A:VAL:HG22	2	0.16
(2,1074)	1:158:A:LEU:HD21	1:154:A:MET:HG2	6	0.16
(2,1062)	1:145:A:ARG:HD3	1:145:A:ARG:HA	3	0.16
(2,1014)	1:71:A:THR:HA	1:38:A:THR:HG23	3	0.16
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	1	0.16
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	5	0.16
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	7	0.16
(2,994)	1:161:A:ARG:HB2	1:26:A:ILE:HD13	3	0.16
(2,908)	1:41:A:LEU:HD12	1:27:A:PHE:HZ	7	0.16
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	1	0.16
(2,874)	1:86:A:LYS:HB2	1:86:A:LYS:HA	1	0.16
(2,874)	1:86:A:LYS:HB2	1:86:A:LYS:HA	6	0.16
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	3	0.16
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	6	0.16
(2,826)	1:63:A:GLU:HA	1:63:A:GLU:HB2	1	0.16
(2,826)	1:63:A:GLU:HA	1:63:A:GLU:HB2	4	0.16
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	6	0.16
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	8	0.16
(2,697)	1:12:A:LEU:HD13	1:12:A:LEU:HA	3	0.16
(2,694)	1:41:A:LEU:HD21	1:60:A:MET:HB3	4	0.16
(2,652)	1:48:A:LEU:HD11	1:48:A:LEU:HG	7	0.16
(2,586)	1:9:A:VAL:HG22	1:10:A:GLU:HG3	2	0.16
(2,552)	1:28:A:VAL:HG11	1:24:A:PHE:HD2	2	0.16
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG13	3	0.16
(2,525)	1:13:A:THR:HA	1:13:A:THR:HG21	2	0.16
(2,476)	1:45:A:MET:HE2	1:57:A:LEU:HA	5	0.16
(2,475)	1:45:A:MET:HE2	1:45:A:MET:HA	8	0.16
(2,462)	1:36:A:ILE:HG23	1:72:A:VAL:HB	5	0.16
(2,415)	1:61:A:ILE:HD11	1:72:A:VAL:HB	3	0.16
(2,387)	1:33:A:ASP:HA	1:33:A:ASP:HB2	8	0.16
(2,366)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	3	0.16
(2,250)	1:7:A:ALA:HA	1:10:A:GLU:HB2	8	0.16
(2,214)	1:71:A:THR:HA	1:72:A:VAL:HG22	6	0.16
(2,199)	1:41:A:LEU:HA	1:36:A:ILE:HG12	3	0.16
(2,152)	1:11:A:GLN:HA	1:11:A:GLN:HB3	4	0.16
(2,25)	1:71:A:THR:HB	1:35:A:SER:HB3	8	0.16
(1,356)	1:57:A:LEU:H	1:57:A:LEU:HA	4	0.16
(1,331)	1:83:A:ARG:H	1:82:A:VAL:HB	6	0.16
(1,143)	1:71:A:THR:HG22	1:33:A:ASP:HB3	6	0.16
(1,107)	1:153:A:MET:HE3	1:23:A:ALA:HA	8	0.16
(1,83)	1:86:A:LYS:HE3	1:86:A:LYS:HG2	6	0.16
(1,65)	1:52:A:PRO:HD3	1:146:A:VAL:HG13	7	0.16
(1,63)	1:52:A:PRO:HD3	1:45:A:MET:HG3	2	0.16
(1,44)	1:78:A:LEU:HA	1:78:A:LEU:HG	5	0.16
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB3	3	0.16
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB2	6	0.16
(1,17)	1:15:A:GLU:HA	1:15:A:GLU:HG2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:79:A:VAL:HA	1:8:A:ALA:HB2	3	0.16
(2,1583)	1:154:A:MET:HE3	1:20:A:PHE:HB3	2	0.15
(2,1578)	1:35:A:SER:H	1:28:A:VAL:HG13	2	0.15
(2,1432)	1:155:A:GLN:H	1:156:A:ALA:H	6	0.15
(2,1432)	1:155:A:GLN:H	1:156:A:ALA:H	7	0.15
(2,1293)	1:39:A:LYS:H	1:39:A:LYS:HB3	6	0.15
(2,1265)	1:31:A:ALA:H	1:31:A:ALA:HB1	3	0.15
(2,1197)	1:4:A:ILE:HD13	1:5:A:TYR:HE1	2	0.15
(2,1055)	1:84:A:SER:HA	1:84:A:SER:HB2	5	0.15
(2,989)	1:52:A:PRO:HD3	1:39:A:LYS:HE2	6	0.15
(2,967)	1:44:A:VAL:HA	1:27:A:PHE:HZ	4	0.15
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	1	0.15
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	4	0.15
(2,826)	1:63:A:GLU:HA	1:63:A:GLU:HB2	2	0.15
(2,818)	1:43:A:LYS:HD2	1:43:A:LYS:HG3	2	0.15
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	2	0.15
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	3	0.15
(2,702)	1:155:A:GLN:HA	1:155:A:GLN:HB3	5	0.15
(2,680)	1:157:A:LEU:HG	1:157:A:LEU:HB2	5	0.15
(2,652)	1:48:A:LEU:HD12	1:48:A:LEU:HG	6	0.15
(2,649)	1:48:A:LEU:HD13	1:44:A:VAL:HG21	1	0.15
(2,623)	1:43:A:LYS:HG2	1:43:A:LYS:HD3	8	0.15
(2,603)	1:57:A:LEU:HD22	1:38:A:THR:HA	8	0.15
(2,581)	1:9:A:VAL:HA	1:9:A:VAL:HG21	4	0.15
(2,578)	1:143:A:LEU:HD21	1:59:A:GLU:HB2	2	0.15
(2,558)	1:57:A:LEU:HB2	1:38:A:THR:HG22	1	0.15
(2,550)	1:79:A:VAL:HG13	1:5:A:TYR:HB2	4	0.15
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG13	2	0.15
(2,529)	1:76:A:GLU:HA	1:72:A:VAL:HG13	8	0.15
(2,514)	1:31:A:ALA:HB1	1:28:A:VAL:HG23	6	0.15
(2,510)	1:28:A:VAL:HA	1:31:A:ALA:HB3	5	0.15
(2,489)	1:156:A:ALA:HB3	1:156:A:ALA:HA	3	0.15
(2,483)	1:81:A:MET:HE2	1:154:A:MET:HG3	8	0.15
(2,443)	1:85:A:MET:HE3	1:86:A:LYS:HE2	2	0.15
(2,429)	1:61:A:ILE:HG21	1:58:A:GLN:HA	5	0.15
(2,385)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	1	0.15
(2,351)	1:158:A:LEU:HB2	1:158:A:LEU:HD13	4	0.15
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE2	6	0.15
(2,308)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	3	0.15
(2,298)	1:51:A:ASN:HA	1:52:A:PRO:HD3	2	0.15
(2,283)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	3	0.15
(2,270)	1:31:A:ALA:HA	1:32:A:GLU:HB2	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:31:A:ALA:HA	1:32:A:GLU:HB2	7	0.15
(2,250)	1:7:A:ALA:HA	1:10:A:GLU:HB2	3	0.15
(2,250)	1:7:A:ALA:HA	1:10:A:GLU:HB2	4	0.15
(2,247)	1:158:A:LEU:HA	1:158:A:LEU:HB3	4	0.15
(2,210)	1:58:A:GLN:HA	1:61:A:ILE:HD11	4	0.15
(2,197)	1:41:A:LEU:HA	1:44:A:VAL:HB	5	0.15
(2,179)	1:63:A:GLU:HA	1:63:A:GLU:HG3	3	0.15
(2,177)	1:32:A:GLU:HA	1:32:A:GLU:HB3	2	0.15
(2,117)	1:20:A:PHE:HA	1:154:A:MET:HE3	2	0.15
(2,97)	1:40:A:GLU:HA	1:43:A:LYS:HE2	8	0.15
(2,56)	1:26:A:ILE:HA	1:26:A:ILE:HG23	5	0.15
(1,356)	1:57:A:LEU:H	1:57:A:LEU:HA	5	0.15
(1,329)	1:85:A:MET:H	1:85:A:MET:HA	2	0.15
(1,329)	1:85:A:MET:H	1:85:A:MET:HA	5	0.15
(1,326)	1:87:A:ASP:H	1:86:A:LYS:HA	2	0.15
(1,326)	1:87:A:ASP:H	1:86:A:LYS:HA	5	0.15
(1,290)	1:64:A:VAL:HG23	1:65:A:ASP:HB3	5	0.15
(1,274)	1:74:A:PHE:HB3	1:24:A:PHE:HD2	1	0.15
(1,195)	1:155:A:GLN:HG3	1:152:A:ALA:HA	4	0.15
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD12	2	0.15
(1,151)	1:48:A:LEU:HB3	1:48:A:LEU:HD22	4	0.15
(1,149)	1:12:A:LEU:HD23	1:12:A:LEU:HG	5	0.15
(1,109)	1:154:A:MET:HE2	1:19:A:GLU:HA	6	0.15
(1,58)	1:50:A:GLN:HA	1:45:A:MET:HE2	3	0.15
(1,44)	1:78:A:LEU:HA	1:78:A:LEU:HB2	2	0.15
(1,23)	1:60:A:MET:HA	1:60:A:MET:HG2	8	0.15
(1,18)	1:15:A:GLU:HA	1:15:A:GLU:HB3	7	0.15
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	1	0.14
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	4	0.14
(2,1460)	1:45:A:MET:H	1:45:A:MET:HG3	6	0.14
(2,1432)	1:155:A:GLN:H	1:156:A:ALA:H	1	0.14
(2,1432)	1:155:A:GLN:H	1:156:A:ALA:H	5	0.14
(2,1393)	1:10:A:GLU:H	1:10:A:GLU:HB2	5	0.14
(2,1393)	1:10:A:GLU:H	1:10:A:GLU:HB2	6	0.14
(2,1349)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.14
(2,1209)	1:27:A:PHE:HA	1:27:A:PHE:HD2	3	0.14
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD1	1	0.14
(2,1174)	1:145:A:ARG:HG2	1:145:A:ARG:HA	8	0.14
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD12	6	0.14
(2,1104)	1:143:A:LEU:HD13	1:63:A:GLU:HG3	4	0.14
(2,1101)	1:142:A:THR:HB	1:143:A:LEU:HG	5	0.14
(2,1090)	1:21:A:LYS:HB3	1:74:A:PHE:HZ	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1032)	1:77:A:PHE:HB2	1:74:A:PHE:HD2	8	0.14
(2,1030)	1:75:A:ASP:HA	1:74:A:PHE:HE2	2	0.14
(2,981)	1:51:A:ASN:HA	1:52:A:PRO:HG3	6	0.14
(2,967)	1:44:A:VAL:HA	1:27:A:PHE:HZ	3	0.14
(2,965)	1:43:A:LYS:HG3	1:44:A:VAL:HG21	4	0.14
(2,915)	1:15:A:GLU:HG2	1:15:A:GLU:HB3	3	0.14
(2,915)	1:15:A:GLU:HG3	1:15:A:GLU:HB2	5	0.14
(2,915)	1:15:A:GLU:HG3	1:15:A:GLU:HB2	6	0.14
(2,826)	1:63:A:GLU:HA	1:63:A:GLU:HB2	5	0.14
(2,697)	1:12:A:LEU:HD11	1:12:A:LEU:HA	2	0.14
(2,588)	1:9:A:VAL:HG21	1:9:A:VAL:HB	5	0.14
(2,477)	1:45:A:MET:HE3	1:60:A:MET:HG3	6	0.14
(2,366)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	1	0.14
(2,366)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	7	0.14
(2,359)	1:88:A:ASP:HB2	1:88:A:ASP:HA	7	0.14
(2,310)	1:34:A:GLY:HA3	1:28:A:VAL:HG23	1	0.14
(2,293)	1:52:A:PRO:HD2	1:46:A:ARG:HD2	1	0.14
(2,247)	1:158:A:LEU:HA	1:158:A:LEU:HB3	7	0.14
(2,211)	1:41:A:LEU:HA	1:44:A:VAL:HG23	6	0.14
(2,151)	1:11:A:GLN:HA	1:11:A:GLN:HG2	2	0.14
(2,117)	1:20:A:PHE:HA	1:154:A:MET:HE2	1	0.14
(2,117)	1:20:A:PHE:HA	1:154:A:MET:HE2	4	0.14
(1,293)	1:36:A:ILE:HD13	1:77:A:PHE:HA	7	0.14
(1,290)	1:146:A:VAL:HG21	1:60:A:MET:HG3	7	0.14
(1,274)	1:74:A:PHE:HB3	1:24:A:PHE:HD1	2	0.14
(1,274)	1:74:A:PHE:HB3	1:74:A:PHE:HE2	5	0.14
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	7	0.14
(1,146)	1:12:A:LEU:HD23	1:82:A:VAL:HA	1	0.14
(1,139)	1:38:A:THR:HG22	1:57:A:LEU:HA	4	0.14
(1,130)	1:13:A:THR:HG21	1:16:A:GLN:HG3	7	0.14
(1,122)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	5	0.14
(1,119)	1:150:A:ALA:HA	1:150:A:ALA:HB1	5	0.14
(1,118)	1:150:A:ALA:HB1	1:85:A:MET:HB2	4	0.14
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB1	5	0.14
(1,95)	1:26:A:ILE:HD13	1:157:A:LEU:HB3	1	0.14
(1,49)	1:35:A:SER:HA	1:34:A:GLY:HA2	5	0.14
(1,28)	1:89:A:SER:HA	1:137:A:LYS:HB2	4	0.14
(1,24)	1:46:A:ARG:HA	1:46:A:ARG:HB3	6	0.14
(2,1432)	1:155:A:GLN:H	1:156:A:ALA:H	8	0.13
(2,1391)	1:59:A:GLU:H	1:59:A:GLU:HG3	1	0.13
(2,1349)	1:12:A:LEU:H	1:12:A:LEU:HB2	6	0.13
(2,1153)	1:12:A:LEU:HB3	1:17:A:LYS:HD3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD12	1	0.13
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD12	2	0.13
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD11	8	0.13
(2,1087)	1:78:A:LEU:HD13	1:74:A:PHE:HE1	1	0.13
(2,1076)	1:157:A:LEU:HD11	1:27:A:PHE:HB3	7	0.13
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	2	0.13
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	6	0.13
(2,981)	1:51:A:ASN:HA	1:52:A:PRO:HG3	7	0.13
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	3	0.13
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	7	0.13
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	3	0.13
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	4	0.13
(2,791)	1:41:A:LEU:HD13	1:45:A:MET:HG2	4	0.13
(2,768)	1:11:A:GLN:HG3	1:8:A:ALA:HA	6	0.13
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	7	0.13
(2,751)	1:16:A:GLN:HA	1:16:A:GLN:HG3	1	0.13
(2,727)	1:11:A:GLN:HB2	1:11:A:GLN:HG2	8	0.13
(2,706)	1:55:A:GLU:HA	1:55:A:GLU:HB3	5	0.13
(2,706)	1:55:A:GLU:HA	1:55:A:GLU:HB3	7	0.13
(2,617)	1:78:A:LEU:HD21	1:20:A:PHE:HB2	4	0.13
(2,588)	1:9:A:VAL:HG23	1:9:A:VAL:HB	1	0.13
(2,588)	1:9:A:VAL:HG21	1:9:A:VAL:HB	2	0.13
(2,553)	1:34:A:GLY:HA2	1:28:A:VAL:HG13	2	0.13
(2,525)	1:13:A:THR:HA	1:13:A:THR:HG21	5	0.13
(2,429)	1:61:A:ILE:HG21	1:58:A:GLN:HA	7	0.13
(2,360)	1:2:A:ASP:HB3	1:2:A:ASP:HA	7	0.13
(2,359)	1:88:A:ASP:HB2	1:88:A:ASP:HA	3	0.13
(2,298)	1:51:A:ASN:HA	1:52:A:PRO:HD3	6	0.13
(2,264)	1:73:A:ASP:HA	1:24:A:PHE:HD2	3	0.13
(2,206)	1:58:A:GLN:HA	1:57:A:LEU:HB3	2	0.13
(2,180)	1:155:A:GLN:HA	1:155:A:GLN:HG2	8	0.13
(2,177)	1:32:A:GLU:HA	1:32:A:GLU:HB2	3	0.13
(2,131)	1:39:A:LYS:HA	1:39:A:LYS:HG2	7	0.13
(2,124)	1:19:A:GLU:HA	1:22:A:ALA:HB2	4	0.13
(2,114)	1:6:A:LYS:HA	1:1:A:MET:HG3	2	0.13
(2,82)	1:72:A:VAL:HA	1:61:A:ILE:HG22	7	0.13
(2,45)	1:35:A:SER:HB2	1:73:A:ASP:HA	5	0.13
(2,25)	1:71:A:THR:HB	1:35:A:SER:HB3	2	0.13
(1,329)	1:85:A:MET:H	1:85:A:MET:HA	4	0.13
(1,237)	1:10:A:GLU:HA	1:10:A:GLU:HG2	8	0.13
(1,223)	1:79:A:VAL:HB	1:79:A:VAL:HG22	2	0.13
(1,127)	1:150:A:ALA:HB1	1:85:A:MET:HG2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:150:A:ALA:HB1	1:85:A:MET:HG2	2	0.13
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB3	1	0.13
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB3	2	0.13
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB3	4	0.13
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB3	7	0.13
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB3	8	0.13
(1,6)	1:38:A:THR:HA	1:41:A:LEU:HD23	4	0.13
(2,1578)	1:35:A:SER:H	1:28:A:VAL:HG11	1	0.12
(2,1501)	1:11:A:GLN:H	1:11:A:GLN:HG2	3	0.12
(2,1477)	1:48:A:LEU:H	1:48:A:LEU:HG	1	0.12
(2,1477)	1:48:A:LEU:H	1:48:A:LEU:HG	2	0.12
(2,1475)	1:20:A:PHE:H	1:19:A:GLU:HB3	5	0.12
(2,1438)	1:15:A:GLU:H	1:13:A:THR:HB	6	0.12
(2,1308)	1:56:A:GLU:H	1:52:A:PRO:HA	8	0.12
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD2	3	0.12
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD1	1	0.12
(2,1153)	1:12:A:LEU:HB3	1:17:A:LYS:HD3	2	0.12
(2,1153)	1:12:A:LEU:HB3	1:17:A:LYS:HD3	5	0.12
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE2	4	0.12
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD12	5	0.12
(2,1117)	1:4:A:ILE:HG21	1:4:A:ILE:HG13	5	0.12
(2,1058)	1:149:A:SER:HB2	1:151:A:ASP:HB3	7	0.12
(2,1032)	1:77:A:PHE:HB2	1:74:A:PHE:HD2	3	0.12
(2,1023)	1:35:A:SER:HB2	1:73:A:ASP:HB3	1	0.12
(2,1023)	1:35:A:SER:HB2	1:73:A:ASP:HB3	4	0.12
(2,967)	1:44:A:VAL:HA	1:27:A:PHE:HZ	5	0.12
(2,915)	1:15:A:GLU:HG3	1:15:A:GLU:HB2	1	0.12
(2,906)	1:12:A:LEU:HD23	1:20:A:PHE:HE1	7	0.12
(2,885)	1:3:A:ASP:HB2	1:6:A:LYS:HB3	8	0.12
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	4	0.12
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	5	0.12
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	6	0.12
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	8	0.12
(2,818)	1:43:A:LYS:HD2	1:43:A:LYS:HG3	3	0.12
(2,818)	1:43:A:LYS:HD2	1:43:A:LYS:HG3	4	0.12
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	5	0.12
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	6	0.12
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	7	0.12
(2,767)	1:14:A:GLU:HG2	1:14:A:GLU:HB3	1	0.12
(2,751)	1:16:A:GLN:HA	1:16:A:GLN:HG3	4	0.12
(2,751)	1:16:A:GLN:HA	1:16:A:GLN:HG3	8	0.12
(2,702)	1:155:A:GLN:HA	1:155:A:GLN:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,701)	1:155:A:GLN:HB2	1:152:A:ALA:HA	8	0.12
(2,660)	1:140:A:ARG:HG2	1:141:A:PRO:HD2	6	0.12
(2,605)	1:57:A:LEU:HD23	1:45:A:MET:HG2	2	0.12
(2,588)	1:9:A:VAL:HG21	1:9:A:VAL:HB	4	0.12
(2,581)	1:9:A:VAL:HA	1:9:A:VAL:HG21	2	0.12
(2,578)	1:143:A:LEU:HD23	1:59:A:GLU:HB2	1	0.12
(2,562)	1:82:A:VAL:HG21	1:5:A:TYR:HA	3	0.12
(2,550)	1:79:A:VAL:HG12	1:5:A:TYR:HB2	5	0.12
(2,491)	1:9:A:VAL:HA	1:8:A:ALA:HB2	3	0.12
(2,489)	1:156:A:ALA:HB1	1:156:A:ALA:HA	4	0.12
(2,366)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	5	0.12
(2,344)	1:41:A:LEU:HB3	1:60:A:MET:HE2	1	0.12
(2,277)	1:141:A:PRO:HD3	1:141:A:PRO:HB2	5	0.12
(2,241)	1:3:A:ASP:HA	1:6:A:LYS:HG2	7	0.12
(2,231)	1:37:A:SER:HB3	1:37:A:SER:HA	4	0.12
(2,231)	1:37:A:SER:HB3	1:37:A:SER:HA	6	0.12
(2,196)	1:58:A:GLN:HA	1:58:A:GLN:HB2	7	0.12
(2,187)	1:16:A:GLN:HA	1:12:A:LEU:HD23	7	0.12
(2,177)	1:32:A:GLU:HA	1:32:A:GLU:HB3	8	0.12
(2,153)	1:11:A:GLN:HA	1:11:A:GLN:HB2	3	0.12
(2,131)	1:39:A:LYS:HA	1:39:A:LYS:HG2	4	0.12
(2,119)	1:19:A:GLU:HA	1:19:A:GLU:HB2	5	0.12
(2,117)	1:20:A:PHE:HA	1:154:A:MET:HE2	6	0.12
(2,114)	1:6:A:LYS:HA	1:1:A:MET:HG3	5	0.12
(2,21)	1:82:A:VAL:HA	1:85:A:MET:HE3	7	0.12
(1,274)	1:74:A:PHE:HB3	1:24:A:PHE:HD2	4	0.12
(1,271)	1:61:A:ILE:HD11	1:58:A:GLN:HG3	4	0.12
(1,264)	1:26:A:ILE:HG21	1:29:A:LEU:H	1	0.12
(1,251)	1:9:A:VAL:HG23	1:75:A:ASP:HB3	7	0.12
(1,228)	1:43:A:LYS:HA	1:43:A:LYS:HB2	2	0.12
(1,228)	1:43:A:LYS:HA	1:43:A:LYS:HB2	8	0.12
(1,223)	1:79:A:VAL:HB	1:79:A:VAL:HG23	6	0.12
(1,174)	1:52:A:PRO:HG3	1:57:A:LEU:HD13	3	0.12
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB3	3	0.12
(1,42)	1:16:A:GLN:HA	1:19:A:GLU:HB2	6	0.12
(1,22)	1:14:A:GLU:HA	1:14:A:GLU:HG3	2	0.12
(1,2)	1:38:A:THR:HB	1:41:A:LEU:HB3	5	0.12
(2,1599)	2:201:A:9XG:HAL	1:45:A:MET:HE1	2	0.11
(2,1461)	1:50:A:GLN:H	1:50:A:GLN:HG2	7	0.11
(2,1439)	1:55:A:GLU:H	1:53:A:THR:HB	8	0.11
(2,1438)	1:15:A:GLU:H	1:13:A:THR:HB	3	0.11
(2,1393)	1:10:A:GLU:H	1:10:A:GLU:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1308)	1:56:A:GLU:H	1:52:A:PRO:HA	6	0.11
(2,1229)	1:74:A:PHE:HE2	1:20:A:PHE:HB2	7	0.11
(2,1196)	1:4:A:ILE:HG21	1:5:A:TYR:HE1	6	0.11
(2,1182)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	2	0.11
(2,1090)	1:21:A:LYS:HB3	1:74:A:PHE:HZ	1	0.11
(2,1087)	1:78:A:LEU:HD11	1:74:A:PHE:HE2	5	0.11
(2,1058)	1:149:A:SER:HB2	1:151:A:ASP:HB3	3	0.11
(2,1047)	1:79:A:VAL:HG13	1:5:A:TYR:HE2	7	0.11
(2,967)	1:44:A:VAL:HA	1:27:A:PHE:HZ	6	0.11
(2,915)	1:15:A:GLU:HG3	1:15:A:GLU:HB2	7	0.11
(2,895)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	8	0.11
(2,872)	1:50:A:GLN:HA	1:50:A:GLN:HG2	5	0.11
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	1	0.11
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	2	0.11
(2,865)	1:57:A:LEU:HB2	1:57:A:LEU:HA	3	0.11
(2,806)	1:80:A:MET:HG3	1:84:A:SER:HB2	5	0.11
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	1	0.11
(2,706)	1:55:A:GLU:HA	1:55:A:GLU:HB3	4	0.11
(2,706)	1:55:A:GLU:HA	1:55:A:GLU:HB3	8	0.11
(2,705)	1:46:A:ARG:HA	1:46:A:ARG:HG2	8	0.11
(2,697)	1:12:A:LEU:HD13	1:12:A:LEU:HA	1	0.11
(2,594)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	7	0.11
(2,588)	1:9:A:VAL:HG22	1:9:A:VAL:HB	3	0.11
(2,588)	1:9:A:VAL:HG21	1:9:A:VAL:HB	6	0.11
(2,586)	1:9:A:VAL:HG21	1:10:A:GLU:HG3	1	0.11
(2,558)	1:57:A:LEU:HB2	1:38:A:THR:HG21	3	0.11
(2,513)	1:31:A:ALA:HB3	1:36:A:ILE:HG22	4	0.11
(2,493)	1:151:A:ASP:HB2	1:152:A:ALA:HB2	8	0.11
(2,462)	1:36:A:ILE:HG22	1:72:A:VAL:HB	1	0.11
(2,366)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	8	0.11
(2,359)	1:88:A:ASP:HB2	1:88:A:ASP:HA	8	0.11
(2,277)	1:141:A:PRO:HD3	1:141:A:PRO:HB2	8	0.11
(2,263)	1:162:A:ALA:HA	1:162:A:ALA:HB2	4	0.11
(2,250)	1:7:A:ALA:HA	1:10:A:GLU:HB2	5	0.11
(2,237)	1:86:A:LYS:HA	1:86:A:LYS:HD2	5	0.11
(2,187)	1:16:A:GLN:HA	1:12:A:LEU:HD23	2	0.11
(2,180)	1:155:A:GLN:HA	1:155:A:GLN:HG2	6	0.11
(2,131)	1:39:A:LYS:HA	1:39:A:LYS:HG2	5	0.11
(1,338)	1:86:A:LYS:H	1:86:A:LYS:HA	6	0.11
(1,228)	1:43:A:LYS:HA	1:43:A:LYS:HB2	1	0.11
(1,228)	1:43:A:LYS:HA	1:43:A:LYS:HB2	3	0.11
(1,228)	1:43:A:LYS:HA	1:43:A:LYS:HB2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:43:A:LYS:HA	1:43:A:LYS:HB2	6	0.11
(1,223)	1:79:A:VAL:HB	1:79:A:VAL:HG21	5	0.11
(1,134)	1:9:A:VAL:HA	1:82:A:VAL:HG11	4	0.11
(1,128)	1:153:A:MET:HA	1:44:A:VAL:HG12	2	0.11
(1,119)	1:150:A:ALA:HA	1:150:A:ALA:HB3	2	0.11
(1,119)	1:150:A:ALA:HA	1:150:A:ALA:HB2	4	0.11
(1,111)	1:22:A:ALA:HA	1:22:A:ALA:HB2	6	0.11
(1,98)	1:85:A:MET:HE2	1:150:A:ALA:HB3	8	0.11
(1,97)	1:148:A:ILE:HD12	1:146:A:VAL:HB	7	0.11
(1,71)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	6	0.11
(1,65)	1:52:A:PRO:HD3	1:146:A:VAL:HG11	3	0.11
(1,60)	1:31:A:ALA:HA	1:40:A:GLU:HG2	7	0.11
(1,59)	1:160:A:ALA:HA	1:163:A:LYS:HD2	2	0.11
(1,49)	1:71:A:THR:HB	1:35:A:SER:HA	8	0.11
(1,48)	1:29:A:LEU:HA	1:29:A:LEU:HG	3	0.11
(1,41)	1:16:A:GLN:HA	1:16:A:GLN:HB2	3	0.11
(1,22)	1:14:A:GLU:HA	1:14:A:GLU:HG3	5	0.11
(2,1477)	1:48:A:LEU:H	1:48:A:LEU:HG	5	0.1
(2,1385)	1:17:A:LYS:H	1:16:A:GLN:HB2	5	0.1
(2,1265)	1:31:A:ALA:H	1:31:A:ALA:HB1	2	0.1
(2,1207)	1:74:A:PHE:HB2	1:74:A:PHE:HD1	4	0.1
(2,1143)	1:50:A:GLN:HA	1:45:A:MET:HE1	7	0.1
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD13	3	0.1
(2,1127)	1:78:A:LEU:HG	1:78:A:LEU:HD13	4	0.1
(2,1107)	1:60:A:MET:HE2	1:41:A:LEU:HD22	7	0.1
(2,1055)	1:84:A:SER:HA	1:84:A:SER:HB2	6	0.1
(2,995)	1:16:A:GLN:HG2	1:16:A:GLN:HB2	3	0.1
(2,914)	1:16:A:GLN:HA	1:16:A:GLN:HB3	2	0.1
(2,885)	1:3:A:ASP:HB2	1:6:A:LYS:HB3	7	0.1
(2,882)	1:83:A:ARG:HA	1:86:A:LYS:HB3	4	0.1
(2,874)	1:86:A:LYS:HB2	1:86:A:LYS:HA	3	0.1
(2,856)	1:32:A:GLU:HB2	1:33:A:ASP:HB2	8	0.1
(2,800)	1:85:A:MET:HG2	1:85:A:MET:HB2	2	0.1
(2,768)	1:11:A:GLN:HG3	1:8:A:ALA:HA	3	0.1
(2,761)	1:19:A:GLU:HG2	1:19:A:GLU:HB2	6	0.1
(2,761)	1:19:A:GLU:HG2	1:19:A:GLU:HB2	7	0.1
(2,706)	1:55:A:GLU:HA	1:55:A:GLU:HB3	3	0.1
(2,702)	1:155:A:GLN:HA	1:155:A:GLN:HB3	6	0.1
(2,695)	1:41:A:LEU:HB3	1:41:A:LEU:HD21	8	0.1
(2,531)	1:77:A:PHE:HB3	1:72:A:VAL:HG11	2	0.1
(2,358)	1:137:A:LYS:HE2	1:137:A:LYS:HG2	5	0.1
(2,252)	1:50:A:GLN:HA	1:50:A:GLN:HB3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,249)	1:48:A:LEU:HA	1:156:A:ALA:HB3	8	0.1
(2,192)	1:66:A:GLU:HA	1:66:A:GLU:HG2	3	0.1
(2,152)	1:11:A:GLN:HA	1:11:A:GLN:HB3	1	0.1
(2,115)	1:19:A:GLU:HA	1:19:A:GLU:HG2	8	0.1
(2,25)	1:71:A:THR:HB	1:35:A:SER:HB3	5	0.1
(1,226)	1:48:A:LEU:HB3	1:48:A:LEU:HA	6	0.1
(1,169)	1:157:A:LEU:HD12	1:26:A:ILE:HB	5	0.1
(1,119)	1:150:A:ALA:HA	1:150:A:ALA:HB1	3	0.1
(1,40)	1:155:A:GLN:HA	1:158:A:LEU:HD21	3	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found