



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 11:42 AM UTC

PDB ID : 5VLN / pdb_00005vln
BMRB ID : 30288
Title : NMR structure of the N-domain of troponin C bound to switch region of troponin I
Authors : Cai, F.; Hwang, P.M.; Sykes, B.D.
Deposited on : 2017-04-25

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

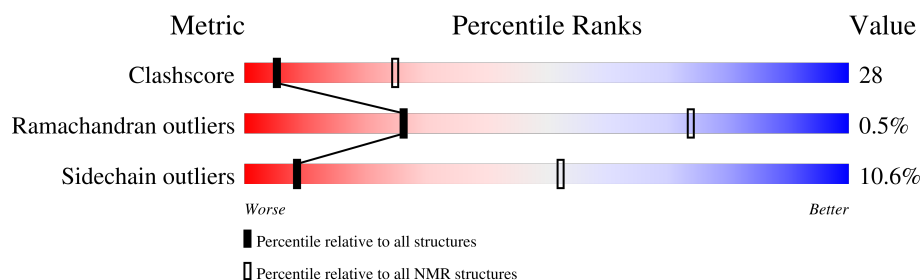
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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 3 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:3-A:84, A:148-A:159 (94)	0.53	3

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1875 atoms, of which 936 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Troponin C, slow skeletal and cardiac muscles,Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms						Trace
1	A	120	Total	C	H	N	O	S	0
			1875	582	936	160	188	9	

There are 4 discrepancies between the modelled and reference sequences:

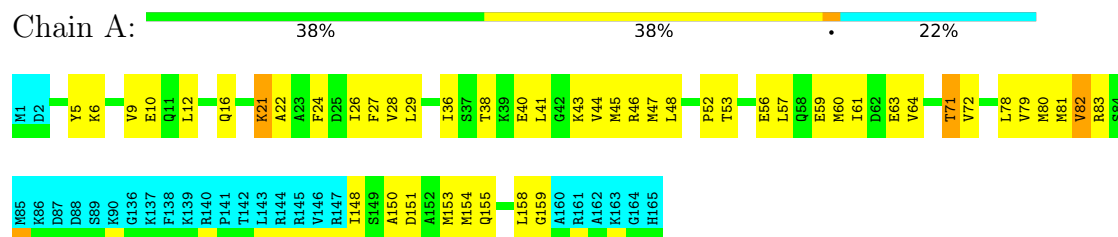
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	CYS	engineered mutation	UNP P63316
A	84	SER	CYS	engineered mutation	UNP P63316
A	164	GLY	-	expression tag	UNP P19429
A	165	HIS	-	expression tag	UNP P19429

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, slow skeletal and cardiac muscles, Troponin I, cardiac muscle

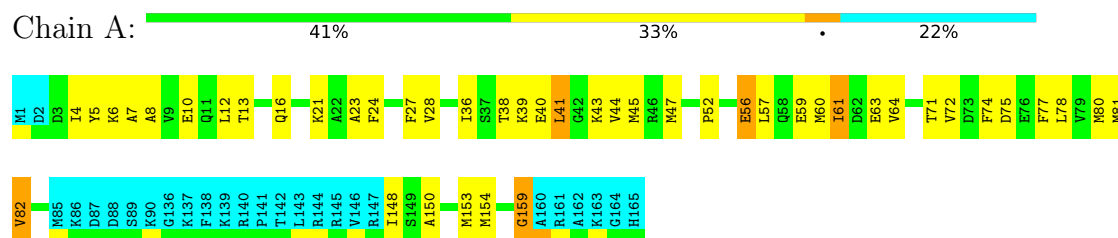


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

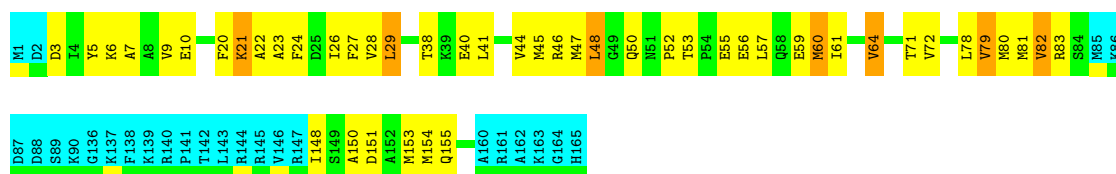
- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle



4.2.2 Score per residue for model 2

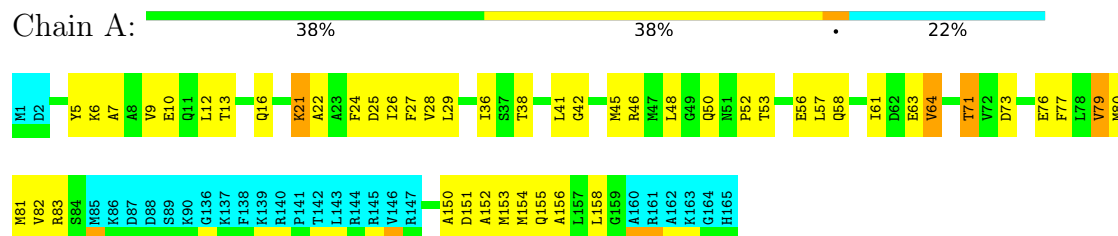
- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle





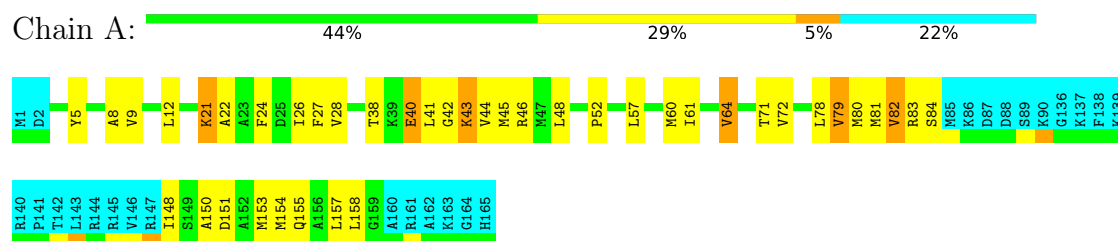
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle



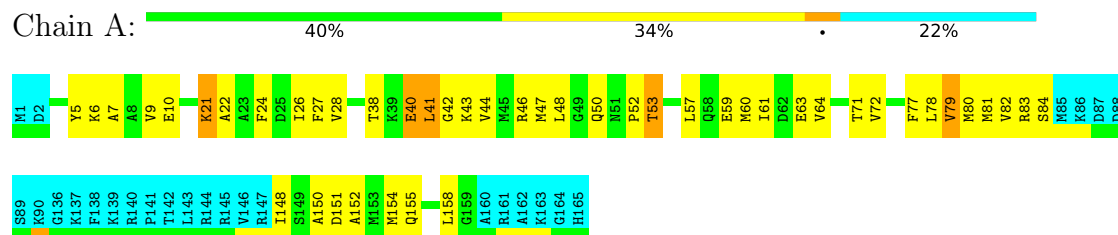
4.2.4 Score per residue for model 4

- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle



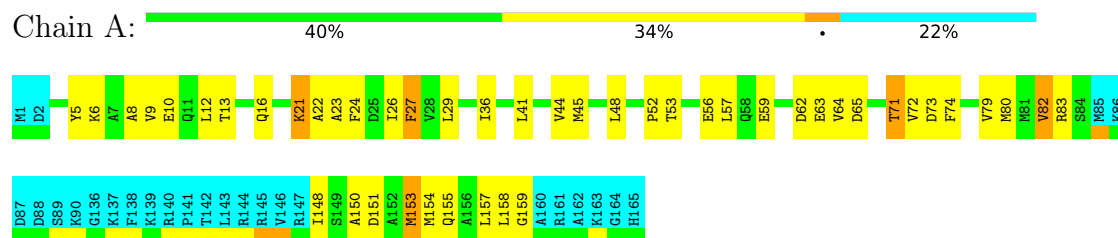
4.2.5 Score per residue for model 5

- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle



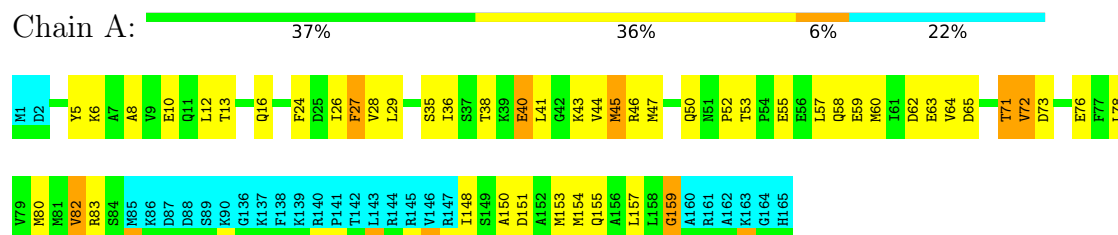
4.2.6 Score per residue for model 6

- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle



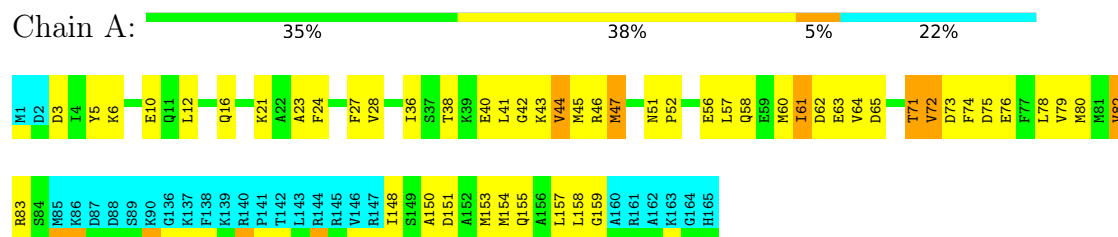
4.2.7 Score per residue for model 7

- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle



4.2.8 Score per residue for model 8

- Molecule 1: Troponin C, slow skeletal and cardiac muscles, Troponin I, cardiac muscle



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	refinement	
ARIA2	structure calculation	

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	1411
Number of shifts mapped to atoms	1411
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

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	724	702	702	40±5
All	All	5792	5616	5616	322

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PRO:HG2	1:A:57:LEU:HD21	0.93	1.41	6	4
1:A:64:VAL:HG11	1:A:80:MET:HB2	0.83	1.47	3	7
1:A:64:VAL:HG12	1:A:79:VAL:HG12	0.79	1.54	2	3
1:A:42:GLY:O	1:A:46:ARG:HG3	0.79	1.76	3	4
1:A:41:LEU:HG	1:A:57:LEU:HD22	0.78	1.56	8	3
1:A:153:MET:HE2	1:A:157:LEU:HG	0.73	1.58	7	2
1:A:41:LEU:HD12	1:A:57:LEU:HD22	0.73	1.60	5	1
1:A:153:MET:HE3	1:A:153:MET:HA	0.72	1.58	8	2
1:A:79:VAL:O	1:A:83:ARG:HG3	0.70	1.87	5	6
1:A:64:VAL:HG23	1:A:72:VAL:HG21	0.69	1.63	7	4
1:A:150:ALA:O	1:A:154:MET:HG2	0.69	1.87	8	8
1:A:41:LEU:HD12	1:A:57:LEU:CD2	0.69	2.18	5	1
1:A:64:VAL:CG1	1:A:80:MET:HB2	0.68	2.18	3	2
1:A:64:VAL:HG21	1:A:80:MET:HB2	0.68	1.63	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:HG11	1:A:80:MET:CB	0.67	2.18	2	6
1:A:41:LEU:HD21	1:A:60:MET:SD	0.67	2.30	1	1
1:A:22:ALA:O	1:A:26:ILE:HG13	0.66	1.91	4	5
1:A:5:TYR:HB2	1:A:79:VAL:HG22	0.65	1.65	2	4
1:A:153:MET:O	1:A:153:MET:HE2	0.65	1.91	6	1
1:A:64:VAL:HG11	1:A:80:MET:CA	0.64	2.22	5	6
1:A:44:VAL:HG13	1:A:153:MET:HE1	0.64	1.70	7	2
1:A:6:LYS:O	1:A:10:GLU:HG3	0.64	1.93	2	4
1:A:44:VAL:O	1:A:48:LEU:HB2	0.64	1.92	2	2
1:A:5:TYR:CB	1:A:79:VAL:HG22	0.62	2.24	2	4
1:A:84:SER:HB3	1:A:148:ILE:O	0.62	1.94	5	2
1:A:60:MET:SD	1:A:148:ILE:HG13	0.62	2.35	1	1
1:A:36:ILE:O	1:A:71:THR:HA	0.61	1.95	1	5
1:A:7:ALA:HA	1:A:10:GLU:CG	0.61	2.24	5	4
1:A:57:LEU:O	1:A:61:ILE:HG12	0.61	1.96	2	4
1:A:21:LYS:O	1:A:24:PHE:HB3	0.60	1.96	3	6
1:A:24:PHE:O	1:A:28:VAL:HG22	0.60	1.96	1	7
1:A:46:ARG:HA	1:A:50:GLN:O	0.60	1.97	7	4
1:A:153:MET:HE2	1:A:157:LEU:CG	0.59	2.27	7	2
1:A:6:LYS:O	1:A:9:VAL:HB	0.59	1.98	2	3
1:A:40:GLU:O	1:A:43:LYS:HB3	0.59	1.98	4	4
1:A:7:ALA:HA	1:A:10:GLU:HG3	0.58	1.74	3	4
1:A:27:PHE:CE2	1:A:41:LEU:HA	0.58	2.34	2	4
1:A:12:LEU:HA	1:A:16:GLN:OE1	0.58	1.98	8	2
1:A:60:MET:O	1:A:63:GLU:HB2	0.58	1.98	7	2
1:A:5:TYR:CE2	1:A:83:ARG:HG2	0.57	2.35	7	3
1:A:53:THR:OG1	1:A:56:GLU:HG3	0.57	1.99	6	1
1:A:151:ASP:O	1:A:155:GLN:HG3	0.56	1.99	7	2
1:A:13:THR:HG23	1:A:16:GLN:HE21	0.56	1.59	7	1
1:A:44:VAL:O	1:A:47:MET:HB2	0.56	2.01	8	1
1:A:64:VAL:CG1	1:A:79:VAL:HG12	0.56	2.30	2	4
1:A:27:PHE:CD2	1:A:157:LEU:HD11	0.56	2.36	7	2
1:A:23:ALA:O	1:A:27:PHE:HB2	0.56	2.01	6	3
1:A:72:VAL:HG22	1:A:76:GLU:HB3	0.55	1.78	7	1
1:A:5:TYR:HB3	1:A:82:VAL:CG1	0.55	2.32	1	1
1:A:59:GLU:O	1:A:63:GLU:HG2	0.55	2.01	5	1
1:A:45:MET:CB	1:A:52:PRO:HG3	0.54	2.32	1	1
1:A:52:PRO:CG	1:A:57:LEU:HD21	0.54	2.33	3	1
1:A:50:GLN:HB3	1:A:52:PRO:HD3	0.54	1.79	3	1
1:A:45:MET:HA	1:A:45:MET:HE2	0.54	1.80	4	2
1:A:64:VAL:HG12	1:A:79:VAL:CG1	0.54	2.31	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD11	1:A:148:ILE:HD11	0.53	1.78	6	1
1:A:57:LEU:O	1:A:61:ILE:HG13	0.53	2.03	8	1
1:A:154:MET:HE2	1:A:154:MET:HA	0.53	1.80	1	4
1:A:80:MET:HE3	1:A:148:ILE:HD12	0.53	1.79	1	1
1:A:6:LYS:O	1:A:10:GLU:HG2	0.53	2.04	6	3
1:A:53:THR:O	1:A:57:LEU:HG	0.53	2.04	7	3
1:A:27:PHE:HE1	1:A:153:MET:SD	0.52	2.27	1	1
1:A:64:VAL:HG21	1:A:80:MET:SD	0.52	2.44	1	3
1:A:45:MET:HE3	1:A:148:ILE:HD13	0.52	1.81	7	1
1:A:153:MET:HE2	1:A:157:LEU:CD1	0.52	2.34	7	2
1:A:21:LYS:O	1:A:21:LYS:HD2	0.52	2.05	3	4
1:A:43:LYS:O	1:A:47:MET:HG3	0.51	2.05	1	2
1:A:27:PHE:CD1	1:A:44:VAL:HG21	0.51	2.41	7	3
1:A:154:MET:O	1:A:158:LEU:HB2	0.50	2.07	6	1
1:A:36:ILE:HD12	1:A:72:VAL:HG12	0.49	1.83	1	3
1:A:26:ILE:O	1:A:29:LEU:HB2	0.49	2.07	2	1
1:A:153:MET:CE	1:A:157:LEU:HG	0.49	2.34	7	1
1:A:27:PHE:CD2	1:A:44:VAL:HG21	0.49	2.42	6	1
1:A:64:VAL:HG23	1:A:72:VAL:CG2	0.49	2.38	8	4
1:A:26:ILE:HA	1:A:29:LEU:HG	0.49	1.85	6	2
1:A:38:THR:O	1:A:57:LEU:HD13	0.49	2.07	2	6
1:A:151:ASP:HA	1:A:154:MET:HB2	0.48	1.84	2	4
1:A:64:VAL:HG13	1:A:79:VAL:HG12	0.48	1.85	3	1
1:A:77:PHE:CE2	1:A:81:MET:HE3	0.48	2.43	1	1
1:A:27:PHE:CZ	1:A:44:VAL:HG11	0.48	2.43	7	2
1:A:62:ASP:HA	1:A:65:ASP:HB3	0.48	1.85	6	3
1:A:21:LYS:HD2	1:A:21:LYS:C	0.48	2.33	2	4
1:A:13:THR:OG1	1:A:16:GLN:HG3	0.48	2.07	1	2
1:A:81:MET:HE1	1:A:148:ILE:HG21	0.48	1.85	1	1
1:A:155:GLN:HG3	1:A:156:ALA:N	0.48	2.24	3	1
1:A:5:TYR:CZ	1:A:83:ARG:HG2	0.48	2.43	8	5
1:A:26:ILE:C	1:A:157:LEU:HD12	0.48	2.33	6	1
1:A:27:PHE:CD2	1:A:36:ILE:HD13	0.48	2.43	6	1
1:A:77:PHE:O	1:A:81:MET:HG2	0.47	2.08	5	2
1:A:21:LYS:HD3	1:A:74:PHE:CG	0.47	2.45	8	1
1:A:36:ILE:HG21	1:A:41:LEU:HD12	0.47	1.86	1	1
1:A:59:GLU:O	1:A:63:GLU:HG3	0.46	2.11	1	1
1:A:43:LYS:CG	1:A:44:VAL:N	0.46	2.79	1	1
1:A:5:TYR:O	1:A:82:VAL:HG11	0.46	2.10	1	1
1:A:5:TYR:HA	1:A:82:VAL:HG21	0.46	1.87	8	3
1:A:5:TYR:HB3	1:A:82:VAL:HG21	0.46	1.88	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:MET:HE1	1:A:157:LEU:HD23	0.46	1.87	7	1
1:A:24:PHE:CE2	1:A:73:ASP:HA	0.46	2.46	3	2
1:A:41:LEU:O	1:A:45:MET:HG2	0.45	2.11	3	1
1:A:23:ALA:HB2	1:A:154:MET:HE1	0.45	1.88	1	1
1:A:8:ALA:O	1:A:12:LEU:HG	0.45	2.11	7	4
1:A:26:ILE:HB	1:A:157:LEU:HD22	0.45	1.87	7	1
1:A:153:MET:CE	1:A:157:LEU:HD23	0.45	2.41	6	1
1:A:60:MET:CE	1:A:148:ILE:HB	0.45	2.42	8	1
1:A:45:MET:HE2	1:A:148:ILE:CD1	0.45	2.42	8	1
1:A:44:VAL:HA	1:A:47:MET:SD	0.45	2.52	7	1
1:A:36:ILE:HD12	1:A:72:VAL:CG1	0.44	2.42	1	1
1:A:60:MET:SD	1:A:148:ILE:HG12	0.44	2.52	7	1
1:A:60:MET:HE3	1:A:148:ILE:HB	0.44	1.89	2	1
1:A:77:PHE:O	1:A:80:MET:HB3	0.44	2.13	5	1
1:A:44:VAL:HG13	1:A:157:LEU:HD21	0.44	1.87	6	1
1:A:61:ILE:HG23	1:A:72:VAL:HG23	0.44	1.89	1	1
1:A:8:ALA:C	1:A:82:VAL:HG21	0.44	2.37	1	1
1:A:151:ASP:HA	1:A:154:MET:CG	0.44	2.43	4	4
1:A:44:VAL:O	1:A:48:LEU:N	0.44	2.51	5	1
1:A:38:THR:HG21	1:A:58:GLN:HG3	0.44	1.90	8	1
1:A:5:TYR:HB3	1:A:82:VAL:CG2	0.43	2.43	4	1
1:A:9:VAL:HG22	1:A:78:LEU:HG	0.43	1.89	5	1
1:A:20:PHE:CD1	1:A:81:MET:HG3	0.43	2.49	2	1
1:A:23:ALA:HB1	1:A:153:MET:HE1	0.43	1.90	2	1
1:A:36:ILE:HD11	1:A:77:PHE:CD2	0.43	2.48	3	1
1:A:81:MET:HA	1:A:81:MET:HE2	0.43	1.89	3	1
1:A:151:ASP:O	1:A:155:GLN:HG2	0.43	2.14	6	3
1:A:55:GLU:O	1:A:59:GLU:HG2	0.42	2.14	7	1
1:A:41:LEU:HG	1:A:57:LEU:CD2	0.42	2.38	8	1
1:A:51:ASN:N	1:A:52:PRO:HD3	0.42	2.28	8	1
1:A:64:VAL:HB	1:A:76:GLU:O	0.42	2.15	8	1
1:A:80:MET:HE3	1:A:81:MET:HE3	0.42	1.90	3	1
1:A:45:MET:HA	1:A:48:LEU:HB2	0.42	1.91	6	1
1:A:151:ASP:O	1:A:154:MET:HB2	0.42	2.15	3	1
1:A:3:ASP:HA	1:A:6:LYS:CB	0.42	2.45	2	1
1:A:5:TYR:O	1:A:9:VAL:HG23	0.42	2.15	6	1
1:A:25:ASP:O	1:A:29:LEU:HG	0.42	2.14	3	1
1:A:48:LEU:HB3	1:A:50:GLN:OE1	0.42	2.14	5	1
1:A:5:TYR:CE1	1:A:83:ARG:HG2	0.42	2.48	3	1
1:A:7:ALA:HA	1:A:10:GLU:CD	0.42	2.40	5	1
1:A:63:GLU:OE1	1:A:83:ARG:HD3	0.41	2.15	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:CZ	1:A:44:VAL:HB	0.41	2.50	5	1
1:A:26:ILE:CD1	1:A:158:LEU:HA	0.41	2.45	6	1
1:A:77:PHE:CZ	1:A:153:MET:HE1	0.41	2.50	3	1
1:A:13:THR:HG23	1:A:16:GLN:OE1	0.41	2.16	6	2
1:A:36:ILE:HD11	1:A:77:PHE:HD2	0.41	1.74	3	1
1:A:3:ASP:HA	1:A:6:LYS:HB3	0.41	1.92	8	1
1:A:78:LEU:O	1:A:82:VAL:HB	0.41	2.15	1	1
1:A:152:ALA:HA	1:A:155:GLN:HE21	0.41	1.76	5	1
1:A:23:ALA:N	1:A:158:LEU:HD21	0.41	2.31	8	1
1:A:23:ALA:CB	1:A:154:MET:HE1	0.41	2.46	1	1
1:A:48:LEU:HD21	1:A:152:ALA:O	0.41	2.16	3	1
1:A:153:MET:O	1:A:157:LEU:HD23	0.41	2.16	4	1
1:A:24:PHE:CZ	1:A:73:ASP:HA	0.40	2.51	3	1
1:A:21:LYS:HD3	1:A:74:PHE:CD1	0.40	2.51	1	1
1:A:45:MET:HB2	1:A:52:PRO:HG3	0.40	1.92	1	1
1:A:45:MET:HB3	1:A:50:GLN:HB2	0.40	1.93	3	1
1:A:73:ASP:CG	1:A:74:PHE:H	0.40	2.24	8	2

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	94/120 (78%)	90±1 (95±1%)	4±1 (4±1%)	0±0 (1±1%)	26	74
All	All	752/960 (78%)	716 (95%)	32 (4%)	4 (1%)	26	74

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	159	GLY	4

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/101 (78%)	71±2 (89±3%)	8±2 (11±3%)	9	52
All	All	632/808 (78%)	565 (89%)	67 (11%)	9	52

All 29 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	71	THR	7
1	A	82	VAL	6
1	A	40	GLU	5
1	A	21	LYS	5
1	A	78	LEU	4
1	A	79	VAL	4
1	A	47	MET	3
1	A	53	THR	3
1	A	64	VAL	3
1	A	72	VAL	3
1	A	41	LEU	2
1	A	61	ILE	2
1	A	60	MET	2
1	A	58	GLN	2
1	A	27	PHE	2
1	A	4	ILE	1
1	A	39	LYS	1
1	A	56	GLU	1
1	A	29	LEU	1
1	A	48	LEU	1
1	A	55	GLU	1
1	A	76	GLU	1
1	A	9	VAL	1
1	A	43	LYS	1
1	A	59	GLU	1
1	A	153	MET	1
1	A	35	SER	1
1	A	45	MET	1
1	A	44	VAL	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](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 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	1411
Number of shifts mapped to atoms	1411
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	-0.24 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	110	0.11 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	112	-0.46 ± 0.12	None needed (< 0.5 ppm)
^{15}N	114	-0.00 ± 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. 1124 atoms were assigned a chemical shift out of a possible 1233. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	469/473 (99%)	192/193 (99%)	185/188 (98%)	92/92 (100%)
Sidechain	625/701 (89%)	427/455 (94%)	198/228 (87%)	0/18 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	30/59 (51%)	15/29 (52%)	15/30 (50%)	0/0 (—%)
Overall	1124/1233 (91%)	634/677 (94%)	398/446 (89%)	92/110 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1411 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	586/603 (97%)	241/246 (98%)	231/240 (96%)	114/117 (97%)
Sidechain	791/943 (84%)	536/608 (88%)	255/297 (86%)	0/38 (0%)
Aromatic	34/77 (44%)	17/38 (45%)	17/37 (46%)	0/2 (0%)
Overall	1411/1623 (87%)	794/892 (89%)	503/574 (88%)	114/157 (73%)

7.1.4 Statistically unusual chemical shifts [i](#)

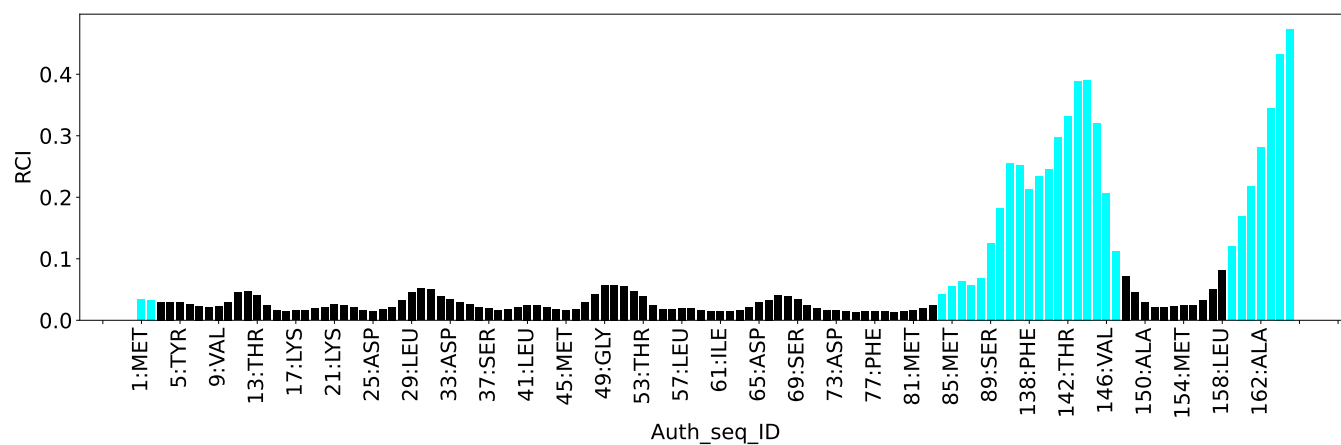
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	21	LYS	HD3	0.37	0.54 – 2.65	-5.8

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2117
Intra-residue ($ i-j =0$)	869
Sequential ($ i-j =1$)	331
Medium range ($ i-j >1$ and $ i-j <5$)	400
Long range ($ i-j \geq 5$)	517
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	17.6
Number of long range restraints per residue ¹	4.3

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)	74.0	0.2
0.2-0.5 (Medium)	148.4	0.5
>0.5 (Large)	137.9	7.64

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 ⓘ

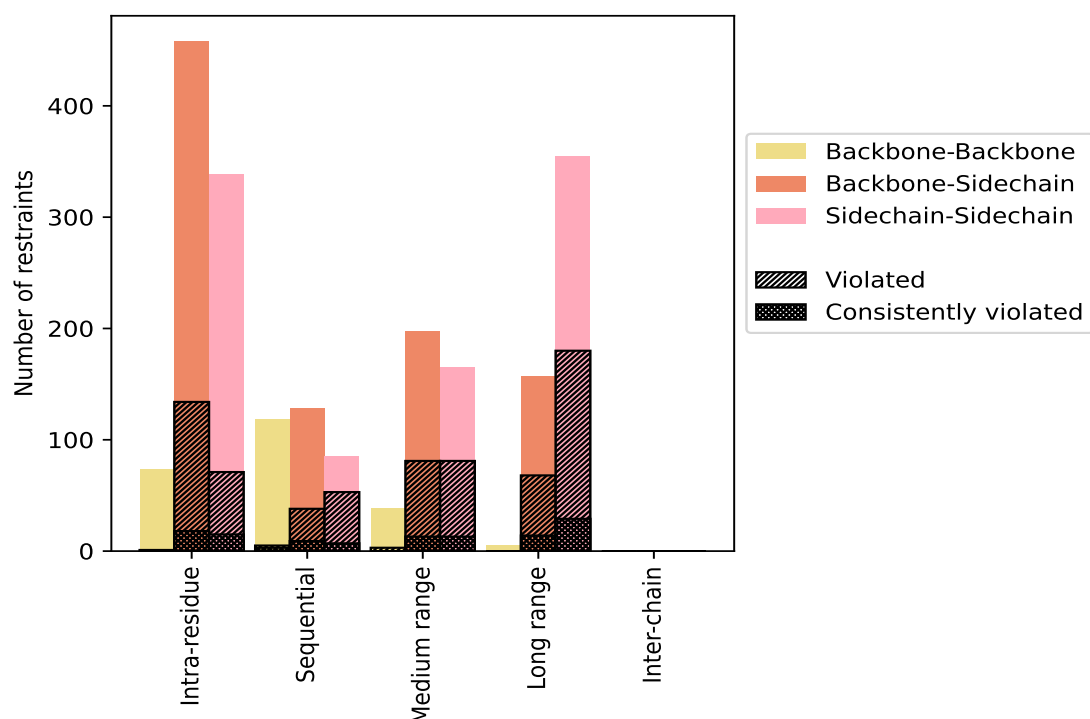
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	869	41.0	206	23.7	9.7	33	3.8	1.6
Backbone-Backbone	73	3.4	1	1.4	0.0	0	0.0	0.0
Backbone-Sidechain	458	21.6	134	29.3	6.3	18	3.9	0.9
Sidechain-Sidechain	338	16.0	71	21.0	3.4	15	4.4	0.7
Sequential (i-j =1)	331	15.6	96	29.0	4.5	19	5.7	0.9
Backbone-Backbone	118	5.6	5	4.2	0.2	3	2.5	0.1
Backbone-Sidechain	128	6.0	38	29.7	1.8	9	7.0	0.4
Sidechain-Sidechain	85	4.0	53	62.4	2.5	7	8.2	0.3
Medium range (i-j >1 & i-j <5)	400	18.9	165	41.2	7.8	26	6.5	1.2
Backbone-Backbone	38	1.8	3	7.9	0.1	0	0.0	0.0
Backbone-Sidechain	197	9.3	81	41.1	3.8	13	6.6	0.6
Sidechain-Sidechain	165	7.8	81	49.1	3.8	13	7.9	0.6
Long range (i-j ≥5)	517	24.4	248	48.0	11.7	43	8.3	2.0
Backbone-Backbone	5	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	157	7.4	68	43.3	3.2	14	8.9	0.7
Sidechain-Sidechain	355	16.8	180	50.7	8.5	29	8.2	1.4
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2117	100.0	715	33.8	33.8	121	5.7	5.7
Backbone-Backbone	234	11.1	9	3.8	0.4	3	1.3	0.1
Backbone-Sidechain	940	44.4	321	34.1	15.2	54	5.7	2.6
Sidechain-Sidechain	943	44.5	385	40.8	18.2	64	6.8	3.0

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

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



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

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

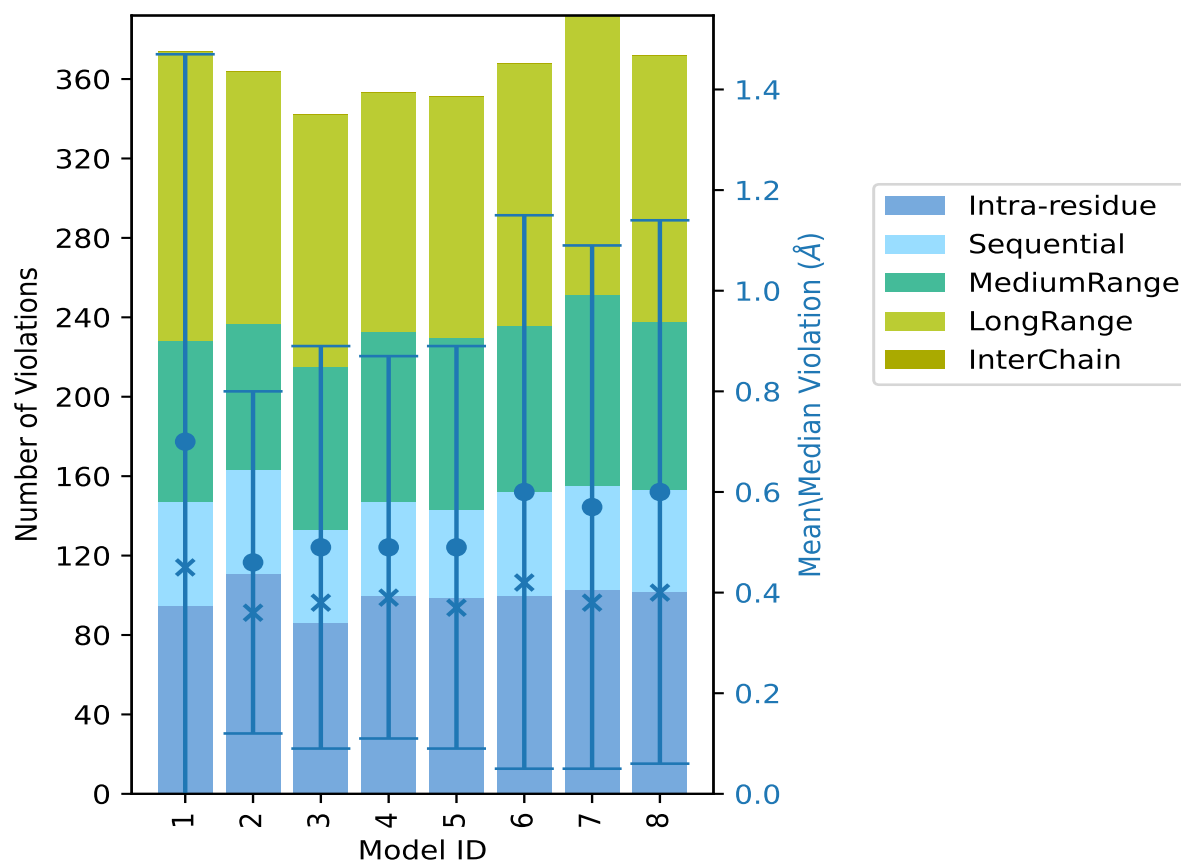
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	95	52	81	146	0	374	0.7	7.64	0.77	0.45
2	111	52	74	127	0	364	0.46	2.59	0.34	0.36
3	86	47	82	127	0	342	0.49	2.72	0.4	0.38
4	100	47	86	120	0	353	0.49	2.3	0.38	0.39
5	99	44	87	121	0	351	0.49	2.63	0.4	0.37
6	100	52	84	132	0	368	0.6	3.8	0.55	0.42
7	103	52	96	141	0	392	0.57	3.73	0.52	0.38
8	102	51	85	134	0	372	0.6	4.23	0.54	0.4

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, 1402(IR:663, SQ:235, MR:235, LR:269, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
61	20	33	53	0	167	1	12.5
26	10	21	26	0	83	2	25.0
22	9	22	33	0	86	3	37.5
20	15	17	39	0	91	4	50.0
18	10	15	20	0	63	5	62.5
11	6	14	19	0	50	6	75.0

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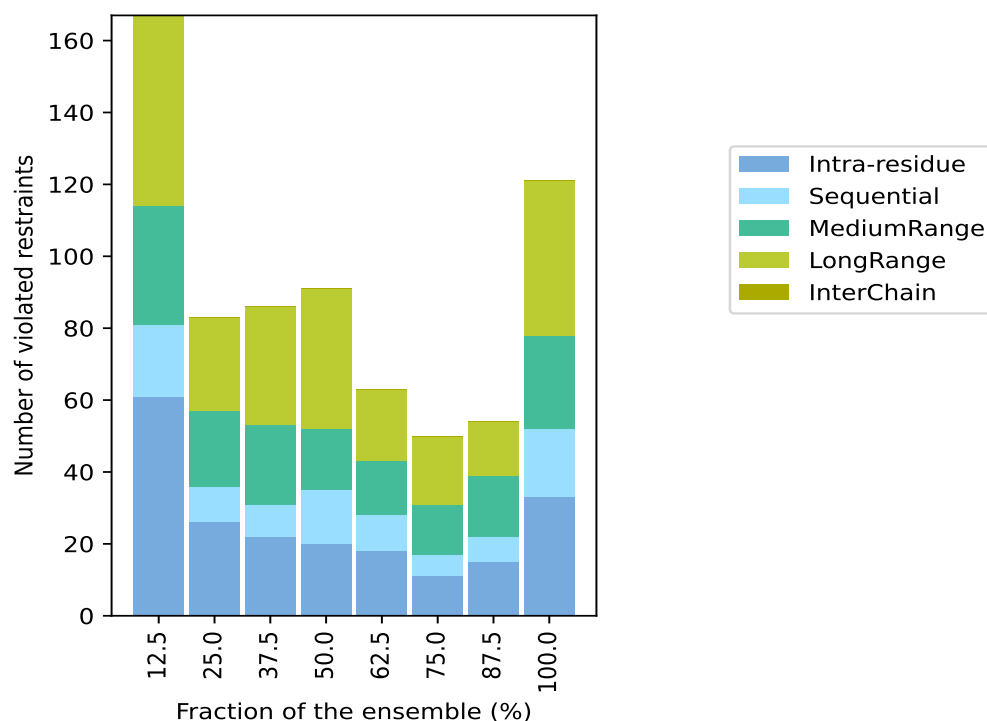
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
15	7	17	15	0	54	7	87.5
33	19	26	43	0	121	8	100.0

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

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

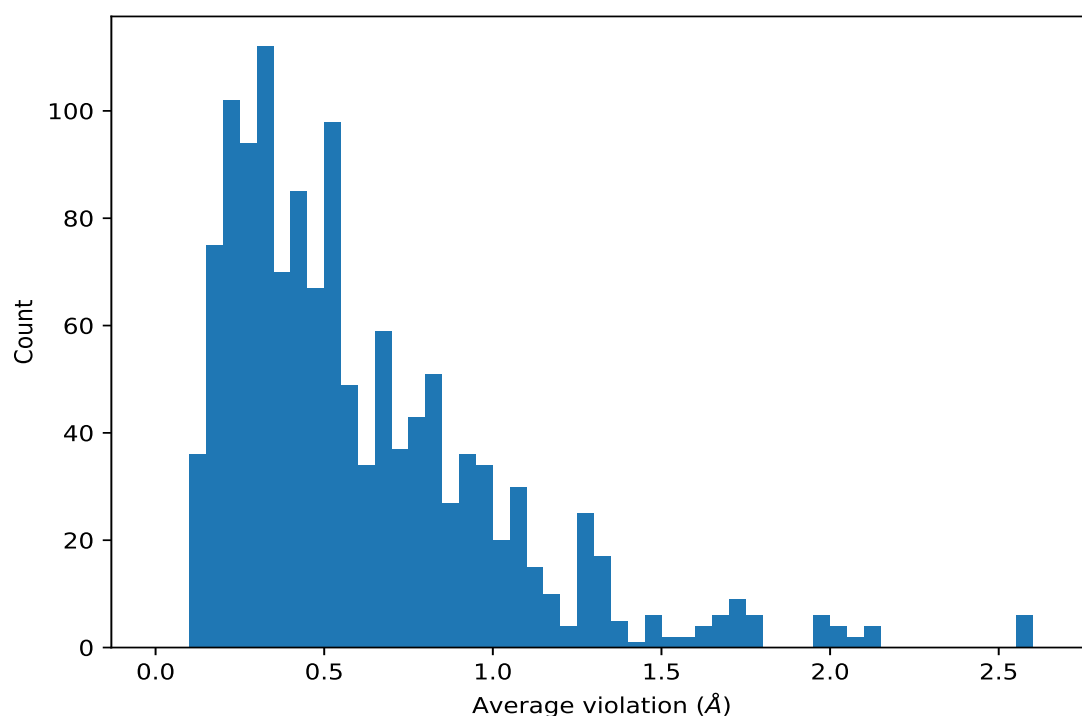
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,76)	1:154:A:MET:HE1	1:163:A:LYS:HE2	8	2.56	0.31	2.55
(1,76)	1:154:A:MET:HE2	1:18:A:ASN:HB2	8	2.56	0.31	2.55
(1,76)	1:154:A:MET:HE3	1:163:A:LYS:HE2	8	2.56	0.31	2.55
(1,76)	1:154:A:MET:HE3	1:18:A:ASN:HB2	8	2.56	0.31	2.55
(1,76)	1:154:A:MET:HE1	1:18:A:ASN:HB2	8	2.56	0.31	2.55
(1,76)	1:154:A:MET:HE2	1:163:A:LYS:HE2	8	2.56	0.31	2.55
(2,337)	1:60:A:MET:HE3	1:84:A:SER:HB3	8	2.1	2.11	0.84
(2,337)	1:60:A:MET:HE2	1:84:A:SER:HB3	8	2.1	2.11	0.84
(2,337)	1:60:A:MET:HE2	1:84:A:SER:HB2	8	2.1	2.11	0.84
(2,337)	1:60:A:MET:HE1	1:84:A:SER:HB3	8	2.1	2.11	0.84
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD13	8	1.98	0.22	1.93
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD11	8	1.98	0.22	1.93
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD12	8	1.98	0.22	1.93
(1,248)	1:24:A:PHE:HA	1:158:A:LEU:HD23	8	1.98	0.22	1.93
(1,248)	1:24:A:PHE:HA	1:158:A:LEU:HD21	8	1.98	0.22	1.93
(1,285)	1:71:A:THR:HG23	1:41:A:LEU:HB3	8	1.78	0.26	1.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,285)	1:71:A:THR:HG21	1:39:A:LYS:HB2	8	1.78	0.26	1.64
(1,285)	1:71:A:THR:HG23	1:39:A:LYS:HB2	8	1.78	0.26	1.64
(1,285)	1:71:A:THR:HG22	1:39:A:LYS:HB2	8	1.78	0.26	1.64
(1,285)	1:71:A:THR:HG22	1:41:A:LEU:HB3	8	1.78	0.26	1.64
(2,323)	1:85:A:MET:HE1	1:78:A:LEU:HD22	8	1.73	0.29	1.74
(2,323)	1:85:A:MET:HE3	1:78:A:LEU:HD23	8	1.73	0.29	1.74
(2,323)	1:85:A:MET:HE1	1:78:A:LEU:HD21	8	1.73	0.29	1.74
(2,323)	1:85:A:MET:HE3	1:78:A:LEU:HD22	8	1.73	0.29	1.74
(2,323)	1:85:A:MET:HE2	1:78:A:LEU:HD21	8	1.73	0.29	1.74
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG23	8	1.64	1.03	1.58
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG22	8	1.64	1.03	1.58
(2,1300)	1:5:A:TYR:HE2	1:79:A:VAL:HG22	8	1.64	1.03	1.58
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG21	8	1.64	1.03	1.58
(1,309)	1:8:A:ALA:HB2	1:4:A:ILE:HG21	8	1.3	0.11	1.35
(1,309)	1:8:A:ALA:HB3	1:4:A:ILE:HG23	8	1.3	0.11	1.35
(1,309)	1:8:A:ALA:HB2	1:4:A:ILE:HG23	8	1.3	0.11	1.35
(1,309)	1:8:A:ALA:HB1	1:4:A:ILE:HG22	8	1.3	0.11	1.35
(1,309)	1:8:A:ALA:HB3	1:4:A:ILE:HG22	8	1.3	0.11	1.35
(1,309)	1:8:A:ALA:HB1	1:4:A:ILE:HG21	8	1.3	0.11	1.35
(1,299)	1:158:A:LEU:HD22	1:26:A:ILE:HA	8	1.27	0.17	1.28
(1,299)	1:48:A:LEU:HD23	1:49:A:GLY:HA2	8	1.27	0.17	1.28
(1,299)	1:48:A:LEU:HD21	1:49:A:GLY:HA2	8	1.27	0.17	1.28
(1,299)	1:158:A:LEU:HD21	1:26:A:ILE:HA	8	1.27	0.17	1.28
(2,578)	1:36:A:ILE:HG21	1:41:A:LEU:HG	8	1.26	0.89	1.0
(2,578)	1:36:A:ILE:HG23	1:41:A:LEU:HG	8	1.26	0.89	1.0
(2,578)	1:36:A:ILE:HG22	1:41:A:LEU:HG	8	1.26	0.89	1.0
(1,95)	1:28:A:VAL:HG12	1:157:A:LEU:HD22	8	1.25	0.18	1.25
(1,95)	1:28:A:VAL:HG13	1:61:A:ILE:HD12	8	1.25	0.18	1.25
(1,95)	1:28:A:VAL:HG11	1:61:A:ILE:HD13	8	1.25	0.18	1.25
(1,95)	1:28:A:VAL:HG11	1:61:A:ILE:HD11	8	1.25	0.18	1.25
(1,95)	1:28:A:VAL:HG13	1:157:A:LEU:HD23	8	1.25	0.18	1.25
(1,95)	1:28:A:VAL:HG13	1:157:A:LEU:HD22	8	1.25	0.18	1.25
(2,1029)	1:31:A:ALA:HB1	1:36:A:ILE:HG22	8	1.19	0.21	1.22
(2,1029)	1:31:A:ALA:HB2	1:36:A:ILE:HG21	8	1.19	0.21	1.22
(2,1029)	1:31:A:ALA:HB1	1:36:A:ILE:HG23	8	1.19	0.21	1.22
(2,1029)	1:31:A:ALA:HB3	1:36:A:ILE:HG22	8	1.19	0.21	1.22
(2,1029)	1:31:A:ALA:HB3	1:36:A:ILE:HG21	8	1.19	0.21	1.22
(2,831)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	8	1.19	0.86	0.73
(2,831)	1:9:A:VAL:HG12	1:10:A:GLU:HG3	8	1.19	0.86	0.73
(2,831)	1:9:A:VAL:HG11	1:10:A:GLU:HG3	8	1.19	0.86	0.73
(2,342)	1:80:A:MET:HE1	1:77:A:PHE:HD1	8	1.12	0.67	1.04
(2,342)	1:80:A:MET:HE2	1:77:A:PHE:HD1	8	1.12	0.67	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,342)	1:80:A:MET:HE3	1:77:A:PHE:HD1	8	1.12	0.67	1.04
(1,182)	1:80:A:MET:HB3	1:77:A:PHE:HB3	8	1.12	0.26	1.08
(1,182)	1:50:A:GLN:HG2	1:52:A:PRO:HD2	8	1.12	0.26	1.08
(1,182)	1:80:A:MET:HB3	1:78:A:LEU:HA	8	1.12	0.26	1.08
(2,1092)	1:53:A:THR:HG22	1:54:A:PRO:HA	8	1.11	0.28	1.13
(2,1092)	1:53:A:THR:HG23	1:54:A:PRO:HA	8	1.11	0.28	1.13
(1,252)	1:28:A:VAL:HG22	1:26:A:ILE:HG13	8	1.09	0.27	1.06
(1,252)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	8	1.09	0.27	1.06
(1,252)	1:28:A:VAL:HG21	1:26:A:ILE:HG13	8	1.09	0.27	1.06
(1,340)	1:150:A:ALA:HB2	1:20:A:PHE:HD2	8	1.06	0.28	0.98
(1,340)	1:81:A:MET:HE2	1:20:A:PHE:HD1	8	1.06	0.28	0.98
(1,340)	1:81:A:MET:HE3	1:20:A:PHE:HD2	8	1.06	0.28	0.98
(1,340)	1:150:A:ALA:HB2	1:20:A:PHE:HD1	8	1.06	0.28	0.98
(1,340)	1:81:A:MET:HE1	1:20:A:PHE:HD1	8	1.06	0.28	0.98
(1,340)	1:150:A:ALA:HB1	1:20:A:PHE:HD2	8	1.06	0.28	0.98
(1,340)	1:81:A:MET:HE1	1:20:A:PHE:HD2	8	1.06	0.28	0.98
(2,362)	1:154:A:MET:HE3	1:81:A:MET:HE3	8	1.05	0.3	1.04
(2,362)	1:154:A:MET:HE3	1:81:A:MET:HE2	8	1.05	0.3	1.04
(2,362)	1:154:A:MET:HE2	1:81:A:MET:HE3	8	1.05	0.3	1.04
(2,362)	1:154:A:MET:HE1	1:81:A:MET:HE2	8	1.05	0.3	1.04
(2,362)	1:154:A:MET:HE3	1:81:A:MET:HE1	8	1.05	0.3	1.04
(2,362)	1:154:A:MET:HE1	1:81:A:MET:HE3	8	1.05	0.3	1.04
(2,362)	1:154:A:MET:HE1	1:81:A:MET:HE1	8	1.05	0.3	1.04
(2,1217)	1:146:A:VAL:HG13	1:147:A:ARG:HA	8	1.0	0.68	1.0
(2,1217)	1:146:A:VAL:HG12	1:147:A:ARG:HA	8	1.0	0.68	1.0
(2,1217)	1:146:A:VAL:HG11	1:147:A:ARG:HA	8	1.0	0.68	1.0
(1,103)	1:13:A:THR:HG23	1:15:A:GLU:HB2	8	0.99	0.15	1.0
(1,103)	1:13:A:THR:HG21	1:15:A:GLU:HB2	8	0.99	0.15	1.0
(1,103)	1:53:A:THR:HG23	1:55:A:GLU:HB3	8	0.99	0.15	1.0
(1,103)	1:13:A:THR:HG22	1:15:A:GLU:HB3	8	0.99	0.15	1.0
(1,103)	1:13:A:THR:HG23	1:15:A:GLU:HB3	8	0.99	0.15	1.0
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD11	8	0.98	0.64	0.71
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD13	8	0.98	0.64	0.71
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD12	8	0.98	0.64	0.71
(1,108)	1:158:A:LEU:HD23	1:162:A:ALA:HA	8	0.96	0.3	0.93
(1,108)	1:158:A:LEU:HD21	1:162:A:ALA:HA	8	0.96	0.3	0.93
(1,108)	1:158:A:LEU:HD22	1:162:A:ALA:HA	8	0.96	0.3	0.93
(1,63)	1:60:A:MET:HE1	1:148:A:ILE:HD12	8	0.93	0.73	0.54
(1,63)	1:60:A:MET:HE3	1:148:A:ILE:HD12	8	0.93	0.73	0.54
(1,63)	1:60:A:MET:HE1	1:148:A:ILE:HD13	8	0.93	0.73	0.54
(1,63)	1:60:A:MET:HE2	1:148:A:ILE:HD12	8	0.93	0.73	0.54
(1,63)	1:60:A:MET:HE1	1:148:A:ILE:HD11	8	0.93	0.73	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,63)	1:60:A:MET:HE2	1:148:A:ILE:HG23	8	0.93	0.73	0.54
(1,179)	1:155:A:GLN:HG3	1:162:A:ALA:HB2	8	0.92	0.24	1.0
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG22	8	0.92	0.24	1.0
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG23	8	0.92	0.24	1.0
(1,297)	1:148:A:ILE:HG23	1:147:A:ARG:HA	8	0.92	0.36	0.87
(1,297)	1:148:A:ILE:HG22	1:84:A:SER:HA	8	0.92	0.36	0.87
(1,297)	1:148:A:ILE:HG21	1:147:A:ARG:HA	8	0.92	0.36	0.87
(1,297)	1:148:A:ILE:HG21	1:84:A:SER:HA	8	0.92	0.36	0.87
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HD1	8	0.87	0.49	1.04
(1,272)	1:47:A:MET:HE2	1:27:A:PHE:HD1	8	0.87	0.49	1.04
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HZ	8	0.87	0.49	1.04
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HD2	8	0.87	0.49	1.04
(1,272)	1:47:A:MET:HE2	1:27:A:PHE:HD2	8	0.87	0.49	1.04
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG23	8	0.85	0.11	0.84
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG22	8	0.85	0.11	0.84
(2,1091)	1:13:A:THR:HG22	1:11:A:GLN:HA	8	0.84	0.32	0.74
(2,1091)	1:13:A:THR:HG21	1:11:A:GLN:HA	8	0.84	0.32	0.74
(2,1091)	1:13:A:THR:HG23	1:11:A:GLN:HA	8	0.84	0.32	0.74
(2,510)	1:12:A:LEU:HD22	1:9:A:VAL:HA	8	0.83	0.06	0.86
(2,510)	1:12:A:LEU:HD23	1:9:A:VAL:HA	8	0.83	0.06	0.86
(2,510)	1:12:A:LEU:HD21	1:9:A:VAL:HA	8	0.83	0.06	0.86
(1,85)	1:160:A:ALA:HB1	1:161:A:ARG:HB3	8	0.82	0.5	0.68
(1,85)	1:160:A:ALA:HB1	1:158:A:LEU:HB3	8	0.82	0.5	0.68
(1,85)	1:160:A:ALA:HB3	1:158:A:LEU:HB3	8	0.82	0.5	0.68
(1,85)	1:160:A:ALA:HB2	1:161:A:ARG:HB3	8	0.82	0.5	0.68
(1,85)	1:160:A:ALA:HB3	1:161:A:ARG:HB3	8	0.82	0.5	0.68
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG22	8	0.82	0.15	0.8
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG21	8	0.82	0.15	0.8
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG23	8	0.82	0.15	0.8
(1,324)	1:36:A:ILE:HG22	1:27:A:PHE:HA	8	0.82	0.15	0.8
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	8	0.81	0.31	0.77
(1,258)	1:31:A:ALA:HB3	1:29:A:LEU:HD23	8	0.8	0.3	0.77
(1,258)	1:31:A:ALA:HB1	1:29:A:LEU:HD23	8	0.8	0.3	0.77
(1,258)	1:31:A:ALA:HB3	1:29:A:LEU:HD21	8	0.8	0.3	0.77
(1,258)	1:31:A:ALA:HB2	1:29:A:LEU:HD21	8	0.8	0.3	0.77
(1,258)	1:31:A:ALA:HB3	1:29:A:LEU:HD22	8	0.8	0.3	0.77
(1,258)	1:31:A:ALA:HB2	1:29:A:LEU:HD22	8	0.8	0.3	0.77
(1,258)	1:31:A:ALA:HB2	1:29:A:LEU:HD23	8	0.8	0.3	0.77
(1,326)	1:61:A:ILE:HD12	1:57:A:LEU:HA	8	0.79	0.3	0.72
(1,326)	1:61:A:ILE:HD13	1:57:A:LEU:HA	8	0.79	0.3	0.72
(1,326)	1:61:A:ILE:HD11	1:57:A:LEU:HA	8	0.79	0.3	0.72
(2,1277)	1:78:A:LEU:HD11	1:20:A:PHE:HE1	8	0.79	0.81	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1277)	1:78:A:LEU:HD12	1:20:A:PHE:HE2	8	0.79	0.81	0.5
(2,1277)	1:78:A:LEU:HD12	1:20:A:PHE:HE1	8	0.79	0.81	0.5
(2,353)	1:45:A:MET:HE2	1:148:A:ILE:HG22	8	0.76	0.42	0.64
(2,353)	1:45:A:MET:HE2	1:148:A:ILE:HG21	8	0.76	0.42	0.64
(2,353)	1:45:A:MET:HE2	1:148:A:ILE:HG23	8	0.76	0.42	0.64
(2,353)	1:45:A:MET:HE1	1:148:A:ILE:HG23	8	0.76	0.42	0.64
(2,353)	1:45:A:MET:HE3	1:148:A:ILE:HG22	8	0.76	0.42	0.64
(2,353)	1:45:A:MET:HE3	1:148:A:ILE:HG23	8	0.76	0.42	0.64
(2,353)	1:45:A:MET:HE3	1:148:A:ILE:HG21	8	0.76	0.42	0.64
(1,264)	1:42:A:GLY:HA3	1:52:A:PRO:HB2	8	0.75	0.55	0.47
(1,264)	1:42:A:GLY:HA3	1:46:A:ARG:HG2	8	0.75	0.55	0.47
(1,264)	1:42:A:GLY:HA3	1:46:A:ARG:HB2	8	0.75	0.55	0.47
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG12	8	0.72	0.26	0.83
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG21	8	0.72	0.26	0.83
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG22	8	0.72	0.26	0.83
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG23	8	0.72	0.26	0.83
(2,1184)	1:148:A:ILE:HD13	1:44:A:VAL:HG23	8	0.72	0.3	0.79
(2,1184)	1:148:A:ILE:HD13	1:44:A:VAL:HG22	8	0.72	0.3	0.79
(2,1184)	1:148:A:ILE:HD11	1:44:A:VAL:HG21	8	0.72	0.3	0.79
(2,1184)	1:148:A:ILE:HD11	1:44:A:VAL:HG22	8	0.72	0.3	0.79
(2,1184)	1:148:A:ILE:HD12	1:44:A:VAL:HG23	8	0.72	0.3	0.79
(2,710)	1:72:A:VAL:HG21	1:36:A:ILE:HB	8	0.72	0.26	0.57
(2,710)	1:72:A:VAL:HG22	1:36:A:ILE:HB	8	0.72	0.26	0.57
(2,710)	1:72:A:VAL:HG23	1:36:A:ILE:HB	8	0.72	0.26	0.57
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG21	8	0.72	0.02	0.72
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG22	8	0.72	0.02	0.72
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG23	8	0.72	0.02	0.72
(1,87)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	8	0.72	0.02	0.72
(2,1025)	1:28:A:VAL:HG13	1:43:A:LYS:HD2	8	0.68	0.25	0.64
(2,1025)	1:28:A:VAL:HG13	1:43:A:LYS:HD3	8	0.68	0.25	0.64
(2,1025)	1:28:A:VAL:HG11	1:43:A:LYS:HD3	8	0.68	0.25	0.64
(2,1025)	1:28:A:VAL:HG11	1:43:A:LYS:HD2	8	0.68	0.25	0.64
(2,1198)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	8	0.66	0.23	0.6
(2,1198)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	8	0.66	0.23	0.6
(2,1198)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	8	0.66	0.23	0.6
(2,1030)	1:31:A:ALA:HB2	1:71:A:THR:HG23	8	0.65	0.24	0.6
(2,1030)	1:31:A:ALA:HB3	1:71:A:THR:HG21	8	0.65	0.24	0.6
(2,1030)	1:31:A:ALA:HB1	1:71:A:THR:HG23	8	0.65	0.24	0.6
(2,1030)	1:31:A:ALA:HB2	1:71:A:THR:HG21	8	0.65	0.24	0.6
(2,1030)	1:31:A:ALA:HB1	1:71:A:THR:HG22	8	0.65	0.24	0.6
(2,1030)	1:31:A:ALA:HB2	1:71:A:THR:HG22	8	0.65	0.24	0.6
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG23	8	0.65	0.15	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG22	8	0.65	0.15	0.67
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG21	8	0.65	0.15	0.67
(2,1201)	1:28:A:VAL:HG22	1:24:A:PHE:HD1	8	0.65	0.13	0.68
(2,1201)	1:28:A:VAL:HG21	1:24:A:PHE:HD2	8	0.65	0.13	0.68
(2,1201)	1:28:A:VAL:HG23	1:24:A:PHE:HD1	8	0.65	0.13	0.68
(2,1201)	1:28:A:VAL:HG21	1:24:A:PHE:HD1	8	0.65	0.13	0.68
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE2	8	0.65	0.07	0.62
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE1	8	0.65	0.07	0.62
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD13	8	0.64	0.14	0.56
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD12	8	0.64	0.14	0.56
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD11	8	0.64	0.14	0.56
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG22	8	0.62	0.02	0.62
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG21	8	0.62	0.02	0.62
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG23	8	0.62	0.02	0.62
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	8	0.59	0.23	0.56
(1,349)	1:4:A:ILE:HG13	1:5:A:TYR:HE2	8	0.59	0.23	0.56
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE1	8	0.59	0.23	0.56
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD13	8	0.58	0.07	0.61
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD11	8	0.58	0.07	0.61
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD12	8	0.58	0.07	0.61
(1,255)	1:28:A:VAL:HG13	1:72:A:VAL:HB	8	0.58	0.31	0.47
(1,255)	1:28:A:VAL:HG11	1:72:A:VAL:HB	8	0.58	0.31	0.47
(1,255)	1:28:A:VAL:HG12	1:72:A:VAL:HB	8	0.58	0.31	0.47
(1,246)	1:158:A:LEU:HD21	1:22:A:ALA:HA	8	0.58	0.25	0.62
(1,246)	1:26:A:ILE:HD12	1:22:A:ALA:HA	8	0.58	0.25	0.62
(1,246)	1:26:A:ILE:HD11	1:22:A:ALA:HA	8	0.58	0.25	0.62
(1,246)	1:26:A:ILE:HD13	1:22:A:ALA:HA	8	0.58	0.25	0.62
(1,246)	1:158:A:LEU:HD23	1:22:A:ALA:HA	8	0.58	0.25	0.62
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD12	8	0.55	0.09	0.56
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD13	8	0.55	0.09	0.56
(2,365)	1:154:A:MET:HE1	1:158:A:LEU:HD21	8	0.54	0.09	0.54
(2,365)	1:154:A:MET:HE2	1:158:A:LEU:HD21	8	0.54	0.09	0.54
(2,365)	1:154:A:MET:HE1	1:158:A:LEU:HD22	8	0.54	0.09	0.54
(2,365)	1:154:A:MET:HE3	1:158:A:LEU:HD21	8	0.54	0.09	0.54
(2,365)	1:154:A:MET:HE2	1:158:A:LEU:HD23	8	0.54	0.09	0.54
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB2	8	0.54	0.15	0.52
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB3	8	0.54	0.15	0.52
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG22	8	0.52	0.06	0.54
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG21	8	0.52	0.06	0.54
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG23	8	0.52	0.06	0.54
(2,766)	1:36:A:ILE:HG21	1:72:A:VAL:HB	8	0.52	0.22	0.55
(2,766)	1:36:A:ILE:HG23	1:72:A:VAL:HB	8	0.52	0.22	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,766)	1:36:A:ILE:HG22	1:72:A:VAL:HB	8	0.52	0.22	0.55
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG22	8	0.52	0.18	0.57
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG21	8	0.52	0.18	0.57
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG23	8	0.52	0.18	0.57
(2,379)	1:81:A:MET:HE3	1:81:A:MET:HG3	8	0.52	0.03	0.52
(2,379)	1:81:A:MET:HE2	1:81:A:MET:HG3	8	0.52	0.03	0.52
(2,379)	1:81:A:MET:HE1	1:81:A:MET:HG3	8	0.52	0.03	0.52
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	8	0.52	0.36	0.36
(2,485)	1:157:A:LEU:HD22	1:158:A:LEU:HG	8	0.5	0.32	0.38
(2,485)	1:157:A:LEU:HD23	1:158:A:LEU:HG	8	0.5	0.32	0.38
(2,485)	1:157:A:LEU:HD21	1:158:A:LEU:HG	8	0.5	0.32	0.38
(1,51)	1:38:A:THR:HB	1:61:A:ILE:HD12	8	0.5	0.22	0.44
(1,51)	1:61:A:ILE:HD13	1:41:A:LEU:HA	8	0.5	0.22	0.44
(1,51)	1:61:A:ILE:HD11	1:41:A:LEU:HA	8	0.5	0.22	0.44
(1,51)	1:38:A:THR:HB	1:61:A:ILE:HD13	8	0.5	0.22	0.44
(1,51)	1:38:A:THR:HB	1:61:A:ILE:HD11	8	0.5	0.22	0.44
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	8	0.49	0.02	0.5
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD21	8	0.49	0.55	0.3
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD22	8	0.49	0.55	0.3
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD23	8	0.49	0.55	0.3
(1,151)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	8	0.46	0.11	0.48
(1,151)	1:26:A:ILE:HD11	1:157:A:LEU:HB2	8	0.46	0.11	0.48
(1,151)	1:26:A:ILE:HD12	1:157:A:LEU:HB2	8	0.46	0.11	0.48
(2,410)	1:31:A:ALA:HB3	1:28:A:VAL:HG21	8	0.46	0.1	0.45
(2,410)	1:31:A:ALA:HB1	1:28:A:VAL:HG22	8	0.46	0.1	0.45
(2,410)	1:31:A:ALA:HB2	1:28:A:VAL:HG23	8	0.46	0.1	0.45
(2,410)	1:31:A:ALA:HB3	1:28:A:VAL:HG22	8	0.46	0.1	0.45
(2,410)	1:31:A:ALA:HB2	1:28:A:VAL:HG22	8	0.46	0.1	0.45
(2,410)	1:31:A:ALA:HB3	1:28:A:VAL:HG23	8	0.46	0.1	0.45
(2,374)	1:31:A:ALA:HB2	1:32:A:GLU:HB2	8	0.44	0.1	0.44
(2,374)	1:31:A:ALA:HB3	1:32:A:GLU:HB2	8	0.44	0.1	0.44
(2,374)	1:31:A:ALA:HB2	1:32:A:GLU:HB3	8	0.44	0.1	0.44
(2,374)	1:31:A:ALA:HB1	1:32:A:GLU:HB3	8	0.44	0.1	0.44
(2,374)	1:31:A:ALA:HB1	1:32:A:GLU:HB2	8	0.44	0.1	0.44
(1,102)	1:13:A:THR:HG21	1:16:A:GLN:HG2	8	0.44	0.08	0.44
(1,102)	1:13:A:THR:HG22	1:16:A:GLN:HG2	8	0.44	0.08	0.44
(1,102)	1:13:A:THR:HG23	1:16:A:GLN:HG2	8	0.44	0.08	0.44
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE1	8	0.43	0.14	0.4
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE3	8	0.43	0.14	0.4
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE2	8	0.43	0.14	0.4
(2,620)	1:140:A:ARG:HG2	1:140:A:ARG:HD3	8	0.42	0.02	0.42
(2,620)	1:140:A:ARG:HG3	1:140:A:ARG:HD2	8	0.42	0.02	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1266)	1:20:A:PHE:HD1	1:20:A:PHE:HE1	8	0.42	0.0	0.42
(2,1266)	1:20:A:PHE:HD2	1:20:A:PHE:HE2	8	0.42	0.0	0.42
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB2	8	0.42	0.08	0.42
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB3	8	0.42	0.08	0.42
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB1	8	0.42	0.08	0.42
(2,669)	1:90:A:LYS:HE3	1:90:A:LYS:HD2	8	0.41	0.05	0.44
(2,669)	1:90:A:LYS:HE2	1:90:A:LYS:HD3	8	0.41	0.05	0.44
(2,407)	1:36:A:ILE:HG23	1:41:A:LEU:HB3	8	0.41	0.16	0.44
(2,407)	1:36:A:ILE:HG22	1:41:A:LEU:HB3	8	0.41	0.16	0.44
(2,407)	1:36:A:ILE:HG21	1:41:A:LEU:HB3	8	0.41	0.16	0.44
(1,247)	1:23:A:ALA:HB1	1:24:A:PHE:HB3	8	0.39	0.1	0.38
(1,247)	1:23:A:ALA:HB2	1:24:A:PHE:HB3	8	0.39	0.1	0.38
(1,247)	1:23:A:ALA:HB3	1:24:A:PHE:HB3	8	0.39	0.1	0.38
(1,323)	1:8:A:ALA:HB2	1:79:A:VAL:HA	8	0.39	0.11	0.41
(1,323)	1:8:A:ALA:HB1	1:79:A:VAL:HA	8	0.39	0.11	0.41
(1,323)	1:8:A:ALA:HB3	1:79:A:VAL:HA	8	0.39	0.11	0.41
(2,927)	1:8:A:ALA:HB2	1:79:A:VAL:HA	8	0.38	0.11	0.4
(2,927)	1:8:A:ALA:HB1	1:79:A:VAL:HA	8	0.38	0.11	0.4
(2,927)	1:8:A:ALA:HB3	1:79:A:VAL:HA	8	0.38	0.11	0.4
(1,79)	1:31:A:ALA:HB1	1:36:A:ILE:HA	8	0.37	0.13	0.32
(1,79)	1:31:A:ALA:HB2	1:36:A:ILE:HA	8	0.37	0.13	0.32
(1,79)	1:31:A:ALA:HB3	1:36:A:ILE:HA	8	0.37	0.13	0.32
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	8	0.35	0.01	0.35
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	8	0.35	0.13	0.34
(2,516)	1:57:A:LEU:HD21	1:45:A:MET:HG2	8	0.35	0.13	0.35
(2,516)	1:57:A:LEU:HD23	1:45:A:MET:HG2	8	0.35	0.13	0.35
(2,516)	1:57:A:LEU:HD22	1:45:A:MET:HG2	8	0.35	0.13	0.35
(2,1235)	1:5:A:TYR:HD2	1:5:A:TYR:HE2	8	0.35	0.02	0.34
(2,1235)	1:5:A:TYR:HD1	1:5:A:TYR:HE1	8	0.35	0.02	0.34
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG22	8	0.34	0.11	0.34
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG21	8	0.34	0.11	0.34
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB1	8	0.34	0.17	0.3
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB3	8	0.34	0.17	0.3
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB2	8	0.34	0.17	0.3
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	8	0.33	0.16	0.28
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD22	8	0.33	0.16	0.28
(1,136)	1:58:A:GLN:HB3	1:58:A:GLN:HG2	8	0.33	0.05	0.33
(1,136)	1:155:A:GLN:HB3	1:155:A:GLN:HG2	8	0.33	0.05	0.33
(2,459)	1:71:A:THR:HG23	1:36:A:ILE:HA	8	0.33	0.09	0.31
(2,459)	1:71:A:THR:HG21	1:36:A:ILE:HA	8	0.33	0.09	0.31
(2,459)	1:71:A:THR:HG22	1:36:A:ILE:HA	8	0.33	0.09	0.31
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	8	0.32	0.01	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD1	8	0.32	0.07	0.32
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD2	8	0.32	0.07	0.32
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	8	0.31	0.15	0.31
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	8	0.3	0.01	0.3
(2,929)	1:152:A:ALA:HB3	1:149:A:SER:HA	8	0.3	0.09	0.3
(2,929)	1:152:A:ALA:HB1	1:149:A:SER:HA	8	0.3	0.09	0.3
(2,929)	1:152:A:ALA:HB2	1:149:A:SER:HA	8	0.3	0.09	0.3
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HD13	8	0.29	0.09	0.34
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG23	8	0.29	0.09	0.34
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG21	8	0.29	0.09	0.34
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG22	8	0.29	0.09	0.34
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	8	0.29	0.15	0.22
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	8	0.28	0.03	0.28
(2,847)	1:10:A:GLU:HB3	1:10:A:GLU:HG2	8	0.27	0.04	0.26
(2,847)	1:10:A:GLU:HB2	1:10:A:GLU:HG2	8	0.27	0.04	0.26
(1,205)	1:9:A:VAL:HG23	1:9:A:VAL:HB	8	0.27	0.02	0.28
(1,205)	1:9:A:VAL:HG22	1:9:A:VAL:HB	8	0.27	0.02	0.28
(1,205)	1:9:A:VAL:HG12	1:9:A:VAL:HB	8	0.27	0.02	0.28
(1,205)	1:9:A:VAL:HG11	1:9:A:VAL:HB	8	0.27	0.02	0.28
(2,558)	1:12:A:LEU:HD12	1:12:A:LEU:HA	8	0.26	0.04	0.26
(2,558)	1:12:A:LEU:HD11	1:12:A:LEU:HA	8	0.26	0.04	0.26
(2,558)	1:12:A:LEU:HD13	1:12:A:LEU:HA	8	0.26	0.04	0.26
(1,174)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	8	0.26	0.03	0.26
(1,174)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	8	0.26	0.03	0.26
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	8	0.26	0.11	0.23
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	8	0.26	0.04	0.26
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	8	0.25	0.07	0.28
(2,577)	1:41:A:LEU:HD21	1:41:A:LEU:HG	8	0.23	0.03	0.23
(2,577)	1:41:A:LEU:HD22	1:41:A:LEU:HG	8	0.23	0.03	0.23
(2,577)	1:41:A:LEU:HD23	1:41:A:LEU:HG	8	0.23	0.03	0.23
(2,625)	1:161:A:ARG:HD2	1:161:A:ARG:HG3	8	0.22	0.05	0.24
(2,625)	1:161:A:ARG:HD3	1:161:A:ARG:HG2	8	0.22	0.05	0.24
(2,562)	1:12:A:LEU:HD12	1:17:A:LYS:HG3	8	0.22	0.1	0.2
(2,562)	1:12:A:LEU:HD11	1:17:A:LYS:HG3	8	0.22	0.1	0.2
(2,562)	1:12:A:LEU:HD13	1:17:A:LYS:HG3	8	0.22	0.1	0.2
(1,96)	1:13:A:THR:HB	1:13:A:THR:HG23	8	0.22	0.03	0.23
(1,96)	1:53:A:THR:HB	1:53:A:THR:HG22	8	0.22	0.03	0.23
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG21	8	0.22	0.02	0.22
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG22	8	0.22	0.02	0.22
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG23	8	0.22	0.02	0.22
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD22	8	0.22	0.1	0.18
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD12	8	0.22	0.1	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD11	8	0.22	0.1	0.18
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB2	8	0.21	0.01	0.22
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB3	8	0.21	0.01	0.22
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB1	8	0.21	0.01	0.22
(2,557)	1:4:A:ILE:HG13	1:4:A:ILE:HD12	8	0.21	0.01	0.21
(2,557)	1:4:A:ILE:HG12	1:4:A:ILE:HD11	8	0.21	0.01	0.21
(2,557)	1:4:A:ILE:HG12	1:4:A:ILE:HD13	8	0.21	0.01	0.21
(2,557)	1:4:A:ILE:HG13	1:4:A:ILE:HD13	8	0.21	0.01	0.21
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	8	0.2	0.01	0.2
(1,161)	1:25:A:ASP:HA	1:25:A:ASP:HB3	8	0.19	0.04	0.22
(1,161)	1:22:A:ALA:HA	1:25:A:ASP:HB3	8	0.19	0.04	0.22
(2,667)	1:88:A:ASP:HB3	1:88:A:ASP:HA	8	0.19	0.05	0.19
(2,667)	1:88:A:ASP:HB2	1:88:A:ASP:HA	8	0.19	0.05	0.19
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB3	8	0.18	0.04	0.18
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB2	8	0.18	0.04	0.18
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB1	8	0.18	0.04	0.18
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	8	0.17	0.03	0.16
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD13	8	0.17	0.02	0.18
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD11	8	0.17	0.02	0.18
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD12	8	0.17	0.02	0.18
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	8	0.16	0.01	0.16
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	8	0.15	0.02	0.14
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB1	8	0.14	0.01	0.15
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB2	8	0.14	0.01	0.15
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB3	8	0.14	0.01	0.15
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	8	0.13	0.01	0.13
(1,100)	1:79:A:VAL:HG12	1:76:A:GLU:HB2	7	1.66	0.76	2.23
(1,100)	1:79:A:VAL:HG13	1:76:A:GLU:HB2	7	1.66	0.76	2.23
(1,100)	1:79:A:VAL:HG11	1:76:A:GLU:HB2	7	1.66	0.76	2.23
(2,833)	1:64:A:VAL:HG12	1:63:A:GLU:HG2	7	1.53	0.4	1.55
(2,833)	1:64:A:VAL:HG11	1:63:A:GLU:HG2	7	1.53	0.4	1.55
(1,223)	1:4:A:ILE:HD13	1:83:A:ARG:HD2	7	1.31	0.68	1.44
(1,223)	1:4:A:ILE:HD11	1:3:A:ASP:HB3	7	1.31	0.68	1.44
(1,223)	1:4:A:ILE:HD13	1:3:A:ASP:HB3	7	1.31	0.68	1.44
(1,223)	1:4:A:ILE:HD11	1:83:A:ARG:HD2	7	1.31	0.68	1.44
(1,223)	1:4:A:ILE:HD12	1:83:A:ARG:HD2	7	1.31	0.68	1.44
(1,168)	1:56:A:GLU:HG3	1:59:A:GLU:HB2	7	1.3	0.66	1.17
(1,168)	1:56:A:GLU:HG3	1:146:A:VAL:HB	7	1.3	0.66	1.17
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD12	7	1.18	0.65	1.21
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD13	7	1.18	0.65	1.21
(1,331)	1:5:A:TYR:HD2	1:83:A:ARG:HB2	7	1.09	0.22	1.11
(1,331)	1:5:A:TYR:HD2	1:4:A:ILE:HB	7	1.09	0.22	1.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,331)	1:5:A:TYR:HD1	1:4:A:ILE:HB	7	1.09	0.22	1.11
(1,331)	1:5:A:TYR:HD2	1:90:A:LYS:HD2	7	1.09	0.22	1.11
(1,331)	1:5:A:TYR:HD2	1:90:A:LYS:HD3	7	1.09	0.22	1.11
(1,98)	1:72:A:VAL:HG13	1:36:A:ILE:HG21	7	1.04	0.09	1.02
(1,98)	1:72:A:VAL:HG12	1:36:A:ILE:HG23	7	1.04	0.09	1.02
(1,98)	1:72:A:VAL:HG11	1:64:A:VAL:HG13	7	1.04	0.09	1.02
(1,98)	1:72:A:VAL:HG12	1:36:A:ILE:HG22	7	1.04	0.09	1.02
(1,98)	1:72:A:VAL:HG13	1:36:A:ILE:HG23	7	1.04	0.09	1.02
(1,98)	1:72:A:VAL:HG11	1:36:A:ILE:HG21	7	1.04	0.09	1.02
(1,98)	1:72:A:VAL:HG13	1:36:A:ILE:HG22	7	1.04	0.09	1.02
(2,1106)	1:64:A:VAL:HG23	1:76:A:GLU:HG3	7	1.04	0.7	0.65
(2,1106)	1:64:A:VAL:HG22	1:76:A:GLU:HG3	7	1.04	0.7	0.65
(2,1106)	1:64:A:VAL:HG21	1:76:A:GLU:HG3	7	1.04	0.7	0.65
(2,439)	1:146:A:VAL:HG11	1:56:A:GLU:HA	7	0.94	0.56	0.7
(2,439)	1:146:A:VAL:HG12	1:56:A:GLU:HA	7	0.94	0.56	0.7
(2,1073)	1:48:A:LEU:HD22	1:27:A:PHE:HE1	7	0.94	0.28	0.8
(2,1073)	1:48:A:LEU:HD21	1:27:A:PHE:HE1	7	0.94	0.28	0.8
(2,1073)	1:48:A:LEU:HD23	1:27:A:PHE:HE1	7	0.94	0.28	0.8
(2,1073)	1:48:A:LEU:HD23	1:27:A:PHE:HE2	7	0.94	0.28	0.8
(2,332)	1:1:A:MET:HE2	1:79:A:VAL:HG12	7	0.92	0.31	0.9
(2,332)	1:1:A:MET:HE2	1:79:A:VAL:HG13	7	0.92	0.31	0.9
(2,332)	1:1:A:MET:HE3	1:79:A:VAL:HG11	7	0.92	0.31	0.9
(2,332)	1:1:A:MET:HE2	1:79:A:VAL:HG11	7	0.92	0.31	0.9
(2,332)	1:1:A:MET:HE3	1:79:A:VAL:HG12	7	0.92	0.31	0.9
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG22	7	0.9	0.51	0.59
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG21	7	0.9	0.51	0.59
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG23	7	0.9	0.51	0.59
(1,37)	1:57:A:LEU:HA	1:57:A:LEU:HD12	7	0.9	0.51	0.59
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG21	7	0.89	0.5	1.14
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG23	7	0.89	0.5	1.14
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG22	7	0.89	0.5	1.14
(1,209)	1:59:A:GLU:HG2	1:146:A:VAL:HG11	7	0.89	0.5	1.14
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD11	7	0.87	0.14	0.82
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD13	7	0.87	0.14	0.82
(1,274)	1:52:A:PRO:HA	1:146:A:VAL:HG22	7	0.87	0.14	0.82
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD12	7	0.87	0.14	0.82
(1,81)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	7	0.86	0.59	1.24
(1,81)	1:8:A:ALA:HB1	1:10:A:GLU:HG3	7	0.86	0.59	1.24
(1,81)	1:8:A:ALA:HB3	1:10:A:GLU:HG3	7	0.86	0.59	1.24
(1,81)	1:8:A:ALA:HB2	1:11:A:GLN:HG3	7	0.86	0.59	1.24
(1,81)	1:8:A:ALA:HB3	1:11:A:GLN:HG3	7	0.86	0.59	1.24
(1,118)	1:48:A:LEU:HD11	1:48:A:LEU:HA	7	0.84	0.18	0.97

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,118)	1:48:A:LEU:HD13	1:48:A:LEU:HA	7	0.84	0.18	0.97
(1,118)	1:48:A:LEU:HD12	1:48:A:LEU:HA	7	0.84	0.18	0.97
(1,118)	1:154:A:MET:HA	1:157:A:LEU:HD13	7	0.84	0.18	0.97
(1,118)	1:154:A:MET:HA	1:157:A:LEU:HD11	7	0.84	0.18	0.97
(1,67)	1:80:A:MET:HE3	1:148:A:ILE:HG12	7	0.84	0.43	1.12
(1,67)	1:80:A:MET:HE1	1:81:A:MET:HG3	7	0.84	0.43	1.12
(1,67)	1:80:A:MET:HE2	1:81:A:MET:HG3	7	0.84	0.43	1.12
(1,67)	1:80:A:MET:HE1	1:148:A:ILE:HG12	7	0.84	0.43	1.12
(1,67)	1:80:A:MET:HE2	1:148:A:ILE:HG12	7	0.84	0.43	1.12
(2,940)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	7	0.79	0.57	0.58
(2,940)	1:164:A:GLY:HA3	1:163:A:LYS:HE2	7	0.79	0.57	0.58
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	7	0.79	0.19	0.85
(1,244)	1:2:A:ASP:HB2	1:83:A:ARG:HG3	7	0.76	0.29	0.77
(1,244)	1:2:A:ASP:HB2	1:4:A:ILE:HG12	7	0.76	0.29	0.77
(2,400)	1:162:A:ALA:HB1	1:158:A:LEU:HD23	7	0.7	0.24	0.63
(2,400)	1:162:A:ALA:HB2	1:158:A:LEU:HD21	7	0.7	0.24	0.63
(2,400)	1:162:A:ALA:HB3	1:158:A:LEU:HD23	7	0.7	0.24	0.63
(2,400)	1:162:A:ALA:HB1	1:158:A:LEU:HD21	7	0.7	0.24	0.63
(2,400)	1:162:A:ALA:HB2	1:158:A:LEU:HD22	7	0.7	0.24	0.63
(2,400)	1:162:A:ALA:HB2	1:158:A:LEU:HD23	7	0.7	0.24	0.63
(1,219)	1:60:A:MET:HG3	1:57:A:LEU:HA	7	0.68	0.08	0.69
(1,219)	1:154:A:MET:HG3	1:150:A:ALA:HA	7	0.68	0.08	0.69
(1,99)	1:82:A:VAL:HG13	1:90:A:LYS:HB2	7	0.67	0.41	0.47
(1,99)	1:82:A:VAL:HG12	1:86:A:LYS:HB2	7	0.67	0.41	0.47
(1,99)	1:82:A:VAL:HG12	1:80:A:MET:HE1	7	0.67	0.41	0.47
(1,99)	1:82:A:VAL:HG13	1:86:A:LYS:HB2	7	0.67	0.41	0.47
(1,99)	1:82:A:VAL:HG11	1:86:A:LYS:HB2	7	0.67	0.41	0.47
(2,537)	1:78:A:LEU:HD11	1:78:A:LEU:HB3	7	0.66	0.1	0.72
(2,537)	1:78:A:LEU:HD13	1:78:A:LEU:HB3	7	0.66	0.1	0.72
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	7	0.66	0.17	0.62
(2,429)	1:72:A:VAL:HG11	1:76:A:GLU:HG3	7	0.66	0.31	0.47
(2,429)	1:72:A:VAL:HG12	1:76:A:GLU:HG3	7	0.66	0.31	0.47
(2,429)	1:72:A:VAL:HG13	1:76:A:GLU:HG3	7	0.66	0.31	0.47
(1,293)	1:82:A:VAL:HG11	1:85:A:MET:HG2	7	0.6	0.14	0.53
(1,293)	1:82:A:VAL:HG12	1:85:A:MET:HG2	7	0.6	0.14	0.53
(1,293)	1:82:A:VAL:HG13	1:85:A:MET:HG2	7	0.6	0.14	0.53
(1,293)	1:82:A:VAL:HG11	1:83:A:ARG:HD2	7	0.6	0.14	0.53
(1,293)	1:82:A:VAL:HG12	1:83:A:ARG:HD3	7	0.6	0.14	0.53
(1,293)	1:82:A:VAL:HG13	1:83:A:ARG:HD2	7	0.6	0.14	0.53
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	7	0.59	0.32	0.74
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD12	7	0.59	0.32	0.74
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD22	7	0.56	0.09	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD21	7	0.56	0.09	0.58
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD23	7	0.56	0.09	0.58
(2,1101)	1:61:A:ILE:HD13	1:36:A:ILE:HD13	7	0.54	0.29	0.49
(2,1101)	1:61:A:ILE:HD11	1:36:A:ILE:HD12	7	0.54	0.29	0.49
(2,1101)	1:61:A:ILE:HD12	1:36:A:ILE:HD11	7	0.54	0.29	0.49
(2,1101)	1:61:A:ILE:HD11	1:36:A:ILE:HD13	7	0.54	0.29	0.49
(2,1101)	1:61:A:ILE:HD11	1:36:A:ILE:HD11	7	0.54	0.29	0.49
(2,1101)	1:61:A:ILE:HD12	1:36:A:ILE:HD12	7	0.54	0.29	0.49
(2,65)	1:84:A:SER:HB2	1:148:A:ILE:HG23	7	0.52	0.45	0.37
(2,65)	1:84:A:SER:HB3	1:148:A:ILE:HG22	7	0.52	0.45	0.37
(2,65)	1:84:A:SER:HB2	1:148:A:ILE:HG21	7	0.52	0.45	0.37
(2,65)	1:84:A:SER:HB3	1:148:A:ILE:HG21	7	0.52	0.45	0.37
(2,65)	1:84:A:SER:HB3	1:148:A:ILE:HG23	7	0.52	0.45	0.37
(2,65)	1:84:A:SER:HB2	1:148:A:ILE:HG22	7	0.52	0.45	0.37
(1,220)	1:44:A:VAL:HB	1:148:A:ILE:HD13	7	0.51	0.15	0.45
(1,220)	1:44:A:VAL:HB	1:48:A:LEU:HD11	7	0.51	0.15	0.45
(1,220)	1:44:A:VAL:HB	1:48:A:LEU:HD13	7	0.51	0.15	0.45
(1,220)	1:44:A:VAL:HB	1:48:A:LEU:HD12	7	0.51	0.15	0.45
(1,220)	1:44:A:VAL:HB	1:148:A:ILE:HD11	7	0.51	0.15	0.45
(1,220)	1:44:A:VAL:HB	1:148:A:ILE:HD12	7	0.51	0.15	0.45
(2,1254)	1:78:A:LEU:HD13	1:74:A:PHE:HD1	7	0.51	0.09	0.46
(2,1254)	1:78:A:LEU:HD13	1:74:A:PHE:HD2	7	0.51	0.09	0.46
(2,1254)	1:78:A:LEU:HD12	1:74:A:PHE:HD1	7	0.51	0.09	0.46
(2,1254)	1:78:A:LEU:HD12	1:74:A:PHE:HD2	7	0.51	0.09	0.46
(2,519)	1:78:A:LEU:HD22	1:77:A:PHE:HD1	7	0.5	0.2	0.45
(2,519)	1:78:A:LEU:HD23	1:77:A:PHE:HD1	7	0.5	0.2	0.45
(2,519)	1:78:A:LEU:HD21	1:77:A:PHE:HD1	7	0.5	0.2	0.45
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	7	0.47	0.13	0.49
(2,434)	1:82:A:VAL:HG12	1:5:A:TYR:HD2	7	0.46	0.25	0.5
(2,434)	1:82:A:VAL:HG13	1:5:A:TYR:HD2	7	0.46	0.25	0.5
(2,434)	1:82:A:VAL:HG11	1:5:A:TYR:HD1	7	0.46	0.25	0.5
(2,434)	1:82:A:VAL:HG11	1:5:A:TYR:HD2	7	0.46	0.25	0.5
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG22	7	0.45	0.19	0.46
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG23	7	0.45	0.19	0.46
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG21	7	0.45	0.19	0.46
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG13	7	0.43	0.25	0.49
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG11	7	0.43	0.25	0.49
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG12	7	0.43	0.25	0.49
(2,338)	1:60:A:MET:HE2	1:60:A:MET:HA	7	0.4	0.18	0.31
(2,338)	1:60:A:MET:HE1	1:60:A:MET:HA	7	0.4	0.18	0.31
(2,338)	1:60:A:MET:HE3	1:60:A:MET:HA	7	0.4	0.18	0.31
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	7	0.4	0.21	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,122)	1:45:A:MET:HE3	1:48:A:LEU:HD13	7	0.4	0.21	0.35
(1,122)	1:45:A:MET:HE1	1:48:A:LEU:HD11	7	0.4	0.21	0.35
(1,122)	1:45:A:MET:HE2	1:48:A:LEU:HD11	7	0.4	0.21	0.35
(1,122)	1:157:A:LEU:HD11	1:157:A:LEU:HB3	7	0.4	0.21	0.35
(1,122)	1:45:A:MET:HE2	1:48:A:LEU:HD12	7	0.4	0.21	0.35
(1,122)	1:157:A:LEU:HD13	1:157:A:LEU:HB3	7	0.4	0.21	0.35
(2,521)	1:78:A:LEU:HD22	1:20:A:PHE:HB2	7	0.39	0.06	0.41
(2,521)	1:78:A:LEU:HD23	1:20:A:PHE:HB2	7	0.39	0.06	0.41
(2,521)	1:78:A:LEU:HD21	1:20:A:PHE:HB2	7	0.39	0.06	0.41
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	7	0.38	0.21	0.38
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG21	7	0.37	0.11	0.39
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG23	7	0.37	0.11	0.39
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG22	7	0.37	0.11	0.39
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB2	7	0.33	0.07	0.32
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB1	7	0.33	0.07	0.32
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB3	7	0.33	0.07	0.32
(2,1229)	1:81:A:MET:HE3	1:77:A:PHE:HD1	7	0.3	0.05	0.3
(2,1229)	1:81:A:MET:HE2	1:77:A:PHE:HD1	7	0.3	0.05	0.3
(2,1229)	1:81:A:MET:HE1	1:77:A:PHE:HD1	7	0.3	0.05	0.3
(2,344)	1:80:A:MET:HE1	1:80:A:MET:HA	7	0.24	0.08	0.21
(2,344)	1:80:A:MET:HE2	1:80:A:MET:HA	7	0.24	0.08	0.21
(2,344)	1:80:A:MET:HE3	1:80:A:MET:HA	7	0.24	0.08	0.21
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	7	0.24	0.08	0.24
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD1	7	0.24	0.08	0.24
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG23	7	0.2	0.07	0.18
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	7	0.2	0.07	0.18
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG22	7	0.2	0.07	0.18
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD1	7	0.2	0.06	0.23
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD2	7	0.2	0.06	0.23
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	7	0.17	0.02	0.17
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	7	0.16	0.03	0.16
(2,538)	1:78:A:LEU:HD11	1:78:A:LEU:HG	7	0.13	0.01	0.14
(2,538)	1:78:A:LEU:HD13	1:78:A:LEU:HG	7	0.13	0.01	0.14
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	7	0.11	0.01	0.11
(1,55)	1:148:A:ILE:HD11	1:153:A:MET:HE3	6	1.36	1.25	0.99
(1,55)	1:148:A:ILE:HD11	1:153:A:MET:HB3	6	1.36	1.25	0.99
(1,55)	1:148:A:ILE:HD13	1:153:A:MET:HE1	6	1.36	1.25	0.99
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD21	6	1.31	1.34	0.88
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD11	6	1.31	1.34	0.88
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD13	6	1.31	1.34	0.88
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD12	6	1.31	1.34	0.88
(1,325)	1:61:A:ILE:HD12	1:58:A:GLN:HG3	6	1.08	0.53	1.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,325)	1:61:A:ILE:HD12	1:64:A:VAL:HB	6	1.08	0.53	1.1
(1,325)	1:61:A:ILE:HD13	1:58:A:GLN:HG3	6	1.08	0.53	1.1
(2,1230)	1:162:A:ALA:HB3	1:155:A:GLN:HB3	6	1.03	0.62	1.06
(2,1230)	1:162:A:ALA:HB2	1:155:A:GLN:HB3	6	1.03	0.62	1.06
(2,1230)	1:162:A:ALA:HB1	1:155:A:GLN:HB3	6	1.03	0.62	1.06
(2,349)	1:45:A:MET:HE3	1:52:A:PRO:HD3	6	1.03	0.43	1.02
(2,349)	1:45:A:MET:HE1	1:52:A:PRO:HD3	6	1.03	0.43	1.02
(2,349)	1:45:A:MET:HE2	1:52:A:PRO:HD3	6	1.03	0.43	1.02
(2,465)	1:82:A:VAL:HG23	1:78:A:LEU:HB3	6	0.97	0.6	0.88
(2,465)	1:82:A:VAL:HG21	1:78:A:LEU:HB3	6	0.97	0.6	0.88
(2,465)	1:82:A:VAL:HG22	1:78:A:LEU:HB3	6	0.97	0.6	0.88
(1,312)	1:80:A:MET:HE2	1:60:A:MET:HG3	6	0.96	0.43	0.97
(1,312)	1:80:A:MET:HE2	1:27:A:PHE:HB2	6	0.96	0.43	0.97
(1,312)	1:80:A:MET:HE3	1:60:A:MET:HG3	6	0.96	0.43	0.97
(1,312)	1:80:A:MET:HE1	1:60:A:MET:HG3	6	0.96	0.43	0.97
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD21	6	0.92	0.5	1.02
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD23	6	0.92	0.5	1.02
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD22	6	0.92	0.5	1.02
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD11	6	0.79	0.18	0.9
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD12	6	0.79	0.18	0.9
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD13	6	0.79	0.18	0.9
(2,11)	1:142:A:THR:HB	1:143:A:LEU:HB2	6	0.77	0.75	0.34
(2,363)	1:154:A:MET:HE3	1:162:A:ALA:HB2	6	0.72	0.35	0.74
(2,363)	1:154:A:MET:HE2	1:162:A:ALA:HB3	6	0.72	0.35	0.74
(2,363)	1:154:A:MET:HE3	1:162:A:ALA:HB1	6	0.72	0.35	0.74
(2,363)	1:154:A:MET:HE1	1:162:A:ALA:HB2	6	0.72	0.35	0.74
(2,363)	1:154:A:MET:HE2	1:162:A:ALA:HB2	6	0.72	0.35	0.74
(2,1225)	1:64:A:VAL:HG11	1:76:A:GLU:HA	6	0.7	0.24	0.74
(2,1225)	1:64:A:VAL:HG12	1:76:A:GLU:HA	6	0.7	0.24	0.74
(2,1225)	1:64:A:VAL:HG13	1:76:A:GLU:HA	6	0.7	0.24	0.74
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD21	6	0.68	0.34	0.67
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD23	6	0.68	0.34	0.67
(2,1034)	1:35:A:SER:HA	1:73:A:ASP:HB3	6	0.68	0.36	0.79
(1,277)	1:61:A:ILE:HD11	1:58:A:GLN:HB2	6	0.68	0.26	0.6
(1,277)	1:58:A:GLN:HB2	1:61:A:ILE:HG22	6	0.68	0.26	0.6
(1,277)	1:58:A:GLN:HB2	1:61:A:ILE:HG23	6	0.68	0.26	0.6
(1,277)	1:61:A:ILE:HD13	1:58:A:GLN:HB3	6	0.68	0.26	0.6
(2,310)	1:148:A:ILE:HD11	1:148:A:ILE:HA	6	0.68	0.03	0.68
(2,310)	1:148:A:ILE:HD12	1:148:A:ILE:HA	6	0.68	0.03	0.68
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD3	6	0.67	0.46	0.57
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD2	6	0.67	0.46	0.57
(1,237)	1:44:A:VAL:HA	1:46:A:ARG:HG3	6	0.67	0.23	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,237)	1:52:A:PRO:HD3	1:46:A:ARG:HG3	6	0.67	0.23	0.65
(2,956)	1:50:A:GLN:HB3	1:45:A:MET:HB3	6	0.64	0.3	0.67
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG11	6	0.63	0.3	0.6
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG13	6	0.63	0.3	0.6
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD23	6	0.62	0.43	0.5
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD22	6	0.62	0.43	0.5
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD21	6	0.62	0.43	0.5
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG23	6	0.6	0.19	0.56
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG22	6	0.6	0.19	0.56
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG21	6	0.6	0.19	0.56
(2,397)	1:160:A:ALA:HB2	1:159:A:GLY:HA3	6	0.57	0.08	0.58
(2,397)	1:160:A:ALA:HB3	1:159:A:GLY:HA3	6	0.57	0.08	0.58
(2,397)	1:160:A:ALA:HB1	1:159:A:GLY:HA3	6	0.57	0.08	0.58
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD13	6	0.54	0.37	0.42
(1,316)	1:57:A:LEU:HA	1:143:A:LEU:HD12	6	0.54	0.37	0.42
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD12	6	0.54	0.37	0.42
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD11	6	0.54	0.37	0.42
(1,311)	1:85:A:MET:HE2	1:150:A:ALA:HB3	6	0.52	0.37	0.48
(1,311)	1:85:A:MET:HE2	1:8:A:ALA:HB3	6	0.52	0.37	0.48
(1,311)	1:85:A:MET:HE1	1:8:A:ALA:HB2	6	0.52	0.37	0.48
(1,311)	1:85:A:MET:HE2	1:150:A:ALA:HB1	6	0.52	0.37	0.48
(2,275)	1:56:A:GLU:HA	1:56:A:GLU:HG3	6	0.5	0.24	0.55
(2,1147)	1:140:A:ARG:HG3	1:141:A:PRO:HD3	6	0.49	0.15	0.54
(2,1147)	1:140:A:ARG:HG2	1:141:A:PRO:HD3	6	0.49	0.15	0.54
(1,83)	1:152:A:ALA:HB2	1:48:A:LEU:HD21	6	0.47	0.18	0.54
(1,83)	1:152:A:ALA:HB3	1:48:A:LEU:HD13	6	0.47	0.18	0.54
(1,83)	1:152:A:ALA:HB2	1:48:A:LEU:HD22	6	0.47	0.18	0.54
(1,83)	1:152:A:ALA:HB1	1:48:A:LEU:HD22	6	0.47	0.18	0.54
(1,83)	1:152:A:ALA:HB3	1:48:A:LEU:HD22	6	0.47	0.18	0.54
(2,1167)	1:53:A:THR:HB	1:54:A:PRO:HG3	6	0.45	0.11	0.46
(1,165)	1:18:A:ASN:HB2	1:17:A:LYS:HB2	6	0.44	0.13	0.42
(1,59)	1:47:A:MET:HE2	1:43:A:LYS:HA	6	0.41	0.31	0.24
(1,59)	1:47:A:MET:HE3	1:43:A:LYS:HA	6	0.41	0.31	0.24
(1,59)	1:47:A:MET:HE3	1:153:A:MET:HA	6	0.41	0.31	0.24
(1,59)	1:47:A:MET:HE1	1:153:A:MET:HA	6	0.41	0.31	0.24
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG23	6	0.41	0.07	0.41
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG21	6	0.41	0.07	0.41
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG22	6	0.41	0.07	0.41
(2,1100)	1:61:A:ILE:HD12	1:40:A:GLU:HB2	6	0.4	0.26	0.33
(2,1100)	1:61:A:ILE:HD13	1:40:A:GLU:HB2	6	0.4	0.26	0.33
(2,1100)	1:61:A:ILE:HD11	1:40:A:GLU:HB2	6	0.4	0.26	0.33
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HD11	6	0.34	0.14	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HG22	6	0.34	0.14	0.4
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HG23	6	0.34	0.14	0.4
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HD13	6	0.34	0.14	0.4
(2,427)	1:72:A:VAL:HG12	1:77:A:PHE:HB3	6	0.31	0.13	0.27
(2,427)	1:72:A:VAL:HG13	1:77:A:PHE:HB3	6	0.31	0.13	0.27
(2,427)	1:72:A:VAL:HG11	1:77:A:PHE:HB3	6	0.31	0.13	0.27
(1,139)	1:161:A:ARG:HD2	1:161:A:ARG:HB3	6	0.3	0.22	0.18
(1,139)	1:46:A:ARG:HD2	1:46:A:ARG:HG2	6	0.3	0.22	0.18
(1,139)	1:161:A:ARG:HD3	1:161:A:ARG:HB3	6	0.3	0.22	0.18
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD1	6	0.29	0.1	0.28
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD2	6	0.29	0.1	0.28
(2,188)	1:63:A:GLU:HA	1:63:A:GLU:HB2	6	0.29	0.02	0.29
(2,1122)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	6	0.29	0.13	0.24
(2,1122)	1:72:A:VAL:HG13	1:76:A:GLU:HG2	6	0.29	0.13	0.24
(2,1122)	1:72:A:VAL:HG12	1:76:A:GLU:HG2	6	0.29	0.13	0.24
(2,1131)	1:79:A:VAL:HA	1:83:A:ARG:HG2	6	0.28	0.13	0.33
(1,330)	1:2:A:ASP:HB3	1:5:A:TYR:HD1	6	0.25	0.08	0.24
(1,330)	1:83:A:ARG:HD2	1:5:A:TYR:HD2	6	0.25	0.08	0.24
(1,330)	1:83:A:ARG:HD2	1:5:A:TYR:HD1	6	0.25	0.08	0.24
(1,249)	1:77:A:PHE:HB3	1:75:A:ASP:HA	6	0.23	0.06	0.24
(1,286)	1:72:A:VAL:HG21	1:58:A:GLN:HA	6	0.23	0.15	0.14
(1,286)	1:72:A:VAL:HG22	1:58:A:GLN:HA	6	0.23	0.15	0.14
(2,1541)	1:40:A:GLU:H	1:39:A:LYS:HB2	6	0.22	0.08	0.24
(2,767)	1:45:A:MET:HA	1:45:A:MET:HG3	6	0.19	0.05	0.21
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	6	0.19	0.04	0.21
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB1	6	0.19	0.04	0.21
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB2	6	0.19	0.04	0.21
(1,401)	1:58:A:GLN:H	1:57:A:LEU:HA	6	0.18	0.02	0.19
(1,401)	1:58:A:GLN:H	1:55:A:GLU:HA	6	0.18	0.02	0.19
(1,207)	1:52:A:PRO:HG2	1:52:A:PRO:HB3	6	0.17	0.03	0.18
(1,207)	1:52:A:PRO:HB3	1:56:A:GLU:HB3	6	0.17	0.03	0.18
(2,918)	1:66:A:GLU:HA	1:66:A:GLU:HB2	6	0.13	0.01	0.13
(2,952)	1:33:A:ASP:HB2	1:33:A:ASP:HA	6	0.12	0.01	0.12
(1,318)	1:63:A:GLU:HG3	1:143:A:LEU:HD11	5	1.65	0.88	1.51
(1,318)	1:143:A:LEU:HD11	1:60:A:MET:HG2	5	1.65	0.88	1.51
(1,318)	1:63:A:GLU:HG3	1:143:A:LEU:HD12	5	1.65	0.88	1.51
(2,788)	1:86:A:LYS:HB3	1:90:A:LYS:HA	5	1.44	0.61	1.62
(1,73)	1:153:A:MET:HE1	1:157:A:LEU:HD13	5	1.25	0.25	1.12
(1,73)	1:148:A:ILE:HD11	1:153:A:MET:HE2	5	1.25	0.25	1.12
(1,73)	1:148:A:ILE:HG22	1:153:A:MET:HE3	5	1.25	0.25	1.12
(1,73)	1:153:A:MET:HE3	1:157:A:LEU:HD12	5	1.25	0.25	1.12
(1,73)	1:153:A:MET:HE2	1:157:A:LEU:HD12	5	1.25	0.25	1.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,138)	1:145:A:ARG:HD3	1:50:A:GLN:HG3	5	1.1	1.05	0.54
(1,138)	1:145:A:ARG:HD2	1:50:A:GLN:HG2	5	1.1	1.05	0.54
(2,1012)	1:24:A:PHE:HA	1:21:A:LYS:HD3	5	1.0	0.63	1.36
(2,490)	1:41:A:LEU:HD13	1:38:A:THR:HA	5	0.98	0.42	1.23
(2,490)	1:41:A:LEU:HD12	1:38:A:THR:HA	5	0.98	0.42	1.23
(2,498)	1:79:A:VAL:HG23	1:83:A:ARG:HD2	5	0.94	0.12	1.02
(2,498)	1:79:A:VAL:HG22	1:83:A:ARG:HD2	5	0.94	0.12	1.02
(2,498)	1:79:A:VAL:HG21	1:83:A:ARG:HD2	5	0.94	0.12	1.02
(2,1111)	1:71:A:THR:HG21	1:73:A:ASP:HB2	5	0.85	0.59	1.14
(2,1111)	1:71:A:THR:HG23	1:73:A:ASP:HB2	5	0.85	0.59	1.14
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG11	5	0.84	0.37	0.73
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG13	5	0.84	0.37	0.73
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG12	5	0.84	0.37	0.73
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HE3	5	0.81	0.46	0.97
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HB3	5	0.81	0.46	0.97
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HE1	5	0.81	0.46	0.97
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HE2	5	0.81	0.46	0.97
(1,117)	1:26:A:ILE:H	1:157:A:LEU:HD12	5	0.79	0.1	0.83
(1,117)	1:48:A:LEU:HD12	1:27:A:PHE:HE1	5	0.79	0.1	0.83
(1,117)	1:26:A:ILE:H	1:157:A:LEU:HD11	5	0.79	0.1	0.83
(1,97)	1:72:A:VAL:HG11	1:64:A:VAL:HB	5	0.79	0.35	1.06
(1,97)	1:72:A:VAL:HG13	1:64:A:VAL:HB	5	0.79	0.35	1.06
(1,97)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	5	0.79	0.35	1.06
(1,97)	1:72:A:VAL:HG12	1:76:A:GLU:HG2	5	0.79	0.35	1.06
(1,64)	1:80:A:MET:HE2	1:27:A:PHE:HE2	5	0.77	0.23	0.79
(1,64)	1:80:A:MET:HE3	1:27:A:PHE:HE2	5	0.77	0.23	0.79
(1,64)	1:80:A:MET:HE1	1:27:A:PHE:HE1	5	0.77	0.23	0.79
(2,1093)	1:13:A:THR:HG22	1:11:A:GLN:HG2	5	0.73	1.11	0.18
(1,338)	1:153:A:MET:HE2	1:20:A:PHE:HD1	5	0.71	0.15	0.72
(1,338)	1:153:A:MET:HE1	1:20:A:PHE:HD2	5	0.71	0.15	0.72
(1,338)	1:153:A:MET:HE1	1:20:A:PHE:HD1	5	0.71	0.15	0.72
(1,338)	1:20:A:PHE:HD1	1:19:A:GLU:HG2	5	0.71	0.15	0.72
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG23	5	0.69	0.35	0.7
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG22	5	0.69	0.35	0.7
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG21	5	0.69	0.35	0.7
(1,265)	1:146:A:VAL:HA	1:145:A:ARG:HG2	5	0.67	0.27	0.81
(1,265)	1:146:A:VAL:HA	1:143:A:LEU:HB3	5	0.67	0.27	0.81
(1,265)	1:146:A:VAL:HA	1:143:A:LEU:HB2	5	0.67	0.27	0.81
(1,265)	1:146:A:VAL:HA	1:145:A:ARG:HG3	5	0.67	0.27	0.81
(2,1699)	1:146:A:VAL:HG22	1:52:A:PRO:HA	5	0.59	0.25	0.57
(2,1699)	1:146:A:VAL:HG21	1:52:A:PRO:HA	5	0.59	0.25	0.57
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG11	5	0.59	0.27	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG12	5	0.59	0.27	0.67
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG13	5	0.59	0.27	0.67
(2,1162)	1:157:A:LEU:HD22	1:27:A:PHE:HB3	5	0.56	0.1	0.49
(2,1162)	1:157:A:LEU:HD23	1:27:A:PHE:HB3	5	0.56	0.1	0.49
(2,1162)	1:157:A:LEU:HD21	1:27:A:PHE:HB3	5	0.56	0.1	0.49
(2,274)	1:60:A:MET:HA	1:60:A:MET:HG2	5	0.55	0.27	0.58
(2,466)	1:82:A:VAL:HG21	1:83:A:ARG:HB2	5	0.53	0.69	0.19
(2,466)	1:82:A:VAL:HG23	1:83:A:ARG:HB2	5	0.53	0.69	0.19
(2,466)	1:82:A:VAL:HG22	1:83:A:ARG:HB2	5	0.53	0.69	0.19
(1,350)	1:4:A:ILE:HD13	1:5:A:TYR:HE2	5	0.5	0.12	0.46
(1,350)	1:79:A:VAL:HG13	1:5:A:TYR:HE1	5	0.5	0.12	0.46
(1,350)	1:79:A:VAL:HG11	1:5:A:TYR:HE1	5	0.5	0.12	0.46
(1,350)	1:4:A:ILE:HD13	1:5:A:TYR:HE1	5	0.5	0.12	0.46
(2,866)	1:137:A:LYS:HB2	1:138:A:PHE:HD1	5	0.49	0.1	0.49
(2,866)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	5	0.49	0.1	0.49
(2,866)	1:137:A:LYS:HB3	1:138:A:PHE:HD1	5	0.49	0.1	0.49
(2,1434)	1:56:A:GLU:H	1:56:A:GLU:HB3	5	0.49	0.05	0.47
(1,405)	1:60:A:MET:H	1:60:A:MET:HG2	5	0.45	0.18	0.5
(1,405)	1:60:A:MET:H	1:59:A:GLU:HG3	5	0.45	0.18	0.5
(1,298)	1:148:A:ILE:HG21	1:27:A:PHE:HZ	5	0.45	0.3	0.28
(1,298)	1:148:A:ILE:HG23	1:27:A:PHE:HZ	5	0.45	0.3	0.28
(1,298)	1:148:A:ILE:HG22	1:27:A:PHE:HZ	5	0.45	0.3	0.28
(2,1170)	1:161:A:ARG:HD2	1:26:A:ILE:HD11	5	0.44	0.22	0.41
(2,1170)	1:161:A:ARG:HD2	1:26:A:ILE:HD12	5	0.44	0.22	0.41
(2,1170)	1:161:A:ARG:HD3	1:26:A:ILE:HD11	5	0.44	0.22	0.41
(2,1170)	1:161:A:ARG:HD2	1:26:A:ILE:HD13	5	0.44	0.22	0.41
(2,1007)	1:22:A:ALA:HB2	1:25:A:ASP:HB2	5	0.4	0.08	0.4
(2,1007)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	5	0.4	0.08	0.4
(2,1007)	1:22:A:ALA:HB3	1:25:A:ASP:HB2	5	0.4	0.08	0.4
(1,287)	1:75:A:ASP:HB2	1:78:A:LEU:HB2	5	0.37	0.12	0.36
(2,1135)	1:82:A:VAL:HG12	1:5:A:TYR:HE2	5	0.37	0.17	0.3
(2,1135)	1:82:A:VAL:HG13	1:5:A:TYR:HE2	5	0.37	0.17	0.3
(2,1135)	1:82:A:VAL:HG11	1:5:A:TYR:HE1	5	0.37	0.17	0.3
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG12	5	0.37	0.13	0.4
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG13	5	0.37	0.13	0.4
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG11	5	0.37	0.13	0.4
(1,14)	1:142:A:THR:HA	1:143:A:LEU:HB2	5	0.36	0.17	0.29
(2,417)	1:146:A:VAL:HA	1:146:A:VAL:HG21	5	0.36	0.11	0.41
(2,417)	1:146:A:VAL:HA	1:146:A:VAL:HG23	5	0.36	0.11	0.41
(2,505)	1:72:A:VAL:HG22	1:64:A:VAL:HB	5	0.36	0.19	0.32
(2,505)	1:72:A:VAL:HG21	1:64:A:VAL:HB	5	0.36	0.19	0.32
(2,505)	1:72:A:VAL:HG23	1:64:A:VAL:HB	5	0.36	0.19	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,892)	1:56:A:GLU:HA	1:56:A:GLU:HB2	5	0.34	0.04	0.36
(2,381)	1:7:A:ALA:HB3	1:10:A:GLU:HB2	5	0.33	0.08	0.33
(2,381)	1:7:A:ALA:HB2	1:10:A:GLU:HB2	5	0.33	0.08	0.33
(2,381)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	5	0.33	0.08	0.33
(2,1617)	1:48:A:LEU:H	1:48:A:LEU:HD12	5	0.32	0.19	0.25
(2,1617)	1:48:A:LEU:H	1:48:A:LEU:HD11	5	0.32	0.19	0.25
(2,619)	1:46:A:ARG:HD3	1:46:A:ARG:HG3	5	0.31	0.02	0.31
(2,1153)	1:154:A:MET:HE3	1:150:A:ALA:HA	5	0.3	0.04	0.3
(2,1153)	1:154:A:MET:HE2	1:150:A:ALA:HA	5	0.3	0.04	0.3
(2,1153)	1:154:A:MET:HE1	1:150:A:ALA:HA	5	0.3	0.04	0.3
(2,1006)	1:22:A:ALA:HB2	1:25:A:ASP:HB3	5	0.29	0.1	0.26
(2,1006)	1:22:A:ALA:HB1	1:25:A:ASP:HB3	5	0.29	0.1	0.26
(2,1006)	1:22:A:ALA:HB3	1:25:A:ASP:HB3	5	0.29	0.1	0.26
(1,190)	1:155:A:GLN:HG3	1:155:A:GLN:HA	5	0.28	0.04	0.29
(1,34)	1:16:A:GLN:HA	1:19:A:GLU:HB2	5	0.28	0.11	0.25
(1,334)	1:27:A:PHE:HD2	1:40:A:GLU:HG2	5	0.28	0.11	0.22
(1,334)	1:40:A:GLU:HB2	1:27:A:PHE:HD2	5	0.28	0.11	0.22
(1,334)	1:27:A:PHE:HD1	1:40:A:GLU:HG2	5	0.28	0.11	0.22
(2,177)	1:43:A:LYS:HA	1:43:A:LYS:HG2	5	0.28	0.25	0.17
(2,467)	1:9:A:VAL:HG11	1:6:A:LYS:HA	5	0.27	0.09	0.26
(2,467)	1:9:A:VAL:HG12	1:6:A:LYS:HA	5	0.27	0.09	0.26
(2,467)	1:9:A:VAL:HG13	1:6:A:LYS:HA	5	0.27	0.09	0.26
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HD12	5	0.26	0.07	0.29
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HG22	5	0.26	0.07	0.29
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HG23	5	0.26	0.07	0.29
(2,787)	1:139:A:LYS:HB2	1:139:A:LYS:HA	5	0.24	0.01	0.24
(2,996)	1:157:A:LEU:HG	1:157:A:LEU:HA	5	0.23	0.03	0.24
(2,24)	1:54:A:PRO:HA	1:54:A:PRO:HD3	5	0.23	0.12	0.18
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD21	5	0.23	0.05	0.25
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD22	5	0.23	0.05	0.25
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD23	5	0.23	0.05	0.25
(2,328)	1:47:A:MET:HE1	1:47:A:MET:HG3	5	0.22	0.03	0.22
(2,328)	1:47:A:MET:HE2	1:47:A:MET:HG3	5	0.22	0.03	0.22
(1,362)	1:19:A:GLU:H	1:18:A:ASN:HB2	5	0.22	0.08	0.18
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD23	5	0.21	0.1	0.15
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD21	5	0.21	0.1	0.15
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD22	5	0.21	0.1	0.15
(2,385)	1:156:A:ALA:HB1	1:153:A:MET:HA	5	0.2	0.05	0.22
(2,385)	1:156:A:ALA:HB3	1:153:A:MET:HA	5	0.2	0.05	0.22
(1,404)	1:55:A:GLU:H	1:55:A:GLU:HG2	5	0.2	0.04	0.21
(1,404)	1:55:A:GLU:H	1:54:A:PRO:HG3	5	0.2	0.04	0.21
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD23	5	0.19	0.02	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD21	5	0.19	0.02	0.19
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD22	5	0.19	0.02	0.19
(2,883)	1:1:A:MET:HG3	1:6:A:LYS:HB2	5	0.19	0.07	0.17
(2,1088)	1:51:A:ASN:HB3	1:52:A:PRO:HD3	5	0.19	0.04	0.18
(2,136)	1:15:A:GLU:HA	1:15:A:GLU:HG2	5	0.18	0.04	0.18
(2,136)	1:15:A:GLU:HA	1:15:A:GLU:HG3	5	0.18	0.04	0.18
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB1	5	0.16	0.01	0.17
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB2	5	0.16	0.01	0.17
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB3	5	0.16	0.01	0.17
(2,923)	1:63:A:GLU:HB2	1:63:A:GLU:HG2	5	0.15	0.0	0.15
(1,26)	1:89:A:SER:HB3	1:89:A:SER:HA	5	0.14	0.02	0.13
(1,26)	1:89:A:SER:HB2	1:89:A:SER:HA	5	0.14	0.02	0.13
(2,168)	1:89:A:SER:HA	1:137:A:LYS:HB2	4	2.06	3.22	0.25
(2,168)	1:89:A:SER:HA	1:137:A:LYS:HB3	4	2.06	3.22	0.25
(2,507)	1:48:A:LEU:HD23	1:155:A:GLN:HG3	4	2.02	0.71	1.92
(2,507)	1:48:A:LEU:HD22	1:155:A:GLN:HG3	4	2.02	0.71	1.92
(2,387)	1:156:A:ALA:HB1	1:155:A:GLN:HG3	4	2.0	0.41	1.88
(2,387)	1:156:A:ALA:HB2	1:155:A:GLN:HG3	4	2.0	0.41	1.88
(2,840)	1:47:A:MET:HG2	1:48:A:LEU:HG	4	1.98	0.17	2.0
(1,208)	1:63:A:GLU:HG3	1:64:A:VAL:HG23	4	1.74	0.34	1.7
(1,208)	1:63:A:GLU:HG3	1:64:A:VAL:HG21	4	1.74	0.34	1.7
(1,208)	1:63:A:GLU:HG3	1:143:A:LEU:HD12	4	1.74	0.34	1.7
(1,208)	1:59:A:GLU:HG3	1:146:A:VAL:HG23	4	1.74	0.34	1.7
(1,29)	1:60:A:MET:HA	1:64:A:VAL:HG23	4	1.48	0.31	1.32
(1,29)	1:60:A:MET:HA	1:64:A:VAL:HG21	4	1.48	0.31	1.32
(1,29)	1:60:A:MET:HA	1:143:A:LEU:HD12	4	1.48	0.31	1.32
(1,29)	1:60:A:MET:HA	1:64:A:VAL:HG22	4	1.48	0.31	1.32
(1,156)	1:137:A:LYS:HE2	1:86:A:LYS:HB3	4	1.45	0.9	1.44
(1,156)	1:137:A:LYS:HE3	1:86:A:LYS:HB3	4	1.45	0.9	1.44
(1,62)	1:60:A:MET:HE1	1:142:A:THR:HG21	4	1.28	0.13	1.23
(1,62)	1:60:A:MET:HE2	1:142:A:THR:HG21	4	1.28	0.13	1.23
(1,62)	1:60:A:MET:HE1	1:142:A:THR:HG22	4	1.28	0.13	1.23
(1,62)	1:60:A:MET:HE2	1:142:A:THR:HG22	4	1.28	0.13	1.23
(2,14)	1:79:A:VAL:HA	1:82:A:VAL:HG21	4	1.23	0.3	1.09
(2,14)	1:79:A:VAL:HA	1:82:A:VAL:HG22	4	1.23	0.3	1.09
(1,141)	1:145:A:ARG:HD2	1:146:A:VAL:HG12	4	1.1	0.45	1.26
(1,141)	1:145:A:ARG:HD2	1:146:A:VAL:HG13	4	1.1	0.45	1.26
(1,141)	1:145:A:ARG:HD3	1:146:A:VAL:HG12	4	1.1	0.45	1.26
(2,1154)	1:151:A:ASP:HB3	1:154:A:MET:HB2	4	1.07	0.2	0.99
(2,1154)	1:151:A:ASP:HB2	1:154:A:MET:HB2	4	1.07	0.2	0.99
(2,1150)	1:142:A:THR:HB	1:143:A:LEU:HD21	4	1.05	1.05	0.6
(2,1150)	1:142:A:THR:HB	1:143:A:LEU:HD22	4	1.05	1.05	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1150)	1:142:A:THR:HB	1:143:A:LEU:HD23	4	1.05	1.05	0.6
(1,107)	1:61:A:ILE:HD13	1:38:A:THR:HG23	4	0.98	0.07	0.99
(1,107)	1:61:A:ILE:HG22	1:38:A:THR:HG21	4	0.98	0.07	0.99
(1,107)	1:61:A:ILE:HG23	1:38:A:THR:HG22	4	0.98	0.07	0.99
(1,107)	1:61:A:ILE:HG23	1:38:A:THR:HG23	4	0.98	0.07	0.99
(2,1242)	1:79:A:VAL:HG22	1:5:A:TYR:HD1	4	0.98	0.26	0.85
(2,1242)	1:79:A:VAL:HG23	1:5:A:TYR:HD1	4	0.98	0.26	0.85
(2,554)	1:41:A:LEU:HD22	1:45:A:MET:HG2	4	0.95	0.31	0.9
(2,554)	1:41:A:LEU:HD21	1:45:A:MET:HG2	4	0.95	0.31	0.9
(2,554)	1:41:A:LEU:HD23	1:45:A:MET:HG2	4	0.95	0.31	0.9
(1,266)	1:153:A:MET:HE1	1:157:A:LEU:HA	4	0.88	0.64	0.57
(1,266)	1:153:A:MET:HE3	1:157:A:LEU:HA	4	0.88	0.64	0.57
(2,1215)	1:60:A:MET:HG3	1:146:A:VAL:HG21	4	0.82	0.41	0.74
(2,1215)	1:60:A:MET:HG3	1:146:A:VAL:HG23	4	0.82	0.41	0.74
(2,1215)	1:60:A:MET:HG3	1:146:A:VAL:HG22	4	0.82	0.41	0.74
(2,22)	1:38:A:THR:HA	1:61:A:ILE:HG13	4	0.76	0.44	0.76
(1,394)	1:79:A:VAL:H	1:79:A:VAL:HG21	4	0.76	0.07	0.78
(1,394)	1:79:A:VAL:H	1:78:A:LEU:HB2	4	0.76	0.07	0.78
(1,283)	1:65:A:ASP:HB3	1:61:A:ILE:HD13	4	0.63	0.21	0.59
(1,283)	1:65:A:ASP:HB3	1:61:A:ILE:HD12	4	0.63	0.21	0.59
(2,1146)	1:161:A:ARG:HB2	1:158:A:LEU:HD23	4	0.63	0.35	0.59
(2,1146)	1:161:A:ARG:HB2	1:158:A:LEU:HD22	4	0.63	0.35	0.59
(2,1008)	1:23:A:ALA:HA	1:26:A:ILE:HG12	4	0.62	0.02	0.62
(2,836)	1:10:A:GLU:HA	1:10:A:GLU:HG3	4	0.61	0.08	0.65
(2,321)	1:85:A:MET:HE3	1:85:A:MET:HG2	4	0.6	0.03	0.6
(2,321)	1:85:A:MET:HE2	1:85:A:MET:HG2	4	0.6	0.03	0.6
(2,321)	1:85:A:MET:HE1	1:85:A:MET:HG2	4	0.6	0.03	0.6
(1,4)	1:38:A:THR:HB	1:61:A:ILE:HD13	4	0.57	0.09	0.62
(1,4)	1:38:A:THR:HB	1:61:A:ILE:HD11	4	0.57	0.09	0.62
(1,130)	1:52:A:PRO:HG3	1:57:A:LEU:HD13	4	0.57	0.3	0.43
(1,130)	1:52:A:PRO:HG3	1:57:A:LEU:HD11	4	0.57	0.3	0.43
(1,130)	1:52:A:PRO:HG3	1:57:A:LEU:HD12	4	0.57	0.3	0.43
(1,130)	1:52:A:PRO:HG3	1:146:A:VAL:HG22	4	0.57	0.3	0.43
(2,1365)	1:152:A:ALA:H	1:151:A:ASP:HB2	4	0.56	0.12	0.62
(2,1365)	1:152:A:ALA:H	1:151:A:ASP:HB3	4	0.56	0.12	0.62
(1,288)	1:75:A:ASP:HB3	1:78:A:LEU:HB2	4	0.54	0.2	0.52
(2,472)	1:9:A:VAL:HG12	1:6:A:LYS:HG2	4	0.54	0.15	0.61
(2,472)	1:9:A:VAL:HG11	1:6:A:LYS:HG2	4	0.54	0.15	0.61
(2,472)	1:9:A:VAL:HG13	1:6:A:LYS:HG2	4	0.54	0.15	0.61
(1,269)	1:44:A:VAL:HG23	1:40:A:GLU:HB3	4	0.52	0.17	0.54
(1,269)	1:44:A:VAL:HG22	1:40:A:GLU:HB3	4	0.52	0.17	0.54
(1,269)	1:44:A:VAL:HG22	1:47:A:MET:HB2	4	0.52	0.17	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,86)	1:150:A:ALA:HB3	1:151:A:ASP:HA	4	0.51	0.29	0.38
(1,86)	1:85:A:MET:HA	1:150:A:ALA:HB2	4	0.51	0.29	0.38
(1,86)	1:85:A:MET:HA	1:150:A:ALA:HB1	4	0.51	0.29	0.38
(1,86)	1:85:A:MET:HA	1:150:A:ALA:HB3	4	0.51	0.29	0.38
(1,214)	1:43:A:LYS:HD3	1:40:A:GLU:HG2	4	0.5	0.29	0.49
(1,214)	1:43:A:LYS:HD2	1:40:A:GLU:HG2	4	0.5	0.29	0.49
(1,89)	1:153:A:MET:HE1	1:44:A:VAL:HG11	4	0.49	0.33	0.48
(1,89)	1:153:A:MET:HE1	1:44:A:VAL:HG13	4	0.49	0.33	0.48
(1,89)	1:44:A:VAL:HG11	1:153:A:MET:HB3	4	0.49	0.33	0.48
(1,19)	1:14:A:GLU:HA	1:17:A:LYS:HE2	4	0.47	0.13	0.5
(1,270)	1:44:A:VAL:HG11	1:27:A:PHE:HB2	4	0.45	0.33	0.34
(1,270)	1:44:A:VAL:HG11	1:47:A:MET:HG3	4	0.45	0.33	0.34
(1,270)	1:44:A:VAL:HG12	1:47:A:MET:HG3	4	0.45	0.33	0.34
(2,556)	1:41:A:LEU:HD23	1:41:A:LEU:HB2	4	0.45	0.13	0.48
(2,556)	1:41:A:LEU:HD21	1:41:A:LEU:HB2	4	0.45	0.13	0.48
(1,315)	1:142:A:THR:HG21	1:147:A:ARG:HA	4	0.45	0.17	0.53
(1,315)	1:142:A:THR:HG22	1:147:A:ARG:HA	4	0.45	0.17	0.53
(1,315)	1:142:A:THR:HG23	1:84:A:SER:HA	4	0.45	0.17	0.53
(2,616)	1:140:A:ARG:HD3	1:140:A:ARG:HA	4	0.42	0.09	0.43
(2,616)	1:140:A:ARG:HD2	1:140:A:ARG:HA	4	0.42	0.09	0.43
(2,311)	1:148:A:ILE:HD13	1:45:A:MET:HE2	4	0.42	0.19	0.45
(2,311)	1:148:A:ILE:HD13	1:45:A:MET:HE3	4	0.42	0.19	0.45
(2,311)	1:148:A:ILE:HD11	1:45:A:MET:HE3	4	0.42	0.19	0.45
(1,105)	1:57:A:LEU:HA	1:38:A:THR:HG23	4	0.42	0.06	0.42
(1,105)	1:57:A:LEU:HA	1:38:A:THR:HG22	4	0.42	0.06	0.42
(1,105)	1:57:A:LEU:HA	1:38:A:THR:HG21	4	0.42	0.06	0.42
(2,1196)	1:1:A:MET:HE2	1:6:A:LYS:HG2	4	0.42	0.17	0.4
(2,1196)	1:1:A:MET:HE1	1:6:A:LYS:HG2	4	0.42	0.17	0.4
(2,396)	1:155:A:GLN:HA	1:162:A:ALA:HB2	4	0.42	0.1	0.43
(1,71)	1:153:A:MET:HE1	1:27:A:PHE:HA	4	0.41	0.08	0.41
(1,71)	1:153:A:MET:HE3	1:153:A:MET:HA	4	0.41	0.08	0.41
(1,71)	1:153:A:MET:HE1	1:153:A:MET:HA	4	0.41	0.08	0.41
(2,1145)	1:161:A:ARG:HB3	1:26:A:ILE:HD11	4	0.4	0.19	0.43
(1,337)	1:23:A:ALA:HB1	1:20:A:PHE:HD2	4	0.39	0.25	0.3
(1,337)	1:44:A:VAL:HB	1:27:A:PHE:HE1	4	0.39	0.25	0.3
(1,337)	1:44:A:VAL:HB	1:27:A:PHE:HE2	4	0.39	0.25	0.3
(1,321)	1:146:A:VAL:HG11	1:56:A:GLU:HB2	4	0.39	0.1	0.44
(2,835)	1:7:A:ALA:HB3	1:10:A:GLU:HG3	4	0.39	0.12	0.36
(2,835)	1:7:A:ALA:HB1	1:10:A:GLU:HG3	4	0.39	0.12	0.36
(2,494)	1:79:A:VAL:H	1:79:A:VAL:HG21	4	0.38	0.08	0.4
(2,1436)	1:156:A:ALA:H	1:155:A:GLN:HB2	4	0.38	0.09	0.38
(1,295)	1:142:A:THR:HA	1:147:A:ARG:HD3	4	0.37	0.19	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,295)	1:147:A:ARG:HD2	1:142:A:THR:HA	4	0.37	0.19	0.3
(2,693)	1:27:A:PHE:HB2	1:36:A:ILE:HD13	4	0.35	0.12	0.4
(2,693)	1:27:A:PHE:HB2	1:36:A:ILE:HD11	4	0.35	0.12	0.4
(2,317)	1:61:A:ILE:HG22	1:38:A:THR:HG21	4	0.34	0.11	0.34
(2,317)	1:61:A:ILE:HG21	1:38:A:THR:HG22	4	0.34	0.11	0.34
(2,317)	1:61:A:ILE:HG22	1:38:A:THR:HG22	4	0.34	0.11	0.34
(2,475)	1:38:A:THR:HG22	1:61:A:ILE:HB	4	0.34	0.1	0.36
(2,475)	1:38:A:THR:HG23	1:61:A:ILE:HB	4	0.34	0.1	0.36
(2,1035)	1:35:A:SER:HB2	1:73:A:ASP:HB3	4	0.34	0.19	0.33
(1,317)	1:143:A:LEU:HD13	1:56:A:GLU:HA	4	0.33	0.3	0.18
(1,317)	1:143:A:LEU:HD12	1:56:A:GLU:HA	4	0.33	0.3	0.18
(1,317)	1:143:A:LEU:HD13	1:89:A:SER:HB3	4	0.33	0.3	0.18
(1,52)	1:61:A:ILE:HD12	1:36:A:ILE:HB	4	0.33	0.04	0.32
(1,52)	1:61:A:ILE:HD13	1:36:A:ILE:HB	4	0.33	0.04	0.32
(2,1216)	1:52:A:PRO:HA	1:146:A:VAL:HG21	4	0.33	0.15	0.34
(2,1216)	1:52:A:PRO:HA	1:146:A:VAL:HG22	4	0.33	0.15	0.34
(2,1296)	1:5:A:TYR:HE2	1:90:A:LYS:HD3	4	0.33	0.19	0.24
(2,1296)	1:5:A:TYR:HE1	1:90:A:LYS:HD3	4	0.33	0.19	0.24
(2,1296)	1:5:A:TYR:HE2	1:90:A:LYS:HD2	4	0.33	0.19	0.24
(1,155)	1:14:A:GLU:HA	1:17:A:LYS:HE2	4	0.32	0.07	0.34
(1,155)	1:43:A:LYS:HE2	1:28:A:VAL:HA	4	0.32	0.07	0.34
(2,517)	1:57:A:LEU:HD22	1:41:A:LEU:HB2	4	0.32	0.13	0.34
(2,517)	1:57:A:LEU:HD23	1:41:A:LEU:HB2	4	0.32	0.13	0.34
(1,72)	1:153:A:MET:HE1	1:157:A:LEU:HB2	4	0.32	0.13	0.39
(1,72)	1:153:A:MET:HE3	1:157:A:LEU:HB2	4	0.32	0.13	0.39
(1,72)	1:153:A:MET:HE3	1:81:A:MET:HE3	4	0.32	0.13	0.39
(2,453)	1:79:A:VAL:HG13	1:83:A:ARG:HG2	4	0.31	0.08	0.3
(2,453)	1:79:A:VAL:HG12	1:83:A:ARG:HG2	4	0.31	0.08	0.3
(1,159)	1:151:A:ASP:HB2	1:152:A:ALA:HB3	4	0.3	0.22	0.18
(1,159)	1:150:A:ALA:HB1	1:151:A:ASP:HB2	4	0.3	0.22	0.18
(1,159)	1:150:A:ALA:HB1	1:151:A:ASP:HB3	4	0.3	0.22	0.18
(1,385)	1:46:A:ARG:H	1:46:A:ARG:HG2	4	0.29	0.11	0.34
(1,385)	1:46:A:ARG:H	1:46:A:ARG:HB2	4	0.29	0.11	0.34
(1,226)	1:23:A:ALA:HB1	1:158:A:LEU:HD21	4	0.29	0.07	0.28
(1,226)	1:158:A:LEU:HD23	1:161:A:ARG:HB3	4	0.29	0.07	0.28
(1,226)	1:23:A:ALA:HB3	1:158:A:LEU:HD23	4	0.29	0.07	0.28
(2,15)	1:79:A:VAL:HA	1:79:A:VAL:HG13	4	0.28	0.06	0.29
(2,15)	1:79:A:VAL:HA	1:79:A:VAL:HG11	4	0.28	0.06	0.29
(2,15)	1:79:A:VAL:HA	1:79:A:VAL:HG12	4	0.28	0.06	0.29
(2,916)	1:63:A:GLU:HB3	1:64:A:VAL:HG23	4	0.28	0.15	0.23
(2,916)	1:63:A:GLU:HB3	1:64:A:VAL:HG21	4	0.28	0.15	0.23
(2,916)	1:63:A:GLU:HB3	1:64:A:VAL:HG22	4	0.28	0.15	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,231)	1:23:A:ALA:HB2	1:24:A:PHE:HA	4	0.27	0.11	0.24
(1,231)	1:23:A:ALA:HB3	1:24:A:PHE:HA	4	0.27	0.11	0.24
(1,347)	1:5:A:TYR:HE1	1:2:A:ASP:HB3	4	0.27	0.16	0.23
(1,347)	1:83:A:ARG:HD2	1:5:A:TYR:HE2	4	0.27	0.16	0.23
(2,757)	1:82:A:VAL:HA	1:85:A:MET:HB2	4	0.27	0.17	0.2
(2,1232)	1:44:A:VAL:HG11	1:153:A:MET:HA	4	0.27	0.13	0.21
(2,1232)	1:44:A:VAL:HG12	1:153:A:MET:HA	4	0.27	0.13	0.21
(2,775)	1:155:A:GLN:HA	1:155:A:GLN:HG2	4	0.26	0.03	0.26
(2,1259)	1:77:A:PHE:HA	1:77:A:PHE:HD1	4	0.26	0.02	0.25
(2,682)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	4	0.26	0.11	0.26
(2,361)	1:154:A:MET:HE1	1:154:A:MET:HB3	4	0.23	0.06	0.22
(2,361)	1:154:A:MET:HE3	1:154:A:MET:HB3	4	0.23	0.06	0.22
(2,361)	1:154:A:MET:HE2	1:154:A:MET:HB3	4	0.23	0.06	0.22
(1,403)	1:55:A:GLU:H	1:54:A:PRO:HB3	4	0.23	0.08	0.2
(2,442)	1:79:A:VAL:H	1:79:A:VAL:HG13	4	0.22	0.06	0.25
(2,442)	1:79:A:VAL:H	1:79:A:VAL:HG11	4	0.22	0.06	0.25
(2,442)	1:79:A:VAL:H	1:79:A:VAL:HG12	4	0.22	0.06	0.25
(2,62)	1:89:A:SER:HB2	1:89:A:SER:HA	4	0.2	0.0	0.2
(2,204)	1:10:A:GLU:HA	1:9:A:VAL:HG12	4	0.2	0.08	0.18
(2,204)	1:10:A:GLU:HA	1:9:A:VAL:HG13	4	0.2	0.08	0.18
(2,204)	1:10:A:GLU:HA	1:9:A:VAL:HG11	4	0.2	0.08	0.18
(2,474)	1:38:A:THR:HG23	1:57:A:LEU:HB2	4	0.18	0.06	0.17
(2,474)	1:38:A:THR:HG22	1:57:A:LEU:HB2	4	0.18	0.06	0.17
(2,474)	1:38:A:THR:HG21	1:57:A:LEU:HB2	4	0.18	0.06	0.17
(2,316)	1:61:A:ILE:HG22	1:61:A:ILE:HG12	4	0.18	0.05	0.2
(2,316)	1:61:A:ILE:HG23	1:61:A:ILE:HG12	4	0.18	0.05	0.2
(1,304)	1:51:A:ASN:HB2	1:52:A:PRO:HD2	4	0.17	0.04	0.16
(1,304)	1:52:A:PRO:HD2	1:45:A:MET:HG2	4	0.17	0.04	0.16
(1,310)	1:150:A:ALA:HA	1:148:A:ILE:HG22	4	0.16	0.05	0.16
(1,310)	1:84:A:SER:HB3	1:148:A:ILE:HG21	4	0.16	0.05	0.16
(1,310)	1:84:A:SER:HB3	1:148:A:ILE:HG22	4	0.16	0.05	0.16
(2,1172)	1:43:A:LYS:HG3	1:44:A:VAL:HG21	4	0.16	0.06	0.14
(2,1172)	1:43:A:LYS:HG3	1:44:A:VAL:HG22	4	0.16	0.06	0.14
(2,1172)	1:43:A:LYS:HG3	1:44:A:VAL:HG23	4	0.16	0.06	0.14
(1,133)	1:17:A:LYS:HG2	1:12:A:LEU:HD11	4	0.15	0.04	0.15
(1,133)	1:17:A:LYS:HG2	1:12:A:LEU:HD13	4	0.15	0.04	0.15
(2,73)	1:24:A:PHE:HA	1:74:A:PHE:HD1	4	0.15	0.01	0.15
(2,73)	1:24:A:PHE:HA	1:74:A:PHE:HD2	4	0.15	0.01	0.15
(2,227)	1:7:A:ALA:HA	1:6:A:LYS:HB3	4	0.14	0.01	0.14
(2,164)	1:73:A:ASP:HA	1:73:A:ASP:HB3	4	0.14	0.0	0.14
(2,183)	1:32:A:GLU:HA	1:32:A:GLU:HB2	4	0.14	0.05	0.12
(2,183)	1:32:A:GLU:HA	1:32:A:GLU:HB3	4	0.14	0.05	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,154)	1:6:A:LYS:HE3	1:6:A:LYS:HG2	4	0.12	0.02	0.12
(2,27)	1:54:A:PRO:HA	1:54:A:PRO:HB2	4	0.11	0.0	0.11
(2,222)	1:141:A:PRO:HD3	1:140:A:ARG:HA	3	1.77	0.07	1.78
(2,356)	1:153:A:MET:HE2	1:27:A:PHE:HB2	3	1.56	0.03	1.56
(2,356)	1:153:A:MET:HE1	1:27:A:PHE:HB2	3	1.56	0.03	1.56
(2,441)	1:146:A:VAL:HG12	1:145:A:ARG:HB3	3	1.36	1.14	1.02
(2,441)	1:146:A:VAL:HG13	1:145:A:ARG:HB3	3	1.36	1.14	1.02
(2,377)	1:150:A:ALA:HB1	1:85:A:MET:HG2	3	1.27	1.52	0.25
(2,377)	1:150:A:ALA:HB2	1:85:A:MET:HG2	3	1.27	1.52	0.25
(2,476)	1:38:A:THR:HG22	1:61:A:ILE:HG12	3	1.24	0.62	1.45
(2,476)	1:38:A:THR:HG23	1:61:A:ILE:HG12	3	1.24	0.62	1.45
(2,352)	1:148:A:ILE:HG21	1:153:A:MET:HB3	3	0.93	0.41	0.9
(1,195)	1:148:A:ILE:HG21	1:153:A:MET:HB3	3	0.9	0.41	0.87
(1,169)	1:56:A:GLU:HG3	1:55:A:GLU:HB3	3	0.86	0.44	0.79
(1,169)	1:56:A:GLU:HG3	1:52:A:PRO:HB2	3	0.86	0.44	0.79
(2,18)	1:38:A:THR:HA	1:61:A:ILE:HG12	3	0.84	0.35	0.78
(2,394)	1:156:A:ALA:HB2	1:157:A:LEU:HD21	3	0.83	0.03	0.83
(2,394)	1:156:A:ALA:HB1	1:157:A:LEU:HD21	3	0.83	0.03	0.83
(2,394)	1:156:A:ALA:HB3	1:157:A:LEU:HD21	3	0.83	0.03	0.83
(2,312)	1:148:A:ILE:HD13	1:148:A:ILE:HB	3	0.8	0.41	1.09
(2,312)	1:148:A:ILE:HD11	1:148:A:ILE:HB	3	0.8	0.41	1.09
(1,110)	1:41:A:LEU:HD13	1:60:A:MET:HG2	3	0.8	0.4	1.03
(1,110)	1:41:A:LEU:HD11	1:60:A:MET:HG2	3	0.8	0.4	1.03
(2,340)	1:60:A:MET:HE3	1:60:A:MET:HG2	3	0.79	0.09	0.84
(2,622)	1:145:A:ARG:HA	1:145:A:ARG:HD2	3	0.79	0.19	0.89
(2,622)	1:145:A:ARG:HA	1:145:A:ARG:HD3	3	0.79	0.19	0.89
(2,1183)	1:146:A:VAL:HG23	1:145:A:ARG:HD2	3	0.63	0.14	0.73
(2,1183)	1:146:A:VAL:HG21	1:145:A:ARG:HD2	3	0.63	0.14	0.73
(2,1183)	1:146:A:VAL:HG22	1:145:A:ARG:HD2	3	0.63	0.14	0.73
(2,491)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	3	0.62	0.04	0.59
(2,1210)	1:140:A:ARG:HB3	1:141:A:PRO:HD2	3	0.58	0.06	0.55
(2,350)	1:45:A:MET:HE3	1:44:A:VAL:HG12	3	0.57	0.25	0.69
(2,350)	1:45:A:MET:HE3	1:44:A:VAL:HG13	3	0.57	0.25	0.69
(2,173)	1:27:A:PHE:HA	1:157:A:LEU:HD12	3	0.55	0.16	0.52
(2,173)	1:27:A:PHE:HA	1:157:A:LEU:HD13	3	0.55	0.16	0.52
(2,173)	1:27:A:PHE:HA	1:157:A:LEU:HD11	3	0.55	0.16	0.52
(2,395)	1:156:A:ALA:HB3	1:44:A:VAL:HG11	3	0.55	0.35	0.56
(2,395)	1:156:A:ALA:HB1	1:44:A:VAL:HG12	3	0.55	0.35	0.56
(2,26)	1:54:A:PRO:HA	1:54:A:PRO:HG3	3	0.54	0.03	0.54
(2,1239)	1:5:A:TYR:HD2	1:82:A:VAL:HB	3	0.54	0.55	0.2
(2,300)	1:61:A:ILE:HA	1:61:A:ILE:HD12	3	0.54	0.24	0.66
(2,943)	1:86:A:LYS:HB3	1:90:A:LYS:HE2	3	0.52	0.27	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,943)	1:86:A:LYS:HB3	1:90:A:LYS:HE3	3	0.52	0.27	0.41
(2,1291)	1:41:A:LEU:HD11	1:27:A:PHE:HZ	3	0.51	0.06	0.55
(2,1291)	1:41:A:LEU:HD12	1:27:A:PHE:HZ	3	0.51	0.06	0.55
(2,1291)	1:41:A:LEU:HD13	1:27:A:PHE:HZ	3	0.51	0.06	0.55
(2,330)	1:47:A:MET:HE2	1:47:A:MET:HG2	3	0.51	0.02	0.51
(2,330)	1:47:A:MET:HE1	1:47:A:MET:HG2	3	0.51	0.02	0.51
(1,109)	1:41:A:LEU:HD11	1:27:A:PHE:HZ	3	0.49	0.06	0.53
(1,109)	1:41:A:LEU:HD12	1:27:A:PHE:HZ	3	0.49	0.06	0.53
(1,109)	1:41:A:LEU:HD13	1:27:A:PHE:HZ	3	0.49	0.06	0.53
(2,135)	1:39:A:LYS:HA	1:57:A:LEU:HD12	3	0.49	0.29	0.61
(2,135)	1:39:A:LYS:HA	1:57:A:LEU:HD11	3	0.49	0.29	0.61
(1,186)	1:148:A:ILE:HD13	1:45:A:MET:HG2	3	0.48	0.23	0.42
(1,186)	1:48:A:LEU:HD11	1:45:A:MET:HG2	3	0.48	0.23	0.42
(1,186)	1:148:A:ILE:HD11	1:45:A:MET:HG2	3	0.48	0.23	0.42
(2,749)	1:16:A:GLN:HA	1:16:A:GLN:HG3	3	0.46	0.03	0.48
(1,25)	1:51:A:ASN:HA	1:46:A:ARG:HG3	3	0.46	0.09	0.48
(1,25)	1:51:A:ASN:HA	1:52:A:PRO:HG2	3	0.46	0.09	0.48
(2,486)	1:157:A:LEU:HD22	1:157:A:LEU:HB2	3	0.46	0.02	0.47
(2,209)	1:151:A:ASP:HA	1:154:A:MET:HG2	3	0.46	0.21	0.48
(1,192)	1:41:A:LEU:HD23	1:60:A:MET:HB2	3	0.44	0.09	0.4
(1,192)	1:41:A:LEU:HD22	1:60:A:MET:HB2	3	0.44	0.09	0.4
(1,192)	1:60:A:MET:HB2	1:146:A:VAL:HG23	3	0.44	0.09	0.4
(1,184)	1:45:A:MET:HG3	1:57:A:LEU:HD11	3	0.43	0.16	0.5
(1,184)	1:45:A:MET:HG3	1:57:A:LEU:HD13	3	0.43	0.16	0.5
(1,184)	1:45:A:MET:HG3	1:146:A:VAL:HG13	3	0.43	0.16	0.5
(2,1158)	1:160:A:ALA:HA	1:163:A:LYS:HE2	3	0.43	0.09	0.49
(2,1202)	1:156:A:ALA:HB2	1:47:A:MET:HG2	3	0.4	0.07	0.4
(2,1202)	1:156:A:ALA:HB3	1:47:A:MET:HG2	3	0.4	0.07	0.4
(2,1123)	1:72:A:VAL:HG22	1:76:A:GLU:HG2	3	0.38	0.06	0.38
(2,1123)	1:72:A:VAL:HG23	1:76:A:GLU:HG2	3	0.38	0.06	0.38
(2,804)	1:90:A:LYS:HD3	1:87:A:ASP:HB3	3	0.38	0.22	0.37
(1,82)	1:156:A:ALA:HB3	1:153:A:MET:HB2	3	0.38	0.1	0.37
(1,82)	1:156:A:ALA:HB3	1:47:A:MET:HB3	3	0.38	0.1	0.37
(1,82)	1:156:A:ALA:HB1	1:153:A:MET:HB2	3	0.38	0.1	0.37
(1,234)	1:81:A:MET:HA	1:64:A:VAL:HB	3	0.37	0.19	0.38
(1,218)	1:60:A:MET:HG3	1:146:A:VAL:HG23	3	0.37	0.18	0.44
(1,218)	1:60:A:MET:HG3	1:148:A:ILE:HD13	3	0.37	0.18	0.44
(1,218)	1:60:A:MET:HG3	1:146:A:VAL:HG11	3	0.37	0.18	0.44
(2,973)	1:42:A:GLY:HA2	1:46:A:ARG:HG2	3	0.36	0.26	0.25
(1,328)	1:41:A:LEU:HA	1:44:A:VAL:HG23	3	0.35	0.14	0.36
(1,328)	1:44:A:VAL:HG22	1:157:A:LEU:HA	3	0.35	0.14	0.36
(2,1265)	1:157:A:LEU:HD12	1:27:A:PHE:HD1	3	0.35	0.1	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,267)	1:25:A:ASP:HA	1:28:A:VAL:HG21	3	0.34	0.15	0.44
(2,267)	1:25:A:ASP:HA	1:28:A:VAL:HG22	3	0.34	0.15	0.44
(2,552)	1:38:A:THR:HA	1:41:A:LEU:HD23	3	0.34	0.05	0.34
(1,58)	1:1:A:MET:HE3	1:1:A:MET:HA	3	0.33	0.07	0.32
(1,58)	1:1:A:MET:HE1	1:76:A:GLU:HA	3	0.33	0.07	0.32
(1,386)	1:50:A:GLN:H	1:48:A:LEU:HB2	3	0.33	0.23	0.22
(2,550)	1:41:A:LEU:HD21	1:41:A:LEU:HA	3	0.31	0.13	0.38
(2,550)	1:41:A:LEU:HD22	1:41:A:LEU:HA	3	0.31	0.13	0.38
(2,762)	1:36:A:ILE:HB	1:72:A:VAL:HB	3	0.31	0.11	0.25
(2,1511)	1:59:A:GLU:H	1:59:A:GLU:HG3	3	0.31	0.05	0.32
(2,887)	1:46:A:ARG:HB2	1:46:A:ARG:HD2	3	0.3	0.08	0.31
(2,449)	1:79:A:VAL:HG11	1:64:A:VAL:HB	3	0.3	0.14	0.31
(2,449)	1:79:A:VAL:HG12	1:64:A:VAL:HB	3	0.3	0.14	0.31
(2,449)	1:79:A:VAL:HG13	1:64:A:VAL:HB	3	0.3	0.14	0.31
(2,1016)	1:72:A:VAL:HG11	1:74:A:PHE:HA	3	0.3	0.08	0.31
(2,1016)	1:72:A:VAL:HG12	1:74:A:PHE:HA	3	0.3	0.08	0.31
(2,1096)	1:58:A:GLN:HG2	1:38:A:THR:HG23	3	0.3	0.07	0.26
(2,1096)	1:58:A:GLN:HG2	1:38:A:THR:HG21	3	0.3	0.07	0.26
(1,177)	1:156:A:ALA:HA	1:155:A:GLN:HG3	3	0.29	0.12	0.36
(2,643)	1:162:A:ALA:HB1	1:158:A:LEU:HB3	3	0.29	0.12	0.34
(2,643)	1:162:A:ALA:HB2	1:158:A:LEU:HB3	3	0.29	0.12	0.34
(1,263)	1:42:A:GLY:HA3	1:46:A:ARG:HG3	3	0.29	0.07	0.29
(1,263)	1:42:A:GLY:HA3	1:52:A:PRO:HG2	3	0.29	0.07	0.29
(2,276)	1:14:A:GLU:HA	1:17:A:LYS:HB2	3	0.29	0.06	0.32
(2,610)	1:54:A:PRO:HG2	1:54:A:PRO:HB3	3	0.27	0.02	0.28
(2,1214)	1:146:A:VAL:HG22	1:52:A:PRO:HB3	3	0.27	0.14	0.22
(2,1214)	1:146:A:VAL:HG21	1:52:A:PRO:HB3	3	0.27	0.14	0.22
(2,325)	1:47:A:MET:HE3	1:157:A:LEU:HA	3	0.26	0.02	0.27
(2,325)	1:47:A:MET:HE1	1:157:A:LEU:HA	3	0.26	0.02	0.27
(1,54)	1:148:A:ILE:HD12	1:80:A:MET:HG2	3	0.26	0.13	0.22
(1,54)	1:148:A:ILE:HD13	1:45:A:MET:HG2	3	0.26	0.13	0.22
(2,446)	1:79:A:VAL:HG11	1:5:A:TYR:HB2	3	0.26	0.07	0.26
(2,446)	1:79:A:VAL:HG12	1:5:A:TYR:HB2	3	0.26	0.07	0.26
(2,1182)	1:141:A:PRO:HD3	1:140:A:ARG:HD2	3	0.25	0.14	0.18
(2,1182)	1:141:A:PRO:HD3	1:140:A:ARG:HD3	3	0.25	0.14	0.18
(1,206)	1:43:A:LYS:HB3	1:43:A:LYS:HD3	3	0.24	0.08	0.24
(1,206)	1:17:A:LYS:HG3	1:17:A:LYS:HB2	3	0.24	0.08	0.24
(2,1020)	1:28:A:VAL:HA	1:36:A:ILE:HG22	3	0.23	0.02	0.22
(2,1020)	1:28:A:VAL:HA	1:36:A:ILE:HG23	3	0.23	0.02	0.22
(2,1003)	1:19:A:GLU:HA	1:158:A:LEU:HD23	3	0.22	0.09	0.22
(2,1003)	1:19:A:GLU:HA	1:158:A:LEU:HD21	3	0.22	0.09	0.22
(2,130)	1:19:A:GLU:HA	1:158:A:LEU:HD13	3	0.22	0.04	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,130)	1:19:A:GLU:HA	1:158:A:LEU:HD12	3	0.22	0.04	0.21
(2,1004)	1:21:A:LYS:HG2	1:74:A:PHE:HE2	3	0.22	0.09	0.18
(2,1125)	1:77:A:PHE:HB2	1:74:A:PHE:HD1	3	0.21	0.02	0.22
(2,1125)	1:77:A:PHE:HB2	1:74:A:PHE:HD2	3	0.21	0.02	0.22
(2,249)	1:161:A:ARG:HA	1:161:A:ARG:HG3	3	0.21	0.08	0.21
(2,249)	1:161:A:ARG:HA	1:161:A:ARG:HG2	3	0.21	0.08	0.21
(2,651)	1:41:A:LEU:HB2	1:41:A:LEU:HG	3	0.21	0.02	0.22
(1,411)	1:159:A:GLY:H	1:159:A:GLY:HA3	3	0.17	0.04	0.16
(1,411)	1:159:A:GLY:H	1:155:A:GLN:HA	3	0.17	0.04	0.16
(1,372)	1:16:A:GLN:H	1:17:A:LYS:H	3	0.16	0.01	0.17
(2,307)	1:26:A:ILE:HD12	1:157:A:LEU:HB2	3	0.16	0.03	0.17
(2,307)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	3	0.16	0.03	0.17
(1,47)	1:60:A:MET:HA	1:60:A:MET:HB3	3	0.15	0.03	0.15
(1,47)	1:60:A:MET:HA	1:63:A:GLU:HB2	3	0.15	0.03	0.15
(2,1132)	1:81:A:MET:HA	1:77:A:PHE:HE1	3	0.14	0.02	0.14
(1,245)	1:43:A:LYS:HB2	1:43:A:LYS:HA	3	0.12	0.0	0.12
(2,257)	1:3:A:ASP:HA	1:6:A:LYS:HD3	3	0.12	0.01	0.12
(2,127)	1:19:A:GLU:HA	1:19:A:GLU:HB3	3	0.12	0.0	0.12
(2,1065)	1:43:A:LYS:HG2	1:43:A:LYS:HB3	3	0.11	0.01	0.12
(2,1049)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	3	0.11	0.01	0.1
(2,1623)	1:33:A:ASP:H	1:33:A:ASP:HA	3	0.11	0.0	0.11
(1,412)	1:49:A:GLY:H	1:49:A:GLY:HA3	3	0.1	0.0	0.1
(2,477)	1:38:A:THR:HG23	1:61:A:ILE:HG13	2	1.27	0.39	1.27
(1,120)	1:153:A:MET:HE1	1:157:A:LEU:HD13	2	1.1	0.08	1.1
(1,120)	1:153:A:MET:HE2	1:157:A:LEU:HD12	2	1.1	0.08	1.1
(2,368)	1:23:A:ALA:HB2	1:153:A:MET:HE1	2	0.98	0.12	0.98
(2,368)	1:23:A:ALA:HB2	1:153:A:MET:HE3	2	0.98	0.12	0.98
(2,348)	1:45:A:MET:HA	1:45:A:MET:HE3	2	0.97	0.09	0.97
(1,80)	1:150:A:ALA:HB2	1:154:A:MET:HG3	2	0.95	0.4	0.95
(1,80)	1:150:A:ALA:HB1	1:85:A:MET:HG3	2	0.95	0.4	0.95
(2,968)	1:80:A:MET:HG3	1:64:A:VAL:HG23	2	0.86	0.1	0.86
(2,415)	1:44:A:VAL:HG13	1:47:A:MET:HE1	2	0.79	0.34	0.79
(2,415)	1:44:A:VAL:HG11	1:47:A:MET:HE3	2	0.79	0.34	0.79
(2,588)	1:52:A:PRO:HG2	1:57:A:LEU:HD11	2	0.73	0.33	0.73
(2,588)	1:52:A:PRO:HG2	1:57:A:LEU:HD13	2	0.73	0.33	0.73
(2,1234)	1:148:A:ILE:HB	1:84:A:SER:HB2	2	0.69	0.41	0.69
(2,1234)	1:148:A:ILE:HB	1:84:A:SER:HB3	2	0.69	0.41	0.69
(2,346)	1:45:A:MET:HE2	1:50:A:GLN:HA	2	0.66	0.02	0.66
(2,346)	1:45:A:MET:HE1	1:50:A:GLN:HA	2	0.66	0.02	0.66
(2,1213)	1:143:A:LEU:HD12	1:143:A:LEU:HA	2	0.54	0.02	0.54
(2,1213)	1:143:A:LEU:HD13	1:143:A:LEU:HA	2	0.54	0.02	0.54
(2,492)	1:41:A:LEU:HD12	1:41:A:LEU:HB2	2	0.52	0.38	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,492)	1:41:A:LEU:HD13	1:41:A:LEU:HB2	2	0.52	0.38	0.52
(2,1151)	1:150:A:ALA:HA	1:148:A:ILE:HG22	2	0.52	0.08	0.52
(2,702)	1:59:A:GLU:HA	1:62:A:ASP:HB2	2	0.5	0.18	0.5
(2,1220)	1:148:A:ILE:HG13	1:148:A:ILE:HA	2	0.47	0.07	0.47
(2,733)	1:56:A:GLU:HG2	1:56:A:GLU:HA	2	0.47	0.1	0.47
(2,904)	1:4:A:ILE:HD12	1:5:A:TYR:HE2	2	0.47	0.12	0.47
(2,904)	1:4:A:ILE:HD11	1:5:A:TYR:HE2	2	0.47	0.12	0.47
(2,460)	1:71:A:THR:HG23	1:35:A:SER:HB3	2	0.43	0.01	0.43
(2,1001)	1:17:A:LYS:HE3	1:78:A:LEU:HD12	2	0.42	0.3	0.42
(2,1001)	1:17:A:LYS:HE3	1:78:A:LEU:HD11	2	0.42	0.3	0.42
(1,36)	1:76:A:GLU:HA	1:76:A:GLU:HG2	2	0.42	0.16	0.42
(2,358)	1:153:A:MET:HE1	1:44:A:VAL:HG11	2	0.4	0.08	0.4
(2,358)	1:153:A:MET:HE1	1:44:A:VAL:HG13	2	0.4	0.08	0.4
(2,668)	1:6:A:LYS:HE3	1:10:A:GLU:HG3	2	0.4	0.02	0.4
(2,665)	1:21:A:LYS:HG2	1:21:A:LYS:HE2	2	0.39	0.0	0.39
(1,268)	1:44:A:VAL:HG22	1:47:A:MET:HB3	2	0.38	0.04	0.38
(1,268)	1:44:A:VAL:HG21	1:47:A:MET:HB3	2	0.38	0.04	0.38
(1,60)	1:47:A:MET:HE3	1:26:A:ILE:HG22	2	0.36	0.01	0.36
(1,60)	1:47:A:MET:HE2	1:26:A:ILE:HG23	2	0.36	0.01	0.36
(2,1181)	1:141:A:PRO:HD2	1:140:A:ARG:HD2	2	0.34	0.04	0.34
(2,1181)	1:141:A:PRO:HD2	1:140:A:ARG:HD3	2	0.34	0.04	0.34
(2,1190)	1:37:A:SER:HA	1:61:A:ILE:HG21	2	0.34	0.13	0.34
(2,1190)	1:37:A:SER:HA	1:61:A:ILE:HG22	2	0.34	0.13	0.34
(1,273)	1:51:A:ASN:HB3	1:46:A:ARG:HG3	2	0.34	0.2	0.34
(2,1400)	1:85:A:MET:H	1:84:A:SER:HB2	2	0.34	0.01	0.34
(2,355)	1:153:A:MET:HE2	1:27:A:PHE:HD2	2	0.34	0.07	0.34
(2,355)	1:153:A:MET:HE1	1:27:A:PHE:HD2	2	0.34	0.07	0.34
(2,555)	1:41:A:LEU:HD23	1:60:A:MET:HB2	2	0.34	0.13	0.34
(2,555)	1:41:A:LEU:HD22	1:60:A:MET:HB2	2	0.34	0.13	0.34
(2,246)	1:90:A:LYS:HA	1:90:A:LYS:HG3	2	0.33	0.08	0.33
(1,236)	1:47:A:MET:HG3	1:48:A:LEU:HG	2	0.32	0.16	0.32
(2,1164)	1:158:A:LEU:HD12	1:161:A:ARG:HD3	2	0.32	0.12	0.32
(2,1164)	1:158:A:LEU:HD13	1:161:A:ARG:HD3	2	0.32	0.12	0.32
(1,70)	1:153:A:MET:HE2	1:27:A:PHE:HE2	2	0.32	0.03	0.32
(1,70)	1:153:A:MET:HE1	1:27:A:PHE:HE2	2	0.32	0.03	0.32
(1,91)	1:146:A:VAL:HG21	1:56:A:GLU:HB3	2	0.3	0.1	0.3
(1,91)	1:146:A:VAL:HG22	1:56:A:GLU:HB3	2	0.3	0.1	0.3
(2,126)	1:19:A:GLU:HA	1:19:A:GLU:HG2	2	0.3	0.07	0.3
(2,405)	1:36:A:ILE:HG22	1:40:A:GLU:HB2	2	0.3	0.07	0.3
(2,506)	1:72:A:VAL:HG22	1:76:A:GLU:HB2	2	0.29	0.07	0.29
(2,1027)	1:31:A:ALA:HA	1:43:A:LYS:HB3	2	0.28	0.12	0.28
(2,357)	1:153:A:MET:HE2	1:36:A:ILE:HG22	2	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,357)	1:153:A:MET:HE1	1:36:A:ILE:HG22	2	0.26	0.03	0.26
(2,687)	1:27:A:PHE:HB3	1:24:A:PHE:HA	2	0.26	0.06	0.26
(2,1142)	1:138:A:PHE:HB2	1:137:A:LYS:HB2	2	0.26	0.05	0.26
(2,1142)	1:138:A:PHE:HB2	1:137:A:LYS:HB3	2	0.26	0.05	0.26
(2,965)	1:60:A:MET:HB3	1:60:A:MET:HG2	2	0.25	0.01	0.25
(2,1163)	1:157:A:LEU:HD23	1:27:A:PHE:HE2	2	0.25	0.12	0.25
(2,1163)	1:157:A:LEU:HD21	1:27:A:PHE:HE2	2	0.25	0.12	0.25
(2,1228)	1:83:A:ARG:HD3	1:64:A:VAL:HG21	2	0.25	0.04	0.25
(1,181)	1:50:A:GLN:HG2	1:45:A:MET:HA	2	0.24	0.01	0.24
(1,181)	1:50:A:GLN:HG3	1:49:A:GLY:HA3	2	0.24	0.01	0.24
(2,1204)	1:140:A:ARG:HB2	1:141:A:PRO:HD3	2	0.24	0.01	0.24
(1,215)	1:43:A:LYS:HB3	1:43:A:LYS:HD3	2	0.23	0.06	0.23
(1,215)	1:43:A:LYS:HB3	1:43:A:LYS:HD2	2	0.23	0.06	0.23
(1,53)	1:157:A:LEU:HA	1:26:A:ILE:HD11	2	0.22	0.02	0.22
(1,53)	1:157:A:LEU:HA	1:26:A:ILE:HD12	2	0.22	0.02	0.22
(1,241)	1:48:A:LEU:HG	1:45:A:MET:HA	2	0.22	0.02	0.22
(1,93)	1:28:A:VAL:HG13	1:24:A:PHE:HD2	2	0.22	0.08	0.22
(1,93)	1:28:A:VAL:HG13	1:27:A:PHE:HD1	2	0.22	0.08	0.22
(2,1166)	1:54:A:PRO:HG3	1:53:A:THR:HA	2	0.22	0.03	0.22
(2,1231)	1:162:A:ALA:HB2	1:163:A:LYS:HE2	2	0.22	0.04	0.22
(2,1231)	1:162:A:ALA:HB3	1:163:A:LYS:HE2	2	0.22	0.04	0.22
(2,174)	1:60:A:MET:HA	1:60:A:MET:HG3	2	0.21	0.01	0.21
(1,35)	1:45:A:MET:HA	1:48:A:LEU:HB3	2	0.21	0.0	0.21
(2,61)	1:89:A:SER:HB3	1:89:A:SER:HA	2	0.21	0.0	0.21
(2,544)	1:43:A:LYS:HG2	1:43:A:LYS:HE2	2	0.2	0.06	0.2
(2,544)	1:43:A:LYS:HG2	1:43:A:LYS:HE3	2	0.2	0.06	0.2
(2,931)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	2	0.2	0.06	0.2
(2,28)	1:54:A:PRO:HA	1:57:A:LEU:HG	2	0.2	0.0	0.2
(2,244)	1:23:A:ALA:HA	1:26:A:ILE:HG13	2	0.2	0.02	0.2
(2,926)	1:8:A:ALA:HB1	1:5:A:TYR:HD1	2	0.2	0.04	0.2
(2,926)	1:8:A:ALA:HB1	1:5:A:TYR:HD2	2	0.2	0.04	0.2
(2,503)	1:48:A:LEU:HD21	1:153:A:MET:HA	2	0.19	0.08	0.19
(2,1021)	1:17:A:LYS:HA	1:12:A:LEU:HD12	2	0.18	0.04	0.18
(2,1021)	1:17:A:LYS:HA	1:12:A:LEU:HD13	2	0.18	0.04	0.18
(2,679)	1:33:A:ASP:HB3	1:33:A:ASP:HA	2	0.18	0.0	0.18
(2,583)	1:141:A:PRO:HG3	1:141:A:PRO:HA	2	0.16	0.01	0.16
(1,69)	1:22:A:ALA:HB2	1:158:A:LEU:HD21	2	0.16	0.04	0.16
(1,69)	1:22:A:ALA:HB2	1:158:A:LEU:HD22	2	0.16	0.04	0.16
(2,747)	1:14:A:GLU:HA	1:14:A:GLU:HG3	2	0.16	0.0	0.16
(2,1109)	1:71:A:THR:HA	1:72:A:VAL:HB	2	0.16	0.0	0.16
(2,238)	1:23:A:ALA:HA	1:26:A:ILE:HD13	2	0.16	0.01	0.16
(2,383)	1:4:A:ILE:HG23	1:7:A:ALA:HB2	2	0.16	0.01	0.16

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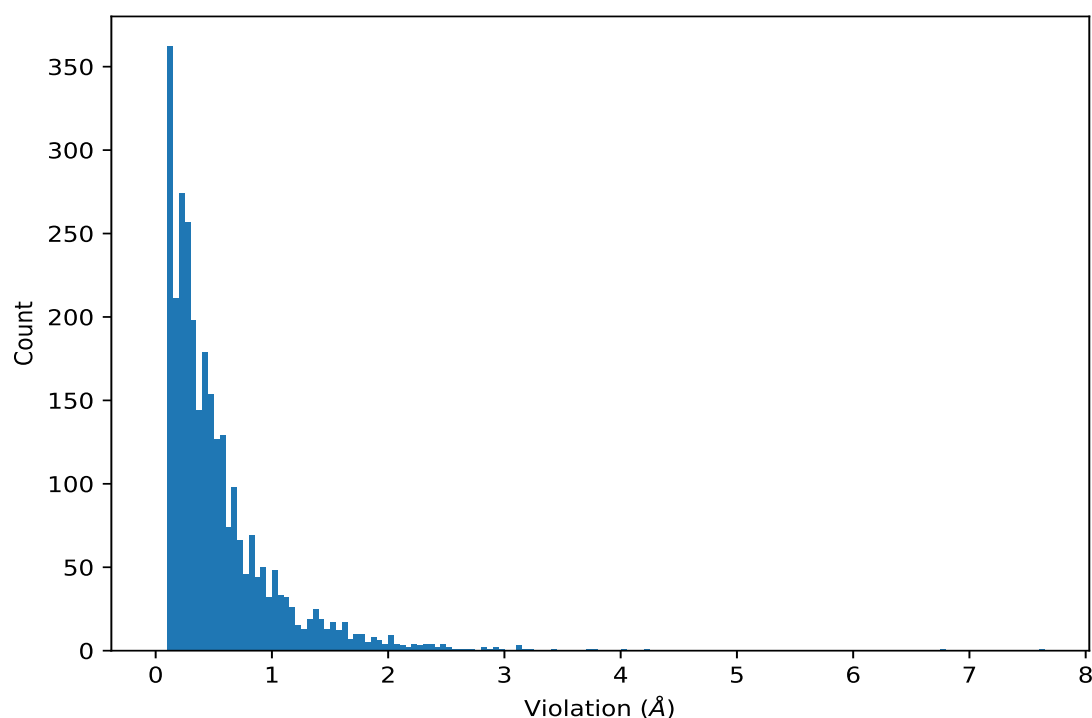
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,383)	1:4:A:ILE:HG22	1:7:A:ALA:HB1	2	0.16	0.01	0.16
(1,162)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	2	0.15	0.02	0.15
(1,162)	1:78:A:LEU:HD22	1:78:A:LEU:HB3	2	0.15	0.02	0.15
(2,617)	1:46:A:ARG:HD3	1:46:A:ARG:HA	2	0.15	0.02	0.15
(2,1195)	1:156:A:ALA:HB2	1:47:A:MET:HE1	2	0.15	0.03	0.15
(2,1195)	1:156:A:ALA:HB3	1:47:A:MET:HE1	2	0.15	0.03	0.15
(2,255)	1:145:A:ARG:HA	1:145:A:ARG:HG2	2	0.14	0.01	0.14
(2,421)	1:31:A:ALA:HB2	1:28:A:VAL:HG13	2	0.12	0.02	0.12
(2,421)	1:31:A:ALA:HB1	1:28:A:VAL:HG11	2	0.12	0.02	0.12
(2,930)	1:141:A:PRO:HB3	1:141:A:PRO:HD2	2	0.12	0.02	0.12
(1,18)	1:40:A:GLU:HA	1:40:A:GLU:HB2	2	0.12	0.01	0.12
(2,423)	1:13:A:THR:HG22	1:16:A:GLN:HG3	2	0.12	0.0	0.12
(2,423)	1:13:A:THR:HG23	1:16:A:GLN:HG3	2	0.12	0.0	0.12
(2,545)	1:43:A:LYS:HG2	1:43:A:LYS:HD3	2	0.12	0.01	0.12
(2,1188)	1:61:A:ILE:HG21	1:65:A:ASP:HA	2	0.12	0.0	0.12
(2,1221)	1:148:A:ILE:HA	1:148:A:ILE:HB	2	0.11	0.01	0.11
(2,950)	1:16:A:GLN:HG2	1:16:A:GLN:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:89:A:SER:HA	1:137:A:LYS:HB2	1	7.64
(2,337)	1:60:A:MET:HE3	1:84:A:SER:HB3	1	6.78
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD21	8	4.23
(2,813)	1:150:A:ALA:HB1	1:85:A:MET:HG3	1	4.03
(1,55)	1:148:A:ILE:HD11	1:153:A:MET:HB3	6	3.8
(2,337)	1:60:A:MET:HE3	1:84:A:SER:HB3	7	3.73
(2,377)	1:150:A:ALA:HB1	1:85:A:MET:HG2	1	3.42
(1,138)	1:145:A:ARG:HD3	1:50:A:GLN:HG3	1	3.2
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG23	1	3.18
(1,76)	1:154:A:MET:HE2	1:163:A:LYS:HE2	8	3.13
(1,318)	1:63:A:GLU:HG3	1:143:A:LEU:HD11	1	3.12
(2,507)	1:48:A:LEU:HD22	1:155:A:GLN:HG3	6	3.1
(2,1093)	1:13:A:THR:HG22	1:11:A:GLN:HG2	1	2.95
(2,1277)	1:78:A:LEU:HD11	1:20:A:PHE:HE1	1	2.93
(2,337)	1:60:A:MET:HE2	1:84:A:SER:HB3	6	2.92
(2,441)	1:146:A:VAL:HG12	1:145:A:ARG:HB3	8	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1150)	1:142:A:THR:HB	1:143:A:LEU:HD23	6	2.84
(1,76)	1:154:A:MET:HE2	1:18:A:ASN:HB2	6	2.81
(1,156)	1:137:A:LYS:HE3	1:86:A:LYS:HB3	3	2.72
(2,387)	1:156:A:ALA:HB2	1:155:A:GLN:HG3	6	2.68
(1,76)	1:154:A:MET:HE1	1:18:A:ASN:HB2	5	2.63
(1,76)	1:154:A:MET:HE2	1:18:A:ASN:HB2	2	2.59
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG22	8	2.52
(1,76)	1:154:A:MET:HE3	1:163:A:LYS:HE2	3	2.52
(1,76)	1:154:A:MET:HE3	1:18:A:ASN:HB2	7	2.48
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG21	6	2.46
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD13	1	2.46
(1,168)	1:56:A:GLU:HG3	1:59:A:GLU:HB2	7	2.45
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG23	7	2.43
(2,578)	1:36:A:ILE:HG22	1:41:A:LEU:HG	6	2.42
(2,831)	1:9:A:VAL:HG11	1:10:A:GLU:HG3	6	2.38
(2,323)	1:85:A:MET:HE2	1:78:A:LEU:HD21	7	2.38
(1,100)	1:79:A:VAL:HG11	1:76:A:GLU:HB2	7	2.38
(1,100)	1:79:A:VAL:HG11	1:76:A:GLU:HB2	8	2.35
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD13	5	2.34
(1,63)	1:60:A:MET:HE1	1:148:A:ILE:HD12	1	2.32
(1,285)	1:71:A:THR:HG23	1:41:A:LEU:HB3	1	2.31
(1,100)	1:79:A:VAL:HG13	1:76:A:GLU:HB2	6	2.31
(2,578)	1:36:A:ILE:HG21	1:41:A:LEU:HG	7	2.3
(1,76)	1:154:A:MET:HE3	1:18:A:ASN:HB2	4	2.3
(2,831)	1:9:A:VAL:HG12	1:10:A:GLU:HG3	8	2.29
(2,578)	1:36:A:ILE:HG21	1:41:A:LEU:HG	8	2.24
(2,1106)	1:64:A:VAL:HG22	1:76:A:GLU:HG3	4	2.23
(1,100)	1:79:A:VAL:HG12	1:76:A:GLU:HB2	1	2.23
(1,223)	1:4:A:ILE:HD11	1:3:A:ASP:HB3	5	2.22
(2,831)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	7	2.16
(2,840)	1:47:A:MET:HG2	1:48:A:LEU:HG	6	2.15
(1,208)	1:63:A:GLU:HG3	1:64:A:VAL:HG23	8	2.14
(2,833)	1:64:A:VAL:HG11	1:63:A:GLU:HG2	4	2.13
(2,840)	1:47:A:MET:HG2	1:48:A:LEU:HG	1	2.11
(1,248)	1:24:A:PHE:HA	1:158:A:LEU:HD21	7	2.09
(1,318)	1:63:A:GLU:HG3	1:143:A:LEU:HD11	7	2.08
(2,507)	1:48:A:LEU:HD23	1:155:A:GLN:HG3	7	2.07
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD11	8	2.07
(2,788)	1:86:A:LYS:HB3	1:90:A:LYS:HA	1	2.05
(2,788)	1:86:A:LYS:HB3	1:90:A:LYS:HA	3	2.04
(1,248)	1:24:A:PHE:HA	1:158:A:LEU:HD23	6	2.04
(1,223)	1:4:A:ILE:HD13	1:83:A:ARG:HD2	4	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:24:A:PHE:HA	1:158:A:LEU:HD21	8	2.02
(1,29)	1:60:A:MET:HA	1:64:A:VAL:HG22	7	2.01
(2,940)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	1	2.0
(1,208)	1:63:A:GLU:HG3	1:143:A:LEU:HD12	6	2.0
(1,76)	1:154:A:MET:HE1	1:163:A:LYS:HE2	1	2.0
(2,342)	1:80:A:MET:HE2	1:77:A:PHE:HD1	7	1.99
(1,285)	1:71:A:THR:HG22	1:39:A:LYS:HB2	4	1.99
(2,11)	1:142:A:THR:HB	1:143:A:LEU:HB2	6	1.98
(1,266)	1:153:A:MET:HE1	1:157:A:LEU:HA	1	1.97
(2,1217)	1:146:A:VAL:HG12	1:147:A:ARG:HA	4	1.95
(2,833)	1:64:A:VAL:HG11	1:63:A:GLU:HG2	3	1.95
(1,85)	1:160:A:ALA:HB3	1:158:A:LEU:HB3	5	1.95
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD21	1	1.94
(2,387)	1:156:A:ALA:HB1	1:155:A:GLN:HG3	7	1.93
(1,285)	1:71:A:THR:HG23	1:39:A:LYS:HB2	5	1.93
(2,840)	1:47:A:MET:HG2	1:48:A:LEU:HG	8	1.9
(2,466)	1:82:A:VAL:HG21	1:83:A:ARG:HB2	1	1.9
(2,476)	1:38:A:THR:HG22	1:61:A:ILE:HG12	6	1.87
(1,264)	1:42:A:GLY:HA3	1:52:A:PRO:HB2	6	1.87
(2,1106)	1:64:A:VAL:HG23	1:76:A:GLU:HG3	3	1.86
(2,1217)	1:146:A:VAL:HG13	1:147:A:ARG:HA	3	1.85
(2,323)	1:85:A:MET:HE1	1:78:A:LEU:HD21	3	1.85
(2,222)	1:141:A:PRO:HD3	1:140:A:ARG:HA	6	1.85
(2,387)	1:156:A:ALA:HB1	1:155:A:GLN:HG3	8	1.84
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD13	5	1.84
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD13	3	1.81
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD12	4	1.81
(1,168)	1:56:A:GLU:HG3	1:146:A:VAL:HB	8	1.8
(2,342)	1:80:A:MET:HE1	1:77:A:PHE:HD1	1	1.79
(2,222)	1:141:A:PRO:HD3	1:140:A:ARG:HA	7	1.78
(2,1066)	1:44:A:VAL:HG23	1:27:A:PHE:HB3	1	1.77
(1,325)	1:61:A:ILE:HD12	1:58:A:GLN:HG3	5	1.77
(2,507)	1:48:A:LEU:HD23	1:155:A:GLN:HG3	8	1.76
(2,323)	1:85:A:MET:HE3	1:78:A:LEU:HD23	2	1.76
(1,55)	1:148:A:ILE:HD11	1:153:A:MET:HE3	8	1.76
(2,463)	1:82:A:VAL:HG22	1:5:A:TYR:HB2	1	1.75
(2,14)	1:79:A:VAL:HA	1:82:A:VAL:HG22	1	1.75
(1,248)	1:24:A:PHE:HA	1:26:A:ILE:HD11	2	1.75
(2,840)	1:47:A:MET:HG2	1:48:A:LEU:HG	7	1.74
(2,465)	1:82:A:VAL:HG21	1:78:A:LEU:HB3	8	1.74
(2,362)	1:154:A:MET:HE3	1:81:A:MET:HE3	1	1.74
(2,342)	1:80:A:MET:HE3	1:77:A:PHE:HD1	8	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:85:A:MET:HE3	1:78:A:LEU:HD22	5	1.74
(2,323)	1:85:A:MET:HE1	1:78:A:LEU:HD21	8	1.73
(2,439)	1:146:A:VAL:HG11	1:56:A:GLU:HA	4	1.72
(1,63)	1:60:A:MET:HE1	1:148:A:ILE:HD11	7	1.72
(2,1230)	1:162:A:ALA:HB1	1:155:A:GLN:HB3	8	1.71
(2,117)	1:78:A:LEU:HA	1:78:A:LEU:HD11	1	1.71
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HD2	7	1.7
(1,168)	1:56:A:GLU:HG3	1:146:A:VAL:HB	3	1.69
(2,222)	1:141:A:PRO:HD3	1:140:A:ARG:HA	8	1.68
(2,477)	1:38:A:THR:HG23	1:61:A:ILE:HG13	6	1.67
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD13	6	1.66
(1,312)	1:80:A:MET:HE1	1:60:A:MET:HG3	8	1.66
(1,285)	1:71:A:THR:HG22	1:41:A:LEU:HB3	6	1.66
(1,37)	1:57:A:LEU:HA	1:57:A:LEU:HD12	8	1.65
(2,719)	1:20:A:PHE:HB2	1:78:A:LEU:HD13	1	1.64
(2,465)	1:82:A:VAL:HG22	1:78:A:LEU:HB3	6	1.64
(2,11)	1:142:A:THR:HB	1:143:A:LEU:HB2	7	1.64
(1,325)	1:61:A:ILE:HD13	1:58:A:GLN:HG3	4	1.64
(1,285)	1:71:A:THR:HG21	1:39:A:LYS:HB2	2	1.63
(1,285)	1:71:A:THR:HG23	1:41:A:LEU:HB3	7	1.63
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD23	5	1.63
(1,73)	1:148:A:ILE:HD11	1:153:A:MET:HE2	3	1.63
(2,1230)	1:162:A:ALA:HB2	1:155:A:GLN:HB3	7	1.62
(2,788)	1:86:A:LYS:HB3	1:90:A:LYS:HA	7	1.62
(1,55)	1:148:A:ILE:HD13	1:153:A:MET:HE1	7	1.62
(2,1230)	1:162:A:ALA:HB1	1:155:A:GLN:HB3	6	1.61
(1,340)	1:150:A:ALA:HB1	1:20:A:PHE:HD2	6	1.61
(2,1012)	1:24:A:PHE:HA	1:21:A:LYS:HD3	7	1.6
(2,356)	1:153:A:MET:HE1	1:27:A:PHE:HB2	7	1.6
(1,285)	1:71:A:THR:HG23	1:39:A:LYS:HB2	3	1.6
(2,833)	1:64:A:VAL:HG12	1:63:A:GLU:HG2	1	1.59
(2,342)	1:80:A:MET:HE2	1:77:A:PHE:HD1	6	1.59
(1,108)	1:158:A:LEU:HD23	1:162:A:ALA:HA	8	1.58
(2,1111)	1:71:A:THR:HG21	1:73:A:ASP:HB2	2	1.57
(2,1012)	1:24:A:PHE:HA	1:21:A:LYS:HD3	1	1.57
(2,387)	1:156:A:ALA:HB2	1:155:A:GLN:HG3	1	1.56
(2,356)	1:153:A:MET:HE2	1:27:A:PHE:HB2	8	1.56
(2,323)	1:85:A:MET:HE3	1:78:A:LEU:HD23	6	1.56
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD13	8	1.55
(2,1073)	1:48:A:LEU:HD22	1:27:A:PHE:HE1	1	1.55
(2,833)	1:64:A:VAL:HG11	1:63:A:GLU:HG2	8	1.55
(1,182)	1:80:A:MET:HB3	1:78:A:LEU:HA	7	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1217)	1:146:A:VAL:HG13	1:147:A:ARG:HA	2	1.54
(2,349)	1:45:A:MET:HE1	1:52:A:PRO:HD3	2	1.54
(2,349)	1:45:A:MET:HE1	1:52:A:PRO:HD3	3	1.54
(1,156)	1:137:A:LYS:HE2	1:86:A:LYS:HB3	8	1.54
(2,439)	1:146:A:VAL:HG11	1:56:A:GLU:HA	1	1.53
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD11	7	1.53
(1,141)	1:145:A:ARG:HD2	1:146:A:VAL:HG12	8	1.53
(1,99)	1:82:A:VAL:HG12	1:80:A:MET:HE1	4	1.53
(2,1029)	1:31:A:ALA:HB1	1:36:A:ILE:HG23	5	1.52
(2,356)	1:153:A:MET:HE1	1:27:A:PHE:HB2	1	1.52
(2,353)	1:45:A:MET:HE3	1:148:A:ILE:HG23	6	1.52
(2,65)	1:84:A:SER:HB2	1:148:A:ILE:HG23	1	1.51
(1,318)	1:63:A:GLU:HG3	1:143:A:LEU:HD12	6	1.51
(1,299)	1:48:A:LEU:HD21	1:49:A:GLY:HA2	5	1.51
(2,1091)	1:13:A:THR:HG22	1:11:A:GLN:HA	1	1.5
(1,326)	1:61:A:ILE:HD12	1:57:A:LEU:HA	1	1.5
(1,95)	1:28:A:VAL:HG11	1:61:A:ILE:HD11	6	1.5
(2,578)	1:36:A:ILE:HG22	1:41:A:LEU:HG	5	1.49
(1,62)	1:60:A:MET:HE2	1:142:A:THR:HG21	3	1.49
(2,1092)	1:53:A:THR:HG22	1:54:A:PRO:HA	6	1.48
(2,439)	1:146:A:VAL:HG11	1:56:A:GLU:HA	2	1.48
(1,285)	1:71:A:THR:HG22	1:39:A:LYS:HB2	8	1.48
(2,1215)	1:60:A:MET:HG3	1:146:A:VAL:HG22	5	1.47
(2,833)	1:64:A:VAL:HG12	1:63:A:GLU:HG2	5	1.47
(1,252)	1:28:A:VAL:HG22	1:26:A:ILE:HG13	1	1.47
(1,81)	1:8:A:ALA:HB3	1:10:A:GLU:HG3	4	1.47
(2,323)	1:85:A:MET:HE1	1:78:A:LEU:HD22	4	1.46
(1,264)	1:42:A:GLY:HA3	1:46:A:ARG:HB2	7	1.46
(1,223)	1:4:A:ILE:HD13	1:3:A:ASP:HB3	3	1.46
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG23	6	1.46
(2,1092)	1:53:A:THR:HG22	1:54:A:PRO:HA	1	1.45
(2,476)	1:38:A:THR:HG23	1:61:A:ILE:HG12	7	1.45
(2,352)	1:148:A:ILE:HG21	1:153:A:MET:HB3	8	1.45
(1,309)	1:8:A:ALA:HB1	1:4:A:ILE:HG22	7	1.45
(1,73)	1:153:A:MET:HE3	1:157:A:LEU:HD12	5	1.45
(1,299)	1:48:A:LEU:HD21	1:49:A:GLY:HA2	3	1.44
(1,223)	1:4:A:ILE:HD11	1:3:A:ASP:HB3	2	1.44
(1,169)	1:56:A:GLU:HG3	1:55:A:GLU:HB3	1	1.43
(2,1242)	1:79:A:VAL:HG23	1:5:A:TYR:HD1	1	1.42
(2,554)	1:41:A:LEU:HD22	1:45:A:MET:HG2	8	1.42
(2,332)	1:1:A:MET:HE2	1:79:A:VAL:HG12	2	1.42
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG11	1	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:48:A:LEU:HD23	1:49:A:GLY:HA2	4	1.42
(1,195)	1:148:A:ILE:HG21	1:153:A:MET:HB3	8	1.42
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD3	7	1.41
(1,208)	1:63:A:GLU:HG3	1:64:A:VAL:HG21	1	1.41
(1,95)	1:28:A:VAL:HG11	1:61:A:ILE:HD13	3	1.41
(1,95)	1:28:A:VAL:HG11	1:61:A:ILE:HD13	5	1.41
(1,63)	1:60:A:MET:HE2	1:148:A:ILE:HG23	8	1.41
(1,297)	1:148:A:ILE:HG23	1:147:A:ARG:HA	1	1.4
(1,208)	1:59:A:GLU:HG3	1:146:A:VAL:HG23	7	1.4
(1,182)	1:80:A:MET:HB3	1:77:A:PHE:HB3	1	1.4
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG23	7	1.4
(2,1154)	1:151:A:ASP:HB2	1:154:A:MET:HB2	1	1.39
(2,323)	1:85:A:MET:HE1	1:78:A:LEU:HD22	1	1.39
(2,22)	1:38:A:THR:HA	1:61:A:ILE:HG13	6	1.39
(1,331)	1:5:A:TYR:HD1	1:4:A:ILE:HB	4	1.39
(2,1068)	1:44:A:VAL:HG23	1:27:A:PHE:HB2	1	1.38
(2,1029)	1:31:A:ALA:HB1	1:36:A:ILE:HG22	1	1.38
(1,81)	1:8:A:ALA:HB2	1:11:A:GLN:HG3	7	1.38
(1,81)	1:8:A:ALA:HB3	1:11:A:GLN:HG3	8	1.38
(1,309)	1:8:A:ALA:HB3	1:4:A:ILE:HG23	2	1.37
(1,309)	1:8:A:ALA:HB1	1:4:A:ILE:HG22	4	1.37
(1,309)	1:8:A:ALA:HB2	1:4:A:ILE:HG23	8	1.37
(1,258)	1:31:A:ALA:HB3	1:29:A:LEU:HD21	8	1.37
(1,252)	1:28:A:VAL:HG21	1:26:A:ILE:HG13	7	1.37
(1,209)	1:59:A:GLU:HG2	1:146:A:VAL:HG11	8	1.37
(2,1012)	1:24:A:PHE:HA	1:21:A:LYS:HD3	8	1.36
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG22	5	1.36
(2,490)	1:41:A:LEU:HD12	1:38:A:THR:HA	6	1.35
(1,156)	1:137:A:LYS:HE2	1:86:A:LYS:HB3	7	1.35
(1,80)	1:150:A:ALA:HB2	1:154:A:MET:HG3	1	1.35
(1,67)	1:80:A:MET:HE2	1:81:A:MET:HG3	5	1.35
(1,29)	1:60:A:MET:HA	1:64:A:VAL:HG23	8	1.35
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD12	7	1.34
(1,340)	1:81:A:MET:HE1	1:20:A:PHE:HD2	7	1.34
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD13	1	1.34
(1,252)	1:28:A:VAL:HG21	1:26:A:ILE:HG13	8	1.34
(2,1029)	1:31:A:ALA:HB3	1:36:A:ILE:HG22	7	1.33
(1,244)	1:2:A:ASP:HB2	1:83:A:ARG:HG3	2	1.33
(1,141)	1:145:A:ARG:HD3	1:146:A:VAL:HG12	7	1.33
(2,490)	1:41:A:LEU:HD12	1:38:A:THR:HA	8	1.32
(2,353)	1:45:A:MET:HE3	1:148:A:ILE:HG21	8	1.32
(1,331)	1:5:A:TYR:HD2	1:4:A:ILE:HB	3	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:8:A:ALA:HB3	1:4:A:ILE:HG22	5	1.32
(1,299)	1:158:A:LEU:HD22	1:26:A:ILE:HA	1	1.32
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD23	3	1.32
(2,1239)	1:5:A:TYR:HD2	1:82:A:VAL:HB	1	1.31
(2,1092)	1:53:A:THR:HG22	1:54:A:PRO:HA	8	1.31
(2,1029)	1:31:A:ALA:HB2	1:36:A:ILE:HG21	2	1.31
(2,390)	1:8:A:ALA:HB2	1:82:A:VAL:HB	1	1.31
(2,18)	1:38:A:THR:HA	1:61:A:ILE:HG12	6	1.3
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HE1	7	1.3
(2,1141)	1:5:A:TYR:HA	1:82:A:VAL:HB	1	1.29
(1,297)	1:148:A:ILE:HG21	1:147:A:ARG:HA	3	1.29
(1,29)	1:60:A:MET:HA	1:64:A:VAL:HG21	1	1.29
(1,62)	1:60:A:MET:HE1	1:142:A:THR:HG21	2	1.28
(2,1106)	1:64:A:VAL:HG23	1:76:A:GLU:HG3	1	1.27
(2,465)	1:82:A:VAL:HG21	1:78:A:LEU:HB3	7	1.27
(1,223)	1:4:A:ILE:HD13	1:83:A:ARG:HD2	1	1.27
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG22	7	1.27
(1,29)	1:60:A:MET:HA	1:143:A:LEU:HD12	6	1.27
(2,1092)	1:53:A:THR:HG23	1:54:A:PRO:HA	7	1.26
(1,297)	1:148:A:ILE:HG23	1:147:A:ARG:HA	5	1.26
(1,95)	1:28:A:VAL:HG13	1:61:A:ILE:HD12	2	1.26
(1,182)	1:80:A:MET:HB3	1:78:A:LEU:HA	8	1.25
(2,1136)	1:82:A:VAL:HG11	1:20:A:PHE:HE1	1	1.24
(2,1111)	1:71:A:THR:HG23	1:73:A:ASP:HB2	4	1.24
(1,299)	1:158:A:LEU:HD22	1:26:A:ILE:HA	7	1.24
(1,95)	1:28:A:VAL:HG12	1:157:A:LEU:HD22	1	1.24
(1,95)	1:28:A:VAL:HG11	1:61:A:ILE:HD13	4	1.24
(1,81)	1:8:A:ALA:HB2	1:11:A:GLN:HG3	6	1.24
(2,490)	1:41:A:LEU:HD13	1:38:A:THR:HA	7	1.23
(1,299)	1:158:A:LEU:HD22	1:26:A:ILE:HA	8	1.23
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD23	1	1.23
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG23	1	1.22
(2,1025)	1:28:A:VAL:HG11	1:43:A:LYS:HD3	3	1.22
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HE2	8	1.22
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD12	4	1.21
(1,309)	1:8:A:ALA:HB2	1:4:A:ILE:HG23	3	1.21
(1,182)	1:80:A:MET:HB3	1:78:A:LEU:HA	6	1.21
(1,312)	1:80:A:MET:HE2	1:60:A:MET:HG3	1	1.2
(1,309)	1:8:A:ALA:HB1	1:4:A:ILE:HG21	6	1.2
(1,277)	1:58:A:GLN:HB2	1:61:A:ILE:HG22	3	1.2
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HZ	5	1.2
(1,252)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	6	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:158:A:LEU:HD23	1:162:A:ALA:HA	1	1.2
(1,103)	1:53:A:THR:HG23	1:55:A:GLU:HB3	4	1.2
(1,98)	1:72:A:VAL:HG12	1:36:A:ILE:HG22	5	1.2
(2,539)	1:29:A:LEU:HD11	1:26:A:ILE:HA	2	1.19
(2,349)	1:45:A:MET:HE3	1:52:A:PRO:HD3	1	1.19
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	6	1.19
(1,325)	1:61:A:ILE:HD12	1:58:A:GLN:HG3	2	1.19
(1,141)	1:145:A:ARG:HD2	1:146:A:VAL:HG12	6	1.19
(1,120)	1:153:A:MET:HE2	1:157:A:LEU:HD12	6	1.19
(1,62)	1:60:A:MET:HE2	1:142:A:THR:HG22	5	1.19
(2,1218)	1:146:A:VAL:HG12	1:52:A:PRO:HD2	6	1.18
(2,710)	1:72:A:VAL:HG21	1:36:A:ILE:HB	7	1.18
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	1	1.18
(1,85)	1:160:A:ALA:HB1	1:161:A:ARG:HB3	2	1.18
(2,14)	1:79:A:VAL:HA	1:82:A:VAL:HG21	8	1.17
(1,168)	1:56:A:GLU:HG3	1:59:A:GLU:HB2	5	1.17
(1,98)	1:72:A:VAL:HG12	1:36:A:ILE:HG23	2	1.17
(1,67)	1:80:A:MET:HE1	1:81:A:MET:HG3	2	1.17
(1,331)	1:5:A:TYR:HD2	1:83:A:ARG:HB2	7	1.16
(1,67)	1:80:A:MET:HE1	1:81:A:MET:HG3	3	1.16
(1,62)	1:60:A:MET:HE1	1:142:A:THR:HG22	4	1.16
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	5	1.15
(1,312)	1:80:A:MET:HE2	1:27:A:PHE:HB2	2	1.15
(1,255)	1:28:A:VAL:HG12	1:72:A:VAL:HB	7	1.15
(2,1111)	1:71:A:THR:HG21	1:73:A:ASP:HB2	5	1.14
(2,507)	1:48:A:LEU:HD22	1:155:A:GLN:HG3	1	1.14
(2,363)	1:154:A:MET:HE2	1:162:A:ALA:HB2	7	1.14
(2,332)	1:1:A:MET:HE2	1:79:A:VAL:HG13	3	1.14
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG21	1	1.14
(2,1146)	1:161:A:ARG:HB2	1:158:A:LEU:HD22	6	1.13
(2,415)	1:44:A:VAL:HG13	1:47:A:MET:HE1	1	1.13
(1,340)	1:81:A:MET:HE2	1:20:A:PHE:HD1	2	1.13
(1,110)	1:41:A:LEU:HD11	1:60:A:MET:HG2	2	1.13
(2,1091)	1:13:A:THR:HG22	1:11:A:GLN:HA	6	1.12
(2,1029)	1:31:A:ALA:HB3	1:36:A:ILE:HG22	4	1.12
(2,551)	1:41:A:LEU:HD22	1:57:A:LEU:HA	5	1.12
(2,400)	1:162:A:ALA:HB2	1:158:A:LEU:HD23	8	1.12
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD2	8	1.12
(1,311)	1:85:A:MET:HE1	1:8:A:ALA:HB2	4	1.12
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	3	1.12
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD12	5	1.12
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD21	8	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:13:A:THR:HG21	1:15:A:GLU:HB2	3	1.12
(1,73)	1:148:A:ILE:HG22	1:153:A:MET:HE3	4	1.12
(1,73)	1:153:A:MET:HE2	1:157:A:LEU:HD12	6	1.12
(1,67)	1:80:A:MET:HE1	1:81:A:MET:HG3	4	1.12
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	4	1.11
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	1	1.11
(1,331)	1:5:A:TYR:HD2	1:90:A:LYS:HD2	5	1.11
(2,1234)	1:148:A:ILE:HB	1:84:A:SER:HB2	1	1.1
(2,833)	1:64:A:VAL:HG12	1:63:A:GLU:HG2	7	1.1
(2,368)	1:23:A:ALA:HB2	1:153:A:MET:HE1	8	1.1
(1,237)	1:52:A:PRO:HD3	1:46:A:ARG:HG3	6	1.1
(2,1184)	1:148:A:ILE:HD13	1:44:A:VAL:HG23	6	1.09
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD12	6	1.09
(2,429)	1:72:A:VAL:HG12	1:76:A:GLU:HG3	7	1.09
(2,312)	1:148:A:ILE:HD13	1:148:A:ILE:HB	7	1.09
(2,312)	1:148:A:ILE:HD13	1:148:A:ILE:HB	8	1.09
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	8	1.09
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG12	7	1.09
(1,309)	1:8:A:ALA:HB2	1:4:A:ILE:HG21	1	1.09
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HD1	6	1.09
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG22	8	1.09
(1,130)	1:52:A:PRO:HG3	1:57:A:LEU:HD12	5	1.09
(1,97)	1:72:A:VAL:HG12	1:76:A:GLU:HG2	7	1.09
(2,1034)	1:35:A:SER:HA	1:73:A:ASP:HB3	7	1.08
(2,362)	1:154:A:MET:HE3	1:81:A:MET:HE2	2	1.08
(1,272)	1:47:A:MET:HE2	1:27:A:PHE:HD2	8	1.08
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD11	4	1.08
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG23	4	1.08
(2,498)	1:79:A:VAL:HG21	1:83:A:ARG:HD2	6	1.07
(2,362)	1:154:A:MET:HE1	1:81:A:MET:HE3	7	1.07
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG23	4	1.07
(1,97)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	8	1.07
(2,1154)	1:151:A:ASP:HB3	1:154:A:MET:HB2	6	1.06
(2,1101)	1:61:A:ILE:HD11	1:36:A:ILE:HD11	7	1.06
(2,588)	1:52:A:PRO:HG2	1:57:A:LEU:HD11	8	1.06
(2,348)	1:45:A:MET:HA	1:45:A:MET:HE3	8	1.06
(1,331)	1:5:A:TYR:HD2	1:83:A:ARG:HB2	1	1.06
(1,103)	1:13:A:THR:HG23	1:15:A:GLU:HB2	6	1.06
(1,97)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	6	1.06
(2,1241)	1:82:A:VAL:HG21	1:5:A:TYR:HD2	1	1.05
(2,1073)	1:48:A:LEU:HD21	1:27:A:PHE:HE1	2	1.05
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD21	4	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,362)	1:154:A:MET:HE2	1:81:A:MET:HE3	5	1.05
(1,107)	1:61:A:ILE:HG23	1:38:A:THR:HG23	5	1.05
(2,956)	1:50:A:GLN:HB3	1:45:A:MET:HB3	7	1.04
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD23	6	1.04
(2,363)	1:154:A:MET:HE2	1:162:A:ALA:HB2	8	1.04
(2,362)	1:154:A:MET:HE1	1:81:A:MET:HE2	4	1.04
(1,258)	1:31:A:ALA:HB3	1:29:A:LEU:HD23	1	1.04
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD21	3	1.04
(1,95)	1:28:A:VAL:HG13	1:157:A:LEU:HD22	8	1.04
(1,64)	1:80:A:MET:HE3	1:27:A:PHE:HE2	3	1.04
(2,1233)	1:27:A:PHE:HA	1:44:A:VAL:HG23	1	1.03
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG13	4	1.03
(2,498)	1:79:A:VAL:HG22	1:83:A:ARG:HD2	8	1.03
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	7	1.03
(1,299)	1:158:A:LEU:HD21	1:26:A:ILE:HA	6	1.03
(1,297)	1:148:A:ILE:HG22	1:84:A:SER:HA	7	1.03
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG22	6	1.03
(1,110)	1:41:A:LEU:HD13	1:60:A:MET:HG2	1	1.03
(1,107)	1:61:A:ILE:HD13	1:38:A:THR:HG23	2	1.03
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	1	1.02
(2,1198)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	7	1.02
(2,1029)	1:31:A:ALA:HB1	1:36:A:ILE:HG23	8	1.02
(2,498)	1:79:A:VAL:HG23	1:83:A:ARG:HD2	7	1.02
(2,441)	1:146:A:VAL:HG12	1:145:A:ARG:HB3	7	1.02
(1,325)	1:61:A:ILE:HD12	1:64:A:VAL:HB	3	1.02
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG23	5	1.02
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD21	2	1.02
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD21	4	1.02
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG23	5	1.02
(1,120)	1:153:A:MET:HE1	1:157:A:LEU:HD13	2	1.02
(1,98)	1:72:A:VAL:HG13	1:36:A:ILE:HG21	1	1.02
(1,98)	1:72:A:VAL:HG11	1:64:A:VAL:HG13	4	1.02
(2,1225)	1:64:A:VAL:HG13	1:76:A:GLU:HA	6	1.01
(2,1034)	1:35:A:SER:HA	1:73:A:ASP:HB3	1	1.01
(2,1030)	1:31:A:ALA:HB1	1:71:A:THR:HG22	6	1.01
(2,710)	1:72:A:VAL:HG23	1:36:A:ILE:HB	6	1.01
(2,485)	1:157:A:LEU:HD23	1:158:A:LEU:HG	7	1.01
(2,429)	1:72:A:VAL:HG11	1:76:A:GLU:HG3	6	1.01
(2,14)	1:79:A:VAL:HA	1:82:A:VAL:HG22	6	1.01
(2,14)	1:79:A:VAL:HA	1:82:A:VAL:HG21	7	1.01
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HD1	1	1.01
(1,108)	1:158:A:LEU:HD21	1:162:A:ALA:HA	5	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:13:A:THR:HG23	1:15:A:GLU:HB3	8	1.01
(2,1217)	1:146:A:VAL:HG13	1:147:A:ARG:HA	1	1.0
(2,1184)	1:148:A:ILE:HD12	1:44:A:VAL:HG23	5	1.0
(2,1092)	1:53:A:THR:HG22	1:54:A:PRO:HA	4	1.0
(2,363)	1:154:A:MET:HE1	1:162:A:ALA:HB2	6	1.0
(2,337)	1:60:A:MET:HE1	1:84:A:SER:HB3	8	1.0
(1,299)	1:48:A:LEU:HD23	1:49:A:GLY:HA2	2	1.0
(1,86)	1:150:A:ALA:HB3	1:151:A:ASP:HA	1	1.0
(2,1217)	1:146:A:VAL:HG11	1:147:A:ARG:HA	5	0.99
(2,788)	1:86:A:LYS:HB3	1:90:A:LYS:HA	6	0.99
(1,324)	1:36:A:ILE:HG22	1:27:A:PHE:HA	7	0.99
(1,265)	1:146:A:VAL:HA	1:143:A:LEU:HB3	4	0.99
(1,103)	1:13:A:THR:HG21	1:15:A:GLU:HB2	2	0.99
(1,99)	1:82:A:VAL:HG12	1:86:A:LYS:HB2	5	0.99
(1,98)	1:72:A:VAL:HG11	1:36:A:ILE:HG21	7	0.99
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG21	3	0.99
(2,1198)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	1	0.98
(2,1073)	1:48:A:LEU:HD21	1:27:A:PHE:HE1	4	0.98
(2,400)	1:162:A:ALA:HB2	1:158:A:LEU:HD23	7	0.98
(1,340)	1:81:A:MET:HE3	1:20:A:PHE:HD2	3	0.98
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG22	1	0.98
(1,270)	1:44:A:VAL:HG11	1:27:A:PHE:HB2	1	0.98
(1,118)	1:48:A:LEU:HD13	1:48:A:LEU:HA	4	0.98
(1,118)	1:48:A:LEU:HD12	1:48:A:LEU:HA	5	0.98
(1,118)	1:48:A:LEU:HD11	1:48:A:LEU:HA	6	0.98
(2,940)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	4	0.97
(2,554)	1:41:A:LEU:HD23	1:45:A:MET:HG2	7	0.97
(2,395)	1:156:A:ALA:HB1	1:44:A:VAL:HG12	1	0.97
(2,332)	1:1:A:MET:HE3	1:79:A:VAL:HG11	5	0.97
(1,340)	1:150:A:ALA:HB2	1:20:A:PHE:HD2	1	0.97
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HB3	6	0.97
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG22	2	0.97
(1,118)	1:48:A:LEU:HD13	1:48:A:LEU:HA	3	0.97
(2,968)	1:80:A:MET:HG3	1:64:A:VAL:HG23	6	0.96
(2,940)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	5	0.96
(2,519)	1:78:A:LEU:HD22	1:77:A:PHE:HD1	6	0.96
(1,340)	1:150:A:ALA:HB2	1:20:A:PHE:HD1	4	0.96
(1,283)	1:65:A:ASP:HB3	1:61:A:ILE:HD13	8	0.96
(1,182)	1:80:A:MET:HB3	1:77:A:PHE:HB3	2	0.96
(1,98)	1:72:A:VAL:HG13	1:36:A:ILE:HG22	8	0.96
(2,1558)	1:44:A:VAL:H	1:44:A:VAL:HG21	1	0.95
(2,1184)	1:148:A:ILE:HD11	1:44:A:VAL:HG21	3	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,622)	1:145:A:ARG:HA	1:145:A:ARG:HD2	6	0.95
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD11	1	0.95
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG22	4	0.95
(1,274)	1:52:A:PRO:HA	1:146:A:VAL:HG22	4	0.95
(1,258)	1:31:A:ALA:HB1	1:29:A:LEU:HD23	2	0.95
(1,108)	1:158:A:LEU:HD22	1:162:A:ALA:HA	6	0.95
(1,107)	1:61:A:ILE:HG22	1:38:A:THR:HG21	3	0.95
(1,103)	1:13:A:THR:HG22	1:15:A:GLU:HB3	5	0.95
(1,98)	1:72:A:VAL:HG13	1:36:A:ILE:HG23	6	0.95
(2,1091)	1:13:A:THR:HG22	1:11:A:GLN:HA	8	0.94
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG11	1	0.94
(2,1029)	1:31:A:ALA:HB3	1:36:A:ILE:HG21	6	0.94
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG12	8	0.94
(2,429)	1:72:A:VAL:HG11	1:76:A:GLU:HG3	8	0.94
(2,362)	1:154:A:MET:HE1	1:81:A:MET:HE1	8	0.94
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	4	0.94
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD12	6	0.94
(1,338)	1:20:A:PHE:HD1	1:19:A:GLU:HG2	8	0.94
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD13	6	0.94
(1,73)	1:153:A:MET:HE1	1:157:A:LEU:HD13	2	0.94
(1,64)	1:80:A:MET:HE1	1:27:A:PHE:HE1	5	0.94
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG23	5	0.94
(2,1184)	1:148:A:ILE:HD13	1:44:A:VAL:HG23	1	0.93
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD21	7	0.93
(2,710)	1:72:A:VAL:HG23	1:36:A:ILE:HB	8	0.93
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG22	7	0.93
(1,59)	1:47:A:MET:HE2	1:43:A:LYS:HA	6	0.93
(2,1154)	1:151:A:ASP:HB2	1:154:A:MET:HB2	7	0.92
(2,831)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	1	0.92
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	1	0.92
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD11	1	0.92
(1,252)	1:28:A:VAL:HG21	1:26:A:ILE:HG13	4	0.92
(1,179)	1:11:A:GLN:HG3	1:13:A:THR:HG22	3	0.92
(2,1030)	1:31:A:ALA:HB3	1:71:A:THR:HG21	2	0.91
(2,1029)	1:31:A:ALA:HB1	1:36:A:ILE:HG23	3	0.91
(2,833)	1:64:A:VAL:HG12	1:63:A:GLU:HG2	6	0.91
(1,108)	1:158:A:LEU:HD23	1:162:A:ALA:HA	7	0.91
(1,103)	1:13:A:THR:HG21	1:15:A:GLU:HB2	7	0.91
(1,95)	1:28:A:VAL:HG13	1:157:A:LEU:HD23	7	0.91
(2,1154)	1:151:A:ASP:HB3	1:154:A:MET:HB2	8	0.9
(2,1100)	1:61:A:ILE:HD12	1:40:A:GLU:HB2	8	0.9
(2,540)	1:29:A:LEU:HD12	1:29:A:LEU:HB2	2	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,492)	1:41:A:LEU:HD13	1:41:A:LEU:HB2	5	0.9
(2,352)	1:148:A:ILE:HG21	1:153:A:MET:HB3	7	0.9
(2,332)	1:1:A:MET:HE2	1:79:A:VAL:HG11	6	0.9
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD12	7	0.9
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD13	8	0.9
(1,340)	1:81:A:MET:HE1	1:20:A:PHE:HD1	5	0.9
(2,1062)	1:43:A:LYS:HD3	1:44:A:VAL:HG21	1	0.89
(2,1030)	1:31:A:ALA:HB2	1:71:A:THR:HG23	1	0.89
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD13	1	0.89
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD12	3	0.89
(2,956)	1:50:A:GLN:HB3	1:45:A:MET:HB3	6	0.89
(2,943)	1:86:A:LYS:HB3	1:90:A:LYS:HE2	8	0.89
(2,622)	1:145:A:ARG:HA	1:145:A:ARG:HD2	8	0.89
(2,198)	1:154:A:MET:HA	1:155:A:GLN:HG3	6	0.89
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG13	1	0.89
(1,252)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	5	0.89
(1,182)	1:80:A:MET:HB3	1:78:A:LEU:HA	4	0.89
(1,89)	1:153:A:MET:HE1	1:44:A:VAL:HG13	2	0.89
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG12	6	0.89
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG22	7	0.89
(2,1225)	1:64:A:VAL:HG12	1:76:A:GLU:HA	8	0.88
(2,647)	1:41:A:LEU:HD23	1:41:A:LEU:HB3	5	0.88
(2,485)	1:157:A:LEU:HD22	1:158:A:LEU:HG	8	0.88
(2,477)	1:38:A:THR:HG23	1:61:A:ILE:HG13	7	0.88
(2,348)	1:45:A:MET:HA	1:45:A:MET:HE3	6	0.88
(2,327)	1:47:A:MET:HE2	1:43:A:LYS:HE3	4	0.88
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG23	1	0.88
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG22	2	0.88
(1,117)	1:26:A:ILE:H	1:157:A:LEU:HD11	5	0.88
(1,85)	1:160:A:ALA:HB1	1:161:A:ARG:HB3	1	0.88
(2,1242)	1:79:A:VAL:HG22	1:5:A:TYR:HD1	8	0.87
(2,510)	1:12:A:LEU:HD21	1:9:A:VAL:HA	4	0.87
(2,510)	1:12:A:LEU:HD23	1:9:A:VAL:HA	7	0.87
(2,394)	1:156:A:ALA:HB1	1:157:A:LEU:HD21	1	0.87
(2,332)	1:1:A:MET:HE3	1:79:A:VAL:HG11	4	0.87
(1,326)	1:61:A:ILE:HD11	1:57:A:LEU:HA	8	0.87
(1,214)	1:43:A:LYS:HD2	1:40:A:GLU:HG2	4	0.87
(1,195)	1:148:A:ILE:HG21	1:153:A:MET:HB3	7	0.87
(1,107)	1:61:A:ILE:HG23	1:38:A:THR:HG22	4	0.87
(1,51)	1:61:A:ILE:HD13	1:41:A:LEU:HA	2	0.87
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB2	6	0.87
(2,510)	1:12:A:LEU:HD23	1:9:A:VAL:HA	2	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,510)	1:12:A:LEU:HD23	1:9:A:VAL:HA	5	0.86
(2,510)	1:12:A:LEU:HD23	1:9:A:VAL:HA	8	0.86
(2,368)	1:23:A:ALA:HB2	1:153:A:MET:HE3	7	0.86
(2,349)	1:45:A:MET:HE2	1:52:A:PRO:HD3	8	0.86
(2,340)	1:60:A:MET:HE3	1:60:A:MET:HG2	1	0.86
(1,318)	1:143:A:LEU:HD11	1:60:A:MET:HG2	8	0.86
(1,255)	1:28:A:VAL:HG11	1:72:A:VAL:HB	6	0.86
(1,182)	1:50:A:GLN:HG2	1:52:A:PRO:HD2	3	0.86
(2,1699)	1:146:A:VAL:HG22	1:52:A:PRO:HA	6	0.85
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG21	8	0.85
(2,1092)	1:53:A:THR:HG22	1:54:A:PRO:HA	5	0.85
(2,1034)	1:35:A:SER:HA	1:73:A:ASP:HB3	6	0.85
(2,510)	1:12:A:LEU:HD21	1:9:A:VAL:HA	3	0.85
(2,498)	1:79:A:VAL:HG23	1:83:A:ARG:HD2	1	0.85
(2,274)	1:60:A:MET:HA	1:60:A:MET:HG2	3	0.85
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	6	0.85
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	8	0.85
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG22	3	0.85
(1,317)	1:143:A:LEU:HD13	1:89:A:SER:HB3	4	0.85
(1,293)	1:82:A:VAL:HG12	1:85:A:MET:HG2	3	0.85
(1,246)	1:26:A:ILE:HD12	1:22:A:ALA:HA	2	0.85
(1,117)	1:48:A:LEU:HD12	1:27:A:PHE:HE1	4	0.85
(1,100)	1:79:A:VAL:HG12	1:76:A:GLU:HB2	3	0.85
(2,1699)	1:146:A:VAL:HG21	1:52:A:PRO:HA	3	0.84
(2,766)	1:36:A:ILE:HG21	1:72:A:VAL:HB	7	0.84
(2,340)	1:60:A:MET:HE3	1:60:A:MET:HG2	8	0.84
(1,311)	1:85:A:MET:HE2	1:150:A:ALA:HB3	2	0.84
(1,298)	1:148:A:ILE:HG21	1:27:A:PHE:HZ	5	0.84
(1,288)	1:75:A:ASP:HB3	1:78:A:LEU:HB2	3	0.84
(1,246)	1:26:A:ILE:HD13	1:22:A:ALA:HA	4	0.84
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG21	5	0.84
(2,1242)	1:79:A:VAL:HG23	1:5:A:TYR:HD1	6	0.83
(2,528)	1:29:A:LEU:HD22	1:29:A:LEU:HB3	2	0.83
(2,434)	1:82:A:VAL:HG11	1:5:A:TYR:HD1	4	0.83
(2,394)	1:156:A:ALA:HB3	1:157:A:LEU:HD21	7	0.83
(1,394)	1:79:A:VAL:H	1:79:A:VAL:HG21	5	0.83
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG22	5	0.83
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG23	8	0.83
(1,252)	1:28:A:VAL:HG23	1:26:A:ILE:HG13	2	0.83
(1,244)	1:2:A:ASP:HB2	1:4:A:ILE:HG12	7	0.83
(1,219)	1:154:A:MET:HG3	1:150:A:ALA:HA	3	0.83
(1,117)	1:26:A:ILE:H	1:157:A:LEU:HD12	2	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,956)	1:50:A:GLN:HB3	1:45:A:MET:HB3	8	0.82
(2,917)	1:64:A:VAL:HG11	1:63:A:GLU:HB3	3	0.82
(2,554)	1:41:A:LEU:HD23	1:45:A:MET:HG2	6	0.82
(2,362)	1:154:A:MET:HE2	1:81:A:MET:HE3	3	0.82
(2,332)	1:1:A:MET:HE2	1:79:A:VAL:HG12	7	0.82
(1,394)	1:79:A:VAL:H	1:78:A:LEU:HB2	4	0.82
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG21	6	0.82
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD13	3	0.82
(1,265)	1:146:A:VAL:HA	1:145:A:ARG:HG2	2	0.82
(1,255)	1:28:A:VAL:HG11	1:72:A:VAL:HB	8	0.82
(1,168)	1:56:A:GLU:HG3	1:59:A:GLU:HB2	4	0.82
(1,118)	1:154:A:MET:HA	1:157:A:LEU:HD13	7	0.82
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG12	2	0.82
(2,1092)	1:53:A:THR:HG23	1:54:A:PRO:HA	3	0.81
(2,350)	1:45:A:MET:HE3	1:44:A:VAL:HG13	5	0.81
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	7	0.81
(2,22)	1:38:A:THR:HA	1:61:A:ILE:HG13	7	0.81
(1,265)	1:146:A:VAL:HA	1:145:A:ARG:HG2	1	0.81
(1,246)	1:26:A:ILE:HD11	1:22:A:ALA:HA	5	0.81
(1,182)	1:80:A:MET:HB3	1:78:A:LEU:HA	5	0.81
(1,100)	1:79:A:VAL:HG13	1:76:A:GLU:HB2	5	0.81
(2,1201)	1:28:A:VAL:HG21	1:24:A:PHE:HD1	5	0.8
(2,1073)	1:48:A:LEU:HD23	1:27:A:PHE:HE2	8	0.8
(2,394)	1:156:A:ALA:HB2	1:157:A:LEU:HD21	8	0.8
(2,275)	1:56:A:GLU:HA	1:56:A:GLU:HG3	6	0.8
(2,274)	1:60:A:MET:HA	1:60:A:MET:HG2	5	0.8
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG23	7	0.8
(1,338)	1:153:A:MET:HE2	1:20:A:PHE:HD1	4	0.8
(1,337)	1:23:A:ALA:HB1	1:20:A:PHE:HD2	1	0.8
(1,258)	1:31:A:ALA:HB2	1:29:A:LEU:HD23	7	0.8
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE2	5	0.8
(1,246)	1:26:A:ILE:HD11	1:22:A:ALA:HA	3	0.8
(1,220)	1:44:A:VAL:HB	1:148:A:ILE:HD13	2	0.8
(1,117)	1:48:A:LEU:HD12	1:27:A:PHE:HE1	3	0.8
(1,61)	1:60:A:MET:HE3	1:147:A:ARG:HD3	8	0.8
(2,1101)	1:61:A:ILE:HD13	1:36:A:ILE:HD13	1	0.79
(2,1025)	1:28:A:VAL:HG11	1:43:A:LYS:HD3	6	0.79
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	3	0.79
(1,331)	1:5:A:TYR:HD2	1:90:A:LYS:HD3	6	0.79
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG23	8	0.79
(1,312)	1:80:A:MET:HE3	1:60:A:MET:HG3	3	0.79
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	2	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:148:A:ILE:HG23	1:27:A:PHE:HZ	2	0.79
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD11	1	0.79
(1,169)	1:56:A:GLU:HG3	1:55:A:GLU:HB3	3	0.79
(1,138)	1:145:A:ARG:HD3	1:50:A:GLN:HG3	2	0.79
(1,64)	1:80:A:MET:HE2	1:27:A:PHE:HE2	4	0.79
(2,1299)	1:82:A:VAL:HG21	1:5:A:TYR:HE2	1	0.78
(2,1242)	1:79:A:VAL:HG23	1:5:A:TYR:HD1	7	0.78
(2,1225)	1:64:A:VAL:HG13	1:76:A:GLU:HA	7	0.78
(2,1201)	1:28:A:VAL:HG21	1:24:A:PHE:HD2	7	0.78
(2,1198)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	8	0.78
(2,537)	1:78:A:LEU:HD11	1:78:A:LEU:HB3	3	0.78
(2,485)	1:157:A:LEU:HD22	1:158:A:LEU:HG	1	0.78
(2,353)	1:45:A:MET:HE2	1:148:A:ILE:HG21	7	0.78
(2,18)	1:38:A:THR:HA	1:61:A:ILE:HG12	7	0.78
(1,331)	1:5:A:TYR:HD2	1:90:A:LYS:HD3	8	0.78
(1,186)	1:48:A:LEU:HD11	1:45:A:MET:HG2	3	0.78
(1,108)	1:158:A:LEU:HD21	1:162:A:ALA:HA	3	0.78
(2,1146)	1:161:A:ARG:HB2	1:158:A:LEU:HD23	8	0.77
(2,510)	1:12:A:LEU:HD23	1:9:A:VAL:HA	6	0.77
(2,177)	1:43:A:LYS:HA	1:43:A:LYS:HG2	1	0.77
(2,135)	1:39:A:LYS:HA	1:57:A:LEU:HD11	6	0.77
(1,326)	1:61:A:ILE:HD13	1:57:A:LEU:HA	2	0.77
(1,244)	1:2:A:ASP:HB2	1:4:A:ILE:HG12	6	0.77
(1,244)	1:2:A:ASP:HB2	1:4:A:ILE:HG12	8	0.77
(2,1215)	1:60:A:MET:HG3	1:146:A:VAL:HG21	8	0.76
(2,1073)	1:48:A:LEU:HD23	1:27:A:PHE:HE1	3	0.76
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE2	7	0.76
(2,968)	1:80:A:MET:HG3	1:64:A:VAL:HG23	8	0.76
(2,300)	1:61:A:ILE:HA	1:61:A:ILE:HD12	6	0.76
(2,173)	1:27:A:PHE:HA	1:157:A:LEU:HD13	1	0.76
(1,293)	1:82:A:VAL:HG11	1:85:A:MET:HG2	2	0.76
(2,1185)	1:36:A:ILE:HD12	1:41:A:LEU:HD12	5	0.75
(2,1091)	1:13:A:THR:HG23	1:11:A:GLN:HA	5	0.75
(2,1025)	1:28:A:VAL:HG11	1:43:A:LYS:HD2	4	0.75
(2,498)	1:79:A:VAL:HG22	1:83:A:ARG:HD2	3	0.75
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	1	0.75
(1,274)	1:52:A:PRO:HA	1:57:A:LEU:HD11	2	0.75
(1,237)	1:44:A:VAL:HA	1:46:A:ARG:HG3	5	0.75
(1,219)	1:154:A:MET:HG3	1:150:A:ALA:HA	7	0.75
(2,1162)	1:157:A:LEU:HD22	1:27:A:PHE:HB3	6	0.74
(2,537)	1:78:A:LEU:HD11	1:78:A:LEU:HB3	5	0.74
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG12	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,353)	1:45:A:MET:HE1	1:148:A:ILE:HG23	4	0.74
(1,394)	1:79:A:VAL:H	1:79:A:VAL:HG21	3	0.74
(1,350)	1:79:A:VAL:HG11	1:5:A:TYR:HE1	5	0.74
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD12	4	0.74
(1,258)	1:31:A:ALA:HB3	1:29:A:LEU:HD22	5	0.74
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG22	2	0.74
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG21	3	0.74
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG12	1	0.74
(2,1300)	1:5:A:TYR:HE2	1:79:A:VAL:HG22	4	0.73
(2,1201)	1:28:A:VAL:HG21	1:24:A:PHE:HD2	6	0.73
(2,1183)	1:146:A:VAL:HG21	1:145:A:ARG:HD2	3	0.73
(2,1183)	1:146:A:VAL:HG22	1:145:A:ARG:HD2	6	0.73
(2,1170)	1:161:A:ARG:HD2	1:26:A:ILE:HD13	4	0.73
(2,1034)	1:35:A:SER:HA	1:73:A:ASP:HB3	8	0.73
(2,537)	1:78:A:LEU:HD13	1:78:A:LEU:HB3	6	0.73
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG11	8	0.73
(1,326)	1:61:A:ILE:HD11	1:57:A:LEU:HA	4	0.73
(1,244)	1:2:A:ASP:HB2	1:4:A:ILE:HG12	5	0.73
(1,168)	1:56:A:GLU:HG3	1:59:A:GLU:HB2	1	0.73
(1,122)	1:157:A:LEU:HD13	1:157:A:LEU:HB3	8	0.73
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG22	6	0.73
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG23	7	0.73
(1,59)	1:47:A:MET:HE3	1:153:A:MET:HA	7	0.73
(1,51)	1:61:A:ILE:HD11	1:41:A:LEU:HA	4	0.73
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	7	0.72
(2,1092)	1:53:A:THR:HG23	1:54:A:PRO:HA	2	0.72
(2,1091)	1:13:A:THR:HG22	1:11:A:GLN:HA	7	0.72
(2,1073)	1:48:A:LEU:HD23	1:27:A:PHE:HE1	5	0.72
(2,1001)	1:17:A:LYS:HE3	1:78:A:LEU:HD12	8	0.72
(2,973)	1:42:A:GLY:HA2	1:46:A:ARG:HG2	1	0.72
(2,935)	1:78:A:LEU:HB2	1:78:A:LEU:HD22	1	0.72
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	7	0.72
(2,537)	1:78:A:LEU:HD11	1:78:A:LEU:HB3	8	0.72
(2,505)	1:72:A:VAL:HG22	1:64:A:VAL:HB	6	0.72
(1,338)	1:153:A:MET:HE2	1:20:A:PHE:HD1	2	0.72
(1,269)	1:44:A:VAL:HG23	1:40:A:GLU:HB3	4	0.72
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE1	7	0.72
(1,237)	1:52:A:PRO:HD3	1:46:A:ARG:HG3	8	0.72
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD12	7	0.72
(1,89)	1:153:A:MET:HE1	1:44:A:VAL:HG11	1	0.72
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD21	6	0.71
(2,1444)	1:146:A:VAL:H	1:146:A:VAL:HG23	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1225)	1:64:A:VAL:HG11	1:76:A:GLU:HA	1	0.71
(2,1215)	1:60:A:MET:HG3	1:146:A:VAL:HG23	3	0.71
(2,1201)	1:28:A:VAL:HG21	1:24:A:PHE:HD1	8	0.71
(2,1147)	1:140:A:ARG:HG3	1:141:A:PRO:HD3	1	0.71
(2,1073)	1:48:A:LEU:HD23	1:27:A:PHE:HE2	7	0.71
(2,1025)	1:28:A:VAL:HG13	1:43:A:LYS:HD3	2	0.71
(2,810)	1:85:A:MET:HG2	1:85:A:MET:HA	1	0.71
(2,563)	1:12:A:LEU:HD13	1:78:A:LEU:HD11	1	0.71
(2,490)	1:41:A:LEU:HD13	1:38:A:THR:HA	5	0.71
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG23	3	0.71
(2,310)	1:148:A:ILE:HD11	1:148:A:ILE:HA	3	0.71
(2,39)	1:44:A:VAL:HA	1:44:A:VAL:HG12	1	0.71
(2,22)	1:38:A:THR:HA	1:61:A:ILE:HG13	8	0.71
(1,326)	1:61:A:ILE:HD13	1:57:A:LEU:HA	7	0.71
(1,297)	1:148:A:ILE:HG22	1:84:A:SER:HA	2	0.71
(1,264)	1:42:A:GLY:HA3	1:52:A:PRO:HB2	2	0.71
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG21	2	0.71
(1,100)	1:79:A:VAL:HG13	1:76:A:GLU:HB2	4	0.71
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG23	4	0.71
(1,87)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	5	0.71
(1,64)	1:80:A:MET:HE2	1:27:A:PHE:HE2	2	0.71
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG22	6	0.7
(2,766)	1:36:A:ILE:HG23	1:72:A:VAL:HB	6	0.7
(2,439)	1:146:A:VAL:HG11	1:56:A:GLU:HA	7	0.7
(2,434)	1:82:A:VAL:HG13	1:5:A:TYR:HD2	5	0.7
(2,365)	1:154:A:MET:HE2	1:158:A:LEU:HD21	2	0.7
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	7	0.7
(2,275)	1:56:A:GLU:HA	1:56:A:GLU:HG3	8	0.7
(2,209)	1:151:A:ASP:HA	1:154:A:MET:HG2	6	0.7
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	6	0.7
(1,326)	1:61:A:ILE:HD11	1:57:A:LEU:HA	3	0.7
(1,277)	1:61:A:ILE:HD13	1:58:A:GLN:HB3	8	0.7
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG22	4	0.7
(1,252)	1:28:A:VAL:HG22	1:26:A:ILE:HG13	3	0.7
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG21	8	0.7
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG22	6	0.7
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG22	7	0.7
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB1	1	0.7
(2,1617)	1:48:A:LEU:H	1:48:A:LEU:HD12	2	0.69
(2,1417)	1:85:A:MET:H	1:85:A:MET:HB2	1	0.69
(2,510)	1:12:A:LEU:HD22	1:9:A:VAL:HA	1	0.69
(2,400)	1:162:A:ALA:HB3	1:158:A:LEU:HD23	4	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,350)	1:45:A:MET:HE3	1:44:A:VAL:HG13	6	0.69
(2,310)	1:148:A:ILE:HD11	1:148:A:ILE:HA	4	0.69
(2,310)	1:148:A:ILE:HD12	1:148:A:ILE:HA	6	0.69
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG23	2	0.69
(1,318)	1:143:A:LEU:HD11	1:60:A:MET:HG2	3	0.69
(1,297)	1:148:A:ILE:HG21	1:84:A:SER:HA	4	0.69
(1,295)	1:142:A:THR:HA	1:147:A:ARG:HD3	4	0.69
(1,274)	1:52:A:PRO:HA	1:146:A:VAL:HG22	7	0.69
(1,219)	1:60:A:MET:HG3	1:57:A:LEU:HA	1	0.69
(1,219)	1:154:A:MET:HG3	1:150:A:ALA:HA	5	0.69
(1,214)	1:43:A:LYS:HD3	1:40:A:GLU:HG2	3	0.69
(1,159)	1:150:A:ALA:HB1	1:151:A:ASP:HB2	3	0.69
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD21	7	0.69
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG22	2	0.69
(1,14)	1:142:A:THR:HA	1:143:A:LEU:HB2	7	0.69
(2,990)	1:45:A:MET:HG2	1:45:A:MET:HE2	5	0.68
(2,907)	1:6:A:LYS:HB3	1:6:A:LYS:HE2	4	0.68
(2,491)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	7	0.68
(2,346)	1:45:A:MET:HE2	1:50:A:GLN:HA	8	0.68
(2,337)	1:60:A:MET:HE2	1:84:A:SER:HB3	5	0.68
(1,297)	1:148:A:ILE:HG22	1:84:A:SER:HA	8	0.68
(1,165)	1:18:A:ASN:HB2	1:17:A:LYS:HB2	2	0.68
(1,108)	1:158:A:LEU:HD23	1:162:A:ALA:HA	4	0.68
(1,85)	1:160:A:ALA:HB3	1:161:A:ARG:HB3	7	0.68
(2,1210)	1:140:A:ARG:HB3	1:141:A:PRO:HD2	2	0.67
(2,1196)	1:1:A:MET:HE1	1:6:A:LYS:HG2	2	0.67
(2,1150)	1:142:A:THR:HB	1:143:A:LEU:HD22	4	0.67
(2,766)	1:36:A:ILE:HG22	1:72:A:VAL:HB	8	0.67
(2,702)	1:59:A:GLU:HA	1:62:A:ASP:HB2	8	0.67
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG11	1	0.67
(2,410)	1:31:A:ALA:HB2	1:28:A:VAL:HG23	7	0.67
(2,397)	1:160:A:ALA:HB1	1:159:A:GLY:HA3	8	0.67
(2,340)	1:60:A:MET:HE3	1:60:A:MET:HG2	7	0.67
(2,338)	1:60:A:MET:HE3	1:60:A:MET:HA	3	0.67
(2,310)	1:148:A:ILE:HD11	1:148:A:ILE:HA	1	0.67
(1,312)	1:80:A:MET:HE3	1:60:A:MET:HG3	6	0.67
(1,258)	1:31:A:ALA:HB2	1:29:A:LEU:HD21	4	0.67
(1,103)	1:13:A:THR:HG23	1:15:A:GLU:HB2	1	0.67
(1,85)	1:160:A:ALA:HB1	1:158:A:LEU:HB3	3	0.67
(1,51)	1:61:A:ILE:HD11	1:41:A:LEU:HA	3	0.67
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	4	0.66
(2,1030)	1:31:A:ALA:HB1	1:71:A:THR:HG23	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,836)	1:10:A:GLU:HA	1:10:A:GLU:HG3	6	0.66
(2,836)	1:10:A:GLU:HA	1:10:A:GLU:HG3	7	0.66
(2,804)	1:90:A:LYS:HD3	1:87:A:ASP:HB3	2	0.66
(2,537)	1:78:A:LEU:HD11	1:78:A:LEU:HB3	4	0.66
(2,472)	1:9:A:VAL:HG13	1:6:A:LYS:HG2	7	0.66
(2,310)	1:148:A:ILE:HD12	1:148:A:ILE:HA	5	0.66
(2,300)	1:61:A:ILE:HA	1:61:A:ILE:HD12	7	0.66
(1,405)	1:60:A:MET:H	1:60:A:MET:HG2	1	0.66
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG21	2	0.66
(1,266)	1:153:A:MET:HE3	1:157:A:LEU:HA	3	0.66
(1,118)	1:154:A:MET:HA	1:157:A:LEU:HD11	8	0.66
(1,87)	1:28:A:VAL:HA	1:28:A:VAL:HG21	1	0.66
(2,1365)	1:152:A:ALA:H	1:151:A:ASP:HB2	2	0.65
(2,1296)	1:5:A:TYR:HE1	1:90:A:LYS:HD3	4	0.65
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD12	1	0.65
(2,1201)	1:28:A:VAL:HG23	1:24:A:PHE:HD1	3	0.65
(2,1184)	1:148:A:ILE:HD13	1:44:A:VAL:HG22	2	0.65
(2,1170)	1:161:A:ARG:HD2	1:26:A:ILE:HD11	1	0.65
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD12	3	0.65
(2,1106)	1:64:A:VAL:HG23	1:76:A:GLU:HG3	5	0.65
(2,346)	1:45:A:MET:HE1	1:50:A:GLN:HA	6	0.65
(2,337)	1:60:A:MET:HE2	1:84:A:SER:HB3	2	0.65
(2,311)	1:148:A:ILE:HD11	1:45:A:MET:HE3	5	0.65
(1,394)	1:79:A:VAL:H	1:79:A:VAL:HG21	2	0.65
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD13	3	0.65
(1,386)	1:50:A:GLN:H	1:48:A:LEU:HB2	2	0.65
(1,349)	1:4:A:ILE:HG13	1:5:A:TYR:HE2	2	0.65
(1,326)	1:61:A:ILE:HD11	1:57:A:LEU:HA	5	0.65
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG23	3	0.65
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE1	8	0.65
(1,219)	1:154:A:MET:HG3	1:150:A:ALA:HA	6	0.65
(1,185)	1:52:A:PRO:HG2	1:45:A:MET:HG2	5	0.65
(1,83)	1:152:A:ALA:HB2	1:48:A:LEU:HD22	3	0.65
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG21	4	0.65
(1,4)	1:38:A:THR:HB	1:61:A:ILE:HD11	3	0.65
(2,1365)	1:152:A:ALA:H	1:151:A:ASP:HB3	4	0.64
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG22	5	0.64
(2,1254)	1:78:A:LEU:HD12	1:74:A:PHE:HD2	7	0.64
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD13	5	0.64
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG13	6	0.64
(2,1008)	1:23:A:ALA:HA	1:26:A:ILE:HG12	1	0.64
(2,1008)	1:23:A:ALA:HA	1:26:A:ILE:HG12	8	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,866)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	5	0.64
(2,836)	1:10:A:GLU:HA	1:10:A:GLU:HG3	8	0.64
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG23	5	0.64
(2,362)	1:154:A:MET:HE3	1:81:A:MET:HE1	6	0.64
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG23	4	0.64
(2,321)	1:85:A:MET:HE2	1:85:A:MET:HG2	6	0.64
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG23	8	0.64
(1,220)	1:44:A:VAL:HB	1:148:A:ILE:HD12	8	0.64
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB2	1	0.64
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	2	0.63
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD13	2	0.63
(2,472)	1:9:A:VAL:HG12	1:6:A:LYS:HG2	8	0.63
(2,407)	1:36:A:ILE:HG21	1:41:A:LEU:HB3	5	0.63
(2,400)	1:162:A:ALA:HB1	1:158:A:LEU:HD23	1	0.63
(2,397)	1:160:A:ALA:HB3	1:159:A:GLY:HA3	6	0.63
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG21	3	0.63
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG23	5	0.63
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG21	8	0.63
(2,310)	1:148:A:ILE:HD11	1:148:A:ILE:HA	2	0.63
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	1	0.63
(2,154)	1:11:A:GLN:HA	1:11:A:GLN:HG3	1	0.63
(2,65)	1:84:A:SER:HB3	1:148:A:ILE:HG23	5	0.63
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD11	2	0.63
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD12	4	0.63
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD13	5	0.63
(1,390)	1:10:A:GLU:H	1:9:A:VAL:HG23	6	0.63
(1,324)	1:28:A:VAL:HA	1:36:A:ILE:HG22	4	0.63
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE2	6	0.63
(1,219)	1:154:A:MET:HG3	1:150:A:ALA:HA	4	0.63
(1,139)	1:46:A:ARG:HD2	1:46:A:ARG:HG2	4	0.63
(1,99)	1:82:A:VAL:HG13	1:90:A:LYS:HB2	2	0.63
(1,83)	1:152:A:ALA:HB1	1:48:A:LEU:HD22	5	0.63
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	5	0.62
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	6	0.62
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD12	2	0.62
(2,1198)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	6	0.62
(2,1145)	1:161:A:ARG:HB3	1:26:A:ILE:HD11	1	0.62
(2,1135)	1:82:A:VAL:HG11	1:5:A:TYR:HE1	4	0.62
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	3	0.62
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG23	4	0.62
(2,397)	1:160:A:ALA:HB2	1:159:A:GLY:HA3	1	0.62
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG21	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG22	6	0.62
(2,337)	1:60:A:MET:HE2	1:84:A:SER:HB2	3	0.62
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	3	0.62
(1,340)	1:150:A:ALA:HB2	1:20:A:PHE:HD1	8	0.62
(1,311)	1:85:A:MET:HE2	1:8:A:ALA:HB3	3	0.62
(1,247)	1:23:A:ALA:HB3	1:24:A:PHE:HB3	5	0.62
(1,85)	1:160:A:ALA:HB1	1:161:A:ARG:HB3	4	0.62
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG21	3	0.62
(1,4)	1:38:A:THR:HB	1:61:A:ILE:HD13	5	0.62
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD21	4	0.61
(2,1091)	1:13:A:THR:HG22	1:11:A:GLN:HA	2	0.61
(2,365)	1:154:A:MET:HE1	1:158:A:LEU:HD22	5	0.61
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG22	1	0.61
(2,321)	1:85:A:MET:HE3	1:85:A:MET:HG2	8	0.61
(2,135)	1:39:A:LYS:HA	1:57:A:LEU:HD12	8	0.61
(1,405)	1:60:A:MET:H	1:59:A:GLU:HG3	5	0.61
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG11	6	0.61
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG23	1	0.61
(1,293)	1:82:A:VAL:HG12	1:83:A:ARG:HD3	7	0.61
(1,288)	1:75:A:ASP:HB3	1:78:A:LEU:HB2	5	0.61
(1,277)	1:58:A:GLN:HB2	1:61:A:ILE:HG23	5	0.61
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE2	4	0.61
(1,122)	1:45:A:MET:HE3	1:48:A:LEU:HD13	5	0.61
(1,19)	1:14:A:GLU:HA	1:17:A:LYS:HE2	4	0.61
(1,4)	1:38:A:THR:HB	1:61:A:ILE:HD11	4	0.61
(2,1201)	1:28:A:VAL:HG22	1:24:A:PHE:HD1	1	0.6
(2,1151)	1:150:A:ALA:HA	1:148:A:ILE:HG22	8	0.6
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG21	8	0.6
(2,1008)	1:23:A:ALA:HA	1:26:A:ILE:HG12	6	0.6
(2,1008)	1:23:A:ALA:HA	1:26:A:ILE:HG12	7	0.6
(2,766)	1:36:A:ILE:HG22	1:72:A:VAL:HB	3	0.6
(2,434)	1:82:A:VAL:HG13	1:5:A:TYR:HD2	3	0.6
(2,407)	1:36:A:ILE:HG23	1:41:A:LEU:HB3	4	0.6
(2,379)	1:81:A:MET:HE1	1:81:A:MET:HG3	3	0.6
(2,365)	1:154:A:MET:HE1	1:158:A:LEU:HD22	3	0.6
(2,321)	1:85:A:MET:HE1	1:85:A:MET:HG2	7	0.6
(2,275)	1:56:A:GLU:HA	1:56:A:GLU:HG3	7	0.6
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD3	3	0.6
(1,283)	1:65:A:ASP:HB3	1:61:A:ILE:HD12	6	0.6
(1,277)	1:58:A:GLN:HB2	1:61:A:ILE:HG23	4	0.6
(1,269)	1:44:A:VAL:HG22	1:47:A:MET:HB2	5	0.6
(1,234)	1:81:A:MET:HA	1:64:A:VAL:HB	3	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:26:A:ILE:H	1:157:A:LEU:HD11	6	0.6
(1,79)	1:31:A:ALA:HB2	1:36:A:ILE:HA	2	0.6
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	3	0.59
(2,1365)	1:152:A:ALA:H	1:151:A:ASP:HB3	5	0.59
(2,1254)	1:78:A:LEU:HD12	1:74:A:PHE:HD1	6	0.59
(2,1162)	1:157:A:LEU:HD21	1:27:A:PHE:HB3	5	0.59
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG22	2	0.59
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD22	2	0.59
(2,904)	1:4:A:ILE:HD12	1:5:A:TYR:HE2	2	0.59
(2,556)	1:41:A:LEU:HD23	1:41:A:LEU:HB2	2	0.59
(2,491)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	6	0.59
(2,491)	1:41:A:LEU:HD13	1:41:A:LEU:HB3	8	0.59
(2,472)	1:9:A:VAL:HG12	1:6:A:LYS:HG2	6	0.59
(2,462)	1:82:A:VAL:HG22	1:5:A:TYR:HB3	1	0.59
(2,400)	1:162:A:ALA:HB1	1:158:A:LEU:HD21	5	0.59
(2,374)	1:31:A:ALA:HB2	1:32:A:GLU:HB2	1	0.59
(2,65)	1:84:A:SER:HB2	1:148:A:ILE:HG21	3	0.59
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD13	6	0.59
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	7	0.59
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE2	1	0.59
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE2	3	0.59
(1,184)	1:45:A:MET:HG3	1:57:A:LEU:HD13	6	0.59
(1,63)	1:60:A:MET:HE3	1:148:A:ILE:HD12	2	0.59
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG22	3	0.59
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD23	5	0.58
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD23	8	0.58
(2,1254)	1:78:A:LEU:HD13	1:74:A:PHE:HD1	8	0.58
(2,1225)	1:64:A:VAL:HG11	1:76:A:GLU:HA	5	0.58
(2,1198)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	2	0.58
(2,1167)	1:53:A:THR:HB	1:54:A:PRO:HG3	3	0.58
(2,940)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	3	0.58
(2,835)	1:7:A:ALA:HB1	1:10:A:GLU:HG3	4	0.58
(2,818)	1:44:A:VAL:HG21	1:43:A:LYS:HB2	1	0.58
(2,710)	1:72:A:VAL:HG22	1:36:A:ILE:HB	5	0.58
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	6	0.58
(2,554)	1:41:A:LEU:HD21	1:45:A:MET:HG2	5	0.58
(2,349)	1:45:A:MET:HE2	1:52:A:PRO:HD3	6	0.58
(2,338)	1:60:A:MET:HE2	1:60:A:MET:HA	1	0.58
(2,324)	1:1:A:MET:HE1	1:6:A:LYS:HA	1	0.58
(2,274)	1:60:A:MET:HA	1:60:A:MET:HG2	6	0.58
(2,26)	1:54:A:PRO:HA	1:54:A:PRO:HG3	1	0.58
(1,283)	1:65:A:ASP:HB3	1:61:A:ILE:HD12	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:58:A:GLN:HB2	1:61:A:ILE:HG22	2	0.58
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG23	3	0.58
(1,251)	1:27:A:PHE:HB3	1:27:A:PHE:HE2	2	0.58
(1,237)	1:52:A:PRO:HD3	1:46:A:ARG:HG3	4	0.58
(1,151)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	5	0.58
(1,139)	1:161:A:ARG:HD3	1:161:A:ARG:HB3	7	0.58
(1,36)	1:76:A:GLU:HA	1:76:A:GLU:HG2	3	0.58
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB3	2	0.58
(2,1699)	1:146:A:VAL:HG21	1:52:A:PRO:HA	2	0.57
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG22	2	0.57
(2,1300)	1:5:A:TYR:HE1	1:79:A:VAL:HG22	3	0.57
(2,1147)	1:140:A:ARG:HG2	1:141:A:PRO:HD3	4	0.57
(2,1101)	1:61:A:ILE:HD11	1:36:A:ILE:HD12	6	0.57
(2,1025)	1:28:A:VAL:HG13	1:43:A:LYS:HD3	7	0.57
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD13	4	0.57
(2,753)	1:11:A:GLN:HG2	1:11:A:GLN:HA	1	0.57
(2,733)	1:56:A:GLU:HG2	1:56:A:GLU:HA	2	0.57
(2,710)	1:72:A:VAL:HG21	1:36:A:ILE:HB	2	0.57
(2,374)	1:31:A:ALA:HB1	1:32:A:GLU:HB2	6	0.57
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD11	4	0.57
(1,315)	1:142:A:THR:HG21	1:147:A:ARG:HA	2	0.57
(1,315)	1:142:A:THR:HG22	1:147:A:ARG:HA	4	0.57
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG22	7	0.57
(1,192)	1:41:A:LEU:HD23	1:60:A:MET:HB2	1	0.57
(1,108)	1:158:A:LEU:HD23	1:162:A:ALA:HA	2	0.57
(1,19)	1:14:A:GLU:HA	1:17:A:LYS:HE2	6	0.57
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG21	7	0.56
(2,1434)	1:56:A:GLU:H	1:56:A:GLU:HB3	7	0.56
(2,1291)	1:41:A:LEU:HD13	1:27:A:PHE:HZ	4	0.56
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD12	7	0.56
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD13	8	0.56
(2,1213)	1:143:A:LEU:HD13	1:143:A:LEU:HA	5	0.56
(2,1147)	1:140:A:ARG:HG3	1:141:A:PRO:HD3	6	0.56
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG22	4	0.56
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG11	5	0.56
(2,1035)	1:35:A:SER:HB2	1:73:A:ASP:HB3	6	0.56
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD11	6	0.56
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	5	0.56
(2,757)	1:82:A:VAL:HA	1:85:A:MET:HB2	1	0.56
(2,395)	1:156:A:ALA:HB3	1:44:A:VAL:HG11	8	0.56
(2,351)	1:4:A:ILE:HA	1:4:A:ILE:HG23	7	0.56
(2,321)	1:85:A:MET:HE3	1:85:A:MET:HG2	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG11	8	0.56
(1,356)	1:66:A:GLU:H	1:65:A:ASP:HB2	2	0.56
(1,338)	1:153:A:MET:HE1	1:20:A:PHE:HD2	3	0.56
(1,244)	1:2:A:ASP:HB2	1:83:A:ARG:HG3	4	0.56
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB2	8	0.56
(1,25)	1:51:A:ASN:HA	1:52:A:PRO:HG2	4	0.56
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD22	3	0.55
(2,1291)	1:41:A:LEU:HD11	1:27:A:PHE:HZ	2	0.55
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD13	4	0.55
(2,1210)	1:140:A:ARG:HB3	1:141:A:PRO:HD2	7	0.55
(2,1167)	1:53:A:THR:HB	1:54:A:PRO:HG3	2	0.55
(2,1122)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	1	0.55
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG21	3	0.55
(2,1091)	1:13:A:THR:HG21	1:11:A:GLN:HA	4	0.55
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD11	7	0.55
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD13	8	0.55
(2,616)	1:140:A:ARG:HD3	1:140:A:ARG:HA	2	0.55
(2,556)	1:41:A:LEU:HD23	1:41:A:LEU:HB2	4	0.55
(2,397)	1:160:A:ALA:HB1	1:159:A:GLY:HA3	7	0.55
(2,353)	1:45:A:MET:HE2	1:148:A:ILE:HG23	3	0.55
(2,338)	1:60:A:MET:HE3	1:60:A:MET:HA	5	0.55
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD3	6	0.55
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD13	7	0.55
(1,219)	1:60:A:MET:HG3	1:57:A:LEU:HA	2	0.55
(1,218)	1:60:A:MET:HG3	1:146:A:VAL:HG11	7	0.55
(1,151)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	6	0.55
(1,102)	1:13:A:THR:HG21	1:16:A:GLN:HG2	8	0.55
(1,80)	1:150:A:ALA:HB1	1:85:A:MET:HG3	6	0.55
(2,1609)	1:45:A:MET:H	1:44:A:VAL:HB	1	0.54
(2,1220)	1:148:A:ILE:HG13	1:148:A:ILE:HA	7	0.54
(2,1145)	1:161:A:ARG:HB3	1:26:A:ILE:HD11	5	0.54
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	6	0.54
(2,866)	1:137:A:LYS:HB2	1:138:A:PHE:HD1	2	0.54
(2,710)	1:72:A:VAL:HG21	1:36:A:ILE:HB	4	0.54
(2,459)	1:71:A:THR:HG23	1:36:A:ILE:HA	1	0.54
(2,427)	1:72:A:VAL:HG12	1:77:A:PHE:HB3	1	0.54
(2,365)	1:154:A:MET:HE3	1:158:A:LEU:HD21	4	0.54
(2,365)	1:154:A:MET:HE3	1:158:A:LEU:HD21	8	0.54
(2,26)	1:54:A:PRO:HA	1:54:A:PRO:HG3	7	0.54
(1,273)	1:51:A:ASN:HB3	1:46:A:ARG:HG3	4	0.54
(1,255)	1:28:A:VAL:HG13	1:72:A:VAL:HB	1	0.54
(1,138)	1:145:A:ARG:HD2	1:50:A:GLN:HG2	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:157:A:LEU:HD11	1:157:A:LEU:HB3	6	0.54
(1,109)	1:41:A:LEU:HD13	1:27:A:PHE:HZ	4	0.54
(1,83)	1:152:A:ALA:HB3	1:48:A:LEU:HD13	4	0.54
(2,1699)	1:146:A:VAL:HG21	1:52:A:PRO:HA	5	0.53
(2,1210)	1:140:A:ARG:HB3	1:141:A:PRO:HD2	6	0.53
(2,1150)	1:142:A:THR:HB	1:143:A:LEU:HD21	2	0.53
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG23	5	0.53
(2,1105)	1:64:A:VAL:HG22	1:77:A:PHE:HB2	3	0.53
(2,1100)	1:61:A:ILE:HD12	1:40:A:GLU:HB2	1	0.53
(2,1030)	1:31:A:ALA:HB2	1:71:A:THR:HG23	3	0.53
(2,831)	1:9:A:VAL:HG12	1:10:A:GLU:HG3	4	0.53
(2,379)	1:81:A:MET:HE1	1:81:A:MET:HG3	7	0.53
(2,365)	1:154:A:MET:HE2	1:158:A:LEU:HD23	6	0.53
(2,330)	1:47:A:MET:HE2	1:47:A:MET:HG2	6	0.53
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	6	0.53
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG21	8	0.53
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	8	0.53
(1,293)	1:82:A:VAL:HG11	1:83:A:ARG:HD2	6	0.53
(1,265)	1:146:A:VAL:HA	1:145:A:ARG:HG3	7	0.53
(1,258)	1:31:A:ALA:HB2	1:29:A:LEU:HD22	6	0.53
(1,220)	1:44:A:VAL:HB	1:148:A:ILE:HD11	7	0.53
(1,109)	1:41:A:LEU:HD11	1:27:A:PHE:HZ	2	0.53
(1,83)	1:152:A:ALA:HB2	1:48:A:LEU:HD21	1	0.53
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB2	8	0.52
(2,1434)	1:56:A:GLU:H	1:56:A:GLU:HB3	6	0.52
(2,1277)	1:78:A:LEU:HD12	1:20:A:PHE:HE2	2	0.52
(2,1213)	1:143:A:LEU:HD12	1:143:A:LEU:HA	2	0.52
(2,1184)	1:148:A:ILE:HD11	1:44:A:VAL:HG22	4	0.52
(2,1025)	1:28:A:VAL:HG11	1:43:A:LYS:HD3	8	0.52
(2,1019)	1:27:A:PHE:HB3	1:157:A:LEU:HD12	5	0.52
(2,956)	1:50:A:GLN:HB3	1:45:A:MET:HB3	1	0.52
(2,916)	1:63:A:GLU:HB3	1:64:A:VAL:HG23	8	0.52
(2,622)	1:145:A:ARG:HA	1:145:A:ARG:HD3	7	0.52
(2,537)	1:78:A:LEU:HD11	1:78:A:LEU:HB3	2	0.52
(2,396)	1:155:A:GLN:HA	1:162:A:ALA:HB2	6	0.52
(2,379)	1:81:A:MET:HE2	1:81:A:MET:HG3	2	0.52
(2,379)	1:81:A:MET:HE3	1:81:A:MET:HG3	4	0.52
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	7	0.52
(2,173)	1:27:A:PHE:HA	1:157:A:LEU:HD12	8	0.52
(2,57)	1:4:A:ILE:HA	1:4:A:ILE:HD11	5	0.52
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD12	8	0.52
(1,338)	1:153:A:MET:HE1	1:20:A:PHE:HD1	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG22	6	0.52
(1,293)	1:82:A:VAL:HG12	1:85:A:MET:HG2	5	0.52
(1,287)	1:75:A:ASP:HB2	1:78:A:LEU:HB2	3	0.52
(1,71)	1:153:A:MET:HE1	1:27:A:PHE:HA	2	0.52
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HG22	3	0.52
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB3	2	0.51
(2,1277)	1:78:A:LEU:HD11	1:20:A:PHE:HE1	6	0.51
(2,1230)	1:162:A:ALA:HB3	1:155:A:GLN:HB3	1	0.51
(2,1201)	1:28:A:VAL:HG21	1:24:A:PHE:HD2	2	0.51
(2,1147)	1:140:A:ARG:HG3	1:141:A:PRO:HD3	7	0.51
(2,1106)	1:64:A:VAL:HG21	1:76:A:GLU:HG3	7	0.51
(2,940)	1:164:A:GLY:HA2	1:163:A:LYS:HE2	2	0.51
(2,927)	1:8:A:ALA:HB1	1:79:A:VAL:HA	8	0.51
(2,766)	1:36:A:ILE:HG21	1:72:A:VAL:HB	4	0.51
(2,710)	1:72:A:VAL:HG21	1:36:A:ILE:HB	1	0.51
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	8	0.51
(2,624)	1:46:A:ARG:HD2	1:43:A:LYS:HA	5	0.51
(2,519)	1:78:A:LEU:HD21	1:77:A:PHE:HD1	5	0.51
(2,516)	1:57:A:LEU:HD21	1:45:A:MET:HG2	1	0.51
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG21	8	0.51
(2,410)	1:31:A:ALA:HB3	1:28:A:VAL:HG23	8	0.51
(2,407)	1:36:A:ILE:HG23	1:41:A:LEU:HB3	1	0.51
(2,400)	1:162:A:ALA:HB2	1:158:A:LEU:HD22	6	0.51
(2,379)	1:81:A:MET:HE2	1:81:A:MET:HG3	8	0.51
(2,330)	1:47:A:MET:HE1	1:47:A:MET:HG2	1	0.51
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	2	0.51
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG13	7	0.51
(1,347)	1:5:A:TYR:HE1	1:2:A:ASP:HB3	3	0.51
(1,328)	1:44:A:VAL:HG22	1:157:A:LEU:HA	5	0.51
(1,325)	1:61:A:ILE:HD13	1:58:A:GLN:HG3	7	0.51
(1,323)	1:8:A:ALA:HB1	1:79:A:VAL:HA	8	0.51
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG21	6	0.51
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	2	0.51
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	7	0.51
(1,253)	1:28:A:VAL:HG21	1:40:A:GLU:HB2	8	0.51
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD21	1	0.51
(1,67)	1:80:A:MET:HE3	1:148:A:ILE:HG12	1	0.51
(2,1277)	1:78:A:LEU:HD12	1:20:A:PHE:HE1	3	0.5
(2,1158)	1:160:A:ALA:HA	1:163:A:LYS:HE2	8	0.5
(2,1135)	1:82:A:VAL:HG13	1:5:A:TYR:HE2	5	0.5
(2,1106)	1:64:A:VAL:HG23	1:76:A:GLU:HG3	2	0.5
(2,1035)	1:35:A:SER:HB2	1:73:A:ASP:HB3	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,578)	1:36:A:ILE:HG21	1:41:A:LEU:HG	1	0.5
(2,537)	1:78:A:LEU:HD13	1:78:A:LEU:HB3	7	0.5
(2,519)	1:78:A:LEU:HD23	1:77:A:PHE:HD1	3	0.5
(2,517)	1:57:A:LEU:HD23	1:41:A:LEU:HB2	6	0.5
(2,465)	1:82:A:VAL:HG23	1:78:A:LEU:HB3	2	0.5
(2,434)	1:82:A:VAL:HG12	1:5:A:TYR:HD2	2	0.5
(2,410)	1:31:A:ALA:HB3	1:28:A:VAL:HG22	5	0.5
(2,407)	1:36:A:ILE:HG22	1:41:A:LEU:HB3	2	0.5
(2,396)	1:155:A:GLN:HA	1:162:A:ALA:HB2	8	0.5
(2,379)	1:81:A:MET:HE2	1:81:A:MET:HG3	6	0.5
(2,342)	1:80:A:MET:HE2	1:77:A:PHE:HD1	3	0.5
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	8	0.5
(2,275)	1:56:A:GLU:HA	1:56:A:GLU:HG3	2	0.5
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	3	0.5
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	4	0.5
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG22	6	0.5
(2,26)	1:54:A:PRO:HA	1:54:A:PRO:HG3	6	0.5
(1,405)	1:60:A:MET:H	1:60:A:MET:HG2	4	0.5
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD11	7	0.5
(1,315)	1:142:A:THR:HG21	1:147:A:ARG:HA	3	0.5
(1,293)	1:82:A:VAL:HG13	1:83:A:ARG:HD2	8	0.5
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	1	0.5
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	4	0.5
(1,184)	1:45:A:MET:HG3	1:57:A:LEU:HD11	1	0.5
(1,151)	1:26:A:ILE:HD12	1:157:A:LEU:HB2	8	0.5
(1,105)	1:57:A:LEU:HA	1:38:A:THR:HG23	2	0.5
(1,102)	1:13:A:THR:HG22	1:16:A:GLN:HG2	2	0.5
(1,102)	1:13:A:THR:HG21	1:16:A:GLN:HG2	7	0.5
(1,82)	1:156:A:ALA:HB3	1:153:A:MET:HB2	2	0.5
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD22	2	0.49
(2,1277)	1:78:A:LEU:HD11	1:20:A:PHE:HE1	7	0.49
(2,1167)	1:53:A:THR:HB	1:54:A:PRO:HG3	1	0.49
(2,1162)	1:157:A:LEU:HD23	1:27:A:PHE:HB3	3	0.49
(2,1162)	1:157:A:LEU:HD21	1:27:A:PHE:HB3	4	0.49
(2,1158)	1:160:A:ALA:HA	1:163:A:LYS:HE2	7	0.49
(2,1101)	1:61:A:ILE:HD11	1:36:A:ILE:HD13	5	0.49
(2,1091)	1:13:A:THR:HG22	1:11:A:GLN:HA	3	0.49
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	2	0.49
(2,1025)	1:28:A:VAL:HG13	1:43:A:LYS:HD3	5	0.49
(2,866)	1:137:A:LYS:HB3	1:138:A:PHE:HD1	8	0.49
(2,788)	1:86:A:LYS:HB3	1:90:A:LYS:HA	8	0.49
(2,749)	1:16:A:GLN:HA	1:16:A:GLN:HG3	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,578)	1:36:A:ILE:HG22	1:41:A:LEU:HG	3	0.49
(2,417)	1:146:A:VAL:HA	1:146:A:VAL:HG21	4	0.49
(2,410)	1:31:A:ALA:HB3	1:28:A:VAL:HG21	3	0.49
(2,397)	1:160:A:ALA:HB2	1:159:A:GLY:HA3	4	0.49
(2,379)	1:81:A:MET:HE1	1:81:A:MET:HG3	5	0.49
(2,358)	1:153:A:MET:HE1	1:44:A:VAL:HG13	2	0.49
(2,330)	1:47:A:MET:HE2	1:47:A:MET:HG2	8	0.49
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	4	0.49
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG11	4	0.49
(2,140)	1:13:A:THR:HA	1:17:A:LYS:HB2	5	0.49
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG12	6	0.49
(1,287)	1:75:A:ASP:HB2	1:78:A:LEU:HB2	6	0.49
(1,269)	1:44:A:VAL:HG23	1:40:A:GLU:HB3	2	0.49
(1,266)	1:153:A:MET:HE1	1:157:A:LEU:HA	4	0.49
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	5	0.49
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	6	0.49
(1,236)	1:47:A:MET:HG3	1:48:A:LEU:HG	6	0.49
(1,138)	1:145:A:ARG:HD2	1:50:A:GLN:HG2	4	0.49
(1,138)	1:145:A:ARG:HD2	1:50:A:GLN:HG2	7	0.49
(1,63)	1:60:A:MET:HE3	1:148:A:ILE:HD12	4	0.49
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG22	1	0.49
(1,34)	1:16:A:GLN:HA	1:19:A:GLU:HB2	1	0.49
(2,1232)	1:44:A:VAL:HG12	1:153:A:MET:HA	1	0.48
(2,1216)	1:52:A:PRO:HA	1:146:A:VAL:HG22	6	0.48
(2,1202)	1:156:A:ALA:HB3	1:47:A:MET:HG2	1	0.48
(2,1190)	1:37:A:SER:HA	1:61:A:ILE:HG21	1	0.48
(2,1162)	1:157:A:LEU:HD22	1:27:A:PHE:HB3	2	0.48
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG13	3	0.48
(2,1007)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	3	0.48
(2,749)	1:16:A:GLN:HA	1:16:A:GLN:HG3	5	0.48
(2,486)	1:157:A:LEU:HD22	1:157:A:LEU:HB2	8	0.48
(2,379)	1:81:A:MET:HE3	1:81:A:MET:HG3	1	0.48
(2,374)	1:31:A:ALA:HB1	1:32:A:GLU:HB3	4	0.48
(2,363)	1:154:A:MET:HE3	1:162:A:ALA:HB1	5	0.48
(2,317)	1:61:A:ILE:HG22	1:38:A:THR:HG22	7	0.48
(2,209)	1:151:A:ASP:HA	1:154:A:MET:HG2	7	0.48
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG22	8	0.48
(2,11)	1:142:A:THR:HB	1:143:A:LEU:HB2	8	0.48
(1,350)	1:4:A:ILE:HD13	1:5:A:TYR:HE2	1	0.48
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG21	7	0.48
(1,323)	1:8:A:ALA:HB3	1:79:A:VAL:HA	6	0.48
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	3	0.48
(1,151)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	7	0.48
(1,118)	1:48:A:LEU:HD11	1:48:A:LEU:HA	2	0.48
(1,102)	1:13:A:THR:HG21	1:16:A:GLN:HG2	6	0.48
(1,79)	1:31:A:ALA:HB1	1:36:A:ILE:HA	1	0.48
(1,79)	1:31:A:ALA:HB3	1:36:A:ILE:HA	7	0.48
(1,51)	1:61:A:ILE:HD13	1:41:A:LEU:HA	5	0.48
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG22	8	0.48
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB2	4	0.48
(1,25)	1:51:A:ASN:HA	1:46:A:ARG:HG3	3	0.48
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB1	2	0.48
(2,1436)	1:156:A:ALA:H	1:155:A:GLN:HB2	3	0.47
(2,1434)	1:56:A:GLU:H	1:56:A:GLU:HB3	8	0.47
(2,1230)	1:162:A:ALA:HB1	1:155:A:GLN:HB3	3	0.47
(2,1216)	1:52:A:PRO:HA	1:146:A:VAL:HG21	3	0.47
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG22	6	0.47
(2,1030)	1:31:A:ALA:HB2	1:71:A:THR:HG22	8	0.47
(2,1007)	1:22:A:ALA:HB3	1:25:A:ASP:HB2	4	0.47
(2,927)	1:8:A:ALA:HB3	1:79:A:VAL:HA	6	0.47
(2,836)	1:10:A:GLU:HA	1:10:A:GLU:HG3	4	0.47
(2,555)	1:41:A:LEU:HD23	1:60:A:MET:HB2	2	0.47
(2,521)	1:78:A:LEU:HD22	1:20:A:PHE:HB2	2	0.47
(2,516)	1:57:A:LEU:HD23	1:45:A:MET:HG2	7	0.47
(2,486)	1:157:A:LEU:HD22	1:157:A:LEU:HB2	7	0.47
(2,485)	1:157:A:LEU:HD23	1:158:A:LEU:HG	6	0.47
(2,475)	1:38:A:THR:HG22	1:61:A:ILE:HB	8	0.47
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG23	1	0.47
(2,449)	1:79:A:VAL:HG12	1:64:A:VAL:HB	3	0.47
(2,429)	1:72:A:VAL:HG11	1:76:A:GLU:HG3	1	0.47
(2,353)	1:45:A:MET:HE2	1:148:A:ILE:HG21	2	0.47
(2,311)	1:148:A:ILE:HD13	1:45:A:MET:HE2	1	0.47
(2,205)	1:76:A:GLU:HA	1:76:A:GLU:HG3	2	0.47
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD11	2	0.47
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE2	5	0.47
(1,316)	1:57:A:LEU:HA	1:143:A:LEU:HD12	2	0.47
(1,270)	1:44:A:VAL:HG12	1:47:A:MET:HG3	6	0.47
(1,264)	1:42:A:GLY:HA3	1:46:A:ARG:HG2	3	0.47
(1,264)	1:42:A:GLY:HA3	1:46:A:ARG:HG2	4	0.47
(1,99)	1:82:A:VAL:HG13	1:86:A:LYS:HB2	8	0.47
(2,1436)	1:156:A:ALA:H	1:155:A:GLN:HB2	2	0.46
(2,1434)	1:56:A:GLU:H	1:56:A:GLU:HB3	4	0.46
(2,1277)	1:78:A:LEU:HD12	1:20:A:PHE:HE2	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1254)	1:78:A:LEU:HD13	1:74:A:PHE:HD2	3	0.46
(2,1214)	1:146:A:VAL:HG21	1:52:A:PRO:HB3	3	0.46
(2,1198)	1:28:A:VAL:HG23	1:25:A:ASP:HB2	5	0.46
(2,1131)	1:79:A:VAL:HA	1:83:A:ARG:HG2	7	0.46
(2,1123)	1:72:A:VAL:HG23	1:76:A:GLU:HG2	2	0.46
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG22	1	0.46
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE3	2	0.46
(2,831)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	3	0.46
(2,762)	1:36:A:ILE:HB	1:72:A:VAL:HB	7	0.46
(2,669)	1:90:A:LYS:HE3	1:90:A:LYS:HD2	1	0.46
(2,669)	1:90:A:LYS:HE2	1:90:A:LYS:HD3	3	0.46
(2,494)	1:79:A:VAL:H	1:79:A:VAL:HG21	4	0.46
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG22	2	0.46
(2,353)	1:45:A:MET:HE3	1:148:A:ILE:HG22	5	0.46
(2,342)	1:80:A:MET:HE1	1:77:A:PHE:HD1	2	0.46
(2,267)	1:25:A:ASP:HA	1:28:A:VAL:HG21	7	0.46
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	3	0.46
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG13	5	0.46
(2,24)	1:54:A:PRO:HA	1:54:A:PRO:HD3	8	0.46
(1,350)	1:79:A:VAL:HG11	1:5:A:TYR:HE1	3	0.46
(1,350)	1:4:A:ILE:HD13	1:5:A:TYR:HE1	4	0.46
(1,321)	1:146:A:VAL:HG11	1:56:A:GLU:HB2	4	0.46
(1,256)	1:31:A:ALA:HA	1:32:A:GLU:HA	8	0.46
(1,183)	1:45:A:MET:HG3	1:52:A:PRO:HG2	2	0.46
(1,165)	1:18:A:ASN:HB2	1:17:A:LYS:HB2	3	0.46
(1,127)	1:41:A:LEU:HD21	1:60:A:MET:HB3	2	0.46
(1,71)	1:153:A:MET:HE3	1:153:A:MET:HA	5	0.46
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG23	8	0.46
(2,1277)	1:78:A:LEU:HD12	1:20:A:PHE:HE2	4	0.45
(2,1196)	1:1:A:MET:HE2	1:6:A:LYS:HG2	1	0.45
(2,1182)	1:141:A:PRO:HD3	1:140:A:ARG:HD2	8	0.45
(2,766)	1:36:A:ILE:HG23	1:72:A:VAL:HB	2	0.45
(2,693)	1:27:A:PHE:HB2	1:36:A:ILE:HD13	2	0.45
(2,669)	1:90:A:LYS:HE3	1:90:A:LYS:HD2	2	0.45
(2,620)	1:140:A:ARG:HG2	1:140:A:ARG:HD3	1	0.45
(2,526)	1:26:A:ILE:HA	1:29:A:LEU:HD22	1	0.45
(2,519)	1:78:A:LEU:HD23	1:77:A:PHE:HD1	8	0.45
(2,516)	1:57:A:LEU:HD23	1:45:A:MET:HG2	4	0.45
(2,494)	1:79:A:VAL:H	1:79:A:VAL:HG21	5	0.45
(2,439)	1:146:A:VAL:HG11	1:56:A:GLU:HA	3	0.45
(2,415)	1:44:A:VAL:HG11	1:47:A:MET:HE3	7	0.45
(2,397)	1:160:A:ALA:HB2	1:159:A:GLY:HA3	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,374)	1:31:A:ALA:HB3	1:32:A:GLU:HB2	2	0.45
(2,349)	1:45:A:MET:HE3	1:52:A:PRO:HD3	4	0.45
(2,342)	1:80:A:MET:HE1	1:77:A:PHE:HD1	4	0.45
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD13	4	0.45
(2,18)	1:38:A:THR:HA	1:61:A:ILE:HG12	8	0.45
(1,393)	1:26:A:ILE:H	1:26:A:ILE:HD13	1	0.45
(1,321)	1:146:A:VAL:HG11	1:56:A:GLU:HB2	3	0.45
(1,286)	1:72:A:VAL:HG21	1:58:A:GLN:HA	8	0.45
(1,246)	1:158:A:LEU:HD23	1:22:A:ALA:HA	6	0.45
(1,237)	1:52:A:PRO:HD3	1:46:A:ARG:HG3	7	0.45
(1,231)	1:23:A:ALA:HB3	1:24:A:PHE:HA	5	0.45
(1,220)	1:44:A:VAL:HB	1:48:A:LEU:HD11	4	0.45
(1,151)	1:26:A:ILE:HD11	1:157:A:LEU:HB2	2	0.45
(1,130)	1:52:A:PRO:HG3	1:146:A:VAL:HG22	7	0.45
(1,99)	1:82:A:VAL:HG11	1:86:A:LYS:HB2	7	0.45
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB2	3	0.44
(2,1277)	1:78:A:LEU:HD12	1:20:A:PHE:HE2	8	0.44
(2,1254)	1:78:A:LEU:HD13	1:74:A:PHE:HD1	2	0.44
(2,1198)	1:28:A:VAL:HG22	1:25:A:ASP:HB2	3	0.44
(2,1164)	1:158:A:LEU:HD13	1:161:A:ARG:HD3	7	0.44
(2,1108)	1:71:A:THR:HA	1:38:A:THR:HG22	7	0.44
(2,1101)	1:61:A:ILE:HD12	1:36:A:ILE:HD12	8	0.44
(2,929)	1:152:A:ALA:HB2	1:149:A:SER:HA	8	0.44
(2,866)	1:137:A:LYS:HB2	1:138:A:PHE:HD1	4	0.44
(2,669)	1:90:A:LYS:HE3	1:90:A:LYS:HD2	5	0.44
(2,620)	1:140:A:ARG:HG2	1:140:A:ARG:HD3	7	0.44
(2,521)	1:78:A:LEU:HD21	1:20:A:PHE:HB2	4	0.44
(2,460)	1:71:A:THR:HG23	1:35:A:SER:HB3	1	0.44
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG23	2	0.44
(2,439)	1:146:A:VAL:HG12	1:56:A:GLU:HA	5	0.44
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG13	7	0.44
(2,365)	1:154:A:MET:HE3	1:158:A:LEU:HD21	7	0.44
(2,352)	1:148:A:ILE:HG21	1:153:A:MET:HB3	6	0.44
(2,342)	1:80:A:MET:HE2	1:77:A:PHE:HD1	5	0.44
(2,337)	1:60:A:MET:HE1	1:84:A:SER:HB3	4	0.44
(2,267)	1:25:A:ASP:HA	1:28:A:VAL:HG22	1	0.44
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	8	0.44
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG21	6	0.44
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB2	4	0.44
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD2	6	0.44
(1,323)	1:8:A:ALA:HB1	1:79:A:VAL:HA	3	0.44
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HE3	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:60:A:MET:HG3	1:148:A:ILE:HD13	5	0.44
(1,168)	1:56:A:GLU:HG3	1:146:A:VAL:HB	6	0.44
(1,165)	1:18:A:ASN:HB2	1:17:A:LYS:HB2	5	0.44
(1,86)	1:85:A:MET:HA	1:150:A:ALA:HB2	2	0.44
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG21	2	0.44
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB1	7	0.43
(2,1434)	1:56:A:GLU:H	1:56:A:GLU:HB3	5	0.43
(2,1291)	1:41:A:LEU:HD12	1:27:A:PHE:HZ	3	0.43
(2,1184)	1:148:A:ILE:HD12	1:44:A:VAL:HG23	8	0.43
(2,1183)	1:146:A:VAL:HG23	1:145:A:ARG:HD2	2	0.43
(2,1167)	1:53:A:THR:HB	1:54:A:PRO:HG3	5	0.43
(2,1151)	1:150:A:ALA:HA	1:148:A:ILE:HG22	6	0.43
(2,1030)	1:31:A:ALA:HB1	1:71:A:THR:HG23	4	0.43
(2,927)	1:8:A:ALA:HB1	1:79:A:VAL:HA	3	0.43
(2,710)	1:72:A:VAL:HG21	1:36:A:ILE:HB	3	0.43
(2,693)	1:27:A:PHE:HB2	1:36:A:ILE:HD11	1	0.43
(2,669)	1:90:A:LYS:HE2	1:90:A:LYS:HD3	7	0.43
(2,668)	1:6:A:LYS:HE3	1:10:A:GLU:HG3	5	0.43
(2,620)	1:140:A:ARG:HG3	1:140:A:ARG:HD2	2	0.43
(2,620)	1:140:A:ARG:HG3	1:140:A:ARG:HD2	4	0.43
(2,616)	1:140:A:ARG:HD3	1:140:A:ARG:HA	6	0.43
(2,616)	1:140:A:ARG:HD3	1:140:A:ARG:HA	7	0.43
(2,502)	1:72:A:VAL:HG21	1:71:A:THR:HA	7	0.43
(2,486)	1:157:A:LEU:HD22	1:157:A:LEU:HB2	1	0.43
(2,453)	1:79:A:VAL:HG13	1:83:A:ARG:HG2	1	0.43
(2,427)	1:72:A:VAL:HG13	1:77:A:PHE:HB3	3	0.43
(2,381)	1:7:A:ALA:HB2	1:10:A:GLU:HB2	4	0.43
(2,374)	1:31:A:ALA:HB2	1:32:A:GLU:HB3	3	0.43
(2,311)	1:148:A:ILE:HD13	1:45:A:MET:HE2	4	0.43
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD1	2	0.43
(1,288)	1:75:A:ASP:HB3	1:78:A:LEU:HB2	4	0.43
(1,286)	1:72:A:VAL:HG21	1:58:A:GLN:HA	7	0.43
(1,268)	1:44:A:VAL:HG22	1:47:A:MET:HB3	6	0.43
(1,247)	1:23:A:ALA:HB2	1:24:A:PHE:HB3	3	0.43
(1,220)	1:44:A:VAL:HB	1:48:A:LEU:HD11	3	0.43
(1,151)	1:26:A:ILE:HD12	1:157:A:LEU:HB2	4	0.43
(1,111)	1:6:A:LYS:HA	1:9:A:VAL:HG22	4	0.43
(1,105)	1:57:A:LEU:HA	1:38:A:THR:HG22	3	0.43
(1,54)	1:148:A:ILE:HD12	1:80:A:MET:HG2	2	0.43
(1,19)	1:14:A:GLU:HA	1:17:A:LYS:HE2	3	0.43
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HG23	5	0.43
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB2	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1266)	1:20:A:PHE:HD2	1:20:A:PHE:HE2	2	0.42
(2,1266)	1:20:A:PHE:HD1	1:20:A:PHE:HE1	3	0.42
(2,1266)	1:20:A:PHE:HD2	1:20:A:PHE:HE2	4	0.42
(2,1266)	1:20:A:PHE:HD2	1:20:A:PHE:HE2	5	0.42
(2,1266)	1:20:A:PHE:HD1	1:20:A:PHE:HE1	7	0.42
(2,1266)	1:20:A:PHE:HD2	1:20:A:PHE:HE2	8	0.42
(2,1265)	1:157:A:LEU:HD12	1:27:A:PHE:HD1	6	0.42
(2,1254)	1:78:A:LEU:HD13	1:74:A:PHE:HD2	4	0.42
(2,1254)	1:78:A:LEU:HD13	1:74:A:PHE:HD1	5	0.42
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD13	3	0.42
(2,1006)	1:22:A:ALA:HB1	1:25:A:ASP:HB3	3	0.42
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE1	4	0.42
(2,749)	1:16:A:GLN:HA	1:16:A:GLN:HG3	4	0.42
(2,620)	1:140:A:ARG:HG2	1:140:A:ARG:HD3	5	0.42
(2,550)	1:41:A:LEU:HD22	1:41:A:LEU:HA	7	0.42
(2,521)	1:78:A:LEU:HD23	1:20:A:PHE:HB2	3	0.42
(2,519)	1:78:A:LEU:HD21	1:77:A:PHE:HD1	4	0.42
(2,460)	1:71:A:THR:HG23	1:35:A:SER:HB3	7	0.42
(2,417)	1:146:A:VAL:HA	1:146:A:VAL:HG23	2	0.42
(2,410)	1:31:A:ALA:HB3	1:28:A:VAL:HG21	1	0.42
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	1	0.42
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	1	0.42
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	5	0.42
(1,323)	1:8:A:ALA:HB2	1:79:A:VAL:HA	2	0.42
(1,321)	1:146:A:VAL:HG11	1:56:A:GLU:HB2	1	0.42
(1,293)	1:82:A:VAL:HG13	1:85:A:MET:HG2	4	0.42
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG21	5	0.42
(1,195)	1:148:A:ILE:HG21	1:153:A:MET:HB3	6	0.42
(1,186)	1:148:A:ILE:HD13	1:45:A:MET:HG2	2	0.42
(1,63)	1:60:A:MET:HE3	1:148:A:ILE:HD12	3	0.42
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB3	3	0.42
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB3	7	0.42
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB2	5	0.41
(2,1515)	1:40:A:GLU:H	1:40:A:GLU:HG2	4	0.41
(2,1443)	1:83:A:ARG:H	1:82:A:VAL:HG21	1	0.41
(2,1266)	1:20:A:PHE:HD1	1:20:A:PHE:HE1	1	0.41
(2,1266)	1:20:A:PHE:HD1	1:20:A:PHE:HE1	6	0.41
(2,1265)	1:157:A:LEU:HD12	1:27:A:PHE:HD1	5	0.41
(2,1201)	1:28:A:VAL:HG22	1:24:A:PHE:HD1	4	0.41
(2,1170)	1:161:A:ARG:HD2	1:26:A:ILE:HD11	5	0.41
(2,1146)	1:161:A:ARG:HB2	1:158:A:LEU:HD22	4	0.41
(2,1094)	1:52:A:PRO:HA	1:57:A:LEU:HD23	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE2	5	0.41
(2,943)	1:86:A:LYS:HB3	1:90:A:LYS:HE2	6	0.41
(2,940)	1:164:A:GLY:HA3	1:163:A:LYS:HE2	6	0.41
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD21	1	0.41
(2,927)	1:8:A:ALA:HB2	1:79:A:VAL:HA	2	0.41
(2,831)	1:9:A:VAL:HG13	1:10:A:GLU:HG3	2	0.41
(2,682)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	1	0.41
(2,643)	1:162:A:ALA:HB1	1:158:A:LEU:HB3	5	0.41
(2,620)	1:140:A:ARG:HG3	1:140:A:ARG:HD2	3	0.41
(2,552)	1:38:A:THR:HA	1:41:A:LEU:HD23	2	0.41
(2,521)	1:78:A:LEU:HD21	1:20:A:PHE:HB2	5	0.41
(2,417)	1:146:A:VAL:HA	1:146:A:VAL:HG21	1	0.41
(2,355)	1:153:A:MET:HE1	1:27:A:PHE:HD2	7	0.41
(2,274)	1:60:A:MET:HA	1:60:A:MET:HG2	4	0.41
(2,246)	1:90:A:LYS:HA	1:90:A:LYS:HG3	7	0.41
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD2	3	0.41
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG21	1	0.41
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	4	0.41
(1,334)	1:40:A:GLU:HB2	1:27:A:PHE:HD2	5	0.41
(1,334)	1:27:A:PHE:HD1	1:40:A:GLU:HG2	7	0.41
(1,330)	1:83:A:ARG:HD2	1:5:A:TYR:HD2	4	0.41
(1,223)	1:4:A:ILE:HD12	1:83:A:ARG:HD2	8	0.41
(1,130)	1:52:A:PRO:HG3	1:57:A:LEU:HD11	4	0.41
(1,109)	1:41:A:LEU:HD12	1:27:A:PHE:HZ	3	0.41
(1,72)	1:153:A:MET:HE3	1:157:A:LEU:HB2	5	0.41
(1,58)	1:1:A:MET:HE1	1:76:A:GLU:HA	6	0.41
(1,44)	1:81:A:MET:HA	1:148:A:ILE:HG23	1	0.41
(1,17)	1:78:A:LEU:HA	1:78:A:LEU:HB2	1	0.41
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD12	8	0.41
(1,4)	1:38:A:THR:HB	1:61:A:ILE:HD13	2	0.41
(2,1224)	1:37:A:SER:HB3	1:61:A:ILE:HD12	6	0.4
(2,1220)	1:148:A:ILE:HG13	1:148:A:ILE:HA	8	0.4
(2,1202)	1:156:A:ALA:HB2	1:47:A:MET:HG2	8	0.4
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD21	4	0.4
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	1	0.4
(2,1027)	1:31:A:ALA:HA	1:43:A:LYS:HB3	1	0.4
(2,1016)	1:72:A:VAL:HG11	1:74:A:PHE:HA	8	0.4
(2,1007)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	2	0.4
(2,956)	1:50:A:GLN:HB3	1:45:A:MET:HB3	2	0.4
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD21	8	0.4
(2,927)	1:8:A:ALA:HB2	1:79:A:VAL:HA	5	0.4
(2,887)	1:46:A:ARG:HB2	1:46:A:ARG:HD2	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,620)	1:140:A:ARG:HG2	1:140:A:ARG:HD3	8	0.4
(2,588)	1:52:A:PRO:HG2	1:57:A:LEU:HD13	7	0.4
(2,556)	1:41:A:LEU:HD21	1:41:A:LEU:HB2	3	0.4
(2,476)	1:38:A:THR:HG22	1:61:A:ILE:HG12	8	0.4
(2,429)	1:72:A:VAL:HG13	1:76:A:GLU:HG3	5	0.4
(2,410)	1:31:A:ALA:HB2	1:28:A:VAL:HG23	4	0.4
(2,317)	1:61:A:ILE:HG22	1:38:A:THR:HG21	8	0.4
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG13	3	0.4
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB2	6	0.4
(1,323)	1:8:A:ALA:HB2	1:79:A:VAL:HA	5	0.4
(1,266)	1:153:A:MET:HE3	1:157:A:LEU:HA	5	0.4
(1,255)	1:28:A:VAL:HG11	1:72:A:VAL:HB	3	0.4
(1,247)	1:23:A:ALA:HB2	1:24:A:PHE:HB3	2	0.4
(1,237)	1:44:A:VAL:HA	1:46:A:ARG:HG3	3	0.4
(1,220)	1:44:A:VAL:HB	1:48:A:LEU:HD12	6	0.4
(1,192)	1:41:A:LEU:HD22	1:60:A:MET:HB2	5	0.4
(1,177)	1:156:A:ALA:HA	1:155:A:GLN:HG3	4	0.4
(1,165)	1:18:A:ASN:HB2	1:17:A:LYS:HB2	4	0.4
(1,140)	1:147:A:ARG:HD3	1:143:A:LEU:HD22	4	0.4
(1,105)	1:57:A:LEU:HA	1:38:A:THR:HG23	4	0.4
(1,102)	1:13:A:THR:HG21	1:16:A:GLN:HG2	3	0.4
(1,102)	1:13:A:THR:HG23	1:16:A:GLN:HG2	5	0.4
(1,99)	1:82:A:VAL:HG12	1:86:A:LYS:HB2	3	0.4
(1,91)	1:146:A:VAL:HG21	1:56:A:GLU:HB3	2	0.4
(1,51)	1:38:A:THR:HB	1:61:A:ILE:HD12	1	0.4
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HG23	4	0.4
(2,1167)	1:53:A:THR:HB	1:54:A:PRO:HG3	4	0.39
(2,1104)	1:64:A:VAL:HG23	1:72:A:VAL:HA	3	0.39
(2,1096)	1:58:A:GLN:HG2	1:38:A:THR:HG21	6	0.39
(2,1007)	1:22:A:ALA:HB1	1:25:A:ASP:HB2	5	0.39
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE1	1	0.39
(2,929)	1:152:A:ALA:HB3	1:149:A:SER:HA	1	0.39
(2,864)	1:86:A:LYS:HB2	1:5:A:TYR:HE2	7	0.39
(2,665)	1:21:A:LYS:HG2	1:21:A:LYS:HE2	1	0.39
(2,665)	1:21:A:LYS:HG2	1:21:A:LYS:HE2	8	0.39
(2,467)	1:9:A:VAL:HG11	1:6:A:LYS:HA	7	0.39
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	2	0.39
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	6	0.39
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG21	5	0.39
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG21	7	0.39
(1,385)	1:46:A:ARG:H	1:46:A:ARG:HB2	4	0.39
(1,283)	1:65:A:ASP:HB3	1:61:A:ILE:HD13	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	1:23:A:ALA:HB3	1:24:A:PHE:HB3	7	0.39
(1,165)	1:18:A:ASN:HB2	1:17:A:LYS:HB2	1	0.39
(1,155)	1:14:A:GLU:HA	1:17:A:LYS:HE2	3	0.39
(1,155)	1:43:A:LYS:HE2	1:28:A:VAL:HA	6	0.39
(1,136)	1:155:A:GLN:HB3	1:155:A:GLN:HG2	7	0.39
(1,72)	1:153:A:MET:HE3	1:157:A:LEU:HB2	3	0.39
(1,72)	1:153:A:MET:HE1	1:157:A:LEU:HB2	8	0.39
(1,51)	1:38:A:THR:HB	1:61:A:ILE:HD13	6	0.39
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HG22	2	0.39
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG21	5	0.39
(2,1556)	1:78:A:LEU:H	1:78:A:LEU:HD23	7	0.38
(2,1229)	1:81:A:MET:HE3	1:77:A:PHE:HD1	4	0.38
(2,1198)	1:28:A:VAL:HG21	1:25:A:ASP:HB2	4	0.38
(2,1181)	1:141:A:PRO:HD2	1:140:A:ARG:HD2	8	0.38
(2,1131)	1:79:A:VAL:HA	1:83:A:ARG:HG2	1	0.38
(2,1123)	1:72:A:VAL:HG22	1:76:A:GLU:HG2	1	0.38
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD22	4	0.38
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE1	3	0.38
(2,929)	1:152:A:ALA:HB1	1:149:A:SER:HA	7	0.38
(2,892)	1:56:A:GLU:HA	1:56:A:GLU:HB2	6	0.38
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	3	0.38
(2,668)	1:6:A:LYS:HE3	1:10:A:GLU:HG3	2	0.38
(2,620)	1:140:A:ARG:HG2	1:140:A:ARG:HD3	6	0.38
(2,550)	1:41:A:LEU:HD22	1:41:A:LEU:HA	6	0.38
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG22	7	0.38
(2,365)	1:154:A:MET:HE1	1:158:A:LEU:HD21	1	0.38
(2,363)	1:154:A:MET:HE2	1:162:A:ALA:HB3	4	0.38
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD11	3	0.38
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	8	0.38
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	8	0.38
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB2	2	0.38
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	2	0.38
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	1	0.38
(1,350)	1:79:A:VAL:HG13	1:5:A:TYR:HE1	2	0.38
(1,326)	1:61:A:ILE:HD13	1:57:A:LEU:HA	6	0.38
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD12	4	0.38
(1,263)	1:42:A:GLY:HA3	1:46:A:ARG:HG3	7	0.38
(1,234)	1:81:A:MET:HA	1:64:A:VAL:HB	4	0.38
(1,226)	1:158:A:LEU:HD23	1:161:A:ARG:HB3	1	0.38
(1,136)	1:58:A:GLN:HB3	1:58:A:GLN:HG2	6	0.38
(1,52)	1:61:A:ILE:HD12	1:36:A:ILE:HB	5	0.38
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG23	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD1	3	0.37
(2,1235)	1:5:A:TYR:HD2	1:5:A:TYR:HE2	1	0.37
(2,1235)	1:5:A:TYR:HD1	1:5:A:TYR:HE1	7	0.37
(2,1163)	1:157:A:LEU:HD21	1:27:A:PHE:HE2	7	0.37
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD22	8	0.37
(2,892)	1:56:A:GLU:HA	1:56:A:GLU:HB2	8	0.37
(2,847)	1:10:A:GLU:HB2	1:10:A:GLU:HG2	4	0.37
(2,835)	1:7:A:ALA:HB3	1:10:A:GLU:HG3	6	0.37
(2,804)	1:90:A:LYS:HD3	1:87:A:ASP:HB3	5	0.37
(2,733)	1:56:A:GLU:HG2	1:56:A:GLU:HA	1	0.37
(2,693)	1:27:A:PHE:HB2	1:36:A:ILE:HD13	4	0.37
(2,475)	1:38:A:THR:HG23	1:61:A:ILE:HB	7	0.37
(2,429)	1:72:A:VAL:HG11	1:76:A:GLU:HG3	4	0.37
(2,407)	1:36:A:ILE:HG21	1:41:A:LEU:HB3	3	0.37
(2,405)	1:36:A:ILE:HG22	1:40:A:GLU:HB2	1	0.37
(2,400)	1:162:A:ALA:HB2	1:158:A:LEU:HD21	3	0.37
(2,381)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	7	0.37
(2,374)	1:31:A:ALA:HB1	1:32:A:GLU:HB2	7	0.37
(2,319)	1:85:A:MET:HE1	1:82:A:VAL:HA	1	0.37
(2,173)	1:27:A:PHE:HA	1:157:A:LEU:HD11	7	0.37
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD2	4	0.37
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG12	2	0.37
(2,126)	1:19:A:GLU:HA	1:19:A:GLU:HG2	6	0.37
(2,65)	1:84:A:SER:HB2	1:148:A:ILE:HG22	7	0.37
(1,362)	1:19:A:GLU:H	1:18:A:ASN:HB2	1	0.37
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HD1	4	0.37
(1,247)	1:23:A:ALA:HB2	1:24:A:PHE:HB3	4	0.37
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	4	0.37
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	5	0.37
(1,136)	1:58:A:GLN:HB3	1:58:A:GLN:HG2	1	0.37
(1,136)	1:155:A:GLN:HB3	1:155:A:GLN:HG2	8	0.37
(1,97)	1:72:A:VAL:HG11	1:64:A:VAL:HB	1	0.37
(1,82)	1:156:A:ALA:HB1	1:153:A:MET:HB2	5	0.37
(1,79)	1:31:A:ALA:HB1	1:36:A:ILE:HA	5	0.37
(1,60)	1:47:A:MET:HE2	1:26:A:ILE:HG23	1	0.37
(2,1695)	1:37:A:SER:H	1:40:A:GLU:HB3	8	0.36
(2,1541)	1:40:A:GLU:H	1:39:A:LYS:HB2	1	0.36
(2,1511)	1:59:A:GLU:H	1:59:A:GLU:HG3	2	0.36
(2,1365)	1:152:A:ALA:H	1:151:A:ASP:HB2	7	0.36
(2,1235)	1:5:A:TYR:HD1	1:5:A:TYR:HE1	6	0.36
(2,1229)	1:81:A:MET:HE3	1:77:A:PHE:HD1	1	0.36
(2,1217)	1:146:A:VAL:HG13	1:147:A:ARG:HA	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1196)	1:1:A:MET:HE1	1:6:A:LYS:HG2	4	0.36
(2,1100)	1:61:A:ILE:HD13	1:40:A:GLU:HB2	2	0.36
(2,1025)	1:28:A:VAL:HG13	1:43:A:LYS:HD2	1	0.36
(2,1006)	1:22:A:ALA:HB1	1:25:A:ASP:HB3	2	0.36
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD22	7	0.36
(2,927)	1:8:A:ALA:HB3	1:79:A:VAL:HA	4	0.36
(2,927)	1:8:A:ALA:HB3	1:79:A:VAL:HA	7	0.36
(2,892)	1:56:A:GLU:HA	1:56:A:GLU:HB2	7	0.36
(2,831)	1:9:A:VAL:HG11	1:10:A:GLU:HG3	5	0.36
(2,669)	1:90:A:LYS:HE2	1:90:A:LYS:HD3	4	0.36
(2,648)	1:57:A:LEU:HD23	1:41:A:LEU:HB3	6	0.36
(2,562)	1:12:A:LEU:HD12	1:17:A:LYS:HG3	2	0.36
(2,562)	1:12:A:LEU:HD13	1:17:A:LYS:HG3	5	0.36
(2,521)	1:78:A:LEU:HD22	1:20:A:PHE:HB2	6	0.36
(2,516)	1:57:A:LEU:HD22	1:45:A:MET:HG2	8	0.36
(2,506)	1:72:A:VAL:HG22	1:76:A:GLU:HB2	3	0.36
(2,505)	1:72:A:VAL:HG22	1:64:A:VAL:HB	8	0.36
(2,494)	1:79:A:VAL:H	1:79:A:VAL:HG21	3	0.36
(2,396)	1:155:A:GLN:HA	1:162:A:ALA:HB2	7	0.36
(2,344)	1:80:A:MET:HE1	1:80:A:MET:HA	1	0.36
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG21	4	0.36
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG22	7	0.36
(1,403)	1:55:A:GLU:H	1:54:A:PRO:HB3	1	0.36
(1,385)	1:46:A:ARG:H	1:46:A:ARG:HG2	3	0.36
(1,337)	1:44:A:VAL:HB	1:27:A:PHE:HE1	3	0.36
(1,329)	1:5:A:TYR:HD1	1:72:A:VAL:HG13	2	0.36
(1,328)	1:41:A:LEU:HA	1:44:A:VAL:HG23	8	0.36
(1,323)	1:8:A:ALA:HB3	1:79:A:VAL:HA	4	0.36
(1,323)	1:8:A:ALA:HB3	1:79:A:VAL:HA	7	0.36
(1,287)	1:75:A:ASP:HB2	1:78:A:LEU:HB2	8	0.36
(1,277)	1:61:A:ILE:HD11	1:58:A:GLN:HB2	1	0.36
(1,192)	1:60:A:MET:HB2	1:146:A:VAL:HG23	7	0.36
(1,177)	1:156:A:ALA:HA	1:155:A:GLN:HG3	5	0.36
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	1	0.36
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	3	0.36
(1,97)	1:72:A:VAL:HG13	1:64:A:VAL:HB	5	0.36
(1,74)	1:154:A:MET:HE3	1:19:A:GLU:HA	8	0.36
(1,71)	1:153:A:MET:HE1	1:153:A:MET:HA	4	0.36
(1,64)	1:80:A:MET:HE1	1:27:A:PHE:HE1	6	0.36
(1,55)	1:148:A:ILE:HD11	1:153:A:MET:HB3	2	0.36
(1,27)	1:89:A:SER:HA	1:88:A:ASP:HB3	5	0.36
(1,14)	1:142:A:THR:HA	1:143:A:LEU:HB2	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG21	4	0.36
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG21	6	0.36
(2,1400)	1:85:A:MET:H	1:84:A:SER:HB2	8	0.35
(2,1235)	1:5:A:TYR:HD2	1:5:A:TYR:HE2	8	0.35
(2,1215)	1:60:A:MET:HG3	1:146:A:VAL:HG23	7	0.35
(2,1153)	1:154:A:MET:HE3	1:150:A:ALA:HA	2	0.35
(2,1004)	1:21:A:LYS:HG2	1:74:A:PHE:HE2	7	0.35
(2,961)	1:81:A:MET:HE2	1:80:A:MET:HG2	7	0.35
(2,904)	1:4:A:ILE:HD11	1:5:A:TYR:HE2	3	0.35
(2,835)	1:7:A:ALA:HB3	1:10:A:GLU:HG3	7	0.35
(2,669)	1:90:A:LYS:HE2	1:90:A:LYS:HD3	6	0.35
(2,669)	1:90:A:LYS:HE2	1:90:A:LYS:HD3	8	0.35
(2,621)	1:147:A:ARG:HD2	1:147:A:ARG:HA	5	0.35
(2,521)	1:78:A:LEU:HD23	1:20:A:PHE:HB2	7	0.35
(2,519)	1:78:A:LEU:HD22	1:77:A:PHE:HD1	2	0.35
(2,517)	1:57:A:LEU:HD22	1:41:A:LEU:HB2	8	0.35
(2,465)	1:82:A:VAL:HG21	1:78:A:LEU:HB3	5	0.35
(2,459)	1:71:A:THR:HG22	1:36:A:ILE:HA	8	0.35
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG21	4	0.35
(2,453)	1:79:A:VAL:HG13	1:83:A:ARG:HG2	7	0.35
(2,446)	1:79:A:VAL:HG11	1:5:A:TYR:HB2	3	0.35
(2,438)	1:146:A:VAL:HA	1:146:A:VAL:HG11	6	0.35
(2,410)	1:31:A:ALA:HB1	1:28:A:VAL:HG22	2	0.35
(2,191)	1:155:A:GLN:HA	1:158:A:LEU:HD12	5	0.35
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	6	0.35
(2,15)	1:79:A:VAL:HA	1:79:A:VAL:HG12	4	0.35
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	3	0.35
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HG22	2	0.35
(1,349)	1:4:A:ILE:HG12	1:5:A:TYR:HE1	4	0.35
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD1	4	0.35
(1,311)	1:85:A:MET:HE1	1:8:A:ALA:HB2	7	0.35
(1,264)	1:42:A:GLY:HA3	1:52:A:PRO:HB2	1	0.35
(1,246)	1:158:A:LEU:HD21	1:22:A:ALA:HA	1	0.35
(1,169)	1:56:A:GLU:HG3	1:52:A:PRO:HB2	2	0.35
(1,122)	1:45:A:MET:HE2	1:48:A:LEU:HD12	7	0.35
(1,70)	1:153:A:MET:HE2	1:27:A:PHE:HE2	8	0.35
(1,37)	1:57:A:LEU:HA	1:146:A:VAL:HG22	4	0.35
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD12	4	0.35
(2,1235)	1:5:A:TYR:HD1	1:5:A:TYR:HE1	2	0.34
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	5	0.34
(2,866)	1:137:A:LYS:HB3	1:138:A:PHE:HD2	7	0.34
(2,643)	1:162:A:ALA:HB2	1:158:A:LEU:HB3	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,578)	1:36:A:ILE:HG21	1:41:A:LEU:HG	4	0.34
(2,558)	1:12:A:LEU:HD12	1:12:A:LEU:HA	2	0.34
(2,552)	1:38:A:THR:HA	1:41:A:LEU:HD23	4	0.34
(2,519)	1:78:A:LEU:HD23	1:77:A:PHE:HD1	7	0.34
(2,516)	1:57:A:LEU:HD21	1:45:A:MET:HG2	2	0.34
(2,475)	1:38:A:THR:HG23	1:61:A:ILE:HB	6	0.34
(2,364)	1:154:A:MET:HE1	1:158:A:LEU:HD13	5	0.34
(2,344)	1:80:A:MET:HE2	1:80:A:MET:HA	7	0.34
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	6	0.34
(2,276)	1:14:A:GLU:HA	1:17:A:LYS:HB2	1	0.34
(2,272)	1:60:A:MET:HA	1:63:A:GLU:HB3	5	0.34
(2,168)	1:89:A:SER:HA	1:137:A:LYS:HB3	4	0.34
(1,349)	1:4:A:ILE:HG13	1:5:A:TYR:HE2	3	0.34
(1,325)	1:61:A:ILE:HD13	1:58:A:GLN:HG3	8	0.34
(1,300)	1:158:A:LEU:HB2	1:155:A:GLN:HA	8	0.34
(1,268)	1:44:A:VAL:HG21	1:47:A:MET:HB3	7	0.34
(1,264)	1:42:A:GLY:HA3	1:46:A:ARG:HG2	5	0.34
(1,247)	1:23:A:ALA:HB3	1:24:A:PHE:HB3	8	0.34
(1,206)	1:17:A:LYS:HG3	1:17:A:LYS:HB2	1	0.34
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	2	0.34
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	6	0.34
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	7	0.34
(1,146)	1:158:A:LEU:HB3	1:158:A:LEU:HG	8	0.34
(1,141)	1:145:A:ARG:HD2	1:146:A:VAL:HG13	5	0.34
(1,105)	1:57:A:LEU:HA	1:38:A:THR:HG21	5	0.34
(1,102)	1:13:A:THR:HG23	1:16:A:GLN:HG2	4	0.34
(1,60)	1:47:A:MET:HE3	1:26:A:ILE:HG22	8	0.34
(1,52)	1:61:A:ILE:HD13	1:36:A:ILE:HB	4	0.34
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	8	0.34
(1,25)	1:51:A:ASN:HA	1:46:A:ARG:HG3	5	0.34
(2,1400)	1:85:A:MET:H	1:84:A:SER:HB2	2	0.33
(2,1235)	1:5:A:TYR:HD1	1:5:A:TYR:HE1	3	0.33
(2,1235)	1:5:A:TYR:HD1	1:5:A:TYR:HE1	5	0.33
(2,1229)	1:81:A:MET:HE2	1:77:A:PHE:HD1	8	0.33
(2,1153)	1:154:A:MET:HE2	1:150:A:ALA:HA	3	0.33
(2,1147)	1:140:A:ARG:HG3	1:141:A:PRO:HD3	2	0.33
(2,1131)	1:79:A:VAL:HA	1:83:A:ARG:HG2	6	0.33
(2,1131)	1:79:A:VAL:HA	1:83:A:ARG:HG2	8	0.33
(2,1003)	1:19:A:GLU:HA	1:158:A:LEU:HD21	1	0.33
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	1	0.33
(2,924)	1:161:A:ARG:HA	1:161:A:ARG:HB2	7	0.33
(2,883)	1:1:A:MET:HG3	1:6:A:LYS:HB2	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,882)	1:1:A:MET:HG3	1:79:A:VAL:HB	8	0.33
(2,619)	1:46:A:ARG:HD3	1:46:A:ARG:HG3	7	0.33
(2,516)	1:57:A:LEU:HD23	1:45:A:MET:HG2	3	0.33
(2,465)	1:82:A:VAL:HG21	1:78:A:LEU:HB3	4	0.33
(2,381)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	6	0.33
(2,381)	1:7:A:ALA:HB1	1:10:A:GLU:HB2	8	0.33
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	6	0.33
(2,204)	1:10:A:GLU:HA	1:9:A:VAL:HG13	1	0.33
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	2	0.33
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD2	5	0.33
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	1	0.33
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG22	1	0.33
(1,327)	1:65:A:ASP:HB3	1:64:A:VAL:HG22	8	0.33
(1,295)	1:142:A:THR:HA	1:147:A:ARG:HD3	7	0.33
(1,264)	1:42:A:GLY:HA3	1:52:A:PRO:HB2	8	0.33
(1,255)	1:28:A:VAL:HG13	1:72:A:VAL:HB	2	0.33
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG23	4	0.33
(1,130)	1:52:A:PRO:HG3	1:57:A:LEU:HD13	3	0.33
(1,86)	1:85:A:MET:HA	1:150:A:ALA:HB3	5	0.33
(1,67)	1:80:A:MET:HE2	1:148:A:ILE:HG12	8	0.33
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	1	0.33
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	3	0.33
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	6	0.33
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	7	0.33
(1,15)	1:28:A:VAL:HA	1:40:A:GLU:HB2	8	0.33
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB2	4	0.33
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB1	5	0.33
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG23	3	0.33
(2,1658)	1:53:A:THR:H	1:53:A:THR:HG22	2	0.32
(2,1511)	1:59:A:GLU:H	1:59:A:GLU:HG3	8	0.32
(2,1235)	1:5:A:TYR:HD2	1:5:A:TYR:HE2	4	0.32
(2,1202)	1:156:A:ALA:HB3	1:47:A:MET:HG2	6	0.32
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD21	6	0.32
(2,929)	1:152:A:ALA:HB2	1:149:A:SER:HA	6	0.32
(2,921)	1:161:A:ARG:HD2	1:161:A:ARG:HB3	4	0.32
(2,702)	1:59:A:GLU:HA	1:62:A:ASP:HB2	5	0.32
(2,687)	1:27:A:PHE:HB3	1:24:A:PHE:HA	5	0.32
(2,619)	1:46:A:ARG:HD3	1:46:A:ARG:HG3	2	0.32
(2,517)	1:57:A:LEU:HD22	1:41:A:LEU:HB2	7	0.32
(2,505)	1:72:A:VAL:HG21	1:64:A:VAL:HB	5	0.32
(2,467)	1:9:A:VAL:HG11	1:6:A:LYS:HA	1	0.32
(2,459)	1:71:A:THR:HG22	1:36:A:ILE:HA	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,429)	1:72:A:VAL:HG12	1:76:A:GLU:HG3	3	0.32
(2,410)	1:31:A:ALA:HB2	1:28:A:VAL:HG22	6	0.32
(2,374)	1:31:A:ALA:HB2	1:32:A:GLU:HB3	8	0.32
(2,358)	1:153:A:MET:HE1	1:44:A:VAL:HG11	1	0.32
(2,332)	1:1:A:MET:HE3	1:79:A:VAL:HG12	8	0.32
(2,276)	1:14:A:GLU:HA	1:17:A:LYS:HB2	6	0.32
(2,188)	1:63:A:GLU:HA	1:63:A:GLU:HB2	1	0.32
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD1	6	0.32
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB2	8	0.32
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HD12	1	0.32
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	2	0.32
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	4	0.32
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD1	8	0.32
(1,312)	1:80:A:MET:HE2	1:60:A:MET:HG3	4	0.32
(1,247)	1:23:A:ALA:HB2	1:24:A:PHE:HB3	6	0.32
(1,246)	1:158:A:LEU:HD21	1:22:A:ALA:HA	7	0.32
(1,228)	1:137:A:LYS:HB2	1:136:A:GLY:HA3	7	0.32
(1,226)	1:23:A:ALA:HB1	1:158:A:LEU:HD21	8	0.32
(1,223)	1:4:A:ILE:HD11	1:83:A:ARG:HD2	6	0.32
(1,190)	1:155:A:GLN:HG3	1:155:A:GLN:HA	5	0.32
(1,85)	1:160:A:ALA:HB2	1:161:A:ARG:HB3	6	0.32
(1,58)	1:1:A:MET:HE3	1:1:A:MET:HA	8	0.32
(1,55)	1:148:A:ILE:HD11	1:153:A:MET:HB3	3	0.32
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	2	0.32
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	5	0.32
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	5	0.32
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB1	4	0.31
(2,1617)	1:48:A:LEU:H	1:48:A:LEU:HD11	4	0.31
(2,1436)	1:156:A:ALA:H	1:155:A:GLN:HB2	4	0.31
(2,1181)	1:141:A:PRO:HD2	1:140:A:ARG:HD3	3	0.31
(2,1145)	1:161:A:ARG:HB3	1:26:A:ILE:HD11	7	0.31
(2,1142)	1:138:A:PHE:HB2	1:137:A:LYS:HB2	2	0.31
(2,1123)	1:72:A:VAL:HG22	1:76:A:GLU:HG2	4	0.31
(2,1122)	1:72:A:VAL:HG13	1:76:A:GLU:HG2	5	0.31
(2,1113)	1:72:A:VAL:HG23	1:77:A:PHE:HB2	3	0.31
(2,1030)	1:31:A:ALA:HB2	1:71:A:THR:HG21	5	0.31
(2,1016)	1:72:A:VAL:HG12	1:74:A:PHE:HA	6	0.31
(2,938)	1:41:A:LEU:HA	1:41:A:LEU:HG	5	0.31
(2,892)	1:56:A:GLU:HA	1:56:A:GLU:HB2	4	0.31
(2,887)	1:46:A:ARG:HB2	1:46:A:ARG:HD2	8	0.31
(2,619)	1:46:A:ARG:HD3	1:46:A:ARG:HG3	1	0.31
(2,619)	1:46:A:ARG:HD3	1:46:A:ARG:HG3	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,571)	1:140:A:ARG:HG3	1:140:A:ARG:HA	2	0.31
(2,558)	1:12:A:LEU:HD12	1:12:A:LEU:HA	1	0.31
(2,459)	1:71:A:THR:HG21	1:36:A:ILE:HA	2	0.31
(2,459)	1:71:A:THR:HG23	1:36:A:ILE:HA	7	0.31
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG23	7	0.31
(2,449)	1:79:A:VAL:HG11	1:64:A:VAL:HB	1	0.31
(2,417)	1:146:A:VAL:HA	1:146:A:VAL:HG21	3	0.31
(2,399)	1:162:A:ALA:HB2	1:158:A:LEU:HD11	8	0.31
(2,361)	1:154:A:MET:HE3	1:154:A:MET:HB3	3	0.31
(2,338)	1:60:A:MET:HE1	1:60:A:MET:HA	2	0.31
(2,249)	1:161:A:ARG:HA	1:161:A:ARG:HG3	4	0.31
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	6	0.31
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	7	0.31
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	2	0.31
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	5	0.31
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG22	2	0.31
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG11	2	0.31
(1,385)	1:46:A:ARG:H	1:46:A:ARG:HB2	5	0.31
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	3	0.31
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	5	0.31
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	5	0.31
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	8	0.31
(1,287)	1:75:A:ASP:HB2	1:78:A:LEU:HB2	5	0.31
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG22	1	0.31
(1,258)	1:31:A:ALA:HB3	1:29:A:LEU:HD21	3	0.31
(1,255)	1:28:A:VAL:HG11	1:72:A:VAL:HB	4	0.31
(1,249)	1:77:A:PHE:HB3	1:75:A:ASP:HA	6	0.31
(1,190)	1:155:A:GLN:HG3	1:155:A:GLN:HA	4	0.31
(1,179)	1:155:A:GLN:HG3	1:162:A:ALA:HB2	1	0.31
(1,102)	1:13:A:THR:HG21	1:16:A:GLN:HG2	1	0.31
(1,71)	1:153:A:MET:HE3	1:153:A:MET:HA	3	0.31
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	6	0.31
(2,1663)	1:35:A:SER:H	1:31:A:ALA:HB1	6	0.3
(2,1259)	1:77:A:PHE:HA	1:77:A:PHE:HD1	1	0.3
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD1	4	0.3
(2,1229)	1:81:A:MET:HE3	1:77:A:PHE:HD1	3	0.3
(2,1158)	1:160:A:ALA:HA	1:163:A:LYS:HE2	1	0.3
(2,1153)	1:154:A:MET:HE1	1:150:A:ALA:HA	4	0.3
(2,1135)	1:82:A:VAL:HG12	1:5:A:TYR:HE2	2	0.3
(2,1100)	1:61:A:ILE:HD13	1:40:A:GLU:HB2	3	0.3
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE3	6	0.3
(2,969)	1:80:A:MET:HG3	1:81:A:MET:HE3	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,578)	1:36:A:ILE:HG23	1:41:A:LEU:HG	2	0.3
(2,457)	1:37:A:SER:HB2	1:71:A:THR:HG21	6	0.3
(2,357)	1:153:A:MET:HE2	1:36:A:ILE:HG22	8	0.3
(2,341)	1:60:A:MET:HE2	1:148:A:ILE:HG12	6	0.3
(2,188)	1:63:A:GLU:HA	1:63:A:GLU:HB2	5	0.3
(2,188)	1:63:A:GLU:HA	1:63:A:GLU:HB2	7	0.3
(2,15)	1:79:A:VAL:HA	1:79:A:VAL:HG13	2	0.3
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	1	0.3
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	6	0.3
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	8	0.3
(1,347)	1:5:A:TYR:HE1	1:2:A:ASP:HB3	5	0.3
(1,288)	1:75:A:ASP:HB3	1:78:A:LEU:HB2	2	0.3
(1,272)	1:47:A:MET:HE1	1:27:A:PHE:HD1	2	0.3
(1,249)	1:77:A:PHE:HB3	1:75:A:ASP:HA	7	0.3
(1,244)	1:2:A:ASP:HB2	1:83:A:ARG:HG3	3	0.3
(1,220)	1:44:A:VAL:HB	1:48:A:LEU:HD13	5	0.3
(1,205)	1:9:A:VAL:HG11	1:9:A:VAL:HB	6	0.3
(1,174)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	4	0.3
(1,174)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	6	0.3
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD23	6	0.3
(1,101)	1:64:A:VAL:HG11	1:80:A:MET:HG3	3	0.3
(1,93)	1:28:A:VAL:HG13	1:24:A:PHE:HD2	5	0.3
(1,85)	1:160:A:ALA:HB3	1:161:A:ARG:HB3	8	0.3
(1,52)	1:61:A:ILE:HD12	1:36:A:ILE:HB	2	0.3
(1,33)	1:16:A:GLN:HA	1:16:A:GLN:HB2	4	0.3
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	4	0.3
(2,1296)	1:5:A:TYR:HE2	1:90:A:LYS:HD3	6	0.29
(2,1228)	1:83:A:ARG:HD3	1:64:A:VAL:HG21	1	0.29
(2,1095)	1:52:A:PRO:HD2	1:57:A:LEU:HD21	1	0.29
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD22	3	0.29
(2,892)	1:56:A:GLU:HA	1:56:A:GLU:HB2	5	0.29
(2,775)	1:155:A:GLN:HA	1:155:A:GLN:HG2	3	0.29
(2,766)	1:36:A:ILE:HG22	1:72:A:VAL:HB	5	0.29
(2,682)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	5	0.29
(2,625)	1:161:A:ARG:HD3	1:161:A:ARG:HG2	8	0.29
(2,616)	1:140:A:ARG:HD2	1:140:A:ARG:HA	5	0.29
(2,610)	1:54:A:PRO:HG2	1:54:A:PRO:HB3	7	0.29
(2,562)	1:12:A:LEU:HD12	1:17:A:LYS:HG3	4	0.29
(2,459)	1:71:A:THR:HG23	1:36:A:ILE:HA	3	0.29
(2,326)	1:44:A:VAL:HA	1:47:A:MET:HE3	7	0.29
(2,317)	1:61:A:ILE:HG21	1:38:A:THR:HG22	6	0.29
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD22	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	3	0.29
(2,33)	1:44:A:VAL:HA	1:47:A:MET:HG2	6	0.29
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	7	0.29
(1,405)	1:60:A:MET:H	1:59:A:GLU:HG3	7	0.29
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HG23	5	0.29
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD11	8	0.29
(1,282)	1:58:A:GLN:HA	1:61:A:ILE:HG12	6	0.29
(1,263)	1:42:A:GLY:HA3	1:52:A:PRO:HG2	6	0.29
(1,215)	1:43:A:LYS:HB3	1:43:A:LYS:HD2	1	0.29
(1,214)	1:43:A:LYS:HD3	1:40:A:GLU:HG2	2	0.29
(1,205)	1:9:A:VAL:HG23	1:9:A:VAL:HB	8	0.29
(1,190)	1:155:A:GLN:HG3	1:155:A:GLN:HA	2	0.29
(1,155)	1:43:A:LYS:HE2	1:28:A:VAL:HA	4	0.29
(1,136)	1:155:A:GLN:HB3	1:155:A:GLN:HG2	2	0.29
(1,136)	1:155:A:GLN:HB3	1:155:A:GLN:HG2	4	0.29
(1,122)	1:45:A:MET:HE2	1:48:A:LEU:HD11	4	0.29
(1,55)	1:148:A:ILE:HD11	1:153:A:MET:HE3	1	0.29
(1,52)	1:61:A:ILE:HD13	1:36:A:ILE:HB	3	0.29
(1,14)	1:142:A:THR:HA	1:143:A:LEU:HB2	6	0.29
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	8	0.29
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	5	0.28
(2,1234)	1:148:A:ILE:HB	1:84:A:SER:HB3	6	0.28
(2,1153)	1:154:A:MET:HE2	1:150:A:ALA:HA	5	0.28
(2,1135)	1:82:A:VAL:HG13	1:5:A:TYR:HE2	3	0.28
(2,1122)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	4	0.28
(2,996)	1:157:A:LEU:HG	1:157:A:LEU:HA	6	0.28
(2,929)	1:152:A:ALA:HB1	1:149:A:SER:HA	4	0.28
(2,610)	1:54:A:PRO:HG2	1:54:A:PRO:HB3	1	0.28
(2,584)	1:52:A:PRO:HG3	1:45:A:MET:HB3	8	0.28
(2,552)	1:38:A:THR:HA	1:41:A:LEU:HD23	5	0.28
(2,485)	1:157:A:LEU:HD22	1:158:A:LEU:HG	5	0.28
(2,482)	1:157:A:LEU:HD21	1:27:A:PHE:HA	5	0.28
(2,472)	1:9:A:VAL:HG11	1:6:A:LYS:HG2	1	0.28
(2,439)	1:146:A:VAL:HG11	1:56:A:GLU:HA	8	0.28
(2,427)	1:72:A:VAL:HG11	1:77:A:PHE:HB3	8	0.28
(2,407)	1:36:A:ILE:HG23	1:41:A:LEU:HB3	7	0.28
(2,396)	1:155:A:GLN:HA	1:162:A:ALA:HB2	3	0.28
(2,374)	1:31:A:ALA:HB2	1:32:A:GLU:HB3	5	0.28
(2,338)	1:60:A:MET:HE2	1:60:A:MET:HA	7	0.28
(2,333)	1:47:A:MET:HE1	1:157:A:LEU:HD21	2	0.28
(2,325)	1:47:A:MET:HE3	1:157:A:LEU:HA	5	0.28
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG22	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:63:A:GLU:HA	1:63:A:GLU:HB2	8	0.28
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD1	1	0.28
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG22	5	0.28
(2,15)	1:79:A:VAL:HA	1:79:A:VAL:HG11	3	0.28
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	8	0.28
(1,298)	1:148:A:ILE:HG22	1:27:A:PHE:HZ	3	0.28
(1,297)	1:148:A:ILE:HG22	1:84:A:SER:HA	6	0.28
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD22	6	0.28
(1,225)	1:140:A:ARG:HB2	1:143:A:LEU:HD13	6	0.28
(1,205)	1:9:A:VAL:HG23	1:9:A:VAL:HB	1	0.28
(1,205)	1:9:A:VAL:HG22	1:9:A:VAL:HB	3	0.28
(1,136)	1:155:A:GLN:HB3	1:155:A:GLN:HG2	5	0.28
(1,70)	1:153:A:MET:HE1	1:27:A:PHE:HE2	7	0.28
(2,1230)	1:162:A:ALA:HB2	1:155:A:GLN:HB3	2	0.27
(2,1229)	1:81:A:MET:HE2	1:77:A:PHE:HD1	6	0.27
(2,1225)	1:64:A:VAL:HG12	1:76:A:GLU:HA	2	0.27
(2,1101)	1:61:A:ILE:HD11	1:36:A:ILE:HD12	2	0.27
(2,1053)	1:40:A:GLU:HG2	1:43:A:LYS:HB3	7	0.27
(2,1034)	1:35:A:SER:HA	1:73:A:ASP:HB3	3	0.27
(2,931)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	3	0.27
(2,929)	1:152:A:ALA:HB3	1:149:A:SER:HA	3	0.27
(2,847)	1:10:A:GLU:HB3	1:10:A:GLU:HG2	2	0.27
(2,847)	1:10:A:GLU:HB3	1:10:A:GLU:HG2	3	0.27
(2,847)	1:10:A:GLU:HB2	1:10:A:GLU:HG2	6	0.27
(2,799)	1:55:A:GLU:HG2	1:55:A:GLU:HB3	2	0.27
(2,775)	1:155:A:GLN:HA	1:155:A:GLN:HG2	2	0.27
(2,667)	1:88:A:ASP:HB2	1:88:A:ASP:HA	3	0.27
(2,577)	1:41:A:LEU:HD21	1:41:A:LEU:HG	1	0.27
(2,577)	1:41:A:LEU:HD22	1:41:A:LEU:HG	8	0.27
(2,558)	1:12:A:LEU:HD11	1:12:A:LEU:HA	7	0.27
(2,544)	1:43:A:LYS:HG2	1:43:A:LYS:HE2	1	0.27
(2,521)	1:78:A:LEU:HD23	1:20:A:PHE:HB2	8	0.27
(2,503)	1:48:A:LEU:HD21	1:153:A:MET:HA	2	0.27
(2,494)	1:79:A:VAL:H	1:79:A:VAL:HG21	2	0.27
(2,490)	1:41:A:LEU:HD13	1:38:A:THR:HA	3	0.27
(2,485)	1:157:A:LEU:HD21	1:158:A:LEU:HG	3	0.27
(2,459)	1:71:A:THR:HG21	1:36:A:ILE:HA	5	0.27
(2,434)	1:82:A:VAL:HG11	1:5:A:TYR:HD2	7	0.27
(2,385)	1:156:A:ALA:HB1	1:153:A:MET:HA	1	0.27
(2,361)	1:154:A:MET:HE3	1:154:A:MET:HB3	5	0.27
(2,344)	1:80:A:MET:HE2	1:80:A:MET:HA	6	0.27
(2,325)	1:47:A:MET:HE1	1:157:A:LEU:HA	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD23	5	0.27
(2,188)	1:63:A:GLU:HA	1:63:A:GLU:HB2	4	0.27
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	3	0.27
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG21	2	0.27
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	6	0.27
(2,130)	1:19:A:GLU:HA	1:158:A:LEU:HD12	3	0.27
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB3	5	0.27
(1,365)	1:22:A:ALA:H	1:21:A:LYS:HA	7	0.27
(1,330)	1:83:A:ARG:HD2	1:5:A:TYR:HD1	7	0.27
(1,316)	1:59:A:GLU:HA	1:143:A:LEU:HD13	6	0.27
(1,295)	1:147:A:ARG:HD2	1:142:A:THR:HA	5	0.27
(1,269)	1:44:A:VAL:HG22	1:40:A:GLU:HB3	3	0.27
(1,205)	1:9:A:VAL:HG22	1:9:A:VAL:HB	2	0.27
(1,190)	1:155:A:GLN:HG3	1:155:A:GLN:HA	3	0.27
(1,174)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	3	0.27
(1,174)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	7	0.27
(1,136)	1:155:A:GLN:HB3	1:155:A:GLN:HG2	3	0.27
(1,79)	1:31:A:ALA:HB3	1:36:A:ILE:HA	4	0.27
(1,63)	1:60:A:MET:HE1	1:148:A:ILE:HD13	5	0.27
(1,51)	1:38:A:THR:HB	1:61:A:ILE:HD13	7	0.27
(1,34)	1:16:A:GLN:HA	1:19:A:GLU:HB2	6	0.27
(1,19)	1:14:A:GLU:HA	1:17:A:LYS:HE2	1	0.27
(1,14)	1:142:A:THR:HA	1:143:A:LEU:HB2	1	0.27
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB2	7	0.27
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	3	0.27
(2,1436)	1:156:A:ALA:H	1:155:A:GLN:HB2	5	0.26
(2,1186)	1:72:A:VAL:HG23	1:36:A:ILE:HD13	3	0.26
(2,1172)	1:43:A:LYS:HG3	1:44:A:VAL:HG21	6	0.26
(2,1167)	1:53:A:THR:HB	1:54:A:PRO:HG3	8	0.26
(2,1147)	1:140:A:ARG:HG2	1:141:A:PRO:HD3	5	0.26
(2,1106)	1:64:A:VAL:HG22	1:76:A:GLU:HG3	8	0.26
(2,1096)	1:58:A:GLN:HG2	1:38:A:THR:HG21	5	0.26
(2,1088)	1:51:A:ASN:HB3	1:52:A:PRO:HD3	3	0.26
(2,1012)	1:24:A:PHE:HA	1:21:A:LYS:HD3	5	0.26
(2,1006)	1:22:A:ALA:HB2	1:25:A:ASP:HB3	1	0.26
(2,965)	1:60:A:MET:HB3	1:60:A:MET:HG2	2	0.26
(2,847)	1:10:A:GLU:HB3	1:10:A:GLU:HG2	5	0.26
(2,847)	1:10:A:GLU:HB2	1:10:A:GLU:HG2	8	0.26
(2,775)	1:155:A:GLN:HA	1:155:A:GLN:HG2	5	0.26
(2,625)	1:161:A:ARG:HD3	1:161:A:ARG:HG2	2	0.26
(2,619)	1:46:A:ARG:HD3	1:46:A:ARG:HG3	4	0.26
(2,558)	1:12:A:LEU:HD13	1:12:A:LEU:HA	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,505)	1:72:A:VAL:HG22	1:64:A:VAL:HB	1	0.26
(2,474)	1:38:A:THR:HG23	1:57:A:LEU:HB2	2	0.26
(2,467)	1:9:A:VAL:HG13	1:6:A:LYS:HA	8	0.26
(2,446)	1:79:A:VAL:HG12	1:5:A:TYR:HB2	4	0.26
(2,442)	1:79:A:VAL:H	1:79:A:VAL:HG12	6	0.26
(2,442)	1:79:A:VAL:H	1:79:A:VAL:HG13	8	0.26
(2,427)	1:72:A:VAL:HG12	1:77:A:PHE:HB3	7	0.26
(2,363)	1:154:A:MET:HE3	1:162:A:ALA:HB2	3	0.26
(2,355)	1:153:A:MET:HE2	1:27:A:PHE:HD2	8	0.26
(2,328)	1:47:A:MET:HE1	1:47:A:MET:HG3	2	0.26
(2,328)	1:47:A:MET:HE2	1:47:A:MET:HG3	5	0.26
(2,230)	1:50:A:GLN:HA	1:50:A:GLN:HG2	1	0.26
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	2	0.26
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	7	0.26
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	8	0.26
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD2	5	0.26
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	4	0.26
(1,276)	1:155:A:GLN:HB2	1:48:A:LEU:HD21	7	0.26
(1,249)	1:77:A:PHE:HB3	1:75:A:ASP:HA	4	0.26
(1,165)	1:18:A:ASN:HB2	1:17:A:LYS:HB2	6	0.26
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD22	5	0.26
(1,86)	1:85:A:MET:HA	1:150:A:ALA:HB1	4	0.26
(1,83)	1:152:A:ALA:HB3	1:48:A:LEU:HD13	2	0.26
(1,82)	1:156:A:ALA:HB3	1:47:A:MET:HB3	4	0.26
(1,79)	1:31:A:ALA:HB1	1:36:A:ILE:HA	3	0.26
(1,36)	1:76:A:GLU:HA	1:76:A:GLU:HG2	2	0.26
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB3	3	0.26
(2,1617)	1:48:A:LEU:H	1:48:A:LEU:HD11	3	0.25
(2,1541)	1:40:A:GLU:H	1:39:A:LYS:HB2	6	0.25
(2,1259)	1:77:A:PHE:HA	1:77:A:PHE:HD1	6	0.25
(2,1259)	1:77:A:PHE:HA	1:77:A:PHE:HD1	8	0.25
(2,1232)	1:44:A:VAL:HG11	1:153:A:MET:HA	8	0.25
(2,1231)	1:162:A:ALA:HB3	1:163:A:LYS:HE2	5	0.25
(2,1204)	1:140:A:ARG:HB2	1:141:A:PRO:HD3	3	0.25
(2,1166)	1:54:A:PRO:HG3	1:53:A:THR:HA	6	0.25
(2,1093)	1:13:A:THR:HG22	1:11:A:GLN:HG2	8	0.25
(2,1020)	1:28:A:VAL:HA	1:36:A:ILE:HG23	5	0.25
(2,1007)	1:22:A:ALA:HB2	1:25:A:ASP:HB2	1	0.25
(2,1006)	1:22:A:ALA:HB1	1:25:A:ASP:HB3	5	0.25
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD21	2	0.25
(2,973)	1:42:A:GLY:HA2	1:46:A:ARG:HG2	6	0.25
(2,943)	1:86:A:LYS:HB3	1:90:A:LYS:HE3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,916)	1:63:A:GLU:HB3	1:64:A:VAL:HG21	1	0.25
(2,847)	1:10:A:GLU:HB3	1:10:A:GLU:HG2	1	0.25
(2,835)	1:7:A:ALA:HB3	1:10:A:GLU:HG3	8	0.25
(2,787)	1:139:A:LYS:HB2	1:139:A:LYS:HA	7	0.25
(2,767)	1:45:A:MET:HA	1:45:A:MET:HG3	1	0.25
(2,762)	1:36:A:ILE:HB	1:72:A:VAL:HB	6	0.25
(2,625)	1:161:A:ARG:HD2	1:161:A:ARG:HG3	5	0.25
(2,625)	1:161:A:ARG:HD2	1:161:A:ARG:HG3	6	0.25
(2,610)	1:54:A:PRO:HG2	1:54:A:PRO:HB3	6	0.25
(2,558)	1:12:A:LEU:HD11	1:12:A:LEU:HA	3	0.25
(2,556)	1:41:A:LEU:HD23	1:41:A:LEU:HB2	1	0.25
(2,467)	1:9:A:VAL:HG12	1:6:A:LYS:HA	6	0.25
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG21	6	0.25
(2,377)	1:150:A:ALA:HB2	1:85:A:MET:HG2	3	0.25
(2,301)	1:61:A:ILE:HD12	1:72:A:VAL:HB	7	0.25
(2,275)	1:56:A:GLU:HA	1:56:A:GLU:HG3	5	0.25
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD23	4	0.25
(2,246)	1:90:A:LYS:HA	1:90:A:LYS:HG3	3	0.25
(2,188)	1:63:A:GLU:HA	1:63:A:GLU:HB2	6	0.25
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	7	0.25
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB1	3	0.25
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	2	0.25
(1,344)	1:77:A:PHE:HZ	1:148:A:ILE:HG22	4	0.25
(1,330)	1:83:A:ARG:HD2	1:5:A:TYR:HD1	8	0.25
(1,320)	1:56:A:GLU:HB2	1:146:A:VAL:HG22	5	0.25
(1,247)	1:23:A:ALA:HB1	1:24:A:PHE:HB3	1	0.25
(1,205)	1:9:A:VAL:HG12	1:9:A:VAL:HB	4	0.25
(1,205)	1:9:A:VAL:HG23	1:9:A:VAL:HB	7	0.25
(1,181)	1:50:A:GLN:HG3	1:49:A:GLY:HA3	6	0.25
(1,174)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	8	0.25
(1,96)	1:53:A:THR:HB	1:53:A:THR:HG22	4	0.25
(1,96)	1:53:A:THR:HB	1:53:A:THR:HG22	5	0.25
(1,89)	1:44:A:VAL:HG11	1:153:A:MET:HB3	5	0.25
(1,58)	1:1:A:MET:HE1	1:76:A:GLU:HA	7	0.25
(1,53)	1:157:A:LEU:HA	1:26:A:ILE:HD11	2	0.25
(1,34)	1:16:A:GLN:HA	1:19:A:GLU:HB2	7	0.25
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	2	0.25
(2,1541)	1:40:A:GLU:H	1:39:A:LYS:HB2	4	0.24
(2,1541)	1:40:A:GLU:H	1:39:A:LYS:HB2	8	0.24
(2,1511)	1:59:A:GLU:H	1:59:A:GLU:HG3	1	0.24
(2,1259)	1:77:A:PHE:HA	1:77:A:PHE:HD1	7	0.24
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1229)	1:81:A:MET:HE2	1:77:A:PHE:HD1	2	0.24
(2,1219)	1:146:A:VAL:HG12	1:52:A:PRO:HB3	6	0.24
(2,1153)	1:154:A:MET:HE3	1:150:A:ALA:HA	1	0.24
(2,1125)	1:77:A:PHE:HB2	1:74:A:PHE:HD2	4	0.24
(2,1096)	1:58:A:GLN:HG2	1:38:A:THR:HG23	4	0.24
(2,996)	1:157:A:LEU:HG	1:157:A:LEU:HA	2	0.24
(2,996)	1:157:A:LEU:HG	1:157:A:LEU:HA	4	0.24
(2,965)	1:60:A:MET:HB3	1:60:A:MET:HG2	8	0.24
(2,926)	1:8:A:ALA:HB1	1:5:A:TYR:HD2	7	0.24
(2,847)	1:10:A:GLU:HB2	1:10:A:GLU:HG2	7	0.24
(2,787)	1:139:A:LYS:HB2	1:139:A:LYS:HA	6	0.24
(2,787)	1:139:A:LYS:HB2	1:139:A:LYS:HA	8	0.24
(2,577)	1:41:A:LEU:HD23	1:41:A:LEU:HG	7	0.24
(2,558)	1:12:A:LEU:HD12	1:12:A:LEU:HA	6	0.24
(2,558)	1:12:A:LEU:HD11	1:12:A:LEU:HA	8	0.24
(2,453)	1:79:A:VAL:HG12	1:83:A:ARG:HG2	6	0.24
(2,442)	1:79:A:VAL:H	1:79:A:VAL:HG13	7	0.24
(2,325)	1:47:A:MET:HE3	1:157:A:LEU:HA	2	0.24
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD1	1	0.24
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD2	4	0.24
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD1	8	0.24
(2,136)	1:15:A:GLU:HA	1:15:A:GLU:HG2	2	0.24
(2,133)	1:6:A:LYS:HA	1:6:A:LYS:HB2	8	0.24
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG22	2	0.24
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG21	3	0.24
(2,50)	1:149:A:SER:HB3	1:152:A:ALA:HB1	7	0.24
(1,404)	1:55:A:GLU:H	1:55:A:GLU:HG2	5	0.24
(1,362)	1:19:A:GLU:H	1:18:A:ASN:HB2	2	0.24
(1,337)	1:44:A:VAL:HB	1:27:A:PHE:HE1	4	0.24
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD1	1	0.24
(1,241)	1:48:A:LEU:HG	1:45:A:MET:HA	3	0.24
(1,231)	1:23:A:ALA:HB2	1:24:A:PHE:HA	3	0.24
(1,231)	1:23:A:ALA:HB2	1:24:A:PHE:HA	4	0.24
(1,226)	1:23:A:ALA:HB1	1:158:A:LEU:HD21	7	0.24
(1,209)	1:63:A:GLU:HG2	1:64:A:VAL:HG21	3	0.24
(1,206)	1:43:A:LYS:HB3	1:43:A:LYS:HD3	8	0.24
(1,174)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	1	0.24
(1,161)	1:25:A:ASP:HA	1:25:A:ASP:HB3	1	0.24
(1,96)	1:13:A:THR:HB	1:13:A:THR:HG23	2	0.24
(1,79)	1:31:A:ALA:HB3	1:36:A:ILE:HA	6	0.24
(1,79)	1:31:A:ALA:HB1	1:36:A:ILE:HA	8	0.24
(1,59)	1:47:A:MET:HE2	1:43:A:LYS:HA	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:47:A:MET:HE2	1:43:A:LYS:HA	5	0.24
(2,1229)	1:81:A:MET:HE1	1:77:A:PHE:HD1	7	0.23
(2,1204)	1:140:A:ARG:HB2	1:141:A:PRO:HD3	4	0.23
(2,1012)	1:24:A:PHE:HA	1:21:A:LYS:HD3	3	0.23
(2,928)	1:9:A:VAL:HA	1:8:A:ALA:HB2	1	0.23
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	4	0.23
(2,787)	1:139:A:LYS:HB2	1:139:A:LYS:HA	3	0.23
(2,767)	1:45:A:MET:HA	1:45:A:MET:HG3	3	0.23
(2,767)	1:45:A:MET:HA	1:45:A:MET:HG3	4	0.23
(2,682)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	2	0.23
(2,667)	1:88:A:ASP:HB3	1:88:A:ASP:HA	2	0.23
(2,625)	1:161:A:ARG:HD2	1:161:A:ARG:HG3	1	0.23
(2,577)	1:41:A:LEU:HD22	1:41:A:LEU:HG	2	0.23
(2,577)	1:41:A:LEU:HD23	1:41:A:LEU:HG	3	0.23
(2,562)	1:12:A:LEU:HD11	1:17:A:LYS:HG3	3	0.23
(2,557)	1:4:A:ILE:HG13	1:4:A:ILE:HD12	2	0.23
(2,466)	1:82:A:VAL:HG21	1:83:A:ARG:HB2	8	0.23
(2,459)	1:71:A:THR:HG22	1:36:A:ILE:HA	4	0.23
(2,453)	1:79:A:VAL:HG13	1:83:A:ARG:HG2	8	0.23
(2,405)	1:36:A:ILE:HG22	1:40:A:GLU:HB2	7	0.23
(2,385)	1:156:A:ALA:HB3	1:153:A:MET:HA	7	0.23
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB3	3	0.23
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB1	5	0.23
(2,357)	1:153:A:MET:HE1	1:36:A:ILE:HG22	7	0.23
(2,338)	1:60:A:MET:HE1	1:60:A:MET:HA	6	0.23
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	3	0.23
(2,233)	1:48:A:LEU:HA	1:48:A:LEU:HB3	2	0.23
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB2	4	0.23
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	1	0.23
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	1	0.23
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	5	0.23
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD1	2	0.23
(2,126)	1:19:A:GLU:HA	1:19:A:GLU:HG2	7	0.23
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG22	6	0.23
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG23	7	0.23
(1,411)	1:159:A:GLY:H	1:159:A:GLY:HA3	5	0.23
(1,403)	1:55:A:GLU:H	1:54:A:PRO:HB3	6	0.23
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD1	3	0.23
(1,330)	1:83:A:ARG:HD2	1:5:A:TYR:HD1	6	0.23
(1,310)	1:84:A:SER:HB3	1:148:A:ILE:HG22	6	0.23
(1,304)	1:51:A:ASN:HB2	1:52:A:PRO:HD2	3	0.23
(1,255)	1:28:A:VAL:HG11	1:72:A:VAL:HB	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:77:A:PHE:HB3	1:75:A:ASP:HA	2	0.23
(1,186)	1:148:A:ILE:HD11	1:45:A:MET:HG2	5	0.23
(1,181)	1:50:A:GLN:HG2	1:45:A:MET:HA	8	0.23
(1,155)	1:14:A:GLU:HA	1:17:A:LYS:HE2	1	0.23
(1,139)	1:161:A:ARG:HD2	1:161:A:ARG:HB3	1	0.23
(1,110)	1:41:A:LEU:HD13	1:60:A:MET:HG2	4	0.23
(1,99)	1:82:A:VAL:HG13	1:86:A:LYS:HB2	6	0.23
(1,96)	1:13:A:THR:HB	1:13:A:THR:HG23	6	0.23
(1,96)	1:13:A:THR:HB	1:13:A:THR:HG23	8	0.23
(2,1214)	1:146:A:VAL:HG22	1:52:A:PRO:HB3	1	0.22
(2,1209)	1:140:A:ARG:HB3	1:141:A:PRO:HD3	2	0.22
(2,1146)	1:161:A:ARG:HB2	1:158:A:LEU:HD23	1	0.22
(2,1125)	1:77:A:PHE:HB2	1:74:A:PHE:HD1	2	0.22
(2,1021)	1:17:A:LYS:HA	1:12:A:LEU:HD12	2	0.22
(2,1020)	1:28:A:VAL:HA	1:36:A:ILE:HG22	7	0.22
(2,1003)	1:19:A:GLU:HA	1:158:A:LEU:HD21	3	0.22
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD22	3	0.22
(2,939)	1:143:A:LEU:HA	1:143:A:LEU:HD21	3	0.22
(2,787)	1:139:A:LYS:HB2	1:139:A:LYS:HA	5	0.22
(2,775)	1:155:A:GLN:HA	1:155:A:GLN:HG2	4	0.22
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	4	0.22
(2,667)	1:88:A:ASP:HB3	1:88:A:ASP:HA	1	0.22
(2,651)	1:41:A:LEU:HB2	1:41:A:LEU:HG	6	0.22
(2,651)	1:41:A:LEU:HB2	1:41:A:LEU:HG	7	0.22
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD23	2	0.22
(2,557)	1:4:A:ILE:HG12	1:4:A:ILE:HD11	3	0.22
(2,557)	1:4:A:ILE:HG13	1:4:A:ILE:HD12	4	0.22
(2,506)	1:72:A:VAL:HG22	1:76:A:GLU:HB2	4	0.22
(2,456)	1:82:A:VAL:HG22	1:5:A:TYR:HA	1	0.22
(2,385)	1:156:A:ALA:HB1	1:153:A:MET:HA	6	0.22
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB2	4	0.22
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB2	8	0.22
(2,353)	1:45:A:MET:HE2	1:148:A:ILE:HG22	1	0.22
(2,350)	1:45:A:MET:HE3	1:44:A:VAL:HG12	8	0.22
(2,334)	1:47:A:MET:HE1	1:44:A:VAL:HG21	7	0.22
(2,328)	1:47:A:MET:HE2	1:47:A:MET:HG3	3	0.22
(2,316)	1:61:A:ILE:HG22	1:61:A:ILE:HG12	3	0.22
(2,312)	1:148:A:ILE:HD11	1:148:A:ILE:HB	1	0.22
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	5	0.22
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB2	7	0.22
(2,244)	1:23:A:ALA:HA	1:26:A:ILE:HG13	8	0.22
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB1	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB1	8	0.22
(2,203)	1:10:A:GLU:HA	1:10:A:GLU:HG2	7	0.22
(2,183)	1:32:A:GLU:HA	1:32:A:GLU:HB3	2	0.22
(2,174)	1:60:A:MET:HA	1:60:A:MET:HG3	2	0.22
(2,149)	1:35:A:SER:HA	1:24:A:PHE:HD2	7	0.22
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	1	0.22
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	2	0.22
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG22	5	0.22
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	5	0.22
(1,404)	1:55:A:GLU:H	1:55:A:GLU:HG2	3	0.22
(1,386)	1:50:A:GLN:H	1:48:A:LEU:HB2	3	0.22
(1,334)	1:40:A:GLU:HB2	1:27:A:PHE:HD2	6	0.22
(1,321)	1:146:A:VAL:HG11	1:56:A:GLU:HB2	2	0.22
(1,270)	1:44:A:VAL:HG11	1:47:A:MET:HG3	4	0.22
(1,265)	1:146:A:VAL:HA	1:143:A:LEU:HB2	5	0.22
(1,205)	1:9:A:VAL:HG22	1:9:A:VAL:HB	5	0.22
(1,190)	1:155:A:GLN:HG3	1:155:A:GLN:HA	6	0.22
(1,174)	1:14:A:GLU:HG3	1:14:A:GLU:HB2	2	0.22
(1,174)	1:66:A:GLU:HG3	1:66:A:GLU:HB2	5	0.22
(1,161)	1:25:A:ASP:HA	1:25:A:ASP:HB3	2	0.22
(1,161)	1:25:A:ASP:HA	1:25:A:ASP:HB3	3	0.22
(1,161)	1:25:A:ASP:HA	1:25:A:ASP:HB3	4	0.22
(1,161)	1:25:A:ASP:HA	1:25:A:ASP:HB3	5	0.22
(1,81)	1:8:A:ALA:HB1	1:10:A:GLU:HG3	3	0.22
(1,67)	1:80:A:MET:HE1	1:148:A:ILE:HG12	7	0.22
(1,63)	1:60:A:MET:HE2	1:148:A:ILE:HD12	6	0.22
(1,54)	1:148:A:ILE:HD13	1:45:A:MET:HG2	4	0.22
(1,51)	1:38:A:THR:HB	1:61:A:ILE:HD11	8	0.22
(2,1636)	1:67:A:ASP:H	1:66:A:GLU:HB3	1	0.21
(2,1265)	1:157:A:LEU:HD12	1:27:A:PHE:HD1	3	0.21
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	6	0.21
(2,1228)	1:83:A:ARG:HD3	1:64:A:VAL:HG21	5	0.21
(2,1217)	1:146:A:VAL:HG11	1:147:A:ARG:HA	6	0.21
(2,1190)	1:37:A:SER:HA	1:61:A:ILE:HG22	7	0.21
(2,1170)	1:161:A:ARG:HD3	1:26:A:ILE:HD11	3	0.21
(2,1122)	1:72:A:VAL:HG12	1:76:A:GLU:HG2	7	0.21
(2,1100)	1:61:A:ILE:HD11	1:40:A:GLU:HB2	7	0.21
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD23	5	0.21
(2,1020)	1:28:A:VAL:HA	1:36:A:ILE:HG22	1	0.21
(2,996)	1:157:A:LEU:HG	1:157:A:LEU:HA	5	0.21
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD23	4	0.21
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,916)	1:63:A:GLU:HB3	1:64:A:VAL:HG23	6	0.21
(2,762)	1:36:A:ILE:HB	1:72:A:VAL:HB	8	0.21
(2,667)	1:88:A:ASP:HB3	1:88:A:ASP:HA	5	0.21
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD23	6	0.21
(2,577)	1:41:A:LEU:HD23	1:41:A:LEU:HG	6	0.21
(2,558)	1:12:A:LEU:HD12	1:12:A:LEU:HA	4	0.21
(2,557)	1:4:A:ILE:HG13	1:4:A:ILE:HD12	1	0.21
(2,557)	1:4:A:ILE:HG13	1:4:A:ILE:HD12	5	0.21
(2,557)	1:4:A:ILE:HG13	1:4:A:ILE:HD13	7	0.21
(2,474)	1:38:A:THR:HG23	1:57:A:LEU:HB2	4	0.21
(2,434)	1:82:A:VAL:HG13	1:5:A:TYR:HD2	6	0.21
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB3	2	0.21
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB1	6	0.21
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB3	7	0.21
(2,344)	1:80:A:MET:HE1	1:80:A:MET:HA	2	0.21
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG23	1	0.21
(2,276)	1:14:A:GLU:HA	1:17:A:LYS:HB2	8	0.21
(2,249)	1:161:A:ARG:HA	1:161:A:ARG:HG2	7	0.21
(2,204)	1:10:A:GLU:HA	1:9:A:VAL:HG11	6	0.21
(2,187)	1:155:A:GLN:HA	1:155:A:GLN:HB3	4	0.21
(2,130)	1:19:A:GLU:HA	1:158:A:LEU:HD13	2	0.21
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG23	4	0.21
(2,61)	1:89:A:SER:HB3	1:89:A:SER:HA	5	0.21
(2,61)	1:89:A:SER:HB3	1:89:A:SER:HA	8	0.21
(2,24)	1:54:A:PRO:HA	1:54:A:PRO:HD3	4	0.21
(1,405)	1:60:A:MET:H	1:60:A:MET:HG2	2	0.21
(1,404)	1:55:A:GLU:H	1:55:A:GLU:HG2	4	0.21
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	7	0.21
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HD12	3	0.21
(1,334)	1:27:A:PHE:HD2	1:40:A:GLU:HG2	1	0.21
(1,272)	1:47:A:MET:HE2	1:27:A:PHE:HD1	3	0.21
(1,263)	1:42:A:GLY:HA3	1:46:A:ARG:HG3	8	0.21
(1,246)	1:158:A:LEU:HD21	1:22:A:ALA:HA	8	0.21
(1,241)	1:48:A:LEU:HG	1:45:A:MET:HA	4	0.21
(1,229)	1:81:A:MET:HE2	1:20:A:PHE:HB3	2	0.21
(1,226)	1:23:A:ALA:HB3	1:158:A:LEU:HD23	6	0.21
(1,212)	1:17:A:LYS:HD3	1:14:A:GLU:HA	4	0.21
(1,184)	1:45:A:MET:HG3	1:146:A:VAL:HG13	7	0.21
(1,151)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	1	0.21
(1,133)	1:17:A:LYS:HG2	1:12:A:LEU:HD11	5	0.21
(1,96)	1:13:A:THR:HB	1:13:A:THR:HG23	1	0.21
(1,96)	1:13:A:THR:HB	1:13:A:THR:HG23	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:22:A:ALA:HB2	1:158:A:LEU:HD21	2	0.21
(1,59)	1:47:A:MET:HE3	1:43:A:LYS:HA	3	0.21
(1,35)	1:45:A:MET:HA	1:48:A:LEU:HB3	6	0.21
(1,35)	1:45:A:MET:HA	1:48:A:LEU:HB3	8	0.21
(1,34)	1:16:A:GLN:HA	1:19:A:GLU:HB2	8	0.21
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD12	3	0.21
(2,1326)	1:72:A:VAL:H	1:72:A:VAL:HG21	7	0.2
(2,1239)	1:5:A:TYR:HD2	1:82:A:VAL:HB	7	0.2
(2,1216)	1:52:A:PRO:HA	1:146:A:VAL:HG21	2	0.2
(2,1184)	1:148:A:ILE:HD13	1:44:A:VAL:HG22	7	0.2
(2,1170)	1:161:A:ARG:HD2	1:26:A:ILE:HD12	2	0.2
(2,1164)	1:158:A:LEU:HD12	1:161:A:ARG:HD3	4	0.2
(2,1142)	1:138:A:PHE:HB2	1:137:A:LYS:HB3	5	0.2
(2,1016)	1:72:A:VAL:HG12	1:74:A:PHE:HA	7	0.2
(2,1009)	1:24:A:PHE:HB3	1:21:A:LYS:HG2	5	0.2
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	7	0.2
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	8	0.2
(2,996)	1:157:A:LEU:HG	1:157:A:LEU:HA	3	0.2
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	1	0.2
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	2	0.2
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	3	0.2
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	5	0.2
(2,929)	1:152:A:ALA:HB2	1:149:A:SER:HA	5	0.2
(2,887)	1:46:A:ARG:HB2	1:46:A:ARG:HD2	6	0.2
(2,853)	1:43:A:LYS:HD3	1:43:A:LYS:HG3	4	0.2
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	8	0.2
(2,757)	1:82:A:VAL:HA	1:85:A:MET:HB2	6	0.2
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	3	0.2
(2,577)	1:41:A:LEU:HD22	1:41:A:LEU:HG	4	0.2
(2,555)	1:41:A:LEU:HD22	1:60:A:MET:HB2	3	0.2
(2,488)	1:44:A:VAL:HG23	1:27:A:PHE:HD1	1	0.2
(2,427)	1:72:A:VAL:HG11	1:77:A:PHE:HB3	6	0.2
(2,407)	1:36:A:ILE:HG22	1:41:A:LEU:HB3	6	0.2
(2,338)	1:60:A:MET:HE2	1:60:A:MET:HA	4	0.2
(2,317)	1:61:A:ILE:HG21	1:38:A:THR:HG22	1	0.2
(2,316)	1:61:A:ILE:HG23	1:61:A:ILE:HG12	4	0.2
(2,300)	1:61:A:ILE:HA	1:61:A:ILE:HD12	8	0.2
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB1	2	0.2
(2,174)	1:60:A:MET:HA	1:60:A:MET:HG3	8	0.2
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	7	0.2
(2,136)	1:15:A:GLU:HA	1:15:A:GLU:HG2	4	0.2
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG21	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:89:A:SER:HB2	1:89:A:SER:HA	1	0.2
(2,62)	1:89:A:SER:HB2	1:89:A:SER:HA	3	0.2
(2,62)	1:89:A:SER:HB2	1:89:A:SER:HA	7	0.2
(2,28)	1:54:A:PRO:HA	1:57:A:LEU:HG	2	0.2
(2,28)	1:54:A:PRO:HA	1:57:A:LEU:HG	3	0.2
(2,11)	1:142:A:THR:HB	1:143:A:LEU:HB2	3	0.2
(1,406)	1:158:A:LEU:H	1:157:A:LEU:HB3	6	0.2
(1,401)	1:58:A:GLN:H	1:57:A:LEU:HA	5	0.2
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	6	0.2
(1,317)	1:143:A:LEU:HD12	1:56:A:GLU:HA	2	0.2
(1,310)	1:84:A:SER:HB3	1:148:A:ILE:HG21	4	0.2
(1,298)	1:148:A:ILE:HG21	1:27:A:PHE:HZ	1	0.2
(1,91)	1:146:A:VAL:HG22	1:56:A:GLU:HB3	3	0.2
(1,53)	1:157:A:LEU:HA	1:26:A:ILE:HD12	3	0.2
(1,14)	1:142:A:THR:HA	1:143:A:LEU:HB2	8	0.2
(1,11)	1:61:A:ILE:HA	1:61:A:ILE:HG22	6	0.2
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD11	6	0.2
(2,1539)	1:44:A:VAL:H	1:43:A:LYS:HB3	1	0.19
(2,1296)	1:5:A:TYR:HE2	1:90:A:LYS:HD2	7	0.19
(2,1274)	1:20:A:PHE:HE2	1:150:A:ALA:HB1	6	0.19
(2,1247)	1:74:A:PHE:HD1	1:77:A:PHE:HD1	1	0.19
(2,1226)	1:61:A:ILE:HA	1:64:A:VAL:HG23	5	0.19
(2,1196)	1:1:A:MET:HE1	1:6:A:LYS:HG2	3	0.19
(2,1166)	1:54:A:PRO:HG3	1:53:A:THR:HA	7	0.19
(2,1122)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	8	0.19
(2,1088)	1:51:A:ASN:HB3	1:52:A:PRO:HD3	6	0.19
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	6	0.19
(2,767)	1:45:A:MET:HA	1:45:A:MET:HG3	7	0.19
(2,757)	1:82:A:VAL:HA	1:85:A:MET:HB2	8	0.19
(2,687)	1:27:A:PHE:HB3	1:24:A:PHE:HA	7	0.19
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	5	0.19
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD21	3	0.19
(2,625)	1:161:A:ARG:HD2	1:161:A:ARG:HG3	7	0.19
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD13	1	0.19
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD11	8	0.19
(2,557)	1:4:A:ILE:HG12	1:4:A:ILE:HD13	6	0.19
(2,557)	1:4:A:ILE:HG12	1:4:A:ILE:HD11	8	0.19
(2,485)	1:157:A:LEU:HD22	1:158:A:LEU:HG	4	0.19
(2,466)	1:82:A:VAL:HG23	1:83:A:ARG:HB2	2	0.19
(2,432)	1:72:A:VAL:HG12	1:76:A:GLU:HB3	7	0.19
(2,407)	1:36:A:ILE:HG21	1:41:A:LEU:HB3	8	0.19
(2,381)	1:7:A:ALA:HB3	1:10:A:GLU:HB2	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,344)	1:80:A:MET:HE1	1:80:A:MET:HA	4	0.19
(2,328)	1:47:A:MET:HE1	1:47:A:MET:HG3	4	0.19
(2,328)	1:47:A:MET:HE2	1:47:A:MET:HG3	7	0.19
(2,316)	1:61:A:ILE:HG22	1:61:A:ILE:HG12	2	0.19
(2,307)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	5	0.19
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD21	2	0.19
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD2	4	0.19
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB3	7	0.19
(2,209)	1:151:A:ASP:HA	1:154:A:MET:HG2	8	0.19
(2,65)	1:84:A:SER:HB3	1:148:A:ILE:HG22	2	0.19
(2,62)	1:89:A:SER:HB2	1:89:A:SER:HA	6	0.19
(1,404)	1:55:A:GLU:H	1:54:A:PRO:HG3	8	0.19
(1,401)	1:58:A:GLN:H	1:57:A:LEU:HA	2	0.19
(1,401)	1:58:A:GLN:H	1:55:A:GLU:HA	4	0.19
(1,401)	1:58:A:GLN:H	1:57:A:LEU:HA	7	0.19
(1,330)	1:2:A:ASP:HB3	1:5:A:TYR:HD1	5	0.19
(1,287)	1:75:A:ASP:HB2	1:78:A:LEU:HB2	7	0.19
(1,207)	1:52:A:PRO:HG2	1:52:A:PRO:HB3	1	0.19
(1,207)	1:52:A:PRO:HG2	1:52:A:PRO:HB3	2	0.19
(1,176)	1:59:A:GLU:HG2	1:59:A:GLU:HA	2	0.19
(1,156)	1:137:A:LYS:HE3	1:86:A:LYS:HB3	5	0.19
(1,83)	1:152:A:ALA:HB3	1:48:A:LEU:HD22	7	0.19
(1,81)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	5	0.19
(1,34)	1:16:A:GLN:HA	1:19:A:GLU:HB2	4	0.19
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB3	8	0.19
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG22	7	0.19
(2,1296)	1:5:A:TYR:HE2	1:90:A:LYS:HD3	3	0.18
(2,1231)	1:162:A:ALA:HB2	1:163:A:LYS:HE2	2	0.18
(2,1182)	1:141:A:PRO:HD3	1:140:A:ARG:HD2	5	0.18
(2,1125)	1:77:A:PHE:HB2	1:74:A:PHE:HD1	6	0.18
(2,1122)	1:72:A:VAL:HG11	1:76:A:GLU:HG2	6	0.18
(2,1111)	1:71:A:THR:HG23	1:73:A:ASP:HB2	7	0.18
(2,1093)	1:13:A:THR:HG22	1:11:A:GLN:HG2	6	0.18
(2,1088)	1:51:A:ASN:HB3	1:52:A:PRO:HD3	1	0.18
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	8	0.18
(2,1004)	1:21:A:LYS:HG2	1:74:A:PHE:HE2	8	0.18
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	7	0.18
(2,974)	1:55:A:GLU:HA	1:55:A:GLU:HB3	8	0.18
(2,956)	1:50:A:GLN:HB3	1:45:A:MET:HB3	5	0.18
(2,910)	1:52:A:PRO:HB3	1:52:A:PRO:HD2	7	0.18
(2,883)	1:1:A:MET:HG3	1:6:A:LYS:HB2	7	0.18
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	2	0.18
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	2	0.18
(2,679)	1:33:A:ASP:HB3	1:33:A:ASP:HA	3	0.18
(2,651)	1:41:A:LEU:HB2	1:41:A:LEU:HG	8	0.18
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD22	4	0.18
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD11	2	0.18
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD11	5	0.18
(2,516)	1:57:A:LEU:HD21	1:45:A:MET:HG2	6	0.18
(2,475)	1:38:A:THR:HG23	1:61:A:ILE:HB	1	0.18
(2,458)	1:82:A:VAL:HA	1:82:A:VAL:HG23	8	0.18
(2,417)	1:146:A:VAL:HA	1:146:A:VAL:HG21	5	0.18
(2,376)	1:150:A:ALA:HA	1:150:A:ALA:HB2	1	0.18
(2,361)	1:154:A:MET:HE1	1:154:A:MET:HB3	2	0.18
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG22	4	0.18
(2,244)	1:23:A:ALA:HA	1:26:A:ILE:HG13	1	0.18
(2,136)	1:15:A:GLU:HA	1:15:A:GLU:HG3	8	0.18
(2,130)	1:19:A:GLU:HA	1:158:A:LEU:HD12	4	0.18
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB1	2	0.18
(2,24)	1:54:A:PRO:HA	1:54:A:PRO:HD3	3	0.18
(2,15)	1:79:A:VAL:HA	1:79:A:VAL:HG12	5	0.18
(2,11)	1:142:A:THR:HB	1:143:A:LEU:HB2	1	0.18
(1,401)	1:58:A:GLN:H	1:57:A:LEU:HA	8	0.18
(1,362)	1:19:A:GLU:H	1:18:A:ASN:HB2	8	0.18
(1,295)	1:142:A:THR:HA	1:147:A:ARG:HD3	6	0.18
(1,207)	1:52:A:PRO:HG2	1:52:A:PRO:HB3	3	0.18
(1,207)	1:52:A:PRO:HG2	1:52:A:PRO:HB3	6	0.18
(1,159)	1:150:A:ALA:HB1	1:151:A:ASP:HB3	7	0.18
(1,159)	1:151:A:ASP:HB2	1:152:A:ALA:HB3	8	0.18
(1,133)	1:17:A:LYS:HG2	1:12:A:LEU:HD11	7	0.18
(1,47)	1:60:A:MET:HA	1:60:A:MET:HB3	1	0.18
(1,26)	1:89:A:SER:HB2	1:89:A:SER:HA	5	0.18
(2,1617)	1:48:A:LEU:H	1:48:A:LEU:HD11	8	0.17
(2,1232)	1:44:A:VAL:HG12	1:153:A:MET:HA	6	0.17
(2,1232)	1:44:A:VAL:HG11	1:153:A:MET:HA	7	0.17
(2,1195)	1:156:A:ALA:HB2	1:47:A:MET:HE1	2	0.17
(2,1150)	1:142:A:THR:HB	1:143:A:LEU:HD21	5	0.17
(2,1093)	1:13:A:THR:HG22	1:11:A:GLN:HG2	7	0.17
(2,1088)	1:51:A:ASN:HB3	1:52:A:PRO:HD3	2	0.17
(2,1031)	1:33:A:ASP:HB3	1:32:A:GLU:HB3	2	0.17
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	4	0.17
(2,987)	1:75:A:ASP:HA	1:78:A:LEU:HD23	5	0.17
(2,883)	1:1:A:MET:HG3	1:6:A:LYS:HB2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	6	0.17
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	4	0.17
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	5	0.17
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	6	0.17
(2,679)	1:33:A:ASP:HB3	1:33:A:ASP:HA	5	0.17
(2,667)	1:88:A:ASP:HB3	1:88:A:ASP:HA	4	0.17
(2,634)	1:12:A:LEU:HD12	1:12:A:LEU:HB2	3	0.17
(2,625)	1:161:A:ARG:HD3	1:161:A:ARG:HG2	4	0.17
(2,617)	1:46:A:ARG:HD3	1:46:A:ARG:HA	5	0.17
(2,583)	1:141:A:PRO:HG3	1:141:A:PRO:HA	5	0.17
(2,577)	1:41:A:LEU:HD22	1:41:A:LEU:HG	5	0.17
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD12	7	0.17
(2,466)	1:82:A:VAL:HG21	1:83:A:ARG:HB2	5	0.17
(2,446)	1:79:A:VAL:HG11	1:5:A:TYR:HB2	5	0.17
(2,427)	1:72:A:VAL:HG11	1:77:A:PHE:HB3	5	0.17
(2,361)	1:154:A:MET:HE2	1:154:A:MET:HB3	4	0.17
(2,344)	1:80:A:MET:HE3	1:80:A:MET:HA	8	0.17
(2,307)	1:26:A:ILE:HD13	1:157:A:LEU:HB2	6	0.17
(2,302)	1:61:A:ILE:HD12	1:41:A:LEU:HB3	1	0.17
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG22	7	0.17
(2,220)	1:18:A:ASN:HA	1:21:A:LYS:HB3	2	0.17
(2,213)	1:62:A:ASP:HA	1:65:A:ASP:HB2	2	0.17
(2,202)	1:45:A:MET:HA	1:48:A:LEU:HD12	2	0.17
(2,177)	1:43:A:LYS:HA	1:43:A:LYS:HG2	2	0.17
(2,177)	1:43:A:LYS:HA	1:43:A:LYS:HG2	5	0.17
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD2	7	0.17
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	5	0.17
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	6	0.17
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	8	0.17
(2,65)	1:84:A:SER:HB3	1:148:A:ILE:HG22	6	0.17
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB2	3	0.17
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB1	5	0.17
(2,24)	1:54:A:PRO:HA	1:54:A:PRO:HD3	2	0.17
(1,403)	1:55:A:GLU:H	1:54:A:PRO:HB3	4	0.17
(1,372)	1:16:A:GLN:H	1:17:A:LYS:H	7	0.17
(1,372)	1:16:A:GLN:H	1:17:A:LYS:H	8	0.17
(1,330)	1:2:A:ASP:HB3	1:5:A:TYR:HD1	3	0.17
(1,328)	1:41:A:LEU:HA	1:44:A:VAL:HG23	7	0.17
(1,304)	1:51:A:ASN:HB2	1:52:A:PRO:HD2	2	0.17
(1,215)	1:43:A:LYS:HB3	1:43:A:LYS:HD3	8	0.17
(1,162)	1:78:A:LEU:HD22	1:78:A:LEU:HB3	7	0.17
(1,137)	1:46:A:ARG:HD2	1:46:A:ARG:HA	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:45:A:MET:HE1	1:48:A:LEU:HD11	3	0.17
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD12	2	0.17
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HD13	1	0.17
(2,1699)	1:146:A:VAL:HG22	1:52:A:PRO:HA	1	0.16
(2,1617)	1:48:A:LEU:H	1:48:A:LEU:HD12	6	0.16
(2,1425)	1:83:A:ARG:H	1:83:A:ARG:HG2	1	0.16
(2,1399)	1:85:A:MET:H	1:84:A:SER:HA	3	0.16
(2,1311)	1:66:A:GLU:H	1:66:A:GLU:HG3	4	0.16
(2,1216)	1:52:A:PRO:HA	1:146:A:VAL:HG21	5	0.16
(2,1132)	1:81:A:MET:HA	1:77:A:PHE:HE1	7	0.16
(2,1109)	1:71:A:THR:HA	1:72:A:VAL:HB	3	0.16
(2,1109)	1:71:A:THR:HA	1:72:A:VAL:HB	4	0.16
(2,1102)	1:79:A:VAL:HG13	1:5:A:TYR:HE1	1	0.16
(2,1035)	1:35:A:SER:HB2	1:73:A:ASP:HB3	1	0.16
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	3	0.16
(2,999)	1:16:A:GLN:HG2	1:12:A:LEU:HD21	6	0.16
(2,926)	1:8:A:ALA:HB1	1:5:A:TYR:HD1	4	0.16
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	1	0.16
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	7	0.16
(2,790)	1:90:A:LYS:HG2	1:86:A:LYS:HB3	4	0.16
(2,747)	1:14:A:GLU:HA	1:14:A:GLU:HG3	1	0.16
(2,747)	1:14:A:GLU:HA	1:14:A:GLU:HG3	2	0.16
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	2	0.16
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	3	0.16
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	5	0.16
(2,667)	1:88:A:ASP:HB2	1:88:A:ASP:HA	7	0.16
(2,645)	1:157:A:LEU:HB3	1:157:A:LEU:HD22	5	0.16
(2,583)	1:141:A:PRO:HG3	1:141:A:PRO:HA	1	0.16
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD13	4	0.16
(2,562)	1:12:A:LEU:HD12	1:17:A:LYS:HG3	6	0.16
(2,466)	1:82:A:VAL:HG22	1:83:A:ARG:HB2	6	0.16
(2,441)	1:146:A:VAL:HG13	1:145:A:ARG:HB3	5	0.16
(2,383)	1:4:A:ILE:HG23	1:7:A:ALA:HB2	3	0.16
(2,270)	1:29:A:LEU:HA	1:29:A:LEU:HB3	2	0.16
(2,266)	1:157:A:LEU:HA	1:157:A:LEU:HD21	6	0.16
(2,238)	1:23:A:ALA:HA	1:26:A:ILE:HD13	6	0.16
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB3	8	0.16
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB3	3	0.16
(2,227)	1:7:A:ALA:HA	1:6:A:LYS:HB3	3	0.16
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	4	0.16
(2,168)	1:89:A:SER:HA	1:137:A:LYS:HB3	2	0.16
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	7	0.16
(2,95)	1:28:A:VAL:HA	1:28:A:VAL:HG21	1	0.16
(2,73)	1:24:A:PHE:HA	1:74:A:PHE:HD2	3	0.16
(2,34)	1:44:A:VAL:HA	1:47:A:MET:HB3	7	0.16
(2,11)	1:142:A:THR:HB	1:143:A:LEU:HB2	2	0.16
(1,411)	1:159:A:GLY:H	1:155:A:GLN:HA	4	0.16
(1,362)	1:19:A:GLU:H	1:18:A:ASN:HB2	6	0.16
(1,347)	1:5:A:TYR:HE1	1:2:A:ASP:HB3	2	0.16
(1,337)	1:44:A:VAL:HB	1:27:A:PHE:HE2	6	0.16
(1,334)	1:40:A:GLU:HB2	1:27:A:PHE:HD2	2	0.16
(1,236)	1:47:A:MET:HG3	1:48:A:LEU:HG	1	0.16
(1,231)	1:23:A:ALA:HB2	1:24:A:PHE:HA	2	0.16
(1,214)	1:43:A:LYS:HD2	1:40:A:GLU:HG2	5	0.16
(1,210)	1:47:A:MET:HA	1:47:A:MET:HG2	2	0.16
(1,161)	1:22:A:ALA:HA	1:25:A:ASP:HB3	8	0.16
(1,159)	1:151:A:ASP:HB2	1:152:A:ALA:HB3	6	0.16
(1,154)	1:6:A:LYS:HE3	1:6:A:LYS:HG2	1	0.16
(1,1)	1:71:A:THR:HB	1:61:A:ILE:HG22	8	0.16
(2,1541)	1:40:A:GLU:H	1:39:A:LYS:HB2	5	0.15
(2,1172)	1:43:A:LYS:HG3	1:44:A:VAL:HG22	3	0.15
(2,1101)	1:61:A:ILE:HD12	1:36:A:ILE:HD11	4	0.15
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD23	3	0.15
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD22	6	0.15
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	2	0.15
(2,1027)	1:31:A:ALA:HA	1:43:A:LYS:HB3	7	0.15
(2,929)	1:152:A:ALA:HB1	1:149:A:SER:HA	2	0.15
(2,923)	1:63:A:GLU:HB2	1:63:A:GLU:HG2	1	0.15
(2,923)	1:63:A:GLU:HB2	1:63:A:GLU:HG2	3	0.15
(2,923)	1:63:A:GLU:HB2	1:63:A:GLU:HG2	6	0.15
(2,923)	1:63:A:GLU:HB2	1:63:A:GLU:HG2	7	0.15
(2,923)	1:63:A:GLU:HB2	1:63:A:GLU:HG2	8	0.15
(2,918)	1:66:A:GLU:HA	1:66:A:GLU:HB2	1	0.15
(2,883)	1:1:A:MET:HG3	1:6:A:LYS:HB2	3	0.15
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	2	0.15
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	3	0.15
(2,845)	1:10:A:GLU:HA	1:10:A:GLU:HB3	5	0.15
(2,693)	1:27:A:PHE:HB2	1:36:A:ILE:HD13	8	0.15
(2,625)	1:161:A:ARG:HD2	1:161:A:ARG:HG3	3	0.15
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD13	3	0.15
(2,575)	1:57:A:LEU:HG	1:57:A:LEU:HD13	6	0.15
(2,562)	1:12:A:LEU:HD11	1:17:A:LYS:HG3	7	0.15
(2,514)	1:57:A:LEU:HD23	1:38:A:THR:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,485)	1:157:A:LEU:HD23	1:158:A:LEU:HG	2	0.15
(2,478)	1:158:A:LEU:HA	1:158:A:LEU:HD22	2	0.15
(2,435)	1:9:A:VAL:HA	1:82:A:VAL:HG11	4	0.15
(2,385)	1:156:A:ALA:HB3	1:153:A:MET:HA	8	0.15
(2,383)	1:4:A:ILE:HG22	1:7:A:ALA:HB1	5	0.15
(2,377)	1:150:A:ALA:HB1	1:85:A:MET:HG2	7	0.15
(2,255)	1:145:A:ARG:HA	1:145:A:ARG:HG2	8	0.15
(2,247)	1:161:A:ARG:HA	1:161:A:ARG:HD3	5	0.15
(2,238)	1:23:A:ALA:HA	1:26:A:ILE:HD13	7	0.15
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB2	2	0.15
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB1	3	0.15
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB2	4	0.15
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB3	1	0.15
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	2	0.15
(2,177)	1:43:A:LYS:HA	1:43:A:LYS:HG2	8	0.15
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	2	0.15
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	4	0.15
(2,139)	1:64:A:VAL:HA	1:64:A:VAL:HG23	4	0.15
(2,73)	1:24:A:PHE:HA	1:74:A:PHE:HD1	6	0.15
(2,73)	1:24:A:PHE:HA	1:74:A:PHE:HD1	8	0.15
(2,65)	1:84:A:SER:HB3	1:148:A:ILE:HG21	4	0.15
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB3	4	0.15
(2,59)	1:4:A:ILE:HA	1:7:A:ALA:HB2	7	0.15
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG13	4	0.15
(2,22)	1:38:A:THR:HA	1:61:A:ILE:HG13	1	0.15
(1,403)	1:55:A:GLU:H	1:54:A:PRO:HB3	7	0.15
(1,372)	1:16:A:GLN:H	1:17:A:LYS:H	6	0.15
(1,369)	1:148:A:ILE:H	1:148:A:ILE:HD12	4	0.15
(1,317)	1:143:A:LEU:HD13	1:56:A:GLU:HA	3	0.15
(1,315)	1:142:A:THR:HG23	1:84:A:SER:HA	5	0.15
(1,286)	1:72:A:VAL:HG22	1:58:A:GLN:HA	2	0.15
(1,262)	1:42:A:GLY:HA2	1:36:A:ILE:HG23	5	0.15
(1,249)	1:77:A:PHE:HB3	1:75:A:ASP:HA	5	0.15
(1,249)	1:77:A:PHE:HB3	1:75:A:ASP:HA	8	0.15
(1,207)	1:52:A:PRO:HB3	1:56:A:GLU:HB3	4	0.15
(1,196)	1:139:A:LYS:HA	1:139:A:LYS:HB3	1	0.15
(1,161)	1:22:A:ALA:HA	1:25:A:ASP:HB3	6	0.15
(1,96)	1:13:A:THR:HB	1:13:A:THR:HG23	7	0.15
(1,47)	1:60:A:MET:HA	1:63:A:GLU:HB2	3	0.15
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HD11	1	0.15
(1,7)	1:82:A:VAL:HA	1:8:A:ALA:HB2	6	0.15
(2,1655)	1:53:A:THR:H	1:56:A:GLU:HB2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1551)	1:82:A:VAL:H	1:82:A:VAL:HG23	2	0.14
(2,1529)	1:86:A:LYS:H	1:90:A:LYS:HG2	3	0.14
(2,1149)	1:162:A:ALA:HA	1:163:A:LYS:HE2	2	0.14
(2,1135)	1:82:A:VAL:HG12	1:5:A:TYR:HE2	7	0.14
(2,1132)	1:81:A:MET:HA	1:77:A:PHE:HE1	8	0.14
(2,1088)	1:51:A:ASN:HB3	1:52:A:PRO:HD3	4	0.14
(2,1064)	1:43:A:LYS:HG2	1:40:A:GLU:HA	4	0.14
(2,1021)	1:17:A:LYS:HA	1:12:A:LEU:HD13	5	0.14
(2,1006)	1:22:A:ALA:HB3	1:25:A:ASP:HB3	4	0.14
(2,931)	1:141:A:PRO:HB3	1:141:A:PRO:HD3	2	0.14
(2,930)	1:141:A:PRO:HB3	1:141:A:PRO:HD2	7	0.14
(2,918)	1:66:A:GLU:HA	1:66:A:GLU:HB2	6	0.14
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	4	0.14
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	6	0.14
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	1	0.14
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	1	0.14
(2,667)	1:88:A:ASP:HB3	1:88:A:ASP:HA	8	0.14
(2,544)	1:43:A:LYS:HG2	1:43:A:LYS:HE3	4	0.14
(2,538)	1:78:A:LEU:HD11	1:78:A:LEU:HG	3	0.14
(2,538)	1:78:A:LEU:HD11	1:78:A:LEU:HG	4	0.14
(2,538)	1:78:A:LEU:HD13	1:78:A:LEU:HG	7	0.14
(2,538)	1:78:A:LEU:HD11	1:78:A:LEU:HG	8	0.14
(2,505)	1:72:A:VAL:HG23	1:64:A:VAL:HB	7	0.14
(2,421)	1:31:A:ALA:HB2	1:28:A:VAL:HG13	2	0.14
(2,385)	1:156:A:ALA:HB1	1:153:A:MET:HA	5	0.14
(2,378)	1:81:A:MET:HE1	1:80:A:MET:HE2	7	0.14
(2,344)	1:80:A:MET:HE2	1:80:A:MET:HA	5	0.14
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	5	0.14
(2,273)	1:60:A:MET:HA	1:60:A:MET:HB2	8	0.14
(2,257)	1:3:A:ASP:HA	1:6:A:LYS:HD3	1	0.14
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB1	1	0.14
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB2	7	0.14
(2,227)	1:7:A:ALA:HA	1:6:A:LYS:HB3	1	0.14
(2,227)	1:7:A:ALA:HA	1:6:A:LYS:HB3	4	0.14
(2,210)	1:85:A:MET:HA	1:85:A:MET:HB3	5	0.14
(2,204)	1:10:A:GLU:HA	1:9:A:VAL:HG13	7	0.14
(2,177)	1:43:A:LYS:HA	1:43:A:LYS:HG2	6	0.14
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD1	8	0.14
(2,164)	1:73:A:ASP:HA	1:73:A:ASP:HB3	1	0.14
(2,164)	1:73:A:ASP:HA	1:73:A:ASP:HB3	6	0.14
(2,164)	1:73:A:ASP:HA	1:73:A:ASP:HB3	8	0.14
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,142)	1:5:A:TYR:HA	1:5:A:TYR:HB2	5	0.14
(2,137)	1:15:A:GLU:HA	1:15:A:GLU:HB3	2	0.14
(2,136)	1:15:A:GLU:HA	1:15:A:GLU:HG2	3	0.14
(2,136)	1:15:A:GLU:HA	1:15:A:GLU:HG3	5	0.14
(2,101)	1:80:A:MET:HA	1:64:A:VAL:HG22	3	0.14
(2,73)	1:24:A:PHE:HA	1:74:A:PHE:HD1	1	0.14
(2,31)	1:82:A:VAL:HA	1:85:A:MET:HG2	7	0.14
(2,24)	1:54:A:PRO:HA	1:54:A:PRO:HD3	1	0.14
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	8	0.14
(1,333)	1:27:A:PHE:HA	1:27:A:PHE:HD1	2	0.14
(1,323)	1:8:A:ALA:HB2	1:79:A:VAL:HA	1	0.14
(1,304)	1:51:A:ASN:HB2	1:52:A:PRO:HD2	4	0.14
(1,273)	1:51:A:ASN:HB3	1:46:A:ARG:HG3	3	0.14
(1,234)	1:81:A:MET:HA	1:64:A:VAL:HB	2	0.14
(1,206)	1:43:A:LYS:HB3	1:43:A:LYS:HD3	5	0.14
(1,93)	1:28:A:VAL:HG13	1:27:A:PHE:HD1	7	0.14
(1,81)	1:8:A:ALA:HB2	1:10:A:GLU:HG3	2	0.14
(1,43)	1:145:A:ARG:HA	1:146:A:VAL:HG21	4	0.14
(1,16)	1:58:A:GLN:HA	1:61:A:ILE:HD13	8	0.14
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	7	0.14
(2,1367)	1:47:A:MET:H	1:47:A:MET:HB2	2	0.13
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	7	0.13
(2,1237)	1:5:A:TYR:HB3	1:5:A:TYR:HD2	8	0.13
(2,1217)	1:146:A:VAL:HG13	1:147:A:ARG:HA	8	0.13
(2,1214)	1:146:A:VAL:HG21	1:52:A:PRO:HB3	5	0.13
(2,1163)	1:157:A:LEU:HD23	1:27:A:PHE:HE2	8	0.13
(2,1145)	1:161:A:ARG:HB3	1:26:A:ILE:HD11	3	0.13
(2,1059)	1:60:A:MET:HG3	1:146:A:VAL:HG13	2	0.13
(2,1049)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	7	0.13
(2,1035)	1:35:A:SER:HB2	1:73:A:ASP:HB3	7	0.13
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	1	0.13
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	6	0.13
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	7	0.13
(2,1004)	1:21:A:LYS:HG2	1:74:A:PHE:HE2	1	0.13
(2,1001)	1:17:A:LYS:HE3	1:78:A:LEU:HD11	7	0.13
(2,927)	1:8:A:ALA:HB2	1:79:A:VAL:HA	1	0.13
(2,918)	1:66:A:GLU:HA	1:66:A:GLU:HB2	7	0.13
(2,918)	1:66:A:GLU:HA	1:66:A:GLU:HB2	8	0.13
(2,883)	1:1:A:MET:HG3	1:6:A:LYS:HB2	5	0.13
(2,767)	1:45:A:MET:HA	1:45:A:MET:HG3	2	0.13
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	1	0.13
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	5	0.13
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	8	0.13
(2,721)	1:15:A:GLU:HA	1:18:A:ASN:HB2	8	0.13
(2,716)	1:40:A:GLU:HA	1:40:A:GLU:HG2	7	0.13
(2,643)	1:162:A:ALA:HB1	1:158:A:LEU:HB3	1	0.13
(2,617)	1:46:A:ARG:HD3	1:46:A:ARG:HA	8	0.13
(2,545)	1:43:A:LYS:HG2	1:43:A:LYS:HD3	3	0.13
(2,538)	1:78:A:LEU:HD11	1:78:A:LEU:HG	6	0.13
(2,517)	1:57:A:LEU:HD22	1:41:A:LEU:HB2	3	0.13
(2,516)	1:57:A:LEU:HD22	1:45:A:MET:HG2	5	0.13
(2,492)	1:41:A:LEU:HD12	1:41:A:LEU:HB2	8	0.13
(2,474)	1:38:A:THR:HG22	1:57:A:LEU:HB2	3	0.13
(2,474)	1:38:A:THR:HG21	1:57:A:LEU:HB2	5	0.13
(2,449)	1:79:A:VAL:HG13	1:64:A:VAL:HB	4	0.13
(2,434)	1:82:A:VAL:HG12	1:5:A:TYR:HD2	8	0.13
(2,311)	1:148:A:ILE:HD13	1:45:A:MET:HE3	3	0.13
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG21	2	0.13
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB3	1	0.13
(2,295)	1:34:A:GLY:HA3	1:31:A:ALA:HB2	6	0.13
(2,275)	1:56:A:GLU:HA	1:56:A:GLU:HG3	4	0.13
(2,267)	1:25:A:ASP:HA	1:28:A:VAL:HG21	8	0.13
(2,255)	1:145:A:ARG:HA	1:145:A:ARG:HG2	7	0.13
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB3	5	0.13
(2,237)	1:152:A:ALA:HA	1:152:A:ALA:HB3	6	0.13
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB2	5	0.13
(2,227)	1:7:A:ALA:HA	1:6:A:LYS:HB3	8	0.13
(2,164)	1:73:A:ASP:HA	1:73:A:ASP:HB3	7	0.13
(2,58)	1:4:A:ILE:HA	1:4:A:ILE:HG13	2	0.13
(1,411)	1:159:A:GLY:H	1:159:A:GLY:HA3	1	0.13
(1,401)	1:58:A:GLN:H	1:57:A:LEU:HA	6	0.13
(1,362)	1:19:A:GLU:H	1:18:A:ASN:HB2	4	0.13
(1,304)	1:52:A:PRO:HD2	1:45:A:MET:HG2	7	0.13
(1,302)	1:19:A:GLU:HB2	1:158:A:LEU:HD13	7	0.13
(1,298)	1:148:A:ILE:HG22	1:27:A:PHE:HZ	4	0.13
(1,286)	1:72:A:VAL:HG21	1:58:A:GLN:HA	1	0.13
(1,275)	1:53:A:THR:HB	1:55:A:GLU:HB3	6	0.13
(1,245)	1:43:A:LYS:HB2	1:43:A:LYS:HA	6	0.13
(1,191)	1:60:A:MET:HG3	1:60:A:MET:HB2	5	0.13
(1,162)	1:78:A:LEU:HD21	1:78:A:LEU:HB3	2	0.13
(1,157)	1:17:A:LYS:HE2	1:78:A:LEU:HD23	2	0.13
(1,54)	1:148:A:ILE:HD12	1:80:A:MET:HG2	3	0.13
(1,26)	1:89:A:SER:HB3	1:89:A:SER:HA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:89:A:SER:HB3	1:89:A:SER:HA	3	0.13
(1,26)	1:89:A:SER:HB3	1:89:A:SER:HA	6	0.13
(1,18)	1:40:A:GLU:HA	1:40:A:GLU:HB2	8	0.13
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD12	5	0.13
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD11	7	0.13
(1,2)	1:71:A:THR:HB	1:37:A:SER:HA	1	0.13
(2,1416)	1:85:A:MET:H	1:85:A:MET:HG3	7	0.12
(2,1221)	1:148:A:ILE:HA	1:148:A:ILE:HB	7	0.12
(2,1195)	1:156:A:ALA:HB3	1:47:A:MET:HE1	5	0.12
(2,1188)	1:61:A:ILE:HG21	1:65:A:ASP:HA	2	0.12
(2,1182)	1:141:A:PRO:HD3	1:140:A:ARG:HD3	2	0.12
(2,1172)	1:43:A:LYS:HG3	1:44:A:VAL:HG23	7	0.12
(2,1132)	1:81:A:MET:HA	1:77:A:PHE:HE1	1	0.12
(2,1100)	1:61:A:ILE:HD11	1:40:A:GLU:HB2	4	0.12
(2,1093)	1:13:A:THR:HG22	1:11:A:GLN:HG2	3	0.12
(2,1083)	1:52:A:PRO:HB3	1:57:A:LEU:HD21	7	0.12
(2,1065)	1:43:A:LYS:HG2	1:43:A:LYS:HB3	6	0.12
(2,1065)	1:43:A:LYS:HG2	1:43:A:LYS:HB3	7	0.12
(2,1028)	1:31:A:ALA:HA	1:30:A:GLY:HA2	5	0.12
(2,952)	1:33:A:ASP:HB2	1:33:A:ASP:HA	1	0.12
(2,952)	1:33:A:ASP:HB2	1:33:A:ASP:HA	2	0.12
(2,952)	1:33:A:ASP:HB2	1:33:A:ASP:HA	4	0.12
(2,952)	1:33:A:ASP:HB2	1:33:A:ASP:HA	8	0.12
(2,918)	1:66:A:GLU:HA	1:66:A:GLU:HB2	2	0.12
(2,918)	1:66:A:GLU:HA	1:66:A:GLU:HB2	5	0.12
(2,916)	1:63:A:GLU:HB3	1:64:A:VAL:HG22	7	0.12
(2,766)	1:36:A:ILE:HG21	1:72:A:VAL:HB	1	0.12
(2,757)	1:82:A:VAL:HA	1:85:A:MET:HB2	7	0.12
(2,700)	1:61:A:ILE:HG21	1:65:A:ASP:HB3	3	0.12
(2,667)	1:88:A:ASP:HB2	1:88:A:ASP:HA	6	0.12
(2,642)	1:57:A:LEU:HD22	1:57:A:LEU:HB2	4	0.12
(2,562)	1:12:A:LEU:HD12	1:17:A:LYS:HG3	1	0.12
(2,550)	1:41:A:LEU:HD21	1:41:A:LEU:HA	8	0.12
(2,538)	1:78:A:LEU:HD11	1:78:A:LEU:HG	2	0.12
(2,538)	1:78:A:LEU:HD11	1:78:A:LEU:HG	5	0.12
(2,467)	1:9:A:VAL:HG12	1:6:A:LYS:HA	5	0.12
(2,442)	1:79:A:VAL:H	1:79:A:VAL:HG11	1	0.12
(2,423)	1:13:A:THR:HG22	1:16:A:GLN:HG3	2	0.12
(2,423)	1:13:A:THR:HG23	1:16:A:GLN:HG3	4	0.12
(2,395)	1:156:A:ALA:HB3	1:44:A:VAL:HG11	7	0.12
(2,369)	1:23:A:ALA:HB2	1:158:A:LEU:HD21	1	0.12
(2,297)	1:34:A:GLY:HA3	1:28:A:VAL:HG23	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,285)	1:52:A:PRO:HD2	1:50:A:GLN:HB3	4	0.12
(2,278)	1:51:A:ASN:HA	1:52:A:PRO:HD3	3	0.12
(2,257)	1:3:A:ASP:HA	1:6:A:LYS:HD3	7	0.12
(2,228)	1:7:A:ALA:HA	1:7:A:ALA:HB2	2	0.12
(2,224)	1:54:A:PRO:HD2	1:54:A:PRO:HB3	5	0.12
(2,186)	1:63:A:GLU:HA	1:63:A:GLU:HG3	3	0.12
(2,183)	1:32:A:GLU:HA	1:32:A:GLU:HB2	4	0.12
(2,168)	1:89:A:SER:HA	1:137:A:LYS:HB2	8	0.12
(2,131)	1:59:A:GLU:HA	1:59:A:GLU:HB3	5	0.12
(2,127)	1:19:A:GLU:HA	1:19:A:GLU:HB3	4	0.12
(2,127)	1:19:A:GLU:HA	1:19:A:GLU:HB3	7	0.12
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	6	0.12
(2,32)	1:82:A:VAL:HA	1:82:A:VAL:HG12	5	0.12
(1,404)	1:55:A:GLU:H	1:55:A:GLU:HG2	2	0.12
(1,397)	1:70:A:GLY:H	1:69:A:SER:HA	4	0.12
(1,359)	1:147:A:ARG:H	1:146:A:VAL:HG12	3	0.12
(1,345)	1:27:A:PHE:HZ	1:45:A:MET:HE2	1	0.12
(1,317)	1:143:A:LEU:HD13	1:56:A:GLU:HA	1	0.12
(1,310)	1:150:A:ALA:HA	1:148:A:ILE:HG22	2	0.12
(1,286)	1:72:A:VAL:HG21	1:58:A:GLN:HA	3	0.12
(1,286)	1:72:A:VAL:HG21	1:58:A:GLN:HA	6	0.12
(1,270)	1:44:A:VAL:HG11	1:47:A:MET:HG3	7	0.12
(1,245)	1:43:A:LYS:HB2	1:43:A:LYS:HA	1	0.12
(1,245)	1:43:A:LYS:HB2	1:43:A:LYS:HA	8	0.12
(1,218)	1:60:A:MET:HG3	1:146:A:VAL:HG23	1	0.12
(1,177)	1:156:A:ALA:HA	1:155:A:GLN:HG3	2	0.12
(1,161)	1:22:A:ALA:HA	1:25:A:ASP:HB3	7	0.12
(1,154)	1:6:A:LYS:HE3	1:6:A:LYS:HG2	2	0.12
(1,139)	1:161:A:ARG:HD2	1:161:A:ARG:HB3	2	0.12
(1,139)	1:46:A:ARG:HD2	1:46:A:ARG:HG2	6	0.12
(1,133)	1:17:A:LYS:HG2	1:12:A:LEU:HD11	8	0.12
(1,122)	1:45:A:MET:HE3	1:48:A:LEU:HD13	1	0.12
(1,69)	1:22:A:ALA:HB2	1:158:A:LEU:HD22	3	0.12
(1,9)	1:9:A:VAL:HA	1:78:A:LEU:HD22	1	0.12
(2,1623)	1:33:A:ASP:H	1:33:A:ASP:HA	6	0.11
(2,1623)	1:33:A:ASP:H	1:33:A:ASP:HA	7	0.11
(2,1623)	1:33:A:ASP:H	1:33:A:ASP:HA	8	0.11
(2,1544)	1:61:A:ILE:H	1:61:A:ILE:HG12	6	0.11
(2,1541)	1:40:A:GLU:H	1:39:A:LYS:HB2	7	0.11
(2,1428)	1:146:A:VAL:H	1:146:A:VAL:HB	4	0.11
(2,1239)	1:5:A:TYR:HD2	1:82:A:VAL:HB	6	0.11
(2,1203)	1:90:A:LYS:HA	1:87:A:ASP:HB3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1188)	1:61:A:ILE:HG21	1:65:A:ASP:HA	3	0.11
(2,1172)	1:43:A:LYS:HG3	1:44:A:VAL:HG21	8	0.11
(2,1155)	1:147:A:ARG:HD2	1:148:A:ILE:HD12	2	0.11
(2,1131)	1:79:A:VAL:HA	1:83:A:ARG:HG2	2	0.11
(2,1111)	1:71:A:THR:HG21	1:73:A:ASP:HB2	1	0.11
(2,1072)	1:45:A:MET:HE3	1:27:A:PHE:HE1	5	0.11
(2,1055)	1:42:A:GLY:HA3	1:45:A:MET:HB2	8	0.11
(2,1034)	1:35:A:SER:HA	1:73:A:ASP:HB3	5	0.11
(2,1003)	1:19:A:GLU:HA	1:158:A:LEU:HD23	8	0.11
(2,973)	1:42:A:GLY:HA2	1:46:A:ARG:HG2	7	0.11
(2,952)	1:33:A:ASP:HB2	1:33:A:ASP:HA	7	0.11
(2,950)	1:16:A:GLN:HG2	1:16:A:GLN:HB3	4	0.11
(2,804)	1:90:A:LYS:HD3	1:87:A:ASP:HB3	4	0.11
(2,800)	1:46:A:ARG:HA	1:46:A:ARG:HG3	5	0.11
(2,789)	1:86:A:LYS:HB2	1:90:A:LYS:HG2	6	0.11
(2,767)	1:45:A:MET:HA	1:45:A:MET:HG3	8	0.11
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	2	0.11
(2,683)	1:3:A:ASP:HB2	1:6:A:LYS:HD3	1	0.11
(2,657)	1:48:A:LEU:HB2	1:48:A:LEU:HD12	2	0.11
(2,562)	1:12:A:LEU:HD11	1:17:A:LYS:HG3	8	0.11
(2,545)	1:43:A:LYS:HG2	1:43:A:LYS:HD3	6	0.11
(2,503)	1:48:A:LEU:HD21	1:153:A:MET:HA	4	0.11
(2,421)	1:31:A:ALA:HB1	1:28:A:VAL:HG11	3	0.11
(2,307)	1:26:A:ILE:HD12	1:157:A:LEU:HB2	8	0.11
(2,274)	1:60:A:MET:HA	1:60:A:MET:HG2	7	0.11
(2,257)	1:3:A:ASP:HA	1:6:A:LYS:HD3	4	0.11
(2,249)	1:161:A:ARG:HA	1:161:A:ARG:HG3	8	0.11
(2,204)	1:10:A:GLU:HA	1:9:A:VAL:HG12	8	0.11
(2,183)	1:32:A:GLU:HA	1:32:A:GLU:HB2	8	0.11
(2,167)	1:35:A:SER:HB2	1:73:A:ASP:HA	5	0.11
(2,144)	1:5:A:TYR:HA	1:82:A:VAL:HG11	7	0.11
(2,127)	1:19:A:GLU:HA	1:19:A:GLU:HB3	8	0.11
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	2	0.11
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	4	0.11
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	5	0.11
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	8	0.11
(2,77)	1:72:A:VAL:HA	1:72:A:VAL:HG12	7	0.11
(2,27)	1:54:A:PRO:HA	1:54:A:PRO:HB2	2	0.11
(2,27)	1:54:A:PRO:HA	1:54:A:PRO:HB2	3	0.11
(2,27)	1:54:A:PRO:HA	1:54:A:PRO:HB2	5	0.11
(1,386)	1:50:A:GLN:H	1:48:A:LEU:HB2	4	0.11
(1,347)	1:83:A:ARG:HD2	1:5:A:TYR:HE2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:85:A:MET:HE2	1:150:A:ALA:HB1	5	0.11
(1,311)	1:85:A:MET:HE2	1:8:A:ALA:HB3	8	0.11
(1,310)	1:150:A:ALA:HA	1:148:A:ILE:HG22	7	0.11
(1,296)	1:148:A:ILE:HG13	1:153:A:MET:HB3	2	0.11
(1,207)	1:52:A:PRO:HG2	1:52:A:PRO:HB3	7	0.11
(1,154)	1:6:A:LYS:HE3	1:6:A:LYS:HG2	7	0.11
(1,59)	1:47:A:MET:HE1	1:153:A:MET:HA	8	0.11
(1,47)	1:60:A:MET:HA	1:63:A:GLU:HB2	7	0.11
(1,26)	1:89:A:SER:HB2	1:89:A:SER:HA	8	0.11
(1,18)	1:40:A:GLU:HA	1:40:A:GLU:HB2	3	0.11
(2,1221)	1:148:A:ILE:HA	1:148:A:ILE:HB	2	0.1
(2,1131)	1:79:A:VAL:HA	1:83:A:ARG:HG2	3	0.1
(2,1065)	1:43:A:LYS:HG2	1:43:A:LYS:HB3	2	0.1
(2,1049)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	5	0.1
(2,1049)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	8	0.1
(2,1005)	1:21:A:LYS:HG3	1:18:A:ASN:HA	2	0.1
(2,952)	1:33:A:ASP:HB2	1:33:A:ASP:HA	6	0.1
(2,950)	1:16:A:GLN:HG2	1:16:A:GLN:HB3	2	0.1
(2,940)	1:164:A:GLY:HA3	1:163:A:LYS:HE2	8	0.1
(2,930)	1:141:A:PRO:HB3	1:141:A:PRO:HD2	4	0.1
(2,925)	1:145:A:ARG:HB3	1:145:A:ARG:HD2	8	0.1
(2,725)	1:18:A:ASN:HA	1:18:A:ASN:HB3	7	0.1
(2,682)	1:3:A:ASP:HB3	1:6:A:LYS:HB3	4	0.1
(2,628)	1:83:A:ARG:HD3	1:83:A:ARG:HB3	7	0.1
(2,316)	1:61:A:ILE:HG23	1:61:A:ILE:HG12	5	0.1
(2,183)	1:32:A:GLU:HA	1:32:A:GLU:HB3	7	0.1
(2,180)	1:47:A:MET:HA	1:47:A:MET:HB3	4	0.1
(2,179)	1:47:A:MET:HA	1:47:A:MET:HB2	7	0.1
(2,165)	1:73:A:ASP:HA	1:24:A:PHE:HD1	6	0.1
(2,147)	1:35:A:SER:HB2	1:71:A:THR:HA	3	0.1
(2,135)	1:39:A:LYS:HA	1:57:A:LEU:HD11	7	0.1
(2,107)	1:83:A:ARG:HA	1:83:A:ARG:HG3	5	0.1
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	3	0.1
(2,103)	1:83:A:ARG:HA	1:83:A:ARG:HB2	7	0.1
(2,27)	1:54:A:PRO:HA	1:54:A:PRO:HB2	4	0.1
(1,412)	1:49:A:GLY:H	1:49:A:GLY:HA3	2	0.1
(1,412)	1:49:A:GLY:H	1:49:A:GLY:HA3	4	0.1
(1,412)	1:49:A:GLY:H	1:49:A:GLY:HA3	5	0.1
(1,385)	1:46:A:ARG:H	1:46:A:ARG:HB2	6	0.1
(1,154)	1:6:A:LYS:HE3	1:6:A:LYS:HG2	6	0.1
(1,139)	1:46:A:ARG:HD2	1:46:A:ARG:HG2	8	0.1
(1,133)	1:17:A:LYS:HG2	1:12:A:LEU:HD13	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:44:A:VAL:HG11	1:153:A:MET:HB3	3	0.1
(1,72)	1:153:A:MET:HE3	1:81:A:MET:HE3	4	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found