



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:58 AM UTC

PDB ID : 2LKL / pdb_00002lkl
BMRB ID : 16911
Title : Structure of the core intracellular domain of PfEMP1
Authors : Vakonakis, I.; Erat, M.C.
Deposited on : 2011-10-16

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

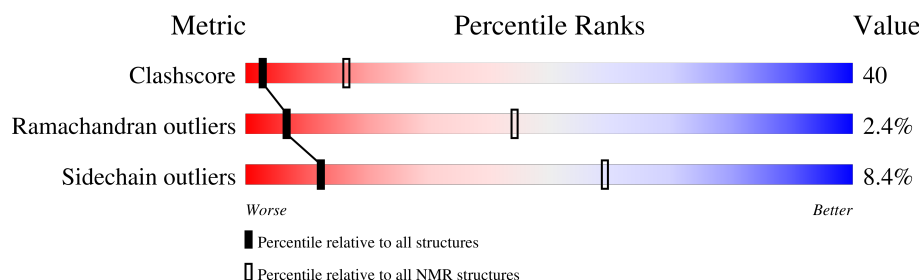
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	81	

2 Ensemble composition and analysis

This entry contains 39 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:8-A:35, A:45-A:81 (65)	0.49	1

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 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 20, 23, 24, 25, 28, 30, 31, 32, 34, 35, 37, 39
2	5, 18, 19, 21, 26, 33
3	6, 17, 29, 36
Single-model clusters	22; 27; 38

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1348 atoms, of which 666 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Erythrocyte membrane protein 1 (PfEMP1).

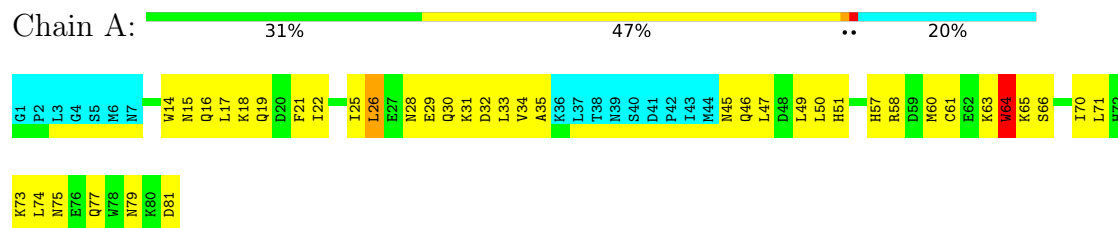
Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1348	427	666	119	132	4	

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: Erythrocyte membrane protein 1 (PfEMP1)

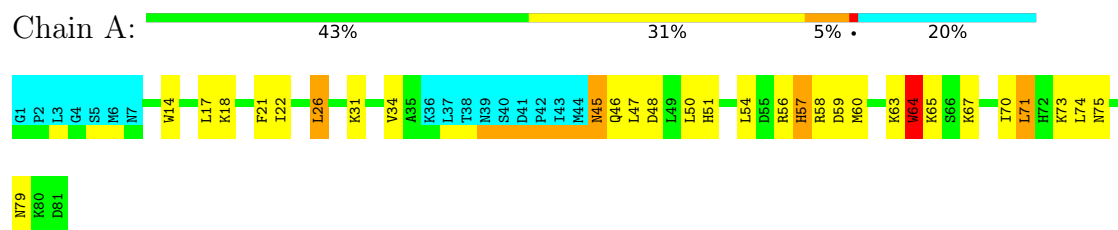


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

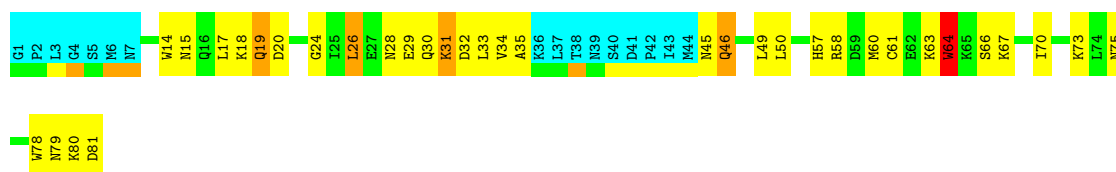
- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



4.2.2 Score per residue for model 2

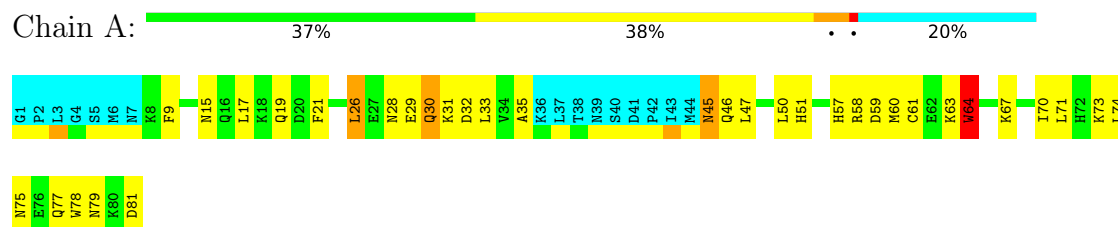
- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)





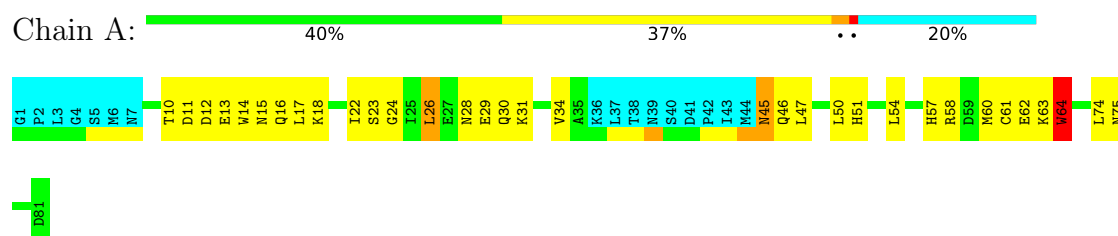
4.2.3 Score per residue for model 3

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



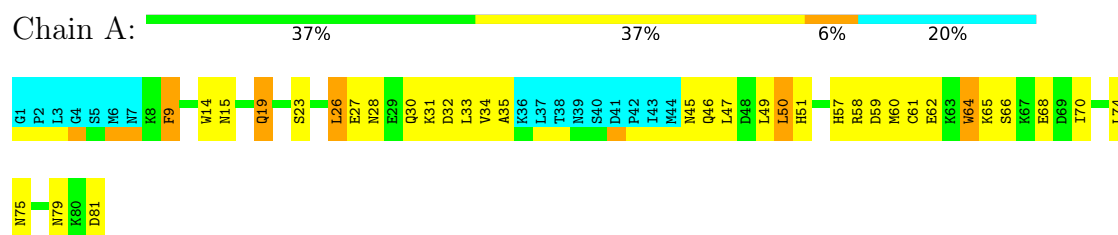
4.2.4 Score per residue for model 4

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



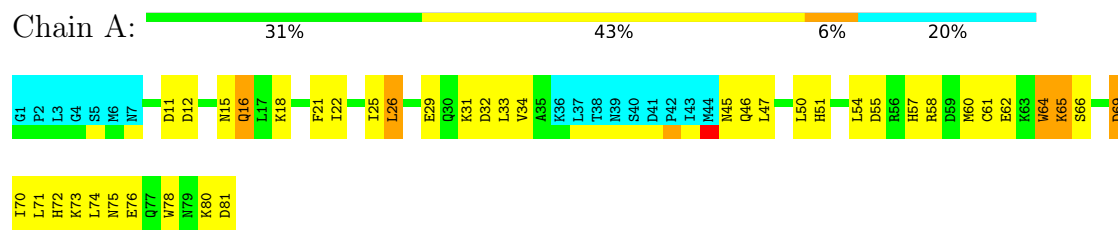
4.2.5 Score per residue for model 5

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



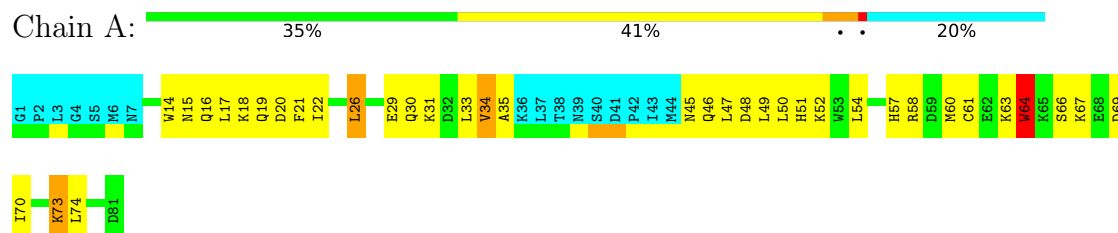
4.2.6 Score per residue for model 6

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



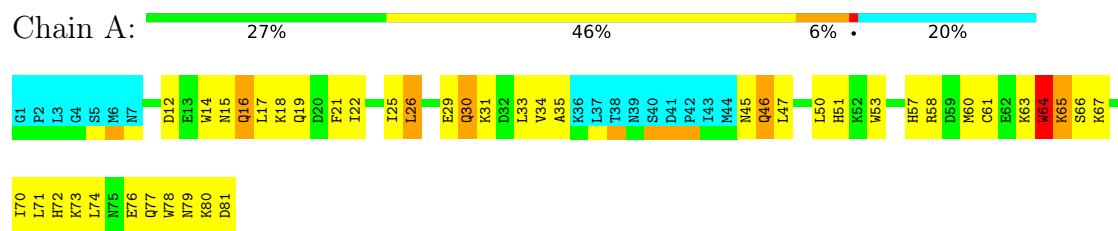
4.2.7 Score per residue for model 7

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



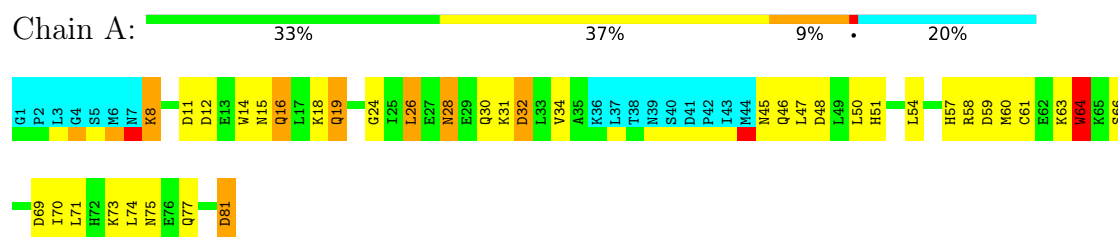
4.2.8 Score per residue for model 8

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



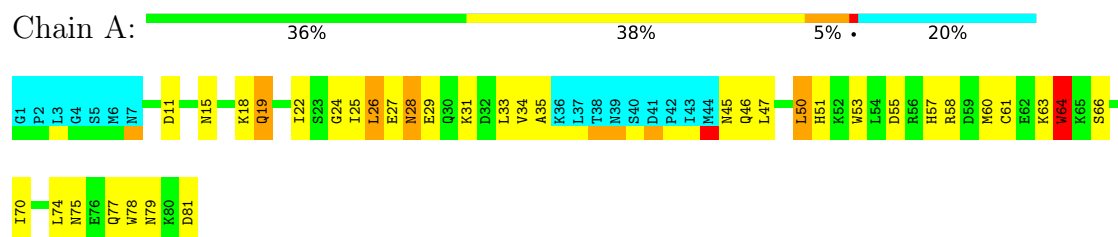
4.2.9 Score per residue for model 9

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



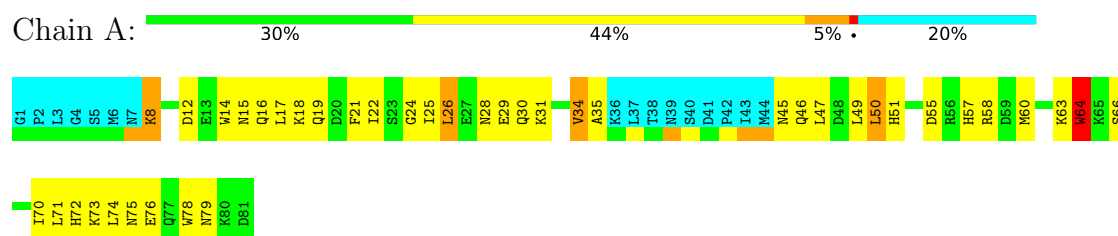
4.2.10 Score per residue for model 10

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



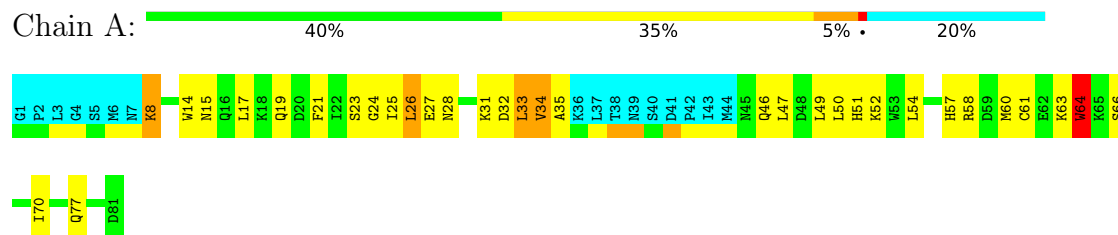
4.2.11 Score per residue for model 11

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



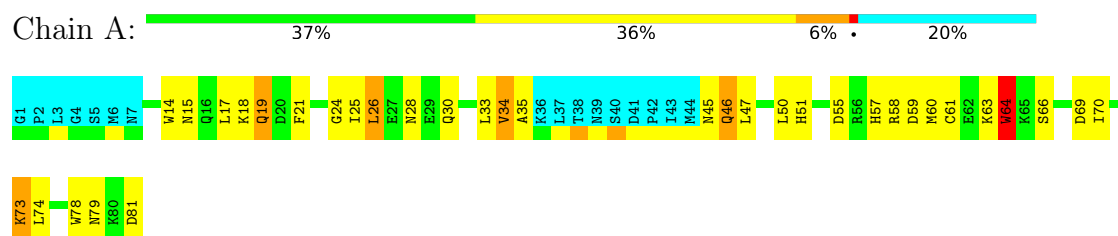
4.2.12 Score per residue for model 12

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



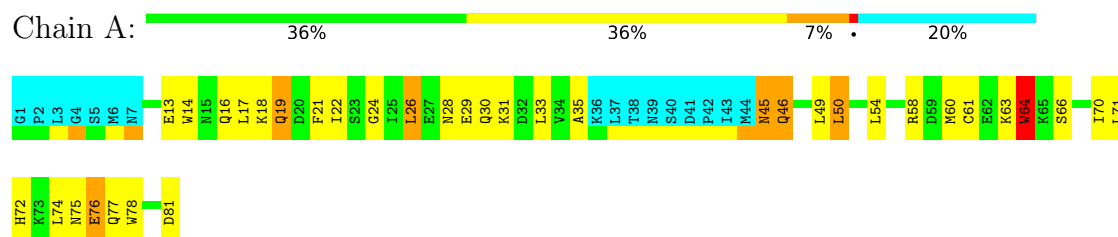
4.2.13 Score per residue for model 13

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



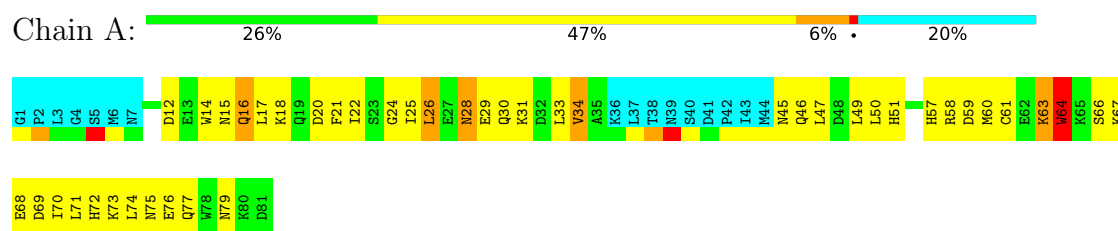
4.2.14 Score per residue for model 14

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



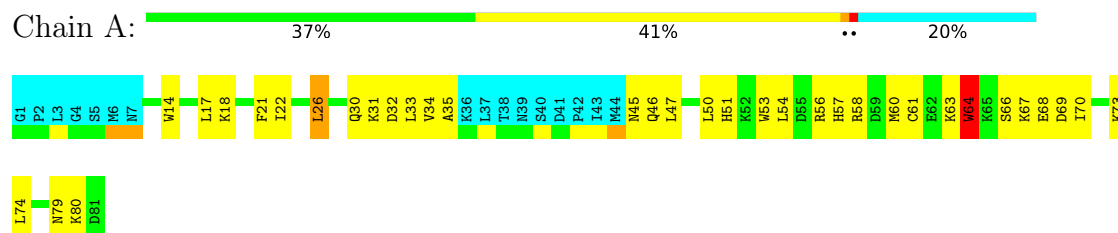
4.2.15 Score per residue for model 15

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



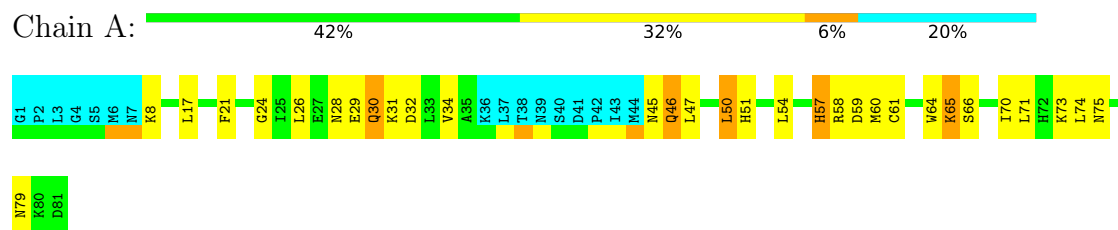
4.2.16 Score per residue for model 16

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



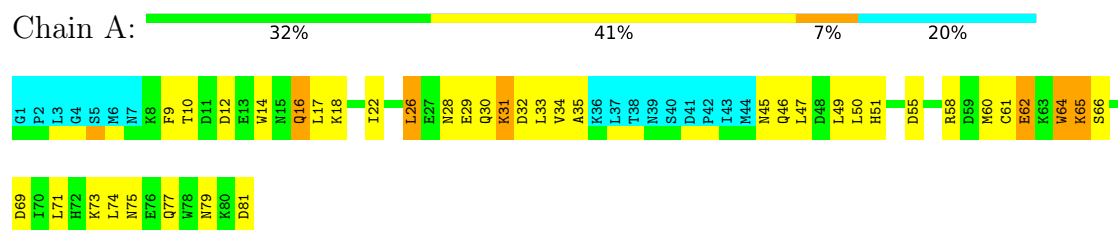
4.2.17 Score per residue for model 17

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



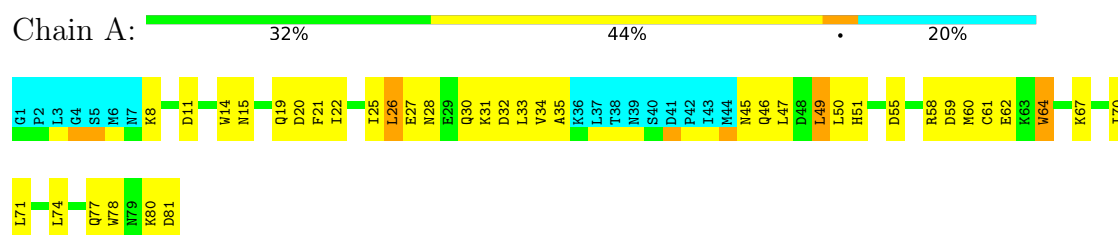
4.2.18 Score per residue for model 18

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



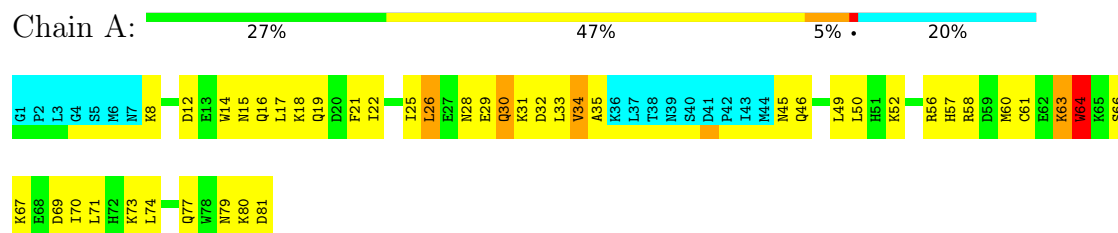
4.2.19 Score per residue for model 19

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



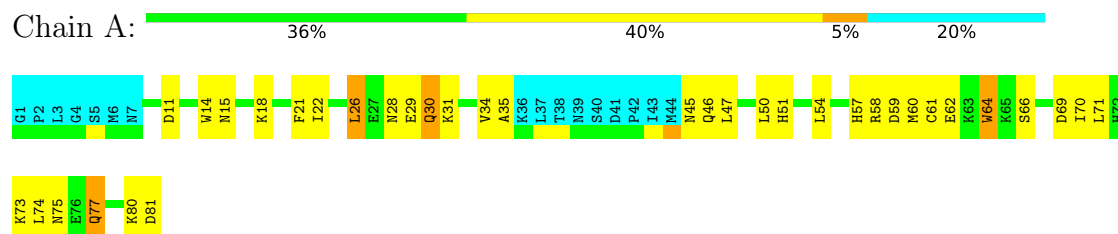
4.2.20 Score per residue for model 20

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



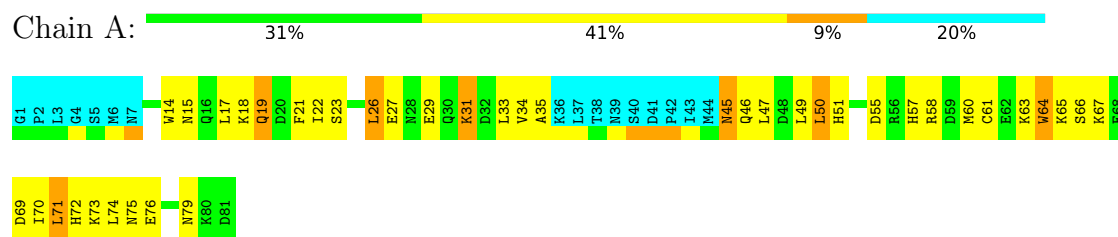
4.2.21 Score per residue for model 21

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



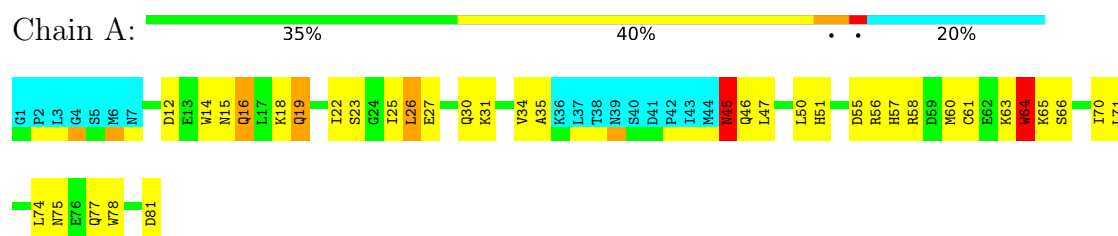
4.2.22 Score per residue for model 22

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



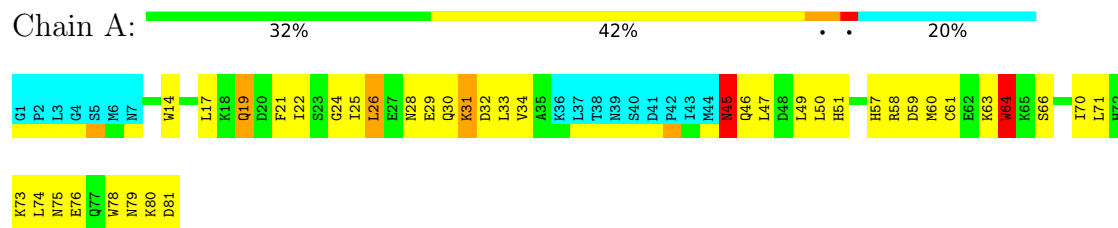
4.2.23 Score per residue for model 23

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



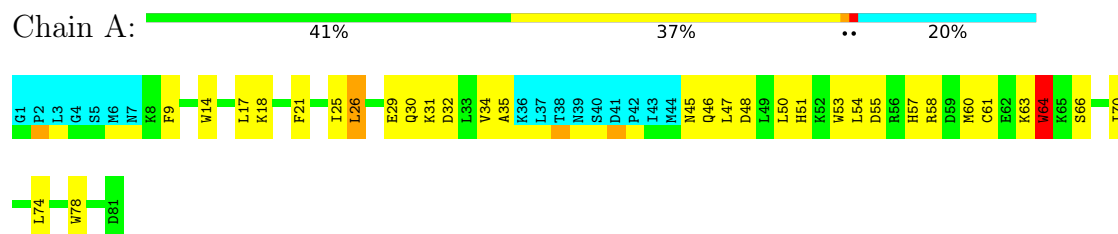
4.2.24 Score per residue for model 24

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



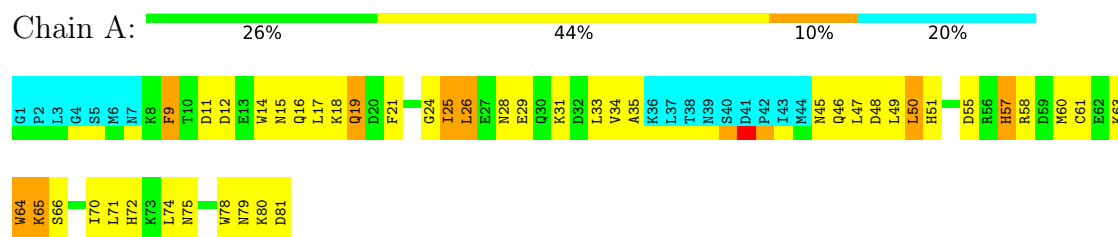
4.2.25 Score per residue for model 25

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



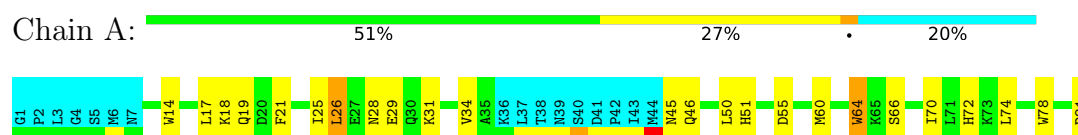
4.2.26 Score per residue for model 26

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



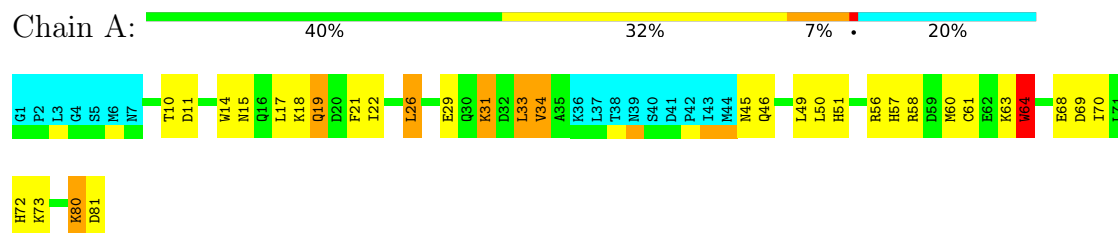
4.2.27 Score per residue for model 27

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



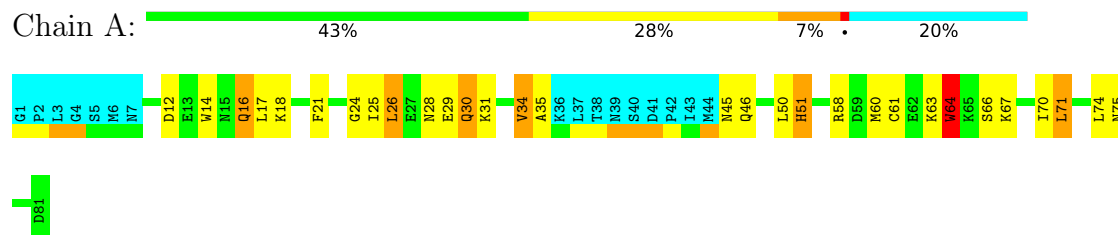
4.2.28 Score per residue for model 28

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



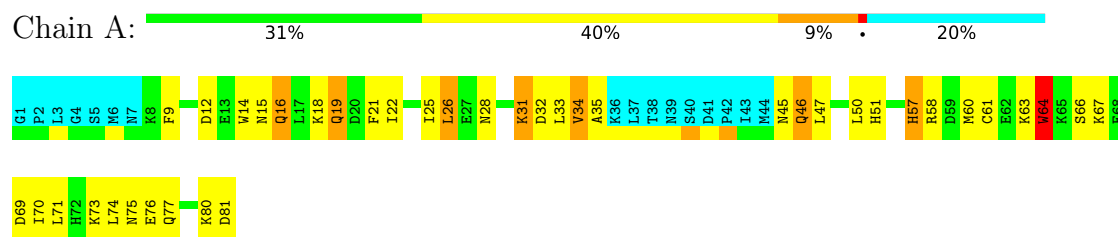
4.2.29 Score per residue for model 29

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



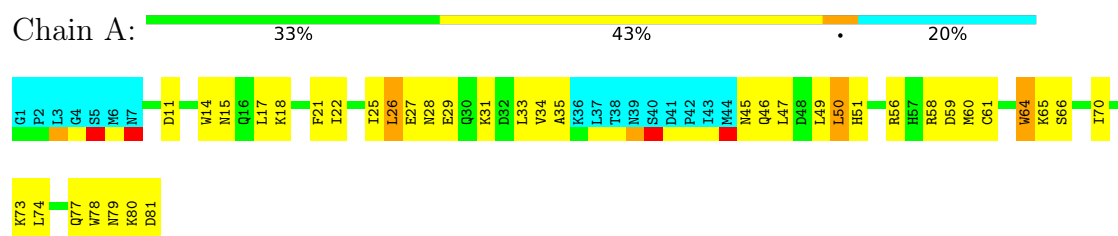
4.2.30 Score per residue for model 30

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



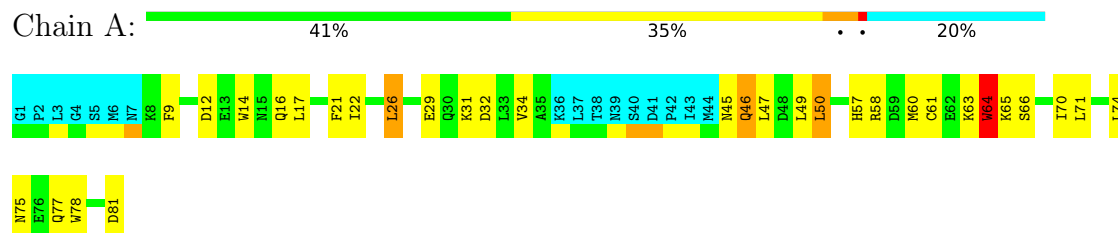
4.2.31 Score per residue for model 31

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



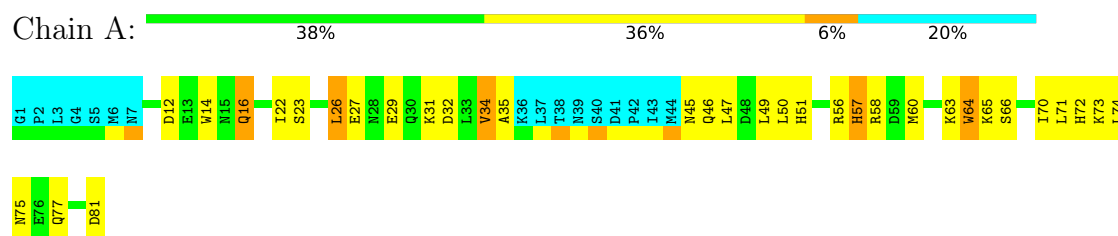
4.2.32 Score per residue for model 32

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



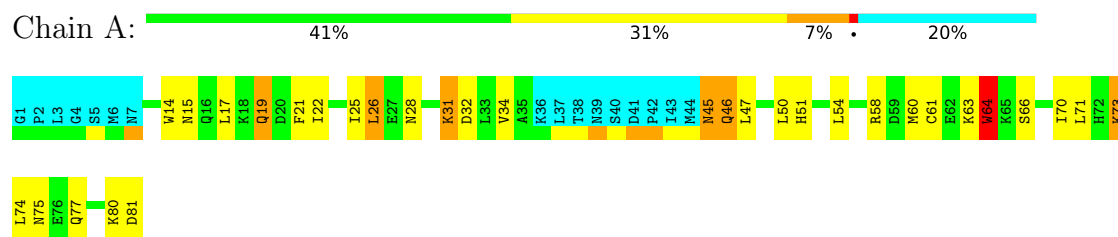
4.2.33 Score per residue for model 33

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



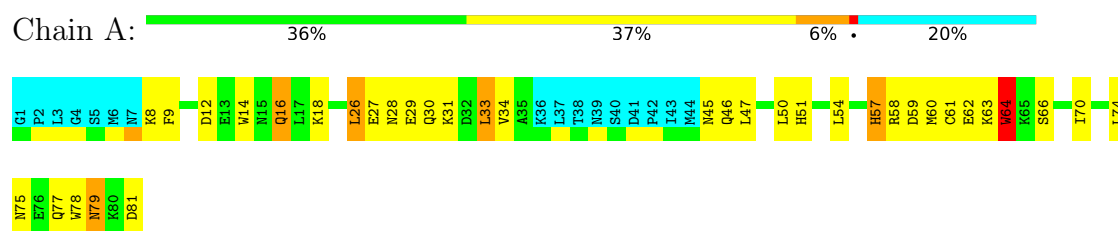
4.2.34 Score per residue for model 34

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



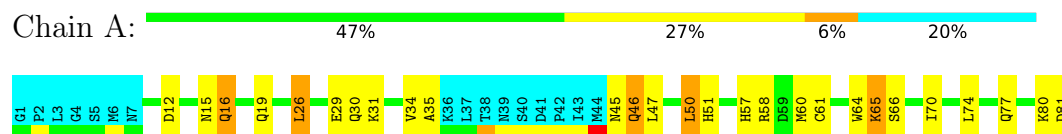
4.2.35 Score per residue for model 35

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



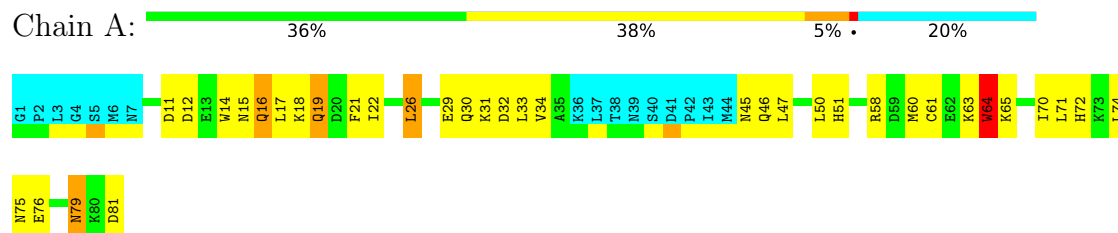
4.2.36 Score per residue for model 36

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



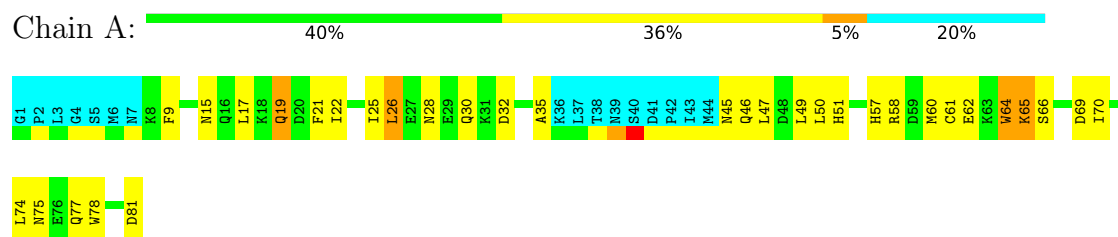
4.2.37 Score per residue for model 37

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



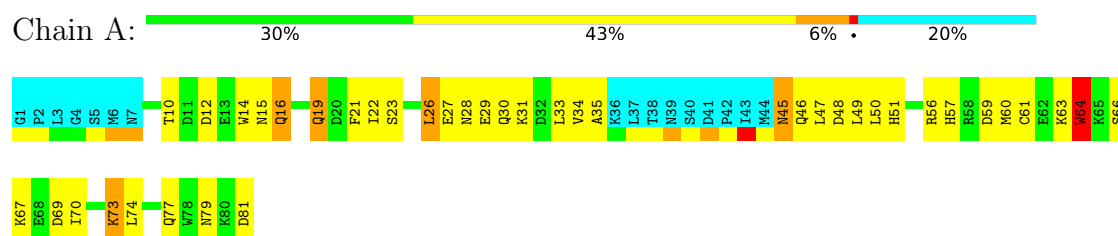
4.2.38 Score per residue for model 38

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



4.2.39 Score per residue for model 39

- Molecule 1: Erythrocyte membrane protein 1 (PfEMP1)



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 39 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.25
X-PLOR NIH	refinement	2.25

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	1063
Number of shifts mapped to atoms	1063
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.64±0.01	0±0/580 (0.0± 0.0%)	1.13±0.01	0±1/777 (0.1± 0.1%)
All	All	0.64	0/22620 (0.0%)	1.13	19/30303 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	51	HIS	CA-CB-CG	-6.01	107.79	113.80	29	2
1	A	57	HIS	CA-CB-CG	-5.94	107.86	113.80	26	6
1	A	9	PHE	CA-CB-CG	-5.63	108.17	113.80	30	9
1	A	72	HIS	CA-CB-CG	-5.18	108.62	113.80	27	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	568	547	544	45±7
All	All	22152	21333	21216	1750

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:O	1:A:26:LEU:HD12	0.93	1.63	23	11
1:A:31:LYS:O	1:A:34:VAL:HG12	0.92	1.64	34	17
1:A:26:LEU:C	1:A:26:LEU:HD12	0.86	1.95	1	28
1:A:26:LEU:HD12	1:A:26:LEU:C	0.81	2.00	21	11
1:A:33:LEU:HD21	1:A:79:ASN:OD1	0.81	1.76	18	1
1:A:14:TRP:CD1	1:A:18:LYS:HZ1	0.80	1.94	2	1
1:A:60:MET:O	1:A:64:TRP:CD1	0.80	2.34	19	10
1:A:34:VAL:HG23	1:A:46:GLN:HE21	0.80	1.37	24	3
1:A:60:MET:HE1	1:A:70:ILE:CG2	0.79	2.08	13	4
1:A:26:LEU:HD12	1:A:26:LEU:O	0.78	1.79	20	28
1:A:60:MET:O	1:A:64:TRP:NE1	0.78	2.18	32	36
1:A:64:TRP:H	1:A:64:TRP:CD1	0.77	1.95	22	3
1:A:50:LEU:HD23	1:A:50:LEU:O	0.75	1.81	4	33
1:A:34:VAL:HG23	1:A:46:GLN:NE2	0.75	1.95	36	4
1:A:22:ILE:HG23	1:A:45:ASN:CG	0.74	2.06	28	8
1:A:66:SER:O	1:A:70:ILE:HD12	0.74	1.83	24	18
1:A:22:ILE:HG23	1:A:45:ASN:OD1	0.74	1.81	8	7
1:A:12:ASP:O	1:A:16:GLN:NE2	0.74	2.20	18	13
1:A:77:GLN:O	1:A:81:ASP:N	0.74	2.21	19	16
1:A:28:ASN:ND2	1:A:30:GLN:OE1	0.74	2.20	14	5
1:A:59:ASP:OD1	1:A:60:MET:N	0.73	2.21	17	9
1:A:64:TRP:O	1:A:66:SER:N	0.73	2.21	26	15
1:A:16:GLN:N	1:A:16:GLN:OE1	0.73	2.21	33	8
1:A:17:LEU:HD11	1:A:21:PHE:CE1	0.73	2.17	32	17
1:A:47:LEU:O	1:A:51:HIS:CD2	0.73	2.42	1	31
1:A:32:ASP:OD1	1:A:33:LEU:N	0.72	2.23	2	5
1:A:45:ASN:O	1:A:46:GLN:NE2	0.72	2.23	8	2
1:A:33:LEU:CD1	1:A:79:ASN:ND2	0.71	2.53	8	6
1:A:31:LYS:NZ	1:A:32:ASP:OD1	0.71	2.24	24	3
1:A:50:LEU:C	1:A:50:LEU:HD23	0.71	2.10	12	3
1:A:64:TRP:CD1	1:A:64:TRP:H	0.71	2.03	33	7
1:A:8:LYS:NZ	1:A:58:ARG:NH2	0.70	2.39	11	1
1:A:50:LEU:HD23	1:A:50:LEU:C	0.70	2.12	30	25
1:A:28:ASN:ND2	1:A:30:GLN:CG	0.69	2.54	13	3
1:A:19:GLN:N	1:A:19:GLN:OE1	0.69	2.25	9	5
1:A:20:ASP:OD2	1:A:67:LYS:NZ	0.69	2.25	2	2
1:A:22:ILE:CG2	1:A:45:ASN:ND2	0.69	2.55	28	3
1:A:60:MET:HE1	1:A:70:ILE:HG21	0.69	1.65	13	4
1:A:30:GLN:CD	1:A:30:GLN:N	0.69	2.51	20	2
1:A:28:ASN:HD22	1:A:28:ASN:C	0.69	1.96	10	2
1:A:30:GLN:HE22	1:A:75:ASN:ND2	0.68	1.87	23	4
1:A:49:LEU:HD22	1:A:49:LEU:N	0.68	2.01	28	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:CYS:SG	1:A:62:GLU:CD	0.68	2.77	5	1
1:A:33:LEU:CD2	1:A:79:ASN:HD22	0.68	2.00	22	2
1:A:63:LYS:C	1:A:64:TRP:CG	0.68	2.71	34	26
1:A:33:LEU:CD2	1:A:79:ASN:ND2	0.68	2.57	22	3
1:A:47:LEU:O	1:A:51:HIS:CG	0.68	2.47	37	12
1:A:64:TRP:CD1	1:A:64:TRP:N	0.68	2.61	22	16
1:A:69:ASP:OD1	1:A:73:LYS:NZ	0.67	2.27	9	3
1:A:58:ARG:O	1:A:61:CYS:SG	0.67	2.51	34	33
1:A:46:GLN:O	1:A:46:GLN:CG	0.67	2.41	36	3
1:A:26:LEU:C	1:A:26:LEU:CD1	0.67	2.67	5	39
1:A:21:PHE:CE2	1:A:74:LEU:CD2	0.67	2.78	6	4
1:A:28:ASN:ND2	1:A:30:GLN:CD	0.67	2.53	24	3
1:A:28:ASN:OD1	1:A:29:GLU:N	0.67	2.28	21	3
1:A:30:GLN:OE1	1:A:33:LEU:HD12	0.67	1.89	13	1
1:A:49:LEU:HD12	1:A:49:LEU:N	0.67	2.04	20	7
1:A:64:TRP:C	1:A:66:SER:H	0.67	1.97	8	26
1:A:49:LEU:CD2	1:A:49:LEU:N	0.67	2.57	19	5
1:A:71:LEU:O	1:A:75:ASN:ND2	0.66	2.28	6	7
1:A:72:HIS:HD1	1:A:72:HIS:C	0.66	1.99	26	2
1:A:64:TRP:O	1:A:65:LYS:C	0.66	2.38	17	3
1:A:66:SER:O	1:A:70:ILE:CD1	0.65	2.44	14	18
1:A:57:HIS:O	1:A:60:MET:CG	0.65	2.44	28	30
1:A:33:LEU:N	1:A:33:LEU:CD2	0.65	2.60	35	2
1:A:11:ASP:O	1:A:15:ASN:ND2	0.65	2.28	10	7
1:A:30:GLN:HE22	1:A:75:ASN:CG	0.65	1.99	3	5
1:A:14:TRP:CZ3	1:A:17:LEU:HD23	0.65	2.27	4	7
1:A:21:PHE:CE1	1:A:74:LEU:HD22	0.65	2.27	24	4
1:A:15:ASN:O	1:A:19:GLN:OE1	0.65	2.14	23	22
1:A:22:ILE:HG23	1:A:45:ASN:CB	0.64	2.23	18	6
1:A:57:HIS:O	1:A:60:MET:SD	0.64	2.55	5	7
1:A:21:PHE:CE1	1:A:74:LEU:CD2	0.64	2.80	17	3
1:A:79:ASN:HD22	1:A:79:ASN:N	0.64	1.90	37	6
1:A:21:PHE:CE2	1:A:74:LEU:HD21	0.64	2.27	6	5
1:A:33:LEU:HD23	1:A:79:ASN:ND2	0.64	2.09	5	1
1:A:54:LEU:O	1:A:58:ARG:N	0.63	2.31	4	11
1:A:25:ILE:O	1:A:28:ASN:OD1	0.63	2.16	30	9
1:A:70:ILE:HG22	1:A:74:LEU:CD1	0.63	2.22	34	9
1:A:30:GLN:NE2	1:A:75:ASN:ND2	0.63	2.46	5	1
1:A:22:ILE:HG23	1:A:45:ASN:HD22	0.63	1.54	21	3
1:A:45:ASN:HD21	1:A:47:LEU:CD2	0.62	2.06	39	2
1:A:14:TRP:NE1	1:A:55:ASP:OD1	0.62	2.31	27	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:TRP:O	1:A:65:LYS:CB	0.62	2.47	18	1
1:A:45:ASN:O	1:A:46:GLN:OE1	0.62	2.17	30	2
1:A:71:LEU:O	1:A:75:ASN:CG	0.62	2.43	15	14
1:A:25:ILE:HD11	1:A:78:TRP:CZ3	0.62	2.29	25	6
1:A:72:HIS:NE2	1:A:76:GLU:OE2	0.62	2.32	15	1
1:A:30:GLN:N	1:A:30:GLN:OE1	0.62	2.33	20	1
1:A:72:HIS:O	1:A:76:GLU:OE1	0.61	2.19	22	4
1:A:77:GLN:NE2	1:A:80:LYS:NZ	0.61	2.48	21	1
1:A:12:ASP:O	1:A:16:GLN:CD	0.61	2.44	11	11
1:A:49:LEU:N	1:A:49:LEU:CD2	0.61	2.63	28	2
1:A:8:LYS:NZ	1:A:58:ARG:CZ	0.61	2.62	11	1
1:A:27:GLU:OE1	1:A:27:GLU:C	0.61	2.44	35	2
1:A:80:LYS:O	1:A:81:ASP:OXT	0.61	2.19	36	3
1:A:72:HIS:C	1:A:72:HIS:ND1	0.61	2.59	26	2
1:A:22:ILE:HG23	1:A:45:ASN:ND2	0.61	2.10	28	6
1:A:73:LYS:O	1:A:77:GLN:OE1	0.61	2.19	15	2
1:A:19:GLN:NE2	1:A:22:ILE:HD12	0.60	2.11	22	6
1:A:72:HIS:CD2	1:A:76:GLU:OE2	0.60	2.55	15	1
1:A:28:ASN:C	1:A:28:ASN:ND2	0.60	2.59	10	2
1:A:81:ASP:OD1	1:A:81:ASP:OXT	0.60	2.19	38	2
1:A:49:LEU:N	1:A:49:LEU:HD22	0.60	2.10	38	5
1:A:49:LEU:HD12	1:A:49:LEU:H	0.60	1.56	20	3
1:A:78:TRP:O	1:A:81:ASP:CG	0.60	2.45	27	3
1:A:76:GLU:OE1	1:A:76:GLU:N	0.60	2.35	22	1
1:A:30:GLN:OE1	1:A:75:ASN:OD1	0.60	2.18	4	3
1:A:12:ASP:O	1:A:16:GLN:OE1	0.60	2.20	36	10
1:A:70:ILE:HG22	1:A:74:LEU:HD13	0.60	1.72	34	13
1:A:28:ASN:HD21	1:A:30:GLN:CD	0.60	2.05	24	1
1:A:68:GLU:H	1:A:68:GLU:CD	0.59	2.05	5	1
1:A:45:ASN:C	1:A:46:GLN:NE2	0.59	2.60	8	1
1:A:14:TRP:CZ3	1:A:17:LEU:CD2	0.59	2.85	22	12
1:A:73:LYS:N	1:A:73:LYS:CD	0.59	2.65	1	9
1:A:45:ASN:C	1:A:46:GLN:CD	0.59	2.69	7	1
1:A:33:LEU:HD12	1:A:33:LEU:N	0.59	2.12	7	8
1:A:19:GLN:N	1:A:19:GLN:CD	0.59	2.61	37	17
1:A:64:TRP:C	1:A:66:SER:N	0.59	2.60	8	24
1:A:77:GLN:O	1:A:81:ASP:CG	0.59	2.45	23	2
1:A:24:GLY:O	1:A:28:ASN:CG	0.59	2.45	14	11
1:A:30:GLN:HE22	1:A:75:ASN:CB	0.59	2.10	17	2
1:A:45:ASN:O	1:A:46:GLN:CG	0.59	2.51	25	13
1:A:46:GLN:O	1:A:47:LEU:C	0.59	2.45	16	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ASN:O	1:A:46:GLN:CD	0.59	2.45	2	4
1:A:30:GLN:OE1	1:A:75:ASN:CG	0.59	2.46	14	3
1:A:64:TRP:N	1:A:64:TRP:CD1	0.58	2.72	8	3
1:A:29:GLU:C	1:A:31:LYS:N	0.58	2.61	35	27
1:A:27:GLU:OE1	1:A:28:ASN:OD1	0.58	2.20	35	1
1:A:78:TRP:O	1:A:81:ASP:OD1	0.58	2.22	27	2
1:A:34:VAL:HG22	1:A:46:GLN:HE22	0.58	1.58	7	1
1:A:27:GLU:OE1	1:A:27:GLU:O	0.58	2.22	19	1
1:A:33:LEU:N	1:A:33:LEU:HD22	0.58	2.13	35	2
1:A:81:ASP:OD1	1:A:81:ASP:C	0.57	2.47	27	5
1:A:70:ILE:O	1:A:74:LEU:HD13	0.57	1.99	25	5
1:A:59:ASP:OD1	1:A:59:ASP:O	0.57	2.22	21	2
1:A:80:LYS:O	1:A:81:ASP:O	0.57	2.21	26	4
1:A:53:TRP:O	1:A:57:HIS:ND1	0.57	2.37	16	1
1:A:64:TRP:O	1:A:66:SER:OG	0.57	2.20	26	2
1:A:45:ASN:C	1:A:46:GLN:OE1	0.57	2.47	34	3
1:A:28:ASN:C	1:A:28:ASN:OD1	0.57	2.48	3	4
1:A:22:ILE:CG2	1:A:45:ASN:OD1	0.57	2.53	19	4
1:A:24:GLY:O	1:A:28:ASN:OD1	0.57	2.21	24	2
1:A:34:VAL:HG23	1:A:46:GLN:HG3	0.57	1.76	19	1
1:A:30:GLN:NE2	1:A:75:ASN:CG	0.57	2.63	14	2
1:A:18:LYS:NZ	1:A:51:HIS:CG	0.57	2.73	28	2
1:A:67:LYS:HZ2	1:A:71:LEU:HD11	0.56	1.60	8	2
1:A:72:HIS:CE1	1:A:76:GLU:OE2	0.56	2.57	8	3
1:A:48:ASP:OD1	1:A:49:LEU:N	0.56	2.38	26	3
1:A:64:TRP:O	1:A:70:ILE:HD11	0.56	2.00	38	2
1:A:29:GLU:C	1:A:31:LYS:H	0.56	2.07	27	15
1:A:67:LYS:NZ	1:A:71:LEU:HD11	0.56	2.16	8	3
1:A:77:GLN:HE21	1:A:80:LYS:NZ	0.56	1.97	21	1
1:A:78:TRP:O	1:A:81:ASP:OD2	0.56	2.24	14	1
1:A:60:MET:O	1:A:64:TRP:CE2	0.56	2.59	7	11
1:A:75:ASN:O	1:A:79:ASN:ND2	0.56	2.39	37	2
1:A:64:TRP:O	1:A:70:ILE:CG1	0.56	2.54	38	1
1:A:17:LEU:HD11	1:A:21:PHE:CZ	0.55	2.36	11	4
1:A:45:ASN:HD21	1:A:47:LEU:HD21	0.55	1.62	39	2
1:A:50:LEU:C	1:A:50:LEU:CD2	0.55	2.79	12	29
1:A:45:ASN:HD22	1:A:45:ASN:N	0.55	1.99	23	3
1:A:16:GLN:OE1	1:A:16:GLN:CA	0.55	2.53	29	4
1:A:46:GLN:O	1:A:50:LEU:N	0.55	2.34	1	9
1:A:77:GLN:OE1	1:A:77:GLN:N	0.55	2.39	33	1
1:A:27:GLU:CD	1:A:27:GLU:C	0.55	2.75	31	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:TRP:O	1:A:81:ASP:OXT	0.55	2.24	31	2
1:A:80:LYS:C	1:A:81:ASP:OD1	0.55	2.50	31	1
1:A:21:PHE:CE2	1:A:54:LEU:HD11	0.55	2.37	17	2
1:A:77:GLN:O	1:A:77:GLN:OE1	0.55	2.24	14	1
1:A:29:GLU:O	1:A:31:LYS:N	0.54	2.41	3	12
1:A:22:ILE:CG2	1:A:45:ASN:HD22	0.54	2.15	4	2
1:A:48:ASP:CG	1:A:49:LEU:HD12	0.54	2.27	7	1
1:A:62:GLU:N	1:A:62:GLU:OE1	0.54	2.39	5	1
1:A:20:ASP:CB	1:A:67:LYS:NZ	0.54	2.70	19	4
1:A:59:ASP:OD1	1:A:59:ASP:C	0.54	2.50	17	6
1:A:80:LYS:O	1:A:81:ASP:C	0.54	2.50	6	5
1:A:25:ILE:CD1	1:A:78:TRP:CZ3	0.54	2.91	23	2
1:A:32:ASP:OD1	1:A:32:ASP:C	0.54	2.48	2	2
1:A:59:ASP:O	1:A:62:GLU:OE1	0.54	2.26	5	1
1:A:17:LEU:CD1	1:A:21:PHE:CE1	0.54	2.91	20	6
1:A:75:ASN:O	1:A:79:ASN:OD1	0.53	2.26	10	3
1:A:11:ASP:O	1:A:15:ASN:CG	0.53	2.52	4	6
1:A:81:ASP:O	1:A:81:ASP:OD1	0.53	2.27	37	1
1:A:45:ASN:OD1	1:A:45:ASN:C	0.53	2.50	1	1
1:A:76:GLU:CD	1:A:76:GLU:N	0.53	2.67	14	1
1:A:18:LYS:HZ2	1:A:51:HIS:CG	0.53	2.22	28	2
1:A:75:ASN:O	1:A:79:ASN:CG	0.53	2.51	26	2
1:A:34:VAL:CG2	1:A:46:GLN:NE2	0.53	2.72	8	1
1:A:79:ASN:N	1:A:79:ASN:ND2	0.53	2.57	37	3
1:A:72:HIS:O	1:A:76:GLU:CD	0.53	2.52	15	1
1:A:30:GLN:CD	1:A:30:GLN:H	0.53	2.11	20	1
1:A:74:LEU:O	1:A:78:TRP:N	0.52	2.38	38	6
1:A:19:GLN:NE2	1:A:19:GLN:N	0.52	2.58	26	2
1:A:46:GLN:OE1	1:A:78:TRP:CZ2	0.52	2.62	32	1
1:A:73:LYS:HD2	1:A:73:LYS:N	0.52	2.20	39	3
1:A:60:MET:O	1:A:63:LYS:CG	0.52	2.58	22	1
1:A:16:GLN:N	1:A:16:GLN:CD	0.52	2.68	29	2
1:A:28:ASN:OD1	1:A:28:ASN:O	0.52	2.28	38	3
1:A:48:ASP:N	1:A:48:ASP:OD1	0.52	2.42	9	2
1:A:21:PHE:CD1	1:A:71:LEU:HD21	0.52	2.40	19	1
1:A:33:LEU:HD23	1:A:79:ASN:HD22	0.52	1.65	26	1
1:A:33:LEU:N	1:A:33:LEU:CD1	0.51	2.73	10	6
1:A:51:HIS:O	1:A:55:ASP:CG	0.51	2.53	23	4
1:A:23:SER:HA	1:A:26:LEU:HD23	0.51	1.81	4	1
1:A:24:GLY:O	1:A:28:ASN:ND2	0.51	2.44	9	2
1:A:81:ASP:OXT	1:A:81:ASP:CG	0.51	2.52	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ILE:HG23	1:A:45:ASN:HB2	0.51	1.81	18	1
1:A:45:ASN:C	1:A:45:ASN:ND2	0.51	2.68	24	1
1:A:14:TRP:CZ3	1:A:17:LEU:HD22	0.51	2.40	29	3
1:A:34:VAL:HG21	1:A:45:ASN:HA	0.51	1.82	1	3
1:A:33:LEU:HD13	1:A:79:ASN:ND2	0.51	2.21	3	4
1:A:14:TRP:CZ2	1:A:58:ARG:CB	0.51	2.94	37	16
1:A:47:LEU:CD2	1:A:51:HIS:NE2	0.51	2.74	35	4
1:A:28:ASN:HD21	1:A:30:GLN:CG	0.51	2.17	13	1
1:A:45:ASN:N	1:A:45:ASN:HD22	0.51	2.03	35	2
1:A:81:ASP:N	1:A:81:ASP:OD1	0.51	2.43	9	1
1:A:68:GLU:CG	1:A:69:ASP:N	0.51	2.74	15	1
1:A:30:GLN:OE1	1:A:30:GLN:CA	0.51	2.58	20	1
1:A:48:ASP:CG	1:A:49:LEU:N	0.51	2.69	39	1
1:A:25:ILE:O	1:A:28:ASN:ND2	0.51	2.44	10	2
1:A:25:ILE:O	1:A:31:LYS:CA	0.50	2.59	12	1
1:A:68:GLU:O	1:A:72:HIS:CD2	0.50	2.63	28	1
1:A:28:ASN:ND2	1:A:28:ASN:C	0.50	2.69	9	1
1:A:73:LYS:HZ2	1:A:73:LYS:HB3	0.50	1.66	13	1
1:A:33:LEU:HD13	1:A:79:ASN:HD22	0.50	1.66	39	1
1:A:21:PHE:CD2	1:A:74:LEU:CD2	0.50	2.95	20	4
1:A:24:GLY:O	1:A:28:ASN:CB	0.50	2.59	12	1
1:A:64:TRP:CD1	1:A:70:ILE:HG12	0.50	2.41	19	29
1:A:33:LEU:HD23	1:A:78:TRP:CD1	0.50	2.41	19	1
1:A:76:GLU:O	1:A:80:LYS:NZ	0.50	2.43	30	1
1:A:49:LEU:N	1:A:49:LEU:CD1	0.50	2.75	20	4
1:A:64:TRP:CD1	1:A:70:ILE:CG1	0.50	2.94	30	1
1:A:34:VAL:CG1	1:A:35:ALA:N	0.50	2.74	23	3
1:A:60:MET:C	1:A:60:MET:SD	0.49	2.95	12	1
1:A:70:ILE:HG22	1:A:74:LEU:HD22	0.49	1.82	30	2
1:A:34:VAL:CG2	1:A:46:GLN:OE1	0.49	2.60	34	2
1:A:45:ASN:O	1:A:46:GLN:HG2	0.49	2.07	27	9
1:A:31:LYS:O	1:A:34:VAL:CG1	0.49	2.61	19	5
1:A:66:SER:OG	1:A:69:ASP:OD2	0.49	2.22	22	2
1:A:73:LYS:N	1:A:73:LYS:HD3	0.49	2.22	2	6
1:A:77:GLN:OE1	1:A:77:GLN:C	0.49	2.56	14	1
1:A:22:ILE:HG23	1:A:45:ASN:HB3	0.49	1.84	19	1
1:A:66:SER:O	1:A:68:GLU:N	0.49	2.44	16	1
1:A:19:GLN:OE1	1:A:19:GLN:N	0.49	2.45	39	1
1:A:70:ILE:O	1:A:74:LEU:CD1	0.49	2.60	22	8
1:A:22:ILE:CG2	1:A:45:ASN:CG	0.49	2.86	19	1
1:A:8:LYS:HZ1	1:A:58:ARG:CZ	0.49	2.21	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:CYS:SG	1:A:62:GLU:OE2	0.49	2.70	5	1
1:A:9:PHE:CE1	1:A:61:CYS:SG	0.48	3.06	5	1
1:A:61:CYS:O	1:A:65:LYS:N	0.48	2.46	38	1
1:A:18:LYS:HD3	1:A:51:HIS:ND1	0.48	2.23	1	6
1:A:66:SER:OG	1:A:69:ASP:CB	0.48	2.61	16	4
1:A:74:LEU:N	1:A:74:LEU:CD1	0.48	2.77	3	19
1:A:63:LYS:C	1:A:64:TRP:CD1	0.48	2.92	8	2
1:A:16:GLN:CD	1:A:16:GLN:N	0.48	2.71	18	1
1:A:66:SER:OG	1:A:69:ASP:CG	0.48	2.57	39	2
1:A:34:VAL:HG23	1:A:46:GLN:OE1	0.48	2.09	1	3
1:A:56:ARG:NE	1:A:57:HIS:NE2	0.48	2.61	1	1
1:A:28:ASN:ND2	1:A:30:GLN:HG2	0.48	2.23	13	1
1:A:56:ARG:NH2	1:A:57:HIS:NE2	0.48	2.61	20	1
1:A:68:GLU:CD	1:A:68:GLU:N	0.48	2.71	5	1
1:A:28:ASN:O	1:A:28:ASN:ND2	0.48	2.42	15	1
1:A:59:ASP:C	1:A:62:GLU:OE1	0.48	2.57	5	1
1:A:28:ASN:OD1	1:A:28:ASN:C	0.48	2.55	38	3
1:A:49:LEU:H	1:A:49:LEU:CD1	0.47	2.22	20	2
1:A:67:LYS:O	1:A:71:LEU:HD23	0.47	2.09	22	3
1:A:61:CYS:SG	1:A:62:GLU:N	0.47	2.88	18	7
1:A:77:GLN:O	1:A:81:ASP:OD1	0.47	2.32	9	1
1:A:56:ARG:CD	1:A:56:ARG:O	0.47	2.63	31	1
1:A:28:ASN:C	1:A:28:ASN:HD22	0.47	2.16	9	1
1:A:33:LEU:HD21	1:A:79:ASN:ND2	0.47	2.24	10	1
1:A:47:LEU:HD23	1:A:51:HIS:NE2	0.47	2.24	35	3
1:A:13:GLU:HA	1:A:16:GLN:NE2	0.47	2.25	4	2
1:A:74:LEU:N	1:A:74:LEU:HD12	0.47	2.24	29	5
1:A:31:LYS:CG	1:A:32:ASP:N	0.47	2.77	32	5
1:A:51:HIS:O	1:A:55:ASP:OD2	0.47	2.33	26	2
1:A:60:MET:HG3	1:A:61:CYS:N	0.47	2.25	31	4
1:A:61:CYS:SG	1:A:62:GLU:OE1	0.47	2.71	5	1
1:A:14:TRP:CZ2	1:A:58:ARG:HB2	0.47	2.45	37	4
1:A:53:TRP:CH2	1:A:77:GLN:OE1	0.47	2.68	10	2
1:A:33:LEU:HD13	1:A:78:TRP:CD1	0.47	2.45	14	1
1:A:46:GLN:O	1:A:46:GLN:HG3	0.47	2.09	27	3
1:A:45:ASN:ND2	1:A:45:ASN:O	0.47	2.45	24	1
1:A:71:LEU:O	1:A:75:ASN:OD1	0.46	2.33	15	2
1:A:57:HIS:HB3	1:A:60:MET:SD	0.46	2.51	23	7
1:A:21:PHE:CZ	1:A:70:ILE:HG21	0.46	2.45	26	3
1:A:25:ILE:CG2	1:A:45:ASN:OD1	0.46	2.63	34	1
1:A:23:SER:OG	1:A:27:GLU:CD	0.46	2.59	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASP:O	1:A:32:ASP:OD1	0.46	2.34	17	1
1:A:77:GLN:NE2	1:A:80:LYS:HZ1	0.46	2.09	21	1
1:A:34:VAL:CG2	1:A:46:GLN:HE21	0.46	2.24	8	2
1:A:34:VAL:HG12	1:A:35:ALA:N	0.46	2.25	13	3
1:A:80:LYS:HB2	1:A:80:LYS:NZ	0.46	2.26	16	1
1:A:81:ASP:O	1:A:81:ASP:CG	0.46	2.58	37	1
1:A:28:ASN:C	1:A:30:GLN:N	0.45	2.73	5	1
1:A:20:ASP:HB3	1:A:67:LYS:NZ	0.45	2.25	19	2
1:A:61:CYS:O	1:A:65:LYS:HB3	0.45	2.12	36	2
1:A:53:TRP:NE1	1:A:81:ASP:OD2	0.45	2.45	10	1
1:A:45:ASN:HD21	1:A:47:LEU:HG	0.45	1.72	11	1
1:A:34:VAL:HG22	1:A:46:GLN:OE1	0.45	2.12	13	1
1:A:30:GLN:C	1:A:32:ASP:N	0.45	2.72	18	5
1:A:33:LEU:CD1	1:A:79:ASN:OD1	0.45	2.63	16	1
1:A:73:LYS:HZ3	1:A:73:LYS:HB3	0.45	1.70	24	1
1:A:45:ASN:O	1:A:46:GLN:C	0.45	2.59	2	1
1:A:30:GLN:HE22	1:A:75:ASN:HA	0.45	1.71	14	2
1:A:21:PHE:CE1	1:A:71:LEU:HD21	0.45	2.45	22	1
1:A:33:LEU:CD1	1:A:79:ASN:HD21	0.45	2.24	31	1
1:A:19:GLN:NE2	1:A:19:GLN:CA	0.45	2.80	26	2
1:A:45:ASN:C	1:A:46:GLN:HG2	0.45	2.37	9	9
1:A:45:ASN:C	1:A:46:GLN:HE21	0.45	2.19	8	1
1:A:30:GLN:HA	1:A:33:LEU:HD13	0.45	1.88	37	1
1:A:45:ASN:C	1:A:46:GLN:CG	0.45	2.90	14	14
1:A:71:LEU:N	1:A:71:LEU:CD2	0.45	2.79	29	2
1:A:14:TRP:CD1	1:A:18:LYS:HE2	0.44	2.47	14	17
1:A:50:LEU:O	1:A:50:LEU:CD2	0.44	2.65	14	5
1:A:15:ASN:HD22	1:A:15:ASN:N	0.44	2.09	15	3
1:A:8:LYS:HZ3	1:A:58:ARG:NE	0.44	2.10	20	1
1:A:34:VAL:CG1	1:A:45:ASN:OD1	0.44	2.65	29	1
1:A:73:LYS:N	1:A:73:LYS:HD2	0.44	2.27	30	1
1:A:19:GLN:NE2	1:A:19:GLN:HA	0.44	2.27	38	1
1:A:56:ARG:CZ	1:A:57:HIS:CE1	0.44	3.00	39	1
1:A:57:HIS:O	1:A:60:MET:HG3	0.44	2.12	7	5
1:A:23:SER:O	1:A:27:GLU:N	0.44	2.50	33	5
1:A:28:ASN:ND2	1:A:30:GLN:HG3	0.44	2.25	13	1
1:A:64:TRP:NE1	1:A:70:ILE:HG12	0.44	2.28	30	1
1:A:33:LEU:CD2	1:A:79:ASN:HD21	0.44	2.25	5	1
1:A:45:ASN:ND2	1:A:47:LEU:HG	0.44	2.27	11	1
1:A:61:CYS:O	1:A:65:LYS:CA	0.44	2.66	38	3
1:A:33:LEU:HD12	1:A:79:ASN:ND2	0.44	2.28	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:HG21	1:A:34:VAL:HG21	0.44	1.88	29	1
1:A:62:GLU:OE1	1:A:62:GLU:O	0.44	2.35	18	1
1:A:60:MET:CG	1:A:61:CYS:N	0.44	2.79	36	3
1:A:9:PHE:O	1:A:58:ARG:NH2	0.44	2.51	26	1
1:A:52:LYS:NZ	1:A:52:LYS:HB2	0.44	2.28	12	1
1:A:76:GLU:HG2	1:A:80:LYS:NZ	0.44	2.27	24	1
1:A:69:ASP:OD1	1:A:69:ASP:N	0.44	2.48	39	1
1:A:18:LYS:HD3	1:A:51:HIS:CE1	0.43	2.48	10	5
1:A:30:GLN:HE22	1:A:75:ASN:HB3	0.43	1.71	17	1
1:A:60:MET:HB2	1:A:64:TRP:CZ2	0.43	2.48	17	1
1:A:20:ASP:CB	1:A:67:LYS:HZ3	0.43	2.27	19	1
1:A:33:LEU:HD22	1:A:79:ASN:ND2	0.43	2.26	22	1
1:A:64:TRP:O	1:A:70:ILE:CD1	0.43	2.64	38	1
1:A:64:TRP:CZ3	1:A:73:LYS:HG3	0.43	2.49	3	3
1:A:45:ASN:ND2	1:A:45:ASN:N	0.43	2.65	32	2
1:A:57:HIS:CB	1:A:60:MET:SD	0.43	3.06	30	1
1:A:53:TRP:O	1:A:57:HIS:CD2	0.43	2.72	25	1
1:A:53:TRP:CZ2	1:A:77:GLN:OE1	0.43	2.72	8	2
1:A:72:HIS:O	1:A:76:GLU:OE2	0.43	2.37	14	1
1:A:48:ASP:OD1	1:A:48:ASP:C	0.43	2.58	1	1
1:A:64:TRP:CH2	1:A:73:LYS:HG3	0.43	2.48	18	2
1:A:56:ARG:NE	1:A:57:HIS:CE1	0.43	2.87	33	1
1:A:77:GLN:NE2	1:A:80:LYS:HZ3	0.43	2.12	21	1
1:A:45:ASN:N	1:A:45:ASN:ND2	0.43	2.67	35	2
1:A:45:ASN:HD21	1:A:47:LEU:CG	0.43	2.27	39	1
1:A:10:THR:O	1:A:14:TRP:N	0.43	2.43	4	4
1:A:46:GLN:HE21	1:A:49:LEU:HB2	0.43	1.73	22	2
1:A:49:LEU:CD2	1:A:49:LEU:H	0.43	2.26	5	1
1:A:22:ILE:HD11	1:A:47:LEU:HD21	0.43	1.91	6	2
1:A:25:ILE:HD11	1:A:78:TRP:CE3	0.43	2.49	25	3
1:A:30:GLN:O	1:A:32:ASP:N	0.43	2.52	18	2
1:A:46:GLN:O	1:A:50:LEU:CB	0.42	2.67	12	1
1:A:60:MET:HG2	1:A:61:CYS:N	0.42	2.29	36	3
1:A:25:ILE:HD13	1:A:28:ASN:HD21	0.42	1.73	20	1
1:A:46:GLN:O	1:A:46:GLN:HG2	0.42	2.15	7	1
1:A:64:TRP:O	1:A:65:LYS:HB2	0.42	2.13	18	1
1:A:27:GLU:OE1	1:A:28:ASN:N	0.42	2.53	31	1
1:A:46:GLN:O	1:A:50:LEU:HB2	0.42	2.14	24	2
1:A:60:MET:HE1	1:A:70:ILE:HG23	0.42	1.85	13	1
1:A:70:ILE:CG2	1:A:74:LEU:CD1	0.42	2.97	36	1
1:A:25:ILE:O	1:A:31:LYS:N	0.42	2.53	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ARG:NH1	1:A:57:HIS:CE1	0.42	2.88	28	1
1:A:76:GLU:C	1:A:80:LYS:NZ	0.42	2.78	30	1
1:A:46:GLN:NE2	1:A:78:TRP:CZ2	0.42	2.88	2	1
1:A:21:PHE:CE2	1:A:54:LEU:CD1	0.42	3.02	6	1
1:A:15:ASN:N	1:A:15:ASN:HD22	0.42	2.11	9	1
1:A:80:LYS:C	1:A:81:ASP:O	0.42	2.62	20	1
1:A:60:MET:SD	1:A:64:TRP:NE1	0.41	2.89	6	1
1:A:30:GLN:NE2	1:A:75:ASN:HA	0.41	2.30	14	1
1:A:30:GLN:CD	1:A:75:ASN:CG	0.41	2.88	14	1
1:A:52:LYS:NZ	1:A:52:LYS:CB	0.41	2.83	12	1
1:A:16:GLN:OE1	1:A:16:GLN:N	0.41	2.53	23	1
1:A:63:LYS:O	1:A:64:TRP:CD2	0.41	2.73	34	1
1:A:31:LYS:HD3	1:A:32:ASP:N	0.41	2.29	34	2
1:A:57:HIS:O	1:A:60:MET:HG2	0.41	2.15	30	1
1:A:27:GLU:C	1:A:27:GLU:OE1	0.41	2.63	31	1
1:A:66:SER:O	1:A:70:ILE:CG1	0.41	2.69	36	1
1:A:45:ASN:O	1:A:46:GLN:HG3	0.41	2.14	5	2
1:A:18:LYS:HD2	1:A:51:HIS:ND1	0.41	2.30	16	1
1:A:45:ASN:C	1:A:46:GLN:HG3	0.41	2.40	2	1
1:A:69:ASP:O	1:A:73:LYS:HD3	0.41	2.15	28	1
1:A:14:TRP:CD1	1:A:18:LYS:NZ	0.41	2.80	2	1
1:A:30:GLN:O	1:A:31:LYS:C	0.41	2.62	16	1
1:A:22:ILE:CD1	1:A:47:LEU:HD21	0.41	2.46	32	1
1:A:8:LYS:NZ	1:A:8:LYS:HB3	0.41	2.31	35	1
1:A:25:ILE:HD13	1:A:78:TRP:CH2	0.41	2.50	23	1
1:A:30:GLN:NE2	1:A:75:ASN:CB	0.41	2.83	24	1
1:A:30:GLN:OE1	1:A:75:ASN:CB	0.41	2.68	29	1
1:A:56:ARG:CD	1:A:56:ARG:C	0.41	2.94	31	1
1:A:63:LYS:O	1:A:64:TRP:CG	0.41	2.73	34	1
1:A:73:LYS:NZ	1:A:73:LYS:HA	0.41	2.31	34	1
1:A:25:ILE:HD11	1:A:78:TRP:CH2	0.41	2.51	10	1
1:A:61:CYS:O	1:A:65:LYS:CB	0.41	2.69	36	1
1:A:26:LEU:HG	1:A:27:GLU:N	0.41	2.31	10	1
1:A:14:TRP:O	1:A:18:LYS:HG3	0.41	2.16	27	1
1:A:60:MET:HB2	1:A:64:TRP:NE1	0.41	2.31	36	1
1:A:45:ASN:O	1:A:46:GLN:HB2	0.40	2.16	4	1
1:A:19:GLN:HA	1:A:19:GLN:NE2	0.40	2.30	37	2
1:A:22:ILE:HG12	1:A:50:LEU:CD1	0.40	2.46	19	1
1:A:79:ASN:ND2	1:A:79:ASN:N	0.40	2.67	24	1
1:A:60:MET:O	1:A:63:LYS:HG3	0.40	2.16	22	1
1:A:78:TRP:CD1	1:A:81:ASP:OD2	0.40	2.74	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PHE:CD2	1:A:74:LEU:HD22	0.40	2.51	8	1
1:A:25:ILE:HA	1:A:28:ASN:ND2	0.40	2.32	10	1
1:A:21:PHE:N	1:A:21:PHE:CD1	0.40	2.89	29	1
1:A:20:ASP:CG	1:A:67:LYS:NZ	0.40	2.78	2	1
1:A:17:LEU:HG	1:A:21:PHE:CE2	0.40	2.52	17	1
1:A:75:ASN:N	1:A:75:ASN:HD22	0.40	2.15	18	1
1:A:66:SER:OG	1:A:69:ASP:HB3	0.40	2.17	21	1
1:A:22:ILE:HD13	1:A:47:LEU:CD2	0.40	2.47	37	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	64/81 (79%)	59±1 (93±2%)	3±1 (5±2%)	2±1 (2±1%)	7	44
All	All	2496/3159 (79%)	2310 (93%)	126 (5%)	60 (2%)	7	44

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	64	TRP	26
1	A	65	LYS	12
1	A	30	GLN	10
1	A	45	ASN	8
1	A	8	LYS	2
1	A	67	LYS	1
1	A	31	LYS	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	63/77 (82%)	58±2 (92±3%)	5±2 (8±3%)	12 59
All	All	2457/3003 (82%)	2251 (92%)	206 (8%)	12 59

All 31 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	26	LEU	38
1	A	64	TRP	37
1	A	34	VAL	18
1	A	19	GLN	17
1	A	50	LEU	15
1	A	16	GLN	14
1	A	46	GLN	9
1	A	31	LYS	6
1	A	73	LYS	6
1	A	65	LYS	4
1	A	63	LYS	4
1	A	71	LEU	3
1	A	28	ASN	3
1	A	33	LEU	3
1	A	77	GLN	3
1	A	45	ASN	3
1	A	69	ASP	2
1	A	52	LYS	2
1	A	30	GLN	2
1	A	8	LYS	2
1	A	56	ARG	2
1	A	80	LYS	2
1	A	67	LYS	2
1	A	79	ASN	2
1	A	32	ASP	1
1	A	81	ASP	1
1	A	76	GLU	1
1	A	62	GLU	1
1	A	49	LEU	1
1	A	59	ASP	1
1	A	25	ILE	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 92% for the well-defined parts and 92% 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	1063
Number of shifts mapped to atoms	1063
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	-0.82 ± 0.12	Should be checked
$^{13}\text{C}_\beta$	78	0.13 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	71	-0.66 ± 0.13	Should be applied
^{15}N	78	0.08 ± 0.14	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 92%, i.e. 880 atoms were assigned a chemical shift out of a possible 956. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	322/326 (99%)	131/131 (100%)	126/130 (97%)	65/65 (100%)
Sidechain	488/538 (91%)	330/339 (97%)	147/174 (84%)	11/25 (44%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	70/92 (76%)	35/46 (76%)	31/36 (86%)	4/10 (40%)
Overall	880/956 (92%)	496/516 (96%)	304/340 (89%)	80/100 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1063 atoms were assigned a chemical shift out of a possible 1154. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	389/404 (96%)	160/163 (98%)	151/162 (93%)	78/79 (99%)
Sidechain	604/658 (92%)	409/418 (98%)	182/212 (86%)	13/28 (46%)
Aromatic	70/92 (76%)	35/46 (76%)	31/36 (86%)	4/10 (40%)
Overall	1063/1154 (92%)	604/627 (96%)	364/410 (89%)	95/117 (81%)

7.1.4 Statistically unusual chemical shifts ⓘ

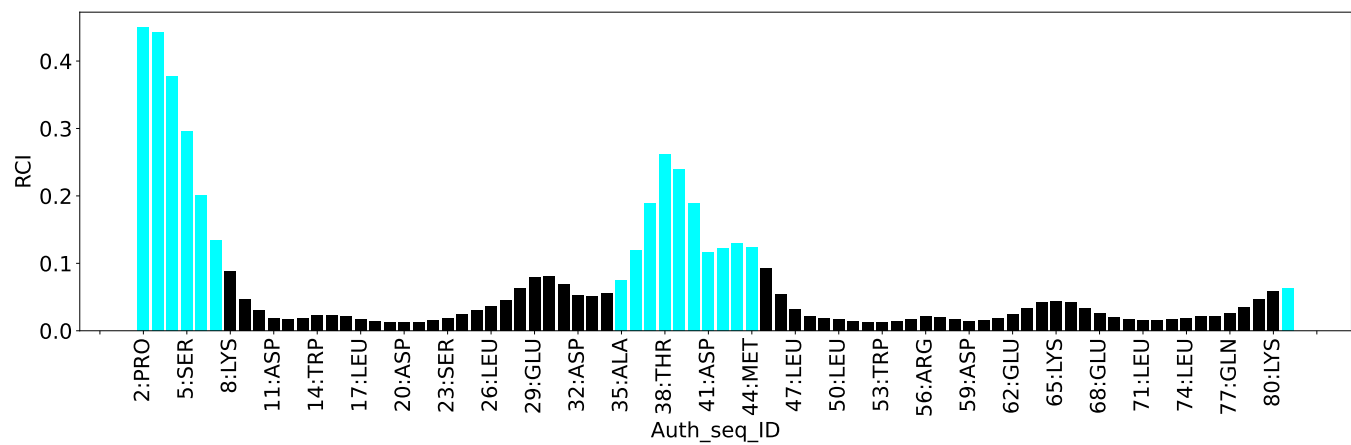
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	58	ARG	HD2	1.48	1.97 – 4.26	-7.2
1	A	58	ARG	HG2	-0.17	0.26 – 2.87	-6.7

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2294
Intra-residue ($ i-j =0$)	768
Sequential ($ i-j =1$)	512
Medium range ($ i-j >1$ and $ i-j <5$)	622
Long range ($ i-j \geq 5$)	392
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	138
Number of unmapped restraints	0
Number of restraints per residue	30.0
Number of long range restraints per residue ¹	4.8

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)	23.2	0.2
0.2-0.5 (Medium)	3.9	0.39
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	6.3	4.52
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

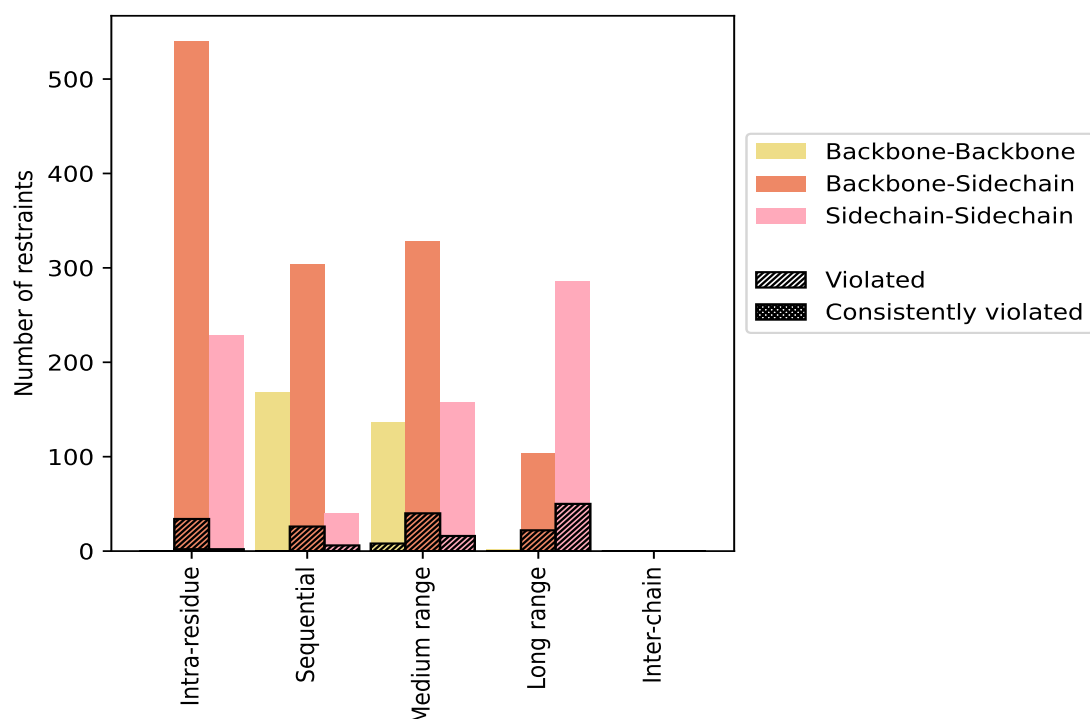
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	768	33.5	36	4.7	1.6	2	0.3	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	540	23.5	34	6.3	1.5	2	0.4	0.1
Sidechain-Sidechain	228	9.9	2	0.9	0.1	0	0.0	0.0
Sequential ($i-j =1$)	512	22.3	32	6.2	1.4	0	0.0	0.0
Backbone-Backbone	168	7.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	304	13.3	26	8.6	1.1	0	0.0	0.0
Sidechain-Sidechain	40	1.7	6	15.0	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	622	27.1	64	10.3	2.8	0	0.0	0.0
Backbone-Backbone	136	5.9	8	5.9	0.3	0	0.0	0.0
Backbone-Sidechain	328	14.3	40	12.2	1.7	0	0.0	0.0
Sidechain-Sidechain	158	6.9	16	10.1	0.7	0	0.0	0.0
Long range ($i-j \geq 5$)	392	17.1	72	18.4	3.1	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	104	4.5	22	21.2	1.0	0	0.0	0.0
Sidechain-Sidechain	286	12.5	50	17.5	2.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2294	100.0	204	8.9	8.9	2	0.1	0.1
Backbone-Backbone	306	13.3	8	2.6	0.3	0	0.0	0.0
Backbone-Sidechain	1276	55.6	122	9.6	5.3	2	0.2	0.1
Sidechain-Sidechain	712	31.0	74	10.4	3.2	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	4	4	8	8	0	24	0.14	0.2	0.03	0.14
2	2	6	14	8	0	30	0.15	0.26	0.04	0.14
3	4	4	10	10	0	28	0.14	0.24	0.03	0.14
4	6	6	14	14	0	40	0.15	0.22	0.03	0.14
5	2	8	8	10	0	28	0.16	0.26	0.05	0.14
6	4	4	6	10	0	24	0.16	0.25	0.04	0.15
7	6	6	18	16	0	46	0.14	0.21	0.03	0.13
8	8	6	12	6	0	32	0.16	0.39	0.07	0.14
9	10	4	8	12	0	34	0.15	0.27	0.05	0.12
10	4	4	4	12	0	24	0.15	0.21	0.03	0.15

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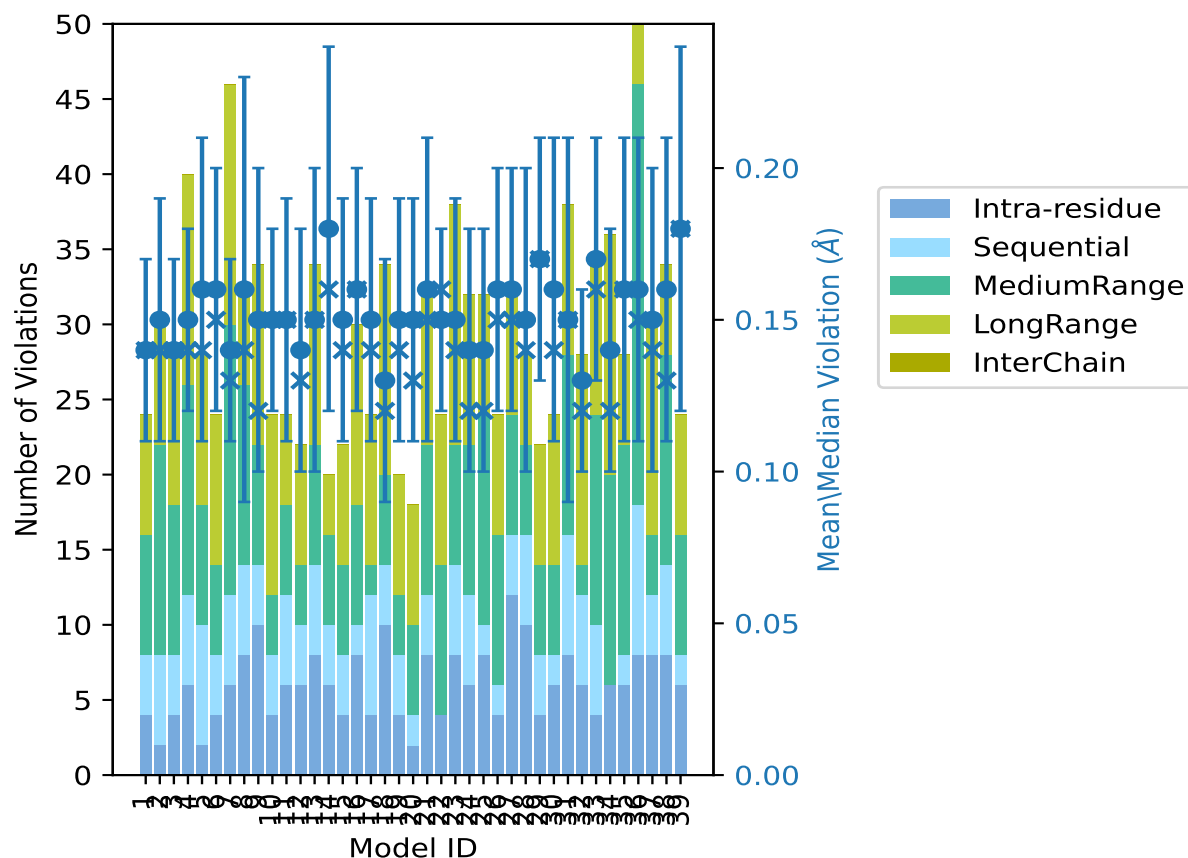
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	6	6	6	6	0	24	0.15	0.23	0.04	0.15
12	6	4	4	8	0	22	0.14	0.22	0.04	0.13
13	8	6	8	12	0	34	0.15	0.31	0.05	0.15
14	6	4	6	4	0	20	0.18	0.28	0.06	0.16
15	4	4	6	8	0	22	0.15	0.23	0.04	0.14
16	8	2	8	12	0	30	0.16	0.24	0.04	0.16
17	4	8	2	10	0	24	0.15	0.23	0.04	0.14
18	10	4	6	14	0	34	0.13	0.24	0.04	0.12
19	4	4	4	8	0	20	0.15	0.21	0.04	0.14
20	2	2	6	8	0	18	0.15	0.2	0.04	0.13
21	8	4	10	10	0	32	0.16	0.27	0.05	0.15
22	4	0	10	10	0	24	0.15	0.21	0.03	0.16
23	8	6	8	16	0	38	0.15	0.23	0.04	0.14
24	6	6	10	10	0	32	0.14	0.22	0.04	0.12
25	8	2	14	8	0	32	0.14	0.25	0.04	0.12
26	4	2	10	8	0	24	0.16	0.23	0.04	0.15
27	12	4	8	8	0	32	0.16	0.23	0.04	0.15
28	10	6	6	6	0	28	0.15	0.28	0.05	0.14
29	4	4	6	8	0	22	0.17	0.22	0.04	0.17
30	6	2	6	10	0	24	0.16	0.3	0.05	0.14
31	8	8	12	10	0	38	0.15	0.37	0.06	0.15
32	6	6	2	14	0	28	0.13	0.2	0.03	0.12
33	4	6	14	10	0	34	0.17	0.27	0.04	0.16
34	6	0	14	16	0	36	0.14	0.26	0.04	0.12
35	6	2	14	6	0	28	0.16	0.26	0.05	0.16
36	8	10	28	4	0	50	0.16	0.26	0.05	0.15
37	8	4	4	14	0	30	0.15	0.3	0.05	0.14
38	8	6	14	6	0	34	0.16	0.27	0.05	0.13
39	6	2	8	8	0	24	0.18	0.27	0.06	0.18

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, 2090(IR:732, SQ:480, MR:558, LR:320, 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	%
14	14	12	20	0	60	1	2.6
4	0	14	4	0	22	2	5.1
4	2	2	10	0	18	3	7.7
2	0	8	8	0	18	4	10.3
2	2	8	2	0	14	5	12.8
0	2	2	6	0	10	6	15.4

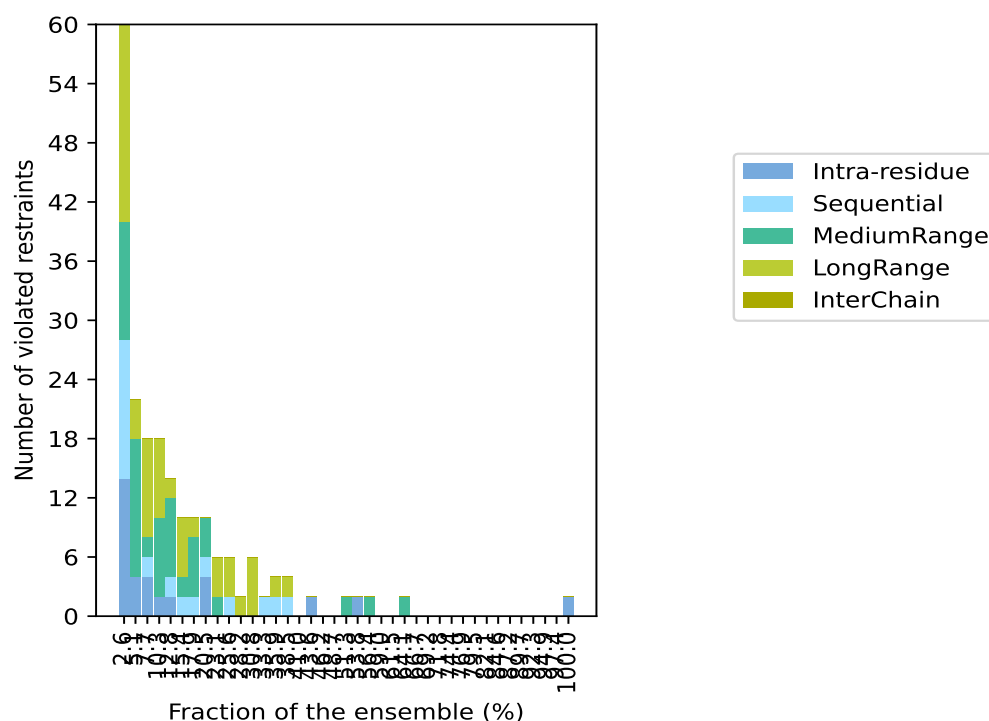
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	2	6	2	0	10	7	17.9
4	2	4	0	0	10	8	20.5
0	0	2	4	0	6	9	23.1
0	2	0	4	0	6	10	25.6
0	0	0	2	0	2	11	28.2
0	0	0	6	0	6	12	30.8
0	2	0	0	0	2	13	33.3
0	2	0	2	0	4	14	35.9
0	2	0	2	0	4	15	38.5
0	0	0	0	0	0	16	41.0
2	0	0	0	0	2	17	43.6
0	0	0	0	0	0	18	46.2
0	0	0	0	0	0	19	48.7
0	0	2	0	0	2	20	51.3
2	0	0	0	0	2	21	53.8
0	0	2	0	0	2	22	56.4
0	0	0	0	0	0	23	59.0
0	0	0	0	0	0	24	61.5
0	0	2	0	0	2	25	64.1
0	0	0	0	0	0	26	66.7
0	0	0	0	0	0	27	69.2
0	0	0	0	0	0	28	71.8
0	0	0	0	0	0	29	74.4
0	0	0	0	0	0	30	76.9
0	0	0	0	0	0	31	79.5
0	0	0	0	0	0	32	82.1
0	0	0	0	0	0	33	84.6
0	0	0	0	0	0	34	87.2
0	0	0	0	0	0	35	89.7
0	0	0	0	0	0	36	92.3
0	0	0	0	0	0	37	94.9
0	0	0	0	0	0	38	97.4
2	0	0	0	0	2	39	100.0

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

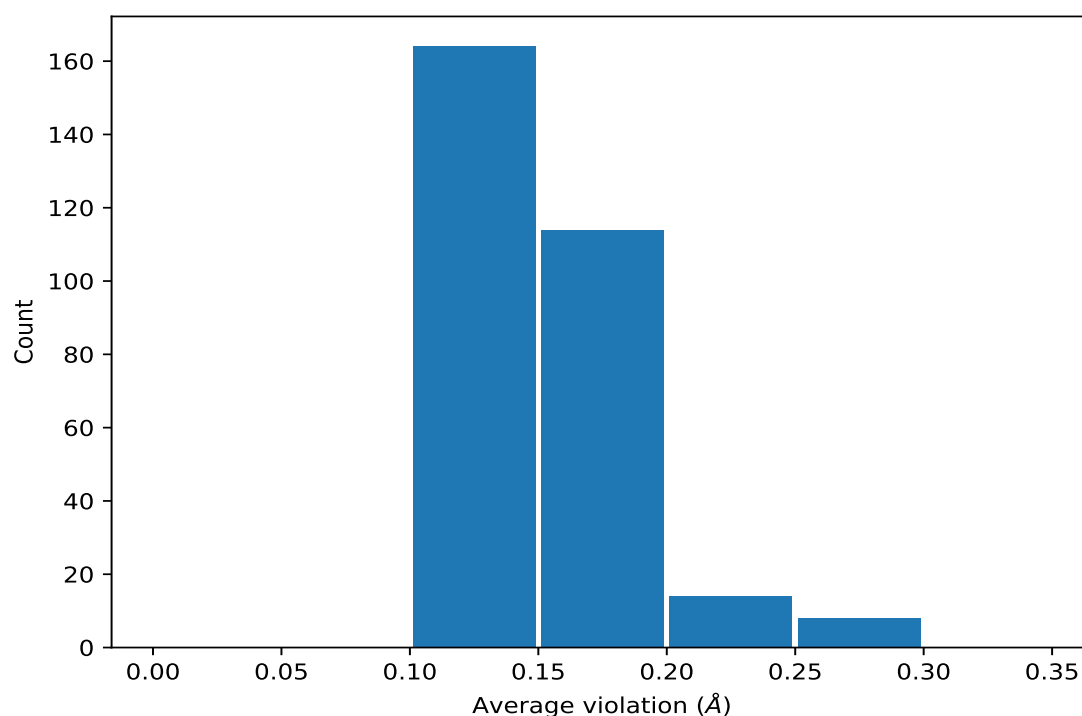
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	39	0.22	0.02	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	39	0.22	0.02	0.21
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	25	0.14	0.03	0.14
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	25	0.14	0.03	0.14
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	22	0.16	0.03	0.16
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	22	0.16	0.03	0.16
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	21	0.14	0.03	0.13
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	21	0.14	0.03	0.13
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	20	0.15	0.03	0.15
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	20	0.15	0.03	0.15
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	20	0.15	0.03	0.15
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	20	0.15	0.03	0.15
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	20	0.15	0.03	0.15
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	20	0.15	0.03	0.15
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	17	0.22	0.07	0.21
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	17	0.22	0.07	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	17	0.22	0.07	0.21
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	17	0.22	0.07	0.21
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	15	0.17	0.04	0.18
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	15	0.17	0.04	0.18
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	15	0.17	0.04	0.18
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	15	0.17	0.04	0.18
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	15	0.13	0.02	0.14
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	15	0.13	0.02	0.14
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	14	0.15	0.03	0.15
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	14	0.15	0.03	0.15
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	14	0.15	0.03	0.15
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	14	0.15	0.03	0.15
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	14	0.15	0.03	0.15
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	14	0.15	0.03	0.15
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	14	0.13	0.02	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	14	0.13	0.02	0.12
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	13	0.12	0.02	0.12
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	13	0.12	0.02	0.12
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	12	0.16	0.05	0.14
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	12	0.16	0.05	0.14
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	12	0.16	0.05	0.14
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	12	0.15	0.04	0.15
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	12	0.15	0.04	0.15
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	12	0.15	0.04	0.15
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	12	0.15	0.04	0.15
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	12	0.15	0.04	0.15
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	12	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	12	0.15	0.04	0.15
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	12	0.15	0.04	0.15
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	12	0.15	0.04	0.15
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	12	0.15	0.04	0.15
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	12	0.14	0.03	0.13
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	12	0.14	0.03	0.13
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	12	0.14	0.03	0.13
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	12	0.14	0.03	0.13
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	12	0.14	0.03	0.13
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	12	0.14	0.03	0.13
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	11	0.12	0.01	0.12
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	11	0.12	0.01	0.12
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	10	0.17	0.04	0.17
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	10	0.17	0.04	0.17
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	10	0.17	0.04	0.17
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	10	0.17	0.04	0.17
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	10	0.17	0.04	0.17
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	10	0.17	0.04	0.17
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	10	0.17	0.04	0.17
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	10	0.17	0.04	0.17
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	10	0.16	0.05	0.16
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	10	0.16	0.05	0.16
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	10	0.16	0.05	0.16
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	10	0.16	0.05	0.16
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	10	0.16	0.05	0.16
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	10	0.16	0.05	0.16
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	10	0.13	0.02	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	10	0.13	0.02	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	10	0.13	0.02	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	10	0.13	0.02	0.12
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	9	0.15	0.05	0.13
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	9	0.15	0.05	0.13
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	9	0.14	0.05	0.12
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	9	0.14	0.05	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	9	0.14	0.04	0.12
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	9	0.14	0.04	0.12
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	9	0.14	0.04	0.12
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	9	0.14	0.04	0.12
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	9	0.14	0.04	0.12
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	9	0.14	0.04	0.12
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	8	0.16	0.05	0.16
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	8	0.16	0.05	0.16
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	8	0.16	0.04	0.16
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	8	0.16	0.04	0.16
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	8	0.15	0.02	0.16
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	8	0.15	0.02	0.16
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	8	0.15	0.02	0.16
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	8	0.15	0.02	0.16
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	8	0.14	0.02	0.15
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	8	0.14	0.02	0.15
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	8	0.14	0.03	0.14
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	8	0.14	0.03	0.14
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	7	0.16	0.05	0.17
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	7	0.16	0.05	0.17
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	7	0.16	0.04	0.15
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	7	0.16	0.04	0.15
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	7	0.14	0.02	0.13
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	7	0.14	0.02	0.13
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	7	0.14	0.02	0.13
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	7	0.14	0.02	0.13
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	7	0.13	0.02	0.13
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	7	0.13	0.02	0.13
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	7	0.13	0.02	0.12
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	7	0.13	0.02	0.12
(1,779)	1:33:A:LEU:HB2	1:34:A:VAL:H	6	0.2	0.02	0.19
(1,1926)	1:33:A:LEU:HB2	1:34:A:VAL:H	6	0.2	0.02	0.19
(1,193)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	6	0.16	0.04	0.17
(1,193)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	6	0.16	0.04	0.17
(1,193)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	6	0.16	0.04	0.17
(1,1340)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	6	0.16	0.04	0.17
(1,1340)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	6	0.16	0.04	0.17
(1,1340)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	6	0.16	0.04	0.17
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	6	0.14	0.01	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	6	0.14	0.01	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	6	0.14	0.01	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	6	0.14	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	6	0.14	0.01	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	6	0.14	0.01	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	6	0.14	0.01	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	6	0.14	0.01	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	6	0.14	0.01	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	6	0.14	0.01	0.15
(1,804)	1:37:A:LEU:HD21	1:49:A:LEU:H	6	0.14	0.02	0.15
(1,804)	1:37:A:LEU:HD22	1:49:A:LEU:H	6	0.14	0.02	0.15
(1,804)	1:37:A:LEU:HD23	1:49:A:LEU:H	6	0.14	0.02	0.15
(1,1951)	1:37:A:LEU:HD21	1:49:A:LEU:H	6	0.14	0.02	0.15
(1,1951)	1:37:A:LEU:HD22	1:49:A:LEU:H	6	0.14	0.02	0.15
(1,1951)	1:37:A:LEU:HD23	1:49:A:LEU:H	6	0.14	0.02	0.15
(1,541)	1:10:A:THR:HB	1:13:A:GLU:H	6	0.14	0.01	0.14
(1,1688)	1:10:A:THR:HB	1:13:A:GLU:H	6	0.14	0.01	0.14
(1,200)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	5	0.16	0.07	0.13
(1,1347)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	5	0.16	0.07	0.13
(1,754)	1:28:A:ASN:HD22	1:30:A:GLN:H	5	0.14	0.03	0.12
(1,1901)	1:28:A:ASN:HD22	1:30:A:GLN:H	5	0.14	0.03	0.12
(1,567)	1:13:A:GLU:H	1:14:A:TRP:HB3	5	0.13	0.01	0.13
(1,1714)	1:13:A:GLU:H	1:14:A:TRP:HB3	5	0.13	0.01	0.13
(1,619)	1:15:A:ASN:H	1:18:A:LYS:HE2	5	0.13	0.01	0.13
(1,708)	1:21:A:PHE:HE1	1:74:A:LEU:H	5	0.13	0.01	0.12
(1,708)	1:21:A:PHE:HE2	1:74:A:LEU:H	5	0.13	0.01	0.12
(1,1766)	1:15:A:ASN:H	1:18:A:LYS:HE2	5	0.13	0.01	0.13
(1,1855)	1:21:A:PHE:HE1	1:74:A:LEU:H	5	0.13	0.01	0.12
(1,1855)	1:21:A:PHE:HE2	1:74:A:LEU:H	5	0.13	0.01	0.12
(1,538)	1:10:A:THR:HB	1:12:A:ASP:H	5	0.11	0.0	0.11
(1,1685)	1:10:A:THR:HB	1:12:A:ASP:H	5	0.11	0.0	0.11
(1,1117)	1:77:A:GLN:HB3	1:77:A:GLN:H	5	0.11	0.01	0.11
(1,2264)	1:77:A:GLN:HB3	1:77:A:GLN:H	5	0.11	0.01	0.11
(1,828)	1:44:A:MET:HG2	1:44:A:MET:H	4	0.18	0.03	0.16
(1,1975)	1:44:A:MET:HG2	1:44:A:MET:H	4	0.18	0.03	0.16
(1,841)	1:45:A:ASN:HA	1:47:A:LEU:H	4	0.16	0.03	0.15
(1,1988)	1:45:A:ASN:HA	1:47:A:LEU:H	4	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	4	0.15	0.03	0.15
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	4	0.15	0.03	0.15
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	4	0.15	0.03	0.15
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	4	0.15	0.03	0.15
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	4	0.15	0.03	0.15
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	4	0.15	0.03	0.15
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	4	0.15	0.03	0.15
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	4	0.15	0.03	0.15
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	4	0.15	0.03	0.15
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	4	0.15	0.03	0.15
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	4	0.15	0.03	0.15
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	4	0.15	0.03	0.15
(1,118)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	4	0.14	0.01	0.15
(1,1265)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	4	0.14	0.01	0.15
(1,266)	1:34:A:VAL:HG21	1:38:A:THR:HB	4	0.13	0.02	0.12
(1,266)	1:34:A:VAL:HG22	1:38:A:THR:HB	4	0.13	0.02	0.12
(1,266)	1:34:A:VAL:HG23	1:38:A:THR:HB	4	0.13	0.02	0.12
(1,1413)	1:34:A:VAL:HG21	1:38:A:THR:HB	4	0.13	0.02	0.12
(1,1413)	1:34:A:VAL:HG22	1:38:A:THR:HB	4	0.13	0.02	0.12
(1,1413)	1:34:A:VAL:HG23	1:38:A:THR:HB	4	0.13	0.02	0.12
(1,267)	1:34:A:VAL:HG21	1:47:A:LEU:HA	4	0.12	0.02	0.12
(1,267)	1:34:A:VAL:HG22	1:47:A:LEU:HA	4	0.12	0.02	0.12
(1,267)	1:34:A:VAL:HG23	1:47:A:LEU:HA	4	0.12	0.02	0.12
(1,1414)	1:34:A:VAL:HG21	1:47:A:LEU:HA	4	0.12	0.02	0.12
(1,1414)	1:34:A:VAL:HG22	1:47:A:LEU:HA	4	0.12	0.02	0.12
(1,1414)	1:34:A:VAL:HG23	1:47:A:LEU:HA	4	0.12	0.02	0.12
(1,531)	1:9:A:PHE:HB3	1:58:A:ARG:HE	4	0.12	0.02	0.12
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD2	4	0.12	0.02	0.12
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD3	4	0.12	0.02	0.12
(1,1678)	1:9:A:PHE:HB3	1:58:A:ARG:HE	4	0.12	0.02	0.12
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD2	4	0.12	0.02	0.12
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD3	4	0.12	0.02	0.12
(1,834)	1:44:A:MET:HG2	1:47:A:LEU:H	4	0.12	0.01	0.12
(1,834)	1:44:A:MET:HG3	1:47:A:LEU:H	4	0.12	0.01	0.12
(1,1981)	1:44:A:MET:HG2	1:47:A:LEU:H	4	0.12	0.01	0.12
(1,1981)	1:44:A:MET:HG3	1:47:A:LEU:H	4	0.12	0.01	0.12
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB2	3	0.26	0.04	0.26
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB3	3	0.26	0.04	0.26
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB2	3	0.26	0.04	0.26
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB3	3	0.26	0.04	0.26
(1,1092)	1:73:A:LYS:HD2	1:77:A:GLN:H	3	0.25	0.03	0.27
(1,1092)	1:73:A:LYS:HD3	1:77:A:GLN:H	3	0.25	0.03	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2239)	1:73:A:LYS:HD2	1:77:A:GLN:H	3	0.25	0.03	0.27
(1,2239)	1:73:A:LYS:HD3	1:77:A:GLN:H	3	0.25	0.03	0.27
(1,783)	1:34:A:VAL:HG11	1:34:A:VAL:H	3	0.23	0.06	0.27
(1,783)	1:34:A:VAL:HG12	1:34:A:VAL:H	3	0.23	0.06	0.27
(1,783)	1:34:A:VAL:HG13	1:34:A:VAL:H	3	0.23	0.06	0.27
(1,1930)	1:34:A:VAL:HG11	1:34:A:VAL:H	3	0.23	0.06	0.27
(1,1930)	1:34:A:VAL:HG12	1:34:A:VAL:H	3	0.23	0.06	0.27
(1,1930)	1:34:A:VAL:HG13	1:34:A:VAL:H	3	0.23	0.06	0.27
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG21	3	0.13	0.01	0.12
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG22	3	0.13	0.01	0.12
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG23	3	0.13	0.01	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG21	3	0.13	0.01	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG22	3	0.13	0.01	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG23	3	0.13	0.01	0.12
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	3	0.12	0.02	0.11
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	3	0.12	0.02	0.11
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	3	0.12	0.02	0.11
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	3	0.12	0.02	0.11
(1,76)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	3	0.12	0.01	0.13
(1,280)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	3	0.12	0.01	0.12
(1,280)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	3	0.12	0.01	0.12
(1,280)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	3	0.12	0.01	0.12
(1,1223)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	3	0.12	0.01	0.13
(1,1427)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	3	0.12	0.01	0.12
(1,1427)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	3	0.12	0.01	0.12
(1,1427)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	3	0.12	0.01	0.12
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	3	0.11	0.02	0.1
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	3	0.11	0.02	0.1
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	3	0.11	0.02	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	3	0.11	0.02	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	3	0.11	0.02	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	3	0.11	0.02	0.1
(1,1063)	1:71:A:LEU:HB3	1:71:A:LEU:H	3	0.11	0.01	0.11
(1,2210)	1:71:A:LEU:HB3	1:71:A:LEU:H	3	0.11	0.01	0.11
(1,1147)	1:81:A:ASP:HB2	1:81:A:ASP:H	2	0.17	0.03	0.17
(1,2294)	1:81:A:ASP:HB2	1:81:A:ASP:H	2	0.17	0.03	0.17
(1,767)	1:31:A:LYS:HG2	1:34:A:VAL:H	2	0.16	0.05	0.16
(1,767)	1:31:A:LYS:HG3	1:34:A:VAL:H	2	0.16	0.05	0.16
(1,1914)	1:31:A:LYS:HG2	1:34:A:VAL:H	2	0.16	0.05	0.16
(1,1914)	1:31:A:LYS:HG3	1:34:A:VAL:H	2	0.16	0.05	0.16
(1,1017)	1:64:A:TRP:HE1	1:60:A:MET:HG3	2	0.15	0.04	0.15
(1,2164)	1:64:A:TRP:HE1	1:60:A:MET:HG3	2	0.15	0.04	0.15

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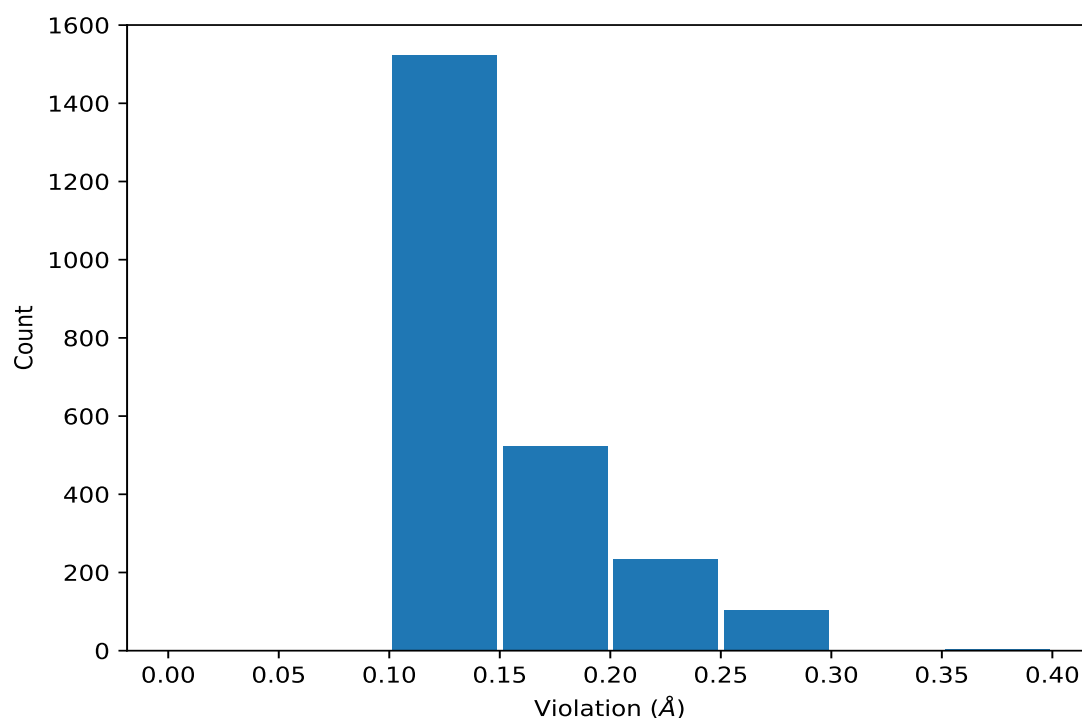
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE1	2	0.13	0.02	0.13
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE2	2	0.13	0.02	0.13
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE3	2	0.13	0.02	0.13
(1,803)	1:37:A:LEU:HG	1:46:A:GLN:HE21	2	0.13	0.01	0.13
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE1	2	0.13	0.02	0.13
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE2	2	0.13	0.02	0.13
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE3	2	0.13	0.02	0.13
(1,1950)	1:37:A:LEU:HG	1:46:A:GLN:HE21	2	0.13	0.01	0.13
(1,827)	1:43:A:ILE:HA	1:45:A:ASN:H	2	0.12	0.02	0.12
(1,962)	1:58:A:ARG:HG3	1:58:A:ARG:H	2	0.12	0.02	0.12
(1,1974)	1:43:A:ILE:HA	1:45:A:ASN:H	2	0.12	0.02	0.12
(1,2109)	1:58:A:ARG:HG3	1:58:A:ARG:H	2	0.12	0.02	0.12
(1,121)	1:18:A:LYS:HD2	1:51:A:HIS:HD2	2	0.12	0.0	0.12
(1,121)	1:18:A:LYS:HD3	1:51:A:HIS:HD2	2	0.12	0.0	0.12
(1,1268)	1:18:A:LYS:HD2	1:51:A:HIS:HD2	2	0.12	0.0	0.12
(1,1268)	1:18:A:LYS:HD3	1:51:A:HIS:HD2	2	0.12	0.0	0.12
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE1	2	0.11	0.01	0.11
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE2	2	0.11	0.01	0.11
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE3	2	0.11	0.01	0.11
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE1	2	0.11	0.01	0.11
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE2	2	0.11	0.01	0.11
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE3	2	0.11	0.01	0.11
(1,678)	1:19:A:GLN:H	1:22:A:ILE:HB	2	0.11	0.01	0.11
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE1	2	0.11	0.01	0.11
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE2	2	0.11	0.01	0.11
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE3	2	0.11	0.01	0.11
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE1	2	0.11	0.01	0.11
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE2	2	0.11	0.01	0.11
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE3	2	0.11	0.01	0.11
(1,1825)	1:19:A:GLN:H	1:22:A:ILE:HB	2	0.11	0.01	0.11
(1,818)	1:41:A:ASP:HB3	1:43:A:ILE:H	2	0.11	0.0	0.11
(1,1965)	1:41:A:ASP:HB3	1:43:A:ILE:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	8	0.39
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	8	0.39
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	31	0.37
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	31	0.37
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	13	0.31
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	13	0.31
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB2	37	0.3
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB3	37	0.3
(1,1347)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	30	0.3
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB2	37	0.3
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB3	37	0.3
(1,200)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	30	0.3
(1,2239)	1:73:A:LYS:HD2	1:77:A:GLN:H	28	0.28
(1,2239)	1:73:A:LYS:HD3	1:77:A:GLN:H	28	0.28
(1,1930)	1:34:A:VAL:HG11	1:34:A:VAL:H	14	0.28
(1,1930)	1:34:A:VAL:HG12	1:34:A:VAL:H	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1930)	1:34:A:VAL:HG13	1:34:A:VAL:H	14	0.28
(1,1092)	1:73:A:LYS:HD2	1:77:A:GLN:H	28	0.28
(1,1092)	1:73:A:LYS:HD3	1:77:A:GLN:H	28	0.28
(1,783)	1:34:A:VAL:HG11	1:34:A:VAL:H	14	0.28
(1,783)	1:34:A:VAL:HG12	1:34:A:VAL:H	14	0.28
(1,783)	1:34:A:VAL:HG13	1:34:A:VAL:H	14	0.28
(1,2239)	1:73:A:LYS:HD2	1:77:A:GLN:H	39	0.27
(1,2239)	1:73:A:LYS:HD3	1:77:A:GLN:H	39	0.27
(1,1930)	1:34:A:VAL:HG11	1:34:A:VAL:H	38	0.27
(1,1930)	1:34:A:VAL:HG12	1:34:A:VAL:H	38	0.27
(1,1930)	1:34:A:VAL:HG13	1:34:A:VAL:H	38	0.27
(1,1908)	1:30:A:GLN:HG2	1:30:A:GLN:H	9	0.27
(1,1908)	1:30:A:GLN:HG3	1:30:A:GLN:H	9	0.27
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	39	0.27
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	33	0.27
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	21	0.27
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	21	0.27
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	21	0.27
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	21	0.27
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	21	0.27
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	21	0.27
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	21	0.27
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	21	0.27
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	21	0.27
(1,1092)	1:73:A:LYS:HD2	1:77:A:GLN:H	39	0.27
(1,1092)	1:73:A:LYS:HD3	1:77:A:GLN:H	39	0.27
(1,783)	1:34:A:VAL:HG11	1:34:A:VAL:H	38	0.27
(1,783)	1:34:A:VAL:HG12	1:34:A:VAL:H	38	0.27
(1,783)	1:34:A:VAL:HG13	1:34:A:VAL:H	38	0.27
(1,761)	1:30:A:GLN:HG2	1:30:A:GLN:H	9	0.27
(1,761)	1:30:A:GLN:HG3	1:30:A:GLN:H	9	0.27
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	39	0.27
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	33	0.27
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	21	0.27
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	21	0.27
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	21	0.27
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	21	0.27
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	21	0.27
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	21	0.27
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	21	0.27
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	21	0.27
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	21	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	34	0.26
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB2	5	0.26
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB3	5	0.26
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	2	0.26
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	36	0.26
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	35	0.26
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	35	0.26
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	35	0.26
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	35	0.26
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	35	0.26
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	35	0.26
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	35	0.26
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	35	0.26
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	35	0.26
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	34	0.26
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB2	5	0.26
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB3	5	0.26
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	2	0.26
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	36	0.26
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	35	0.26
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	35	0.26
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	35	0.26
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	35	0.26
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	35	0.26
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	35	0.26
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	35	0.26
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	35	0.26
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	35	0.26
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	14	0.25
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	6	0.25
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	25	0.25
(1,1926)	1:33:A:LEU:HB2	1:34:A:VAL:H	9	0.25
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	35	0.25
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	36	0.25
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	33	0.25
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	33	0.25
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	33	0.25
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	38	0.25
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	38	0.25
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	38	0.25
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	14	0.25
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	25	0.25
(1,779)	1:33:A:LEU:HB2	1:34:A:VAL:H	9	0.25
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	35	0.25
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	36	0.25
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	33	0.25
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	33	0.25
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	33	0.25
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	38	0.25
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	38	0.25
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	38	0.25
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	3	0.24
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	8	0.24
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	16	0.24
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	18	0.24
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	18	0.24
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	18	0.24
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	3	0.24
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	8	0.24
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	16	0.24
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	18	0.24
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	18	0.24
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	18	0.24
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	21	0.23
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	23	0.23
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	14	0.23
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	36	0.23
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	27	0.23
(1,1975)	1:44:A:MET:HG2	1:44:A:MET:H	39	0.23
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	23	0.23
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	23	0.23
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	27	0.23
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	27	0.23
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	9	0.23
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	11	0.23
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	17	0.23
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	5	0.23
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	5	0.23
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	5	0.23
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	5	0.23
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	5	0.23
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	5	0.23
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	5	0.23
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	5	0.23
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	15	0.23
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	15	0.23
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	15	0.23
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	15	0.23
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	26	0.23
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	26	0.23
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	26	0.23
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	26	0.23
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	26	0.23
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	26	0.23
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	26	0.23
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	26	0.23
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	26	0.23
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	21	0.23
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	23	0.23
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	14	0.23
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	36	0.23
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	27	0.23
(1,828)	1:44:A:MET:HG2	1:44:A:MET:H	39	0.23
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	23	0.23
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	23	0.23
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	27	0.23
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	27	0.23
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	9	0.23
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	11	0.23
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	17	0.23
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	5	0.23
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	5	0.23
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	5	0.23
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	5	0.23
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	5	0.23
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	5	0.23
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	5	0.23
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	5	0.23
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	5	0.23
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	15	0.23
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	15	0.23
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	15	0.23
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	15	0.23
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	26	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	26	0.23
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	26	0.23
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	26	0.23
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	26	0.23
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	26	0.23
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	26	0.23
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	26	0.23
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	26	0.23
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	24	0.22
(1,2186)	1:68:A:GLU:HG2	1:68:A:GLU:H	29	0.22
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	36	0.22
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	39	0.22
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	39	0.22
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	39	0.22
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	39	0.22
(1,1988)	1:45:A:ASN:HA	1:47:A:LEU:H	2	0.22
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	36	0.22
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	12	0.22
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	12	0.22
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	4	0.22
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	23	0.22
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	24	0.22
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	30	0.22
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	24	0.22
(1,1039)	1:68:A:GLU:HG2	1:68:A:GLU:H	29	0.22
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	36	0.22
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	39	0.22
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	39	0.22
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	39	0.22
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	39	0.22
(1,841)	1:45:A:ASN:HA	1:47:A:LEU:H	2	0.22
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	36	0.22
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	12	0.22
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	12	0.22
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	4	0.22
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	23	0.22
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	24	0.22
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	30	0.22
(1,2239)	1:73:A:LYS:HD2	1:77:A:GLN:H	33	0.21
(1,2239)	1:73:A:LYS:HD3	1:77:A:GLN:H	33	0.21
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	10	0.21
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	38	0.21
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	29	0.21
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	29	0.21
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB2	8	0.21
(1,1954)	1:38:A:THR:H	1:39:A:ASN:HB3	8	0.21
(1,1914)	1:31:A:LYS:HG2	1:34:A:VAL:H	36	0.21
(1,1914)	1:31:A:LYS:HG3	1:34:A:VAL:H	36	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	13	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	14	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	18	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	19	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	22	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	25	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	27	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	28	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	29	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	31	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	33	0.21
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	34	0.21
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	7	0.21
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	7	0.21
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	7	0.21
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	7	0.21
(1,1340)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	29	0.21
(1,1340)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	29	0.21
(1,1340)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	29	0.21
(1,1092)	1:73:A:LYS:HD2	1:77:A:GLN:H	33	0.21
(1,1092)	1:73:A:LYS:HD3	1:77:A:GLN:H	33	0.21
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	10	0.21
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	19	0.21
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	38	0.21
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	29	0.21
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	29	0.21
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB2	8	0.21
(1,807)	1:38:A:THR:H	1:39:A:ASN:HB3	8	0.21
(1,767)	1:31:A:LYS:HG2	1:34:A:VAL:H	36	0.21
(1,767)	1:31:A:LYS:HG3	1:34:A:VAL:H	36	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	13	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	14	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	18	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	19	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	22	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	25	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	27	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	28	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	29	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	31	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	33	0.21
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	34	0.21
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	7	0.21
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	7	0.21
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	7	0.21
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	7	0.21
(1,193)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	29	0.21
(1,193)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	29	0.21
(1,193)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	29	0.21
(1,2294)	1:81:A:ASP:HB2	1:81:A:ASP:H	38	0.2
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	12	0.2
(1,2235)	1:73:A:LYS:HD2	1:73:A:LYS:H	27	0.2
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	16	0.2
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	20	0.2
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	13	0.2
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	13	0.2
(1,1926)	1:33:A:LEU:HB2	1:34:A:VAL:H	20	0.2
(1,1901)	1:28:A:ASN:HD22	1:30:A:GLN:H	16	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	1	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	5	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	6	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	12	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	20	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	21	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	26	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	32	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	37	0.2
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	38	0.2
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	7	0.2
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	7	0.2
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	7	0.2
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	7	0.2
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	7	0.2
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	7	0.2
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	11	0.2
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	11	0.2
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	35	0.2
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	35	0.2
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	35	0.2
(1,1147)	1:81:A:ASP:HB2	1:81:A:ASP:H	38	0.2
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	12	0.2
(1,1088)	1:73:A:LYS:HD2	1:73:A:LYS:H	27	0.2
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	16	0.2
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	20	0.2
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	13	0.2
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	13	0.2
(1,779)	1:33:A:LEU:HB2	1:34:A:VAL:H	20	0.2
(1,754)	1:28:A:ASN:HD22	1:30:A:GLN:H	16	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	1	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	5	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	6	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	12	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	20	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	21	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	26	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	32	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	37	0.2
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	38	0.2
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	7	0.2
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	7	0.2
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	7	0.2
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	7	0.2
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	7	0.2
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	7	0.2
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	11	0.2
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	11	0.2
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	11	0.2
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	35	0.2
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	35	0.2
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	35	0.2
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	6	0.19
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	1	0.19
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	37	0.19
(1,2164)	1:64:A:TRP:HE1	1:60:A:MET:HG3	26	0.19
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	35	0.19
(1,2086)	1:56:A:ARG:HB3	1:56:A:ARG:H	23	0.19
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	4	0.19
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1926)	1:33:A:LEU:HB2	1:34:A:VAL:H	4	0.19
(1,1926)	1:33:A:LEU:HB2	1:34:A:VAL:H	29	0.19
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	7	0.19
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	10	0.19
(1,1720)	1:14:A:TRP:HD1	1:14:A:TRP:H	15	0.19
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	17	0.19
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	25	0.19
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	14	0.19
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	14	0.19
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	14	0.19
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	30	0.19
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	30	0.19
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	30	0.19
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	16	0.19
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	16	0.19
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	16	0.19
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	36	0.19
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	36	0.19
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	36	0.19
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	13	0.19
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	13	0.19
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	13	0.19
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	13	0.19
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	39	0.19
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	39	0.19
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	39	0.19
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	39	0.19
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	6	0.19
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	1	0.19
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	37	0.19
(1,1017)	1:64:A:TRP:HE1	1:60:A:MET:HG3	26	0.19
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	35	0.19
(1,939)	1:56:A:ARG:HB3	1:56:A:ARG:H	23	0.19
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	4	0.19
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	4	0.19
(1,779)	1:33:A:LEU:HB2	1:34:A:VAL:H	4	0.19
(1,779)	1:33:A:LEU:HB2	1:34:A:VAL:H	29	0.19
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	7	0.19
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	10	0.19
(1,573)	1:14:A:TRP:HD1	1:14:A:TRP:H	15	0.19
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	17	0.19
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	25	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	14	0.19
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	14	0.19
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	14	0.19
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	30	0.19
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	30	0.19
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	30	0.19
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	16	0.19
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	16	0.19
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	16	0.19
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	36	0.19
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	36	0.19
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	36	0.19
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	13	0.19
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	13	0.19
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	13	0.19
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	13	0.19
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	39	0.19
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	39	0.19
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	39	0.19
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	39	0.19
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	21	0.18
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	27	0.18
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	33	0.18
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	34	0.18
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	6	0.18
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	26	0.18
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	23	0.18
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	11	0.18
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	11	0.18
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	17	0.18
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	17	0.18
(1,1926)	1:33:A:LEU:HB2	1:34:A:VAL:H	6	0.18
(1,1926)	1:33:A:LEU:HB2	1:34:A:VAL:H	36	0.18
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	1	0.18
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	2	0.18
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	35	0.18
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	22	0.18
(1,1633)	1:72:A:HIS:HD2	1:73:A:LYS:HD2	31	0.18
(1,1633)	1:72:A:HIS:HD2	1:73:A:LYS:HD3	31	0.18
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	3	0.18
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	3	0.18
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	5	0.18
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	5	0.18
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	5	0.18
(1,1536)	1:54:A:LEU:HD11	1:74:A:LEU:HD11	15	0.18
(1,1536)	1:54:A:LEU:HD11	1:74:A:LEU:HD12	15	0.18
(1,1536)	1:54:A:LEU:HD11	1:74:A:LEU:HD13	15	0.18
(1,1536)	1:54:A:LEU:HD12	1:74:A:LEU:HD11	15	0.18
(1,1536)	1:54:A:LEU:HD12	1:74:A:LEU:HD12	15	0.18
(1,1536)	1:54:A:LEU:HD12	1:74:A:LEU:HD13	15	0.18
(1,1536)	1:54:A:LEU:HD13	1:74:A:LEU:HD11	15	0.18
(1,1536)	1:54:A:LEU:HD13	1:74:A:LEU:HD12	15	0.18
(1,1536)	1:54:A:LEU:HD13	1:74:A:LEU:HD13	15	0.18
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	35	0.18
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	35	0.18
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	35	0.18
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	17	0.18
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	17	0.18
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	17	0.18
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	17	0.18
(1,1340)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	10	0.18
(1,1340)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	10	0.18
(1,1340)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	10	0.18
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	1	0.18
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	1	0.18
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	1	0.18
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	4	0.18
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	4	0.18
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	4	0.18
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	4	0.18
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	4	0.18
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	4	0.18
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	4	0.18
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	4	0.18
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	4	0.18
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	21	0.18
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	27	0.18
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	33	0.18
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	34	0.18
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	6	0.18
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	26	0.18
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	23	0.18
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	11	0.18
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	17	0.18
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	17	0.18
(1,779)	1:33:A:LEU:HB2	1:34:A:VAL:H	6	0.18
(1,779)	1:33:A:LEU:HB2	1:34:A:VAL:H	36	0.18
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	1	0.18
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	2	0.18
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	35	0.18
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	22	0.18
(1,486)	1:72:A:HIS:HD2	1:73:A:LYS:HD2	31	0.18
(1,486)	1:72:A:HIS:HD2	1:73:A:LYS:HD3	31	0.18
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	3	0.18
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	3	0.18
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	3	0.18
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	5	0.18
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	5	0.18
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	5	0.18
(1,389)	1:54:A:LEU:HD11	1:74:A:LEU:HD11	15	0.18
(1,389)	1:54:A:LEU:HD11	1:74:A:LEU:HD12	15	0.18
(1,389)	1:54:A:LEU:HD11	1:74:A:LEU:HD13	15	0.18
(1,389)	1:54:A:LEU:HD12	1:74:A:LEU:HD11	15	0.18
(1,389)	1:54:A:LEU:HD12	1:74:A:LEU:HD12	15	0.18
(1,389)	1:54:A:LEU:HD12	1:74:A:LEU:HD13	15	0.18
(1,389)	1:54:A:LEU:HD13	1:74:A:LEU:HD11	15	0.18
(1,389)	1:54:A:LEU:HD13	1:74:A:LEU:HD12	15	0.18
(1,389)	1:54:A:LEU:HD13	1:74:A:LEU:HD13	15	0.18
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	35	0.18
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	35	0.18
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	35	0.18
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	17	0.18
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	17	0.18
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	17	0.18
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	17	0.18
(1,193)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	10	0.18
(1,193)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	10	0.18
(1,193)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	10	0.18
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	1	0.18
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	1	0.18
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	1	0.18
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	4	0.18
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	4	0.18
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	4	0.18
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	4	0.18
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	4	0.18
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	4	0.18
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	4	0.18
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	4	0.18
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	5	0.17
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	5	0.17
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	21	0.17
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	21	0.17
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	39	0.17
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	39	0.17
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	32	0.17
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	31	0.17
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	31	0.17
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	8	0.17
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	26	0.17
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	28	0.17
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	21	0.17
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	38	0.17
(1,1975)	1:44:A:MET:HG2	1:44:A:MET:H	11	0.17
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	35	0.17
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	24	0.17
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	24	0.17
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	23	0.17
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	13	0.17
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	19	0.17
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	33	0.17
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	36	0.17
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	7	0.17
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	32	0.17
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	32	0.17
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	32	0.17
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	11	0.17
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	11	0.17
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	11	0.17
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	29	0.17
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	29	0.17
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	29	0.17
(1,1413)	1:34:A:VAL:HG21	1:38:A:THR:HB	15	0.17
(1,1413)	1:34:A:VAL:HG22	1:38:A:THR:HB	15	0.17
(1,1413)	1:34:A:VAL:HG23	1:38:A:THR:HB	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	33	0.17
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	33	0.17
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	33	0.17
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	33	0.17
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	33	0.17
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	33	0.17
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	33	0.17
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	33	0.17
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	33	0.17
(1,1340)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	23	0.17
(1,1340)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	23	0.17
(1,1340)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	23	0.17
(1,1340)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	37	0.17
(1,1340)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	37	0.17
(1,1340)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	37	0.17
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	21	0.17
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	21	0.17
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	21	0.17
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	21	0.17
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	21	0.17
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	21	0.17
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	21	0.17
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	21	0.17
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	21	0.17
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	5	0.17
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	5	0.17
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	21	0.17
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	21	0.17
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	39	0.17
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	39	0.17
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	32	0.17
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	31	0.17
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	31	0.17
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	8	0.17
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	26	0.17
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	28	0.17
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	21	0.17
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	38	0.17
(1,828)	1:44:A:MET:HG2	1:44:A:MET:H	11	0.17
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	35	0.17
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	24	0.17
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	24	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	23	0.17
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	13	0.17
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	19	0.17
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	33	0.17
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	36	0.17
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	7	0.17
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	32	0.17
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	32	0.17
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	32	0.17
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	11	0.17
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	11	0.17
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	11	0.17
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	29	0.17
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	29	0.17
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	29	0.17
(1,266)	1:34:A:VAL:HG21	1:38:A:THR:HB	15	0.17
(1,266)	1:34:A:VAL:HG22	1:38:A:THR:HB	15	0.17
(1,266)	1:34:A:VAL:HG23	1:38:A:THR:HB	15	0.17
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	33	0.17
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	33	0.17
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	33	0.17
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	33	0.17
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	33	0.17
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	33	0.17
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	33	0.17
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	33	0.17
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	33	0.17
(1,193)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	23	0.17
(1,193)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	23	0.17
(1,193)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	23	0.17
(1,193)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	37	0.17
(1,193)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	37	0.17
(1,193)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	37	0.17
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	21	0.17
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	21	0.17
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	21	0.17
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	21	0.17
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	21	0.17
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	21	0.17
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	21	0.17
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	21	0.17
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	21	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	33	0.16
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	33	0.16
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	27	0.16
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	11	0.16
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	22	0.16
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	38	0.16
(1,2162)	1:64:A:TRP:HE1	1:70:A:ILE:HG13	16	0.16
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	16	0.16
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	31	0.16
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	31	0.16
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	31	0.16
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	31	0.16
(1,1988)	1:45:A:ASN:HA	1:47:A:LEU:H	7	0.16
(1,1975)	1:44:A:MET:HG2	1:44:A:MET:H	16	0.16
(1,1951)	1:37:A:LEU:HD21	1:49:A:LEU:H	29	0.16
(1,1951)	1:37:A:LEU:HD22	1:49:A:LEU:H	29	0.16
(1,1951)	1:37:A:LEU:HD23	1:49:A:LEU:H	29	0.16
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	28	0.16
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	37	0.16
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	23	0.16
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	2	0.16
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	2	0.16
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	3	0.16
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	3	0.16
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	4	0.16
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	16	0.16
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	22	0.16
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	24	0.16
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	4	0.16
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	3	0.16
(1,1678)	1:9:A:PHE:HB3	1:58:A:ARG:HE	3	0.16
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	31	0.16
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	22	0.16
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	22	0.16
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	22	0.16
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	22	0.16
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	33	0.16
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	33	0.16
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	33	0.16
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	36	0.16
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	36	0.16
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	36	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	12	0.16
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	12	0.16
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	12	0.16
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	12	0.16
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	12	0.16
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	12	0.16
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	12	0.16
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	12	0.16
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	12	0.16
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	13	0.16
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	13	0.16
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	13	0.16
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	13	0.16
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	13	0.16
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	13	0.16
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	10	0.16
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	10	0.16
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	10	0.16
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	20	0.16
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	20	0.16
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	20	0.16
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	27	0.16
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	27	0.16
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	27	0.16
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	2	0.16
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	2	0.16
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	2	0.16
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	2	0.16
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	10	0.16
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	10	0.16
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	10	0.16
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	10	0.16
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	26	0.16
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	26	0.16
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	26	0.16
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	26	0.16
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	26	0.16
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	26	0.16
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	26	0.16
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	26	0.16
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	26	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	7	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	7	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	7	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	7	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	7	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	7	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	7	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	7	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	17	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	17	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	17	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	17	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	17	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	17	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	17	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	17	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	17	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	24	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	24	0.16
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	24	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	24	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	24	0.16
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	24	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	24	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	24	0.16
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	24	0.16
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	33	0.16
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	33	0.16
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	27	0.16
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	11	0.16
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	22	0.16
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	38	0.16
(1,1015)	1:64:A:TRP:HE1	1:70:A:ILE:HG13	16	0.16
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	16	0.16
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	31	0.16
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	31	0.16
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	31	0.16
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	31	0.16
(1,841)	1:45:A:ASN:HA	1:47:A:LEU:H	7	0.16
(1,828)	1:44:A:MET:HG2	1:44:A:MET:H	16	0.16
(1,804)	1:37:A:LEU:HD21	1:49:A:LEU:H	29	0.16
(1,804)	1:37:A:LEU:HD22	1:49:A:LEU:H	29	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:37:A:LEU:HD23	1:49:A:LEU:H	29	0.16
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	28	0.16
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	37	0.16
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	23	0.16
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	2	0.16
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	2	0.16
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	3	0.16
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	3	0.16
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	4	0.16
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	16	0.16
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	22	0.16
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	24	0.16
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	4	0.16
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	3	0.16
(1,531)	1:9:A:PHE:HB3	1:58:A:ARG:HE	3	0.16
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	31	0.16
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	22	0.16
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	22	0.16
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	22	0.16
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	22	0.16
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	33	0.16
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	33	0.16
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	33	0.16
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	36	0.16
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	36	0.16
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	36	0.16
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	12	0.16
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	12	0.16
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	12	0.16
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	12	0.16
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	12	0.16
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	12	0.16
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	12	0.16
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	12	0.16
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	12	0.16
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	13	0.16
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	13	0.16
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	13	0.16
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	13	0.16
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	13	0.16
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	13	0.16
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	10	0.16
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	10	0.16
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	20	0.16
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	20	0.16
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	20	0.16
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	27	0.16
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	27	0.16
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	27	0.16
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	2	0.16
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	2	0.16
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	2	0.16
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	2	0.16
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	10	0.16
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	10	0.16
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	10	0.16
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	10	0.16
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	26	0.16
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	26	0.16
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	26	0.16
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	26	0.16
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	26	0.16
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	26	0.16
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	26	0.16
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	26	0.16
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	26	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	7	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	7	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	7	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	7	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	7	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	7	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	7	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	7	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	7	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	17	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	17	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	17	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	17	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	17	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	17	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	17	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	17	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	24	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	24	0.16
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	24	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	24	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	24	0.16
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	24	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	24	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	24	0.16
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	24	0.16
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	17	0.15
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	17	0.15
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	18	0.15
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	36	0.15
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	19	0.15
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	36	0.15
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	13	0.15
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	36	0.15
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	38	0.15
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD2	7	0.15
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD3	7	0.15
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	33	0.15
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	37	0.15
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	30	0.15
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	30	0.15
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	9	0.15
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	9	0.15
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	9	0.15
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	27	0.15
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	27	0.15
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	27	0.15
(1,1951)	1:37:A:LEU:HD21	1:49:A:LEU:H	4	0.15
(1,1951)	1:37:A:LEU:HD22	1:49:A:LEU:H	4	0.15
(1,1951)	1:37:A:LEU:HD23	1:49:A:LEU:H	4	0.15
(1,1951)	1:37:A:LEU:HD21	1:49:A:LEU:H	22	0.15
(1,1951)	1:37:A:LEU:HD22	1:49:A:LEU:H	22	0.15
(1,1951)	1:37:A:LEU:HD23	1:49:A:LEU:H	22	0.15
(1,1951)	1:37:A:LEU:HD21	1:49:A:LEU:H	33	0.15
(1,1951)	1:37:A:LEU:HD22	1:49:A:LEU:H	33	0.15
(1,1951)	1:37:A:LEU:HD23	1:49:A:LEU:H	33	0.15
(1,1930)	1:34:A:VAL:HG11	1:34:A:VAL:H	28	0.15
(1,1930)	1:34:A:VAL:HG12	1:34:A:VAL:H	28	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1930)	1:34:A:VAL:HG13	1:34:A:VAL:H	28	0.15
(1,1901)	1:28:A:ASN:HD22	1:30:A:GLN:H	7	0.15
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	8	0.15
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	21	0.15
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	4	0.15
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	1	0.15
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	15	0.15
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	31	0.15
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	28	0.15
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	28	0.15
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	18	0.15
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	25	0.15
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	13	0.15
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	30	0.15
(1,1688)	1:10:A:THR:HB	1:13:A:GLU:H	31	0.15
(1,1688)	1:10:A:THR:HB	1:13:A:GLU:H	36	0.15
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	34	0.15
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	34	0.15
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	34	0.15
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	4	0.15
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	4	0.15
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	4	0.15
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	8	0.15
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	8	0.15
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	8	0.15
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	27	0.15
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	27	0.15
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	27	0.15
(1,1414)	1:34:A:VAL:HG21	1:47:A:LEU:HA	28	0.15
(1,1414)	1:34:A:VAL:HG22	1:47:A:LEU:HA	28	0.15
(1,1414)	1:34:A:VAL:HG23	1:47:A:LEU:HA	28	0.15
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	6	0.15
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	6	0.15
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	6	0.15
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	6	0.15
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	6	0.15
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	6	0.15
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	6	0.15
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	6	0.15
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	6	0.15
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	31	0.15
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	31	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	31	0.15
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	37	0.15
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	37	0.15
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	37	0.15
(1,1347)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	33	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	8	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	8	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	8	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	8	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	8	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	8	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	8	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	8	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	8	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	24	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	24	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	24	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	24	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	24	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	24	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	24	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	24	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	24	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	34	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	34	0.15
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	34	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	34	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	34	0.15
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	34	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	34	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	34	0.15
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	34	0.15
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	10	0.15
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	10	0.15
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	10	0.15
(1,1265)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	7	0.15
(1,1265)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	13	0.15
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	36	0.15
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE1	6	0.15
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE2	6	0.15
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE3	6	0.15
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	17	0.15
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	18	0.15
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	36	0.15
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	19	0.15
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	36	0.15
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	13	0.15
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	36	0.15
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	38	0.15
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD2	7	0.15
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD3	7	0.15
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	33	0.15
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	37	0.15
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	30	0.15
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	30	0.15
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	9	0.15
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	9	0.15
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	9	0.15
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	27	0.15
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	27	0.15
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	27	0.15
(1,804)	1:37:A:LEU:HD21	1:49:A:LEU:H	4	0.15
(1,804)	1:37:A:LEU:HD22	1:49:A:LEU:H	4	0.15
(1,804)	1:37:A:LEU:HD23	1:49:A:LEU:H	4	0.15
(1,804)	1:37:A:LEU:HD21	1:49:A:LEU:H	22	0.15
(1,804)	1:37:A:LEU:HD22	1:49:A:LEU:H	22	0.15
(1,804)	1:37:A:LEU:HD23	1:49:A:LEU:H	22	0.15
(1,804)	1:37:A:LEU:HD21	1:49:A:LEU:H	33	0.15
(1,804)	1:37:A:LEU:HD22	1:49:A:LEU:H	33	0.15
(1,804)	1:37:A:LEU:HD23	1:49:A:LEU:H	33	0.15
(1,783)	1:34:A:VAL:HG11	1:34:A:VAL:H	28	0.15
(1,783)	1:34:A:VAL:HG12	1:34:A:VAL:H	28	0.15
(1,783)	1:34:A:VAL:HG13	1:34:A:VAL:H	28	0.15
(1,754)	1:28:A:ASN:HD22	1:30:A:GLN:H	7	0.15
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	8	0.15
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	21	0.15
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	4	0.15
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	1	0.15
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	15	0.15
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	31	0.15
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	28	0.15
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	28	0.15
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	25	0.15
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	13	0.15
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	30	0.15
(1,541)	1:10:A:THR:HB	1:13:A:GLU:H	31	0.15
(1,541)	1:10:A:THR:HB	1:13:A:GLU:H	36	0.15
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	34	0.15
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	34	0.15
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	34	0.15
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	4	0.15
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	4	0.15
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	4	0.15
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	8	0.15
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	8	0.15
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	8	0.15
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	27	0.15
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	27	0.15
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	27	0.15
(1,267)	1:34:A:VAL:HG21	1:47:A:LEU:HA	28	0.15
(1,267)	1:34:A:VAL:HG22	1:47:A:LEU:HA	28	0.15
(1,267)	1:34:A:VAL:HG23	1:47:A:LEU:HA	28	0.15
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	6	0.15
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	6	0.15
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	6	0.15
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	6	0.15
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	6	0.15
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	6	0.15
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	6	0.15
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	6	0.15
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	6	0.15
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	31	0.15
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	31	0.15
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	31	0.15
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	37	0.15
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	37	0.15
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	37	0.15
(1,200)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	33	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	8	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	8	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	8	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	8	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	8	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	8	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	8	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	8	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	24	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	24	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	24	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	24	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	24	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	24	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	24	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	24	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	24	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	34	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	34	0.15
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	34	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	34	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	34	0.15
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	34	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	34	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	34	0.15
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	34	0.15
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	10	0.15
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	10	0.15
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	10	0.15
(1,118)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	7	0.15
(1,118)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	13	0.15
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	36	0.15
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE1	6	0.15
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE2	6	0.15
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE3	6	0.15
(1,2294)	1:81:A:ASP:HB2	1:81:A:ASP:H	27	0.14
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	9	0.14
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	8	0.14
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	8	0.14
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	10	0.14
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	10	0.14
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	5	0.14
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	24	0.14
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	3	0.14
(1,2000)	1:46:A:GLN:HE22	1:50:A:LEU:HD21	23	0.14
(1,2000)	1:46:A:GLN:HE22	1:50:A:LEU:HD22	23	0.14
(1,2000)	1:46:A:GLN:HE22	1:50:A:LEU:HD23	23	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	15	0.14
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	27	0.14
(1,1988)	1:45:A:ASN:HA	1:47:A:LEU:H	3	0.14
(1,1981)	1:44:A:MET:HG2	1:47:A:LEU:H	35	0.14
(1,1981)	1:44:A:MET:HG3	1:47:A:LEU:H	35	0.14
(1,1975)	1:44:A:MET:HG2	1:44:A:MET:H	37	0.14
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	2	0.14
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	2	0.14
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	14	0.14
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	14	0.14
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	31	0.14
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	31	0.14
(1,1950)	1:37:A:LEU:HG	1:46:A:GLN:HE21	18	0.14
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	5	0.14
(1,1855)	1:21:A:PHE:HE1	1:74:A:LEU:H	29	0.14
(1,1855)	1:21:A:PHE:HE2	1:74:A:LEU:H	29	0.14
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	4	0.14
(1,1766)	1:15:A:ASN:H	1:18:A:LYS:HE2	2	0.14
(1,1766)	1:15:A:ASN:H	1:18:A:LYS:HE2	35	0.14
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	26	0.14
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	4	0.14
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	9	0.14
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	18	0.14
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	32	0.14
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	7	0.14
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	34	0.14
(1,1714)	1:13:A:GLU:H	1:14:A:TRP:HB3	36	0.14
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	21	0.14
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	34	0.14
(1,1688)	1:10:A:THR:HB	1:13:A:GLU:H	9	0.14
(1,1688)	1:10:A:THR:HB	1:13:A:GLU:H	25	0.14
(1,1666)	1:8:A:LYS:HE2	1:58:A:ARG:HE	19	0.14
(1,1666)	1:8:A:LYS:HE3	1:58:A:ARG:HE	19	0.14
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	30	0.14
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	30	0.14
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	30	0.14
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	37	0.14
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	2	0.14
(1,1505)	1:53:A:TRP:HE3	1:54:A:LEU:HG	23	0.14
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	7	0.14
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	7	0.14
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	12	0.14
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	12	0.14
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	12	0.14
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	25	0.14
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	25	0.14
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	25	0.14
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG21	19	0.14
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG22	19	0.14
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG23	19	0.14
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	16	0.14
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	16	0.14
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	16	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	15	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	15	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	15	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	30	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	30	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	30	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	33	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	33	0.14
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	33	0.14
(1,1265)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	1	0.14
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	23	0.14
(1,1147)	1:81:A:ASP:HB2	1:81:A:ASP:H	27	0.14
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	9	0.14
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	8	0.14
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	8	0.14
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	10	0.14
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	10	0.14
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	5	0.14
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	24	0.14
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	3	0.14
(1,853)	1:46:A:GLN:HE22	1:50:A:LEU:HD21	23	0.14
(1,853)	1:46:A:GLN:HE22	1:50:A:LEU:HD22	23	0.14
(1,853)	1:46:A:GLN:HE22	1:50:A:LEU:HD23	23	0.14
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	15	0.14
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	27	0.14
(1,841)	1:45:A:ASN:HA	1:47:A:LEU:H	3	0.14
(1,834)	1:44:A:MET:HG2	1:47:A:LEU:H	35	0.14
(1,834)	1:44:A:MET:HG3	1:47:A:LEU:H	35	0.14
(1,828)	1:44:A:MET:HG2	1:44:A:MET:H	37	0.14
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	2	0.14
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	14	0.14
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	14	0.14
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	31	0.14
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	31	0.14
(1,803)	1:37:A:LEU:HG	1:46:A:GLN:HE21	18	0.14
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	5	0.14
(1,708)	1:21:A:PHE:HE1	1:74:A:LEU:H	29	0.14
(1,708)	1:21:A:PHE:HE2	1:74:A:LEU:H	29	0.14
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	4	0.14
(1,619)	1:15:A:ASN:H	1:18:A:LYS:HE2	2	0.14
(1,619)	1:15:A:ASN:H	1:18:A:LYS:HE2	35	0.14
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	26	0.14
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	4	0.14
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	9	0.14
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	18	0.14
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	32	0.14
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	7	0.14
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	34	0.14
(1,567)	1:13:A:GLU:H	1:14:A:TRP:HB3	36	0.14
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	21	0.14
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	34	0.14
(1,541)	1:10:A:THR:HB	1:13:A:GLU:H	9	0.14
(1,541)	1:10:A:THR:HB	1:13:A:GLU:H	25	0.14
(1,519)	1:8:A:LYS:HE2	1:58:A:ARG:HE	19	0.14
(1,519)	1:8:A:LYS:HE3	1:58:A:ARG:HE	19	0.14
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	30	0.14
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	30	0.14
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	30	0.14
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	37	0.14
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	2	0.14
(1,358)	1:53:A:TRP:HE3	1:54:A:LEU:HG	23	0.14
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	7	0.14
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	7	0.14
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	7	0.14
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	12	0.14
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	12	0.14
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	12	0.14
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	25	0.14
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	25	0.14
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	25	0.14
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG21	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG22	19	0.14
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG23	19	0.14
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	16	0.14
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	16	0.14
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	16	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	15	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	15	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	15	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	30	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	30	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	30	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	33	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	33	0.14
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	33	0.14
(1,118)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	1	0.14
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	23	0.14
(1,2235)	1:73:A:LYS:HD3	1:73:A:LYS:H	4	0.13
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	13	0.13
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	13	0.13
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	7	0.13
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	33	0.13
(1,2201)	1:70:A:ILE:H	1:71:A:LEU:HD21	28	0.13
(1,2201)	1:70:A:ILE:H	1:71:A:LEU:HD22	28	0.13
(1,2201)	1:70:A:ILE:H	1:71:A:LEU:HD23	28	0.13
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	4	0.13
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD2	34	0.13
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD3	34	0.13
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	7	0.13
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	12	0.13
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	22	0.13
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	24	0.13
(1,2109)	1:58:A:ARG:HG3	1:58:A:ARG:H	16	0.13
(1,2105)	1:57:A:HIS:HA	1:61:A:CYS:H	31	0.13
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	14	0.13
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	32	0.13
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	3	0.13
(1,1988)	1:45:A:ASN:HA	1:47:A:LEU:H	25	0.13
(1,1974)	1:43:A:ILE:HA	1:45:A:ASN:H	13	0.13
(1,1911)	1:31:A:LYS:HB2	1:32:A:ASP:H	38	0.13
(1,1911)	1:31:A:LYS:HB3	1:32:A:ASP:H	38	0.13
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	33	0.13
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	38	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:22:A:ILE:HG12	1:22:A:ILE:H	18	0.13
(1,1855)	1:21:A:PHE:HE1	1:74:A:LEU:H	6	0.13
(1,1855)	1:21:A:PHE:HE2	1:74:A:LEU:H	6	0.13
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	30	0.13
(1,1766)	1:15:A:ASN:H	1:18:A:LYS:HE2	26	0.13
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	6	0.13
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	6	0.13
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	36	0.13
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	36	0.13
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	5	0.13
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	8	0.13
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	10	0.13
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	23	0.13
(1,1714)	1:13:A:GLU:H	1:14:A:TRP:HB3	2	0.13
(1,1714)	1:13:A:GLU:H	1:14:A:TRP:HB3	8	0.13
(1,1714)	1:13:A:GLU:H	1:14:A:TRP:HB3	16	0.13
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	20	0.13
(1,1688)	1:10:A:THR:HB	1:13:A:GLU:H	4	0.13
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	11	0.13
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	26	0.13
(1,1484)	1:50:A:LEU:HD11	1:51:A:HIS:HE1	30	0.13
(1,1484)	1:50:A:LEU:HD12	1:51:A:HIS:HE1	30	0.13
(1,1484)	1:50:A:LEU:HD13	1:51:A:HIS:HE1	30	0.13
(1,1427)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	5	0.13
(1,1427)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	5	0.13
(1,1427)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	5	0.13
(1,1414)	1:34:A:VAL:HG21	1:47:A:LEU:HA	38	0.13
(1,1414)	1:34:A:VAL:HG22	1:47:A:LEU:HA	38	0.13
(1,1414)	1:34:A:VAL:HG23	1:47:A:LEU:HA	38	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	2	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	2	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	2	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	2	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	2	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	2	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	2	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	2	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	2	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	4	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	4	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	4	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	4	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	4	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	4	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	4	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	4	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	13	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	13	0.13
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	13	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	13	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	13	0.13
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	13	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	13	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	13	0.13
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	13	0.13
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	4	0.13
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	4	0.13
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	4	0.13
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	4	0.13
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	4	0.13
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	4	0.13
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	6	0.13
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	6	0.13
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	6	0.13
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	17	0.13
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	17	0.13
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	17	0.13
(1,1347)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	38	0.13
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	5	0.13
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	5	0.13
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	5	0.13
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	5	0.13
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	19	0.13
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	19	0.13
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	19	0.13
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	19	0.13
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	39	0.13
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	39	0.13
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	39	0.13
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	39	0.13
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	39	0.13
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	39	0.13
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	39	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	39	0.13
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	39	0.13
(1,1292)	1:78:A:TRP:HH2	1:22:A:ILE:HA	27	0.13
(1,1265)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	10	0.13
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	1	0.13
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	1	0.13
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	1	0.13
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	1	0.13
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	1	0.13
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	1	0.13
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	1	0.13
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	1	0.13
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	1	0.13
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	25	0.13
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	25	0.13
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	25	0.13
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	25	0.13
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	25	0.13
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	25	0.13
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	25	0.13
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	25	0.13
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	25	0.13
(1,1223)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	21	0.13
(1,1223)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	23	0.13
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	9	0.13
(1,1185)	1:9:A:PHE:HD1	1:70:A:ILE:HD11	5	0.13
(1,1185)	1:9:A:PHE:HD1	1:70:A:ILE:HD12	5	0.13
(1,1185)	1:9:A:PHE:HD1	1:70:A:ILE:HD13	5	0.13
(1,1185)	1:9:A:PHE:HD2	1:70:A:ILE:HD11	5	0.13
(1,1185)	1:9:A:PHE:HD2	1:70:A:ILE:HD12	5	0.13
(1,1185)	1:9:A:PHE:HD2	1:70:A:ILE:HD13	5	0.13
(1,1088)	1:73:A:LYS:HD3	1:73:A:LYS:H	4	0.13
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	13	0.13
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	13	0.13
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	7	0.13
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	33	0.13
(1,1054)	1:70:A:ILE:H	1:71:A:LEU:HD21	28	0.13
(1,1054)	1:70:A:ILE:H	1:71:A:LEU:HD22	28	0.13
(1,1054)	1:70:A:ILE:H	1:71:A:LEU:HD23	28	0.13
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	4	0.13
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD2	34	0.13
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD3	34	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	7	0.13
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	12	0.13
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	22	0.13
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	24	0.13
(1,962)	1:58:A:ARG:HG3	1:58:A:ARG:H	16	0.13
(1,958)	1:57:A:HIS:HA	1:61:A:CYS:H	31	0.13
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	14	0.13
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	32	0.13
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	3	0.13
(1,841)	1:45:A:ASN:HA	1:47:A:LEU:H	25	0.13
(1,827)	1:43:A:ILE:HA	1:45:A:ASN:H	13	0.13
(1,764)	1:31:A:LYS:HB2	1:32:A:ASP:H	38	0.13
(1,764)	1:31:A:LYS:HB3	1:32:A:ASP:H	38	0.13
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	33	0.13
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	38	0.13
(1,711)	1:22:A:ILE:HG12	1:22:A:ILE:H	18	0.13
(1,708)	1:21:A:PHE:HE1	1:74:A:LEU:H	6	0.13
(1,708)	1:21:A:PHE:HE2	1:74:A:LEU:H	6	0.13
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	30	0.13
(1,619)	1:15:A:ASN:H	1:18:A:LYS:HE2	26	0.13
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	6	0.13
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	6	0.13
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	36	0.13
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	36	0.13
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	5	0.13
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	8	0.13
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	10	0.13
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	23	0.13
(1,567)	1:13:A:GLU:H	1:14:A:TRP:HB3	2	0.13
(1,567)	1:13:A:GLU:H	1:14:A:TRP:HB3	8	0.13
(1,567)	1:13:A:GLU:H	1:14:A:TRP:HB3	16	0.13
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	20	0.13
(1,541)	1:10:A:THR:HB	1:13:A:GLU:H	4	0.13
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	11	0.13
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	26	0.13
(1,337)	1:50:A:LEU:HD11	1:51:A:HIS:HE1	30	0.13
(1,337)	1:50:A:LEU:HD12	1:51:A:HIS:HE1	30	0.13
(1,337)	1:50:A:LEU:HD13	1:51:A:HIS:HE1	30	0.13
(1,280)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	5	0.13
(1,280)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	5	0.13
(1,280)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	5	0.13
(1,267)	1:34:A:VAL:HG21	1:47:A:LEU:HA	38	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:34:A:VAL:HG22	1:47:A:LEU:HA	38	0.13
(1,267)	1:34:A:VAL:HG23	1:47:A:LEU:HA	38	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	2	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	2	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	2	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	2	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	2	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	2	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	2	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	2	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	2	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	4	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	4	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	4	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	4	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	4	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	4	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	4	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	4	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	4	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	13	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	13	0.13
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	13	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	13	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	13	0.13
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	13	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	13	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	13	0.13
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	13	0.13
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	4	0.13
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	4	0.13
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	4	0.13
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	4	0.13
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	4	0.13
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	4	0.13
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	6	0.13
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	6	0.13
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	6	0.13
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	17	0.13
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	17	0.13
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	17	0.13
(1,200)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	38	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	5	0.13
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	5	0.13
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	5	0.13
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	5	0.13
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	19	0.13
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	19	0.13
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	19	0.13
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	19	0.13
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	39	0.13
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	39	0.13
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	39	0.13
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	39	0.13
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	39	0.13
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	39	0.13
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	39	0.13
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	39	0.13
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	39	0.13
(1,145)	1:78:A:TRP:HH2	1:22:A:ILE:HA	27	0.13
(1,118)	1:18:A:LYS:HE3	1:51:A:HIS:HE1	10	0.13
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	1	0.13
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	1	0.13
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	1	0.13
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	1	0.13
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	1	0.13
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	1	0.13
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	1	0.13
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	1	0.13
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	1	0.13
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	25	0.13
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	25	0.13
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	25	0.13
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	25	0.13
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	25	0.13
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	25	0.13
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	25	0.13
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	25	0.13
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	25	0.13
(1,76)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	21	0.13
(1,76)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	23	0.13
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	9	0.13
(1,38)	1:9:A:PHE:HD1	1:70:A:ILE:HD11	5	0.13
(1,38)	1:9:A:PHE:HD1	1:70:A:ILE:HD12	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:9:A:PHE:HD1	1:70:A:ILE:HD13	5	0.13
(1,38)	1:9:A:PHE:HD2	1:70:A:ILE:HD11	5	0.13
(1,38)	1:9:A:PHE:HD2	1:70:A:ILE:HD12	5	0.13
(1,38)	1:9:A:PHE:HD2	1:70:A:ILE:HD13	5	0.13
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	7	0.12
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	7	0.12
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	11	0.12
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	11	0.12
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG2	36	0.12
(1,2288)	1:79:A:ASN:H	1:80:A:LYS:HG3	36	0.12
(1,2264)	1:77:A:GLN:HB3	1:77:A:GLN:H	27	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	6	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	6	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	9	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	9	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	32	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	32	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	36	0.12
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	36	0.12
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	13	0.12
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	31	0.12
(1,2210)	1:71:A:LEU:HB3	1:71:A:LEU:H	25	0.12
(1,2157)	1:64:A:TRP:HE1	1:60:A:MET:HB2	36	0.12
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	18	0.12
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	27	0.12
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	9	0.12
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	30	0.12
(1,2054)	1:53:A:TRP:HZ2	1:77:A:GLN:H	34	0.12
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	8	0.12
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	8	0.12
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	8	0.12
(1,1981)	1:44:A:MET:HG2	1:47:A:LEU:H	8	0.12
(1,1981)	1:44:A:MET:HG3	1:47:A:LEU:H	8	0.12
(1,1951)	1:37:A:LEU:HD21	1:49:A:LEU:H	8	0.12
(1,1951)	1:37:A:LEU:HD22	1:49:A:LEU:H	8	0.12
(1,1951)	1:37:A:LEU:HD23	1:49:A:LEU:H	8	0.12
(1,1951)	1:37:A:LEU:HD21	1:49:A:LEU:H	23	0.12
(1,1951)	1:37:A:LEU:HD22	1:49:A:LEU:H	23	0.12
(1,1951)	1:37:A:LEU:HD23	1:49:A:LEU:H	23	0.12
(1,1950)	1:37:A:LEU:HG	1:46:A:GLN:HE21	9	0.12
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	21	0.12
(1,1901)	1:28:A:ASN:HD22	1:30:A:GLN:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1855)	1:21:A:PHE:HE1	1:74:A:LEU:H	4	0.12
(1,1855)	1:21:A:PHE:HE2	1:74:A:LEU:H	4	0.12
(1,1855)	1:21:A:PHE:HE1	1:74:A:LEU:H	9	0.12
(1,1855)	1:21:A:PHE:HE2	1:74:A:LEU:H	9	0.12
(1,1855)	1:21:A:PHE:HE1	1:74:A:LEU:H	28	0.12
(1,1855)	1:21:A:PHE:HE2	1:74:A:LEU:H	28	0.12
(1,1831)	1:19:A:GLN:HE21	1:22:A:ILE:HD11	36	0.12
(1,1831)	1:19:A:GLN:HE21	1:22:A:ILE:HD12	36	0.12
(1,1831)	1:19:A:GLN:HE21	1:22:A:ILE:HD13	36	0.12
(1,1825)	1:19:A:GLN:H	1:22:A:ILE:HB	24	0.12
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	17	0.12
(1,1796)	1:18:A:LYS:HE3	1:18:A:LYS:H	26	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	1	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	3	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	10	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	14	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	15	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	24	0.12
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	32	0.12
(1,1745)	1:14:A:TRP:HE1	1:58:A:ARG:HG2	22	0.12
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	7	0.12
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	22	0.12
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	39	0.12
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	39	0.12
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	26	0.12
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	27	0.12
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	37	0.12
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	38	0.12
(1,1714)	1:13:A:GLU:H	1:14:A:TRP:HB3	35	0.12
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	33	0.12
(1,1685)	1:10:A:THR:HB	1:12:A:ASP:H	7	0.12
(1,1678)	1:9:A:PHE:HB3	1:58:A:ARG:HE	30	0.12
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	16	0.12
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	16	0.12
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	16	0.12
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	21	0.12
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	21	0.12
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	21	0.12
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	18	0.12
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	23	0.12
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	21	0.12
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	3	0.12
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	3	0.12
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	3	0.12
(1,1427)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	18	0.12
(1,1427)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	18	0.12
(1,1427)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	18	0.12
(1,1414)	1:34:A:VAL:HG21	1:47:A:LEU:HA	14	0.12
(1,1414)	1:34:A:VAL:HG22	1:47:A:LEU:HA	14	0.12
(1,1414)	1:34:A:VAL:HG23	1:47:A:LEU:HA	14	0.12
(1,1413)	1:34:A:VAL:HG21	1:38:A:THR:HB	22	0.12
(1,1413)	1:34:A:VAL:HG22	1:38:A:THR:HB	22	0.12
(1,1413)	1:34:A:VAL:HG23	1:38:A:THR:HB	22	0.12
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	9	0.12
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	9	0.12
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	9	0.12
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	9	0.12
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	9	0.12
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	9	0.12
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	9	0.12
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	9	0.12
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	9	0.12
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	28	0.12
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	28	0.12
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	28	0.12
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	28	0.12
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	28	0.12
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	28	0.12
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	28	0.12
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	28	0.12
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	28	0.12
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	7	0.12
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	7	0.12
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	7	0.12
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	26	0.12
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	26	0.12
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	26	0.12
(1,1347)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	23	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG21	18	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG22	18	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG23	18	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG21	32	0.12
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG22	32	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:23:A:SER:HA	1:43:A:ILE:HG23	32	0.12
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	16	0.12
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	16	0.12
(1,1333)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	16	0.12
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	16	0.12
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	16	0.12
(1,1333)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	16	0.12
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	16	0.12
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	16	0.12
(1,1333)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	16	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	3	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	3	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	3	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	37	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	37	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	37	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	38	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	38	0.12
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	38	0.12
(1,1276)	1:19:A:GLN:HG2	1:22:A:ILE:HG21	15	0.12
(1,1276)	1:19:A:GLN:HG2	1:22:A:ILE:HG22	15	0.12
(1,1276)	1:19:A:GLN:HG2	1:22:A:ILE:HG23	15	0.12
(1,1276)	1:19:A:GLN:HG3	1:22:A:ILE:HG21	15	0.12
(1,1276)	1:19:A:GLN:HG3	1:22:A:ILE:HG22	15	0.12
(1,1276)	1:19:A:GLN:HG3	1:22:A:ILE:HG23	15	0.12
(1,1268)	1:18:A:LYS:HD2	1:51:A:HIS:HD2	23	0.12
(1,1268)	1:18:A:LYS:HD3	1:51:A:HIS:HD2	23	0.12
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	37	0.12
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	37	0.12
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	37	0.12
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	37	0.12
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	37	0.12
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	37	0.12
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	37	0.12
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	37	0.12
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	37	0.12
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	3	0.12
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	31	0.12
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	32	0.12
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	39	0.12
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE1	11	0.12
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE3	11	0.12
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE1	11	0.12
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE2	11	0.12
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE3	11	0.12
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	7	0.12
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	7	0.12
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	11	0.12
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	11	0.12
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG2	36	0.12
(1,1141)	1:79:A:ASN:H	1:80:A:LYS:HG3	36	0.12
(1,1117)	1:77:A:GLN:HB3	1:77:A:GLN:H	27	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	6	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	6	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	9	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	9	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	32	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	32	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	36	0.12
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	36	0.12
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	13	0.12
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	31	0.12
(1,1063)	1:71:A:LEU:HB3	1:71:A:LEU:H	25	0.12
(1,1010)	1:64:A:TRP:HE1	1:60:A:MET:HB2	36	0.12
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	18	0.12
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	27	0.12
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	9	0.12
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	30	0.12
(1,907)	1:53:A:TRP:HZ2	1:77:A:GLN:H	34	0.12
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	8	0.12
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	8	0.12
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	8	0.12
(1,834)	1:44:A:MET:HG2	1:47:A:LEU:H	8	0.12
(1,834)	1:44:A:MET:HG3	1:47:A:LEU:H	8	0.12
(1,804)	1:37:A:LEU:HD21	1:49:A:LEU:H	8	0.12
(1,804)	1:37:A:LEU:HD22	1:49:A:LEU:H	8	0.12
(1,804)	1:37:A:LEU:HD23	1:49:A:LEU:H	8	0.12
(1,804)	1:37:A:LEU:HD21	1:49:A:LEU:H	23	0.12
(1,804)	1:37:A:LEU:HD22	1:49:A:LEU:H	23	0.12
(1,804)	1:37:A:LEU:HD23	1:49:A:LEU:H	23	0.12
(1,803)	1:37:A:LEU:HG	1:46:A:GLN:HE21	9	0.12
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	21	0.12
(1,754)	1:28:A:ASN:HD22	1:30:A:GLN:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:21:A:PHE:HE1	1:74:A:LEU:H	4	0.12
(1,708)	1:21:A:PHE:HE2	1:74:A:LEU:H	4	0.12
(1,708)	1:21:A:PHE:HE1	1:74:A:LEU:H	9	0.12
(1,708)	1:21:A:PHE:HE2	1:74:A:LEU:H	9	0.12
(1,708)	1:21:A:PHE:HE1	1:74:A:LEU:H	28	0.12
(1,708)	1:21:A:PHE:HE2	1:74:A:LEU:H	28	0.12
(1,684)	1:19:A:GLN:HE21	1:22:A:ILE:HD11	36	0.12
(1,684)	1:19:A:GLN:HE21	1:22:A:ILE:HD12	36	0.12
(1,684)	1:19:A:GLN:HE21	1:22:A:ILE:HD13	36	0.12
(1,678)	1:19:A:GLN:H	1:22:A:ILE:HB	24	0.12
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	17	0.12
(1,649)	1:18:A:LYS:HE3	1:18:A:LYS:H	26	0.12
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	1	0.12
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	3	0.12
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	10	0.12
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	14	0.12
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	15	0.12
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	24	0.12
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	32	0.12
(1,598)	1:14:A:TRP:HE1	1:58:A:ARG:HG2	22	0.12
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	7	0.12
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	22	0.12
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	39	0.12
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	39	0.12
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	26	0.12
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	27	0.12
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	37	0.12
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	38	0.12
(1,567)	1:13:A:GLU:H	1:14:A:TRP:HB3	35	0.12
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	33	0.12
(1,538)	1:10:A:THR:HB	1:12:A:ASP:H	7	0.12
(1,531)	1:9:A:PHE:HB3	1:58:A:ARG:HE	30	0.12
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	16	0.12
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	16	0.12
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	16	0.12
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	21	0.12
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	21	0.12
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	21	0.12
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	18	0.12
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	23	0.12
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	21	0.12
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	3	0.12
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	3	0.12
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	3	0.12
(1,280)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	18	0.12
(1,280)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	18	0.12
(1,280)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	18	0.12
(1,267)	1:34:A:VAL:HG21	1:47:A:LEU:HA	14	0.12
(1,267)	1:34:A:VAL:HG22	1:47:A:LEU:HA	14	0.12
(1,267)	1:34:A:VAL:HG23	1:47:A:LEU:HA	14	0.12
(1,266)	1:34:A:VAL:HG21	1:38:A:THR:HB	22	0.12
(1,266)	1:34:A:VAL:HG22	1:38:A:THR:HB	22	0.12
(1,266)	1:34:A:VAL:HG23	1:38:A:THR:HB	22	0.12
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	9	0.12
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	9	0.12
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	9	0.12
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	9	0.12
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	9	0.12
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	9	0.12
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	9	0.12
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	9	0.12
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	9	0.12
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	28	0.12
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	28	0.12
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	28	0.12
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	28	0.12
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	28	0.12
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	28	0.12
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	28	0.12
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	28	0.12
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	28	0.12
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	7	0.12
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	7	0.12
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	7	0.12
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	26	0.12
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	26	0.12
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	26	0.12
(1,200)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	23	0.12
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG21	18	0.12
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG22	18	0.12
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG23	18	0.12
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG21	32	0.12
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG22	32	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:23:A:SER:HA	1:43:A:ILE:HG23	32	0.12
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD11	16	0.12
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD12	16	0.12
(1,186)	1:22:A:ILE:HG21	1:47:A:LEU:HD13	16	0.12
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD11	16	0.12
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD12	16	0.12
(1,186)	1:22:A:ILE:HG22	1:47:A:LEU:HD13	16	0.12
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD11	16	0.12
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD12	16	0.12
(1,186)	1:22:A:ILE:HG23	1:47:A:LEU:HD13	16	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	3	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	3	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	3	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	37	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	37	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	37	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	38	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	38	0.12
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	38	0.12
(1,129)	1:19:A:GLN:HG2	1:22:A:ILE:HG21	15	0.12
(1,129)	1:19:A:GLN:HG2	1:22:A:ILE:HG22	15	0.12
(1,129)	1:19:A:GLN:HG2	1:22:A:ILE:HG23	15	0.12
(1,129)	1:19:A:GLN:HG3	1:22:A:ILE:HG21	15	0.12
(1,129)	1:19:A:GLN:HG3	1:22:A:ILE:HG22	15	0.12
(1,129)	1:19:A:GLN:HG3	1:22:A:ILE:HG23	15	0.12
(1,121)	1:18:A:LYS:HD2	1:51:A:HIS:HD2	23	0.12
(1,121)	1:18:A:LYS:HD3	1:51:A:HIS:HD2	23	0.12
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	37	0.12
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	37	0.12
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	37	0.12
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	37	0.12
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	37	0.12
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	37	0.12
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	37	0.12
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	37	0.12
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	37	0.12
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	3	0.12
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	31	0.12
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	32	0.12
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	39	0.12
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE1	11	0.12
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE3	11	0.12
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE1	11	0.12
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE2	11	0.12
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE3	11	0.12
(1,2264)	1:77:A:GLN:HB3	1:77:A:GLN:H	9	0.11
(1,2264)	1:77:A:GLN:HB3	1:77:A:GLN:H	28	0.11
(1,2238)	1:73:A:LYS:HB3	1:74:A:LEU:H	18	0.11
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	12	0.11
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	12	0.11
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD2	18	0.11
(1,2229)	1:72:A:HIS:H	1:73:A:LYS:HD3	18	0.11
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	2	0.11
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	3	0.11
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	5	0.11
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	11	0.11
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	17	0.11
(1,2210)	1:71:A:LEU:HB3	1:71:A:LEU:H	36	0.11
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	4	0.11
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	12	0.11
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	20	0.11
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	31	0.11
(1,2164)	1:64:A:TRP:HE1	1:60:A:MET:HG3	36	0.11
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	7	0.11
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD2	24	0.11
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD3	24	0.11
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	1	0.11
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	11	0.11
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	13	0.11
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	25	0.11
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	32	0.11
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	34	0.11
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	7	0.11
(1,2057)	1:53:A:TRP:HH2	1:78:A:TRP:H	22	0.11
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	7	0.11
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	7	0.11
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	11	0.11
(1,2056)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	11	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	16	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	16	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	16	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	29	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	29	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	29	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	33	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	33	0.11
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	33	0.11
(1,1981)	1:44:A:MET:HG2	1:47:A:LEU:H	25	0.11
(1,1981)	1:44:A:MET:HG3	1:47:A:LEU:H	25	0.11
(1,1967)	1:42:A:PRO:HB2	1:43:A:ILE:H	24	0.11
(1,1965)	1:41:A:ASP:HB3	1:43:A:ILE:H	34	0.11
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	1	0.11
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	15	0.11
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	15	0.11
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	25	0.11
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	25	0.11
(1,1924)	1:33:A:LEU:HD21	1:33:A:LEU:H	35	0.11
(1,1924)	1:33:A:LEU:HD22	1:33:A:LEU:H	35	0.11
(1,1924)	1:33:A:LEU:HD23	1:33:A:LEU:H	35	0.11
(1,1914)	1:31:A:LYS:HG2	1:34:A:VAL:H	31	0.11
(1,1914)	1:31:A:LYS:HG3	1:34:A:VAL:H	31	0.11
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	1	0.11
(1,1901)	1:28:A:ASN:HD22	1:30:A:GLN:H	1	0.11
(1,1901)	1:28:A:ASN:HD22	1:30:A:GLN:H	35	0.11
(1,1845)	1:21:A:PHE:HB3	1:21:A:PHE:H	7	0.11
(1,1766)	1:15:A:ASN:H	1:18:A:LYS:HE2	5	0.11
(1,1766)	1:15:A:ASN:H	1:18:A:LYS:HE2	21	0.11
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	38	0.11
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	10	0.11
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	12	0.11
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	17	0.11
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	4	0.11
(1,1733)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	4	0.11
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	15	0.11
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	28	0.11
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	32	0.11
(1,1688)	1:10:A:THR:HB	1:13:A:GLU:H	7	0.11
(1,1685)	1:10:A:THR:HB	1:12:A:ASP:H	8	0.11
(1,1685)	1:10:A:THR:HB	1:12:A:ASP:H	9	0.11
(1,1685)	1:10:A:THR:HB	1:12:A:ASP:H	23	0.11
(1,1685)	1:10:A:THR:HB	1:12:A:ASP:H	34	0.11
(1,1678)	1:9:A:PHE:HB3	1:58:A:ARG:HE	37	0.11
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	6	0.11
(1,1590)	1:64:A:TRP:HE3	1:70:A:ILE:HA	25	0.11
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	2	0.11
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	2	0.11
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	2	0.11
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	10	0.11
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	10	0.11
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	10	0.11
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	19	0.11
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	19	0.11
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	19	0.11
(1,1427)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	20	0.11
(1,1427)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	20	0.11
(1,1427)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	20	0.11
(1,1413)	1:34:A:VAL:HG21	1:38:A:THR:HB	2	0.11
(1,1413)	1:34:A:VAL:HG22	1:38:A:THR:HB	2	0.11
(1,1413)	1:34:A:VAL:HG23	1:38:A:THR:HB	2	0.11
(1,1413)	1:34:A:VAL:HG21	1:38:A:THR:HB	5	0.11
(1,1413)	1:34:A:VAL:HG22	1:38:A:THR:HB	5	0.11
(1,1413)	1:34:A:VAL:HG23	1:38:A:THR:HB	5	0.11
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	24	0.11
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	24	0.11
(1,1369)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	24	0.11
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	24	0.11
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	24	0.11
(1,1369)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	24	0.11
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	24	0.11
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	24	0.11
(1,1369)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	24	0.11
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	34	0.11
(1,1367)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	34	0.11
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	34	0.11
(1,1367)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	34	0.11
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	34	0.11
(1,1367)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	34	0.11
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	19	0.11
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	19	0.11
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	19	0.11
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE2	38	0.11
(1,1345)	1:23:A:SER:HB2	1:67:A:LYS:HE3	38	0.11
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE2	38	0.11
(1,1345)	1:23:A:SER:HB3	1:67:A:LYS:HE3	38	0.11
(1,1340)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	13	0.11
(1,1340)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	13	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	8	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	8	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	8	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	18	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	18	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	18	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	34	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	34	0.11
(1,1293)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	34	0.11
(1,1268)	1:18:A:LYS:HD2	1:51:A:HIS:HD2	27	0.11
(1,1268)	1:18:A:LYS:HD3	1:51:A:HIS:HD2	27	0.11
(1,1252)	1:17:A:LEU:HD11	1:70:A:ILE:HG21	34	0.11
(1,1252)	1:17:A:LEU:HD11	1:70:A:ILE:HG22	34	0.11
(1,1252)	1:17:A:LEU:HD11	1:70:A:ILE:HG23	34	0.11
(1,1252)	1:17:A:LEU:HD12	1:70:A:ILE:HG21	34	0.11
(1,1252)	1:17:A:LEU:HD12	1:70:A:ILE:HG22	34	0.11
(1,1252)	1:17:A:LEU:HD12	1:70:A:ILE:HG23	34	0.11
(1,1252)	1:17:A:LEU:HD13	1:70:A:ILE:HG21	34	0.11
(1,1252)	1:17:A:LEU:HD13	1:70:A:ILE:HG22	34	0.11
(1,1252)	1:17:A:LEU:HD13	1:70:A:ILE:HG23	34	0.11
(1,1251)	1:17:A:LEU:HD21	1:70:A:ILE:HG21	16	0.11
(1,1251)	1:17:A:LEU:HD21	1:70:A:ILE:HG22	16	0.11
(1,1251)	1:17:A:LEU:HD21	1:70:A:ILE:HG23	16	0.11
(1,1251)	1:17:A:LEU:HD22	1:70:A:ILE:HG21	16	0.11
(1,1251)	1:17:A:LEU:HD22	1:70:A:ILE:HG22	16	0.11
(1,1251)	1:17:A:LEU:HD22	1:70:A:ILE:HG23	16	0.11
(1,1251)	1:17:A:LEU:HD23	1:70:A:ILE:HG21	16	0.11
(1,1251)	1:17:A:LEU:HD23	1:70:A:ILE:HG22	16	0.11
(1,1251)	1:17:A:LEU:HD23	1:70:A:ILE:HG23	16	0.11
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	31	0.11
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	31	0.11
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	31	0.11
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	31	0.11
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	31	0.11
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	31	0.11
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	31	0.11
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	31	0.11
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	31	0.11
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	35	0.11
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	35	0.11
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	35	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	35	0.11
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	35	0.11
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	35	0.11
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	35	0.11
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	35	0.11
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	35	0.11
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	13	0.11
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	20	0.11
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	29	0.11
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE1	39	0.11
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE2	39	0.11
(1,1151)	1:3:A:LEU:HA	1:6:A:MET:HE3	39	0.11
(1,1117)	1:77:A:GLN:HB3	1:77:A:GLN:H	9	0.11
(1,1117)	1:77:A:GLN:HB3	1:77:A:GLN:H	28	0.11
(1,1091)	1:73:A:LYS:HB3	1:74:A:LEU:H	18	0.11
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	12	0.11
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	12	0.11
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD2	18	0.11
(1,1082)	1:72:A:HIS:H	1:73:A:LYS:HD3	18	0.11
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	2	0.11
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	3	0.11
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	5	0.11
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	11	0.11
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	17	0.11
(1,1063)	1:71:A:LEU:HB3	1:71:A:LEU:H	36	0.11
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	4	0.11
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	12	0.11
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	20	0.11
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	31	0.11
(1,1017)	1:64:A:TRP:HE1	1:60:A:MET:HG3	36	0.11
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	7	0.11
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD2	24	0.11
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD3	24	0.11
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	1	0.11
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	11	0.11
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	13	0.11
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	25	0.11
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	32	0.11
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	34	0.11
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	7	0.11
(1,910)	1:53:A:TRP:HH2	1:78:A:TRP:H	22	0.11
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	7	0.11
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG2	11	0.11
(1,909)	1:53:A:TRP:HE1	1:77:A:GLN:HG3	11	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	16	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	16	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	16	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	29	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	29	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	29	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	33	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	33	0.11
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	33	0.11
(1,834)	1:44:A:MET:HG2	1:47:A:LEU:H	25	0.11
(1,834)	1:44:A:MET:HG3	1:47:A:LEU:H	25	0.11
(1,820)	1:42:A:PRO:HB2	1:43:A:ILE:H	24	0.11
(1,818)	1:41:A:ASP:HB3	1:43:A:ILE:H	34	0.11
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	1	0.11
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	15	0.11
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	15	0.11
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	25	0.11
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	25	0.11
(1,777)	1:33:A:LEU:HD21	1:33:A:LEU:H	35	0.11
(1,777)	1:33:A:LEU:HD22	1:33:A:LEU:H	35	0.11
(1,777)	1:33:A:LEU:HD23	1:33:A:LEU:H	35	0.11
(1,767)	1:31:A:LYS:HG2	1:34:A:VAL:H	31	0.11
(1,767)	1:31:A:LYS:HG3	1:34:A:VAL:H	31	0.11
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	1	0.11
(1,754)	1:28:A:ASN:HD22	1:30:A:GLN:H	1	0.11
(1,754)	1:28:A:ASN:HD22	1:30:A:GLN:H	35	0.11
(1,698)	1:21:A:PHE:HB3	1:21:A:PHE:H	7	0.11
(1,619)	1:15:A:ASN:H	1:18:A:LYS:HE2	5	0.11
(1,619)	1:15:A:ASN:H	1:18:A:LYS:HE2	21	0.11
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	38	0.11
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	10	0.11
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	12	0.11
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	17	0.11
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD2	4	0.11
(1,586)	1:14:A:TRP:HE1	1:18:A:LYS:HD3	4	0.11
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	15	0.11
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	28	0.11
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	32	0.11
(1,541)	1:10:A:THR:HB	1:13:A:GLU:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:10:A:THR:HB	1:12:A:ASP:H	8	0.11
(1,538)	1:10:A:THR:HB	1:12:A:ASP:H	9	0.11
(1,538)	1:10:A:THR:HB	1:12:A:ASP:H	23	0.11
(1,538)	1:10:A:THR:HB	1:12:A:ASP:H	34	0.11
(1,531)	1:9:A:PHE:HB3	1:58:A:ARG:HE	37	0.11
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	6	0.11
(1,443)	1:64:A:TRP:HE3	1:70:A:ILE:HA	25	0.11
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	12	0.11
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	2	0.11
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	2	0.11
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	2	0.11
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	10	0.11
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	10	0.11
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	10	0.11
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	19	0.11
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	19	0.11
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	19	0.11
(1,280)	1:37:A:LEU:HD11	1:53:A:TRP:HB2	20	0.11
(1,280)	1:37:A:LEU:HD12	1:53:A:TRP:HB2	20	0.11
(1,280)	1:37:A:LEU:HD13	1:53:A:TRP:HB2	20	0.11
(1,266)	1:34:A:VAL:HG21	1:38:A:THR:HB	2	0.11
(1,266)	1:34:A:VAL:HG22	1:38:A:THR:HB	2	0.11
(1,266)	1:34:A:VAL:HG23	1:38:A:THR:HB	2	0.11
(1,266)	1:34:A:VAL:HG21	1:38:A:THR:HB	5	0.11
(1,266)	1:34:A:VAL:HG22	1:38:A:THR:HB	5	0.11
(1,266)	1:34:A:VAL:HG23	1:38:A:THR:HB	5	0.11
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD21	24	0.11
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD22	24	0.11
(1,222)	1:25:A:ILE:HG21	1:50:A:LEU:HD23	24	0.11
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD21	24	0.11
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD22	24	0.11
(1,222)	1:25:A:ILE:HG22	1:50:A:LEU:HD23	24	0.11
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD21	24	0.11
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD22	24	0.11
(1,222)	1:25:A:ILE:HG23	1:50:A:LEU:HD23	24	0.11
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG2	34	0.11
(1,220)	1:25:A:ILE:HG21	1:46:A:GLN:HG3	34	0.11
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG2	34	0.11
(1,220)	1:25:A:ILE:HG22	1:46:A:GLN:HG3	34	0.11
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG2	34	0.11
(1,220)	1:25:A:ILE:HG23	1:46:A:GLN:HG3	34	0.11
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	19	0.11
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	19	0.11
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE2	38	0.11
(1,198)	1:23:A:SER:HB2	1:67:A:LYS:HE3	38	0.11
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE2	38	0.11
(1,198)	1:23:A:SER:HB3	1:67:A:LYS:HE3	38	0.11
(1,193)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	13	0.11
(1,193)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	13	0.11
(1,193)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	13	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	8	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	8	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	8	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	18	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	18	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	18	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG21	34	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG22	34	0.11
(1,146)	1:78:A:TRP:HH2	1:22:A:ILE:HG23	34	0.11
(1,121)	1:18:A:LYS:HD2	1:51:A:HIS:HD2	27	0.11
(1,121)	1:18:A:LYS:HD3	1:51:A:HIS:HD2	27	0.11
(1,105)	1:17:A:LEU:HD11	1:70:A:ILE:HG21	34	0.11
(1,105)	1:17:A:LEU:HD11	1:70:A:ILE:HG22	34	0.11
(1,105)	1:17:A:LEU:HD11	1:70:A:ILE:HG23	34	0.11
(1,105)	1:17:A:LEU:HD12	1:70:A:ILE:HG21	34	0.11
(1,105)	1:17:A:LEU:HD12	1:70:A:ILE:HG22	34	0.11
(1,105)	1:17:A:LEU:HD12	1:70:A:ILE:HG23	34	0.11
(1,105)	1:17:A:LEU:HD13	1:70:A:ILE:HG21	34	0.11
(1,105)	1:17:A:LEU:HD13	1:70:A:ILE:HG22	34	0.11
(1,105)	1:17:A:LEU:HD13	1:70:A:ILE:HG23	34	0.11
(1,104)	1:17:A:LEU:HD21	1:70:A:ILE:HG21	16	0.11
(1,104)	1:17:A:LEU:HD21	1:70:A:ILE:HG22	16	0.11
(1,104)	1:17:A:LEU:HD21	1:70:A:ILE:HG23	16	0.11
(1,104)	1:17:A:LEU:HD22	1:70:A:ILE:HG21	16	0.11
(1,104)	1:17:A:LEU:HD22	1:70:A:ILE:HG22	16	0.11
(1,104)	1:17:A:LEU:HD22	1:70:A:ILE:HG23	16	0.11
(1,104)	1:17:A:LEU:HD23	1:70:A:ILE:HG21	16	0.11
(1,104)	1:17:A:LEU:HD23	1:70:A:ILE:HG22	16	0.11
(1,104)	1:17:A:LEU:HD23	1:70:A:ILE:HG23	16	0.11
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	31	0.11
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	31	0.11
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	31	0.11
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	31	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	31	0.11
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	31	0.11
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	31	0.11
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	31	0.11
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	31	0.11
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	35	0.11
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	35	0.11
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	35	0.11
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	35	0.11
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	35	0.11
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	35	0.11
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	35	0.11
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	35	0.11
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	35	0.11
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	13	0.11
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	20	0.11
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	29	0.11
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE1	39	0.11
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE2	39	0.11
(1,4)	1:3:A:LEU:HA	1:6:A:MET:HE3	39	0.11
(1,2264)	1:77:A:GLN:HB3	1:77:A:GLN:H	8	0.1
(1,2264)	1:77:A:GLN:HB3	1:77:A:GLN:H	31	0.1
(1,2217)	1:71:A:LEU:HB3	1:72:A:HIS:H	32	0.1
(1,2210)	1:71:A:LEU:HB3	1:71:A:LEU:H	28	0.1
(1,2191)	1:69:A:ASP:H	1:67:A:LYS:HG3	18	0.1
(1,2144)	1:62:A:GLU:H	1:65:A:LYS:H	18	0.1
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD2	13	0.1
(1,2136)	1:61:A:CYS:H	1:63:A:LYS:HD3	13	0.1
(1,2110)	1:58:A:ARG:HD2	1:58:A:ARG:H	30	0.1
(1,2109)	1:58:A:ARG:HG3	1:58:A:ARG:H	37	0.1
(1,2052)	1:53:A:TRP:HZ3	1:74:A:LEU:H	32	0.1
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD11	35	0.1
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD12	35	0.1
(1,2033)	1:51:A:HIS:H	1:54:A:LEU:HD13	35	0.1
(1,1997)	1:46:A:GLN:HB2	1:46:A:GLN:HE21	18	0.1
(1,1997)	1:46:A:GLN:HB3	1:46:A:GLN:HE21	18	0.1
(1,1993)	1:46:A:GLN:HA	1:46:A:GLN:HE22	9	0.1
(1,1981)	1:44:A:MET:HG2	1:47:A:LEU:H	38	0.1
(1,1981)	1:44:A:MET:HG3	1:47:A:LEU:H	38	0.1
(1,1974)	1:43:A:ILE:HA	1:45:A:ASN:H	21	0.1
(1,1965)	1:41:A:ASP:HB3	1:43:A:ILE:H	25	0.1
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1964)	1:41:A:ASP:HB2	1:43:A:ILE:H	24	0.1
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG2	28	0.1
(1,1963)	1:41:A:ASP:H	1:42:A:PRO:HG3	28	0.1
(1,1907)	1:29:A:GLU:HB3	1:30:A:GLN:H	7	0.1
(1,1825)	1:19:A:GLN:H	1:22:A:ILE:HB	34	0.1
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	17	0.1
(1,1759)	1:15:A:ASN:HB3	1:16:A:GLN:H	19	0.1
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	20	0.1
(1,1738)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	24	0.1
(1,1716)	1:13:A:GLU:HB2	1:15:A:ASN:H	3	0.1
(1,1707)	1:12:A:ASP:H	1:16:A:GLN:HE22	14	0.1
(1,1691)	1:10:A:THR:H	1:13:A:GLU:HB3	29	0.1
(1,1678)	1:9:A:PHE:HB3	1:58:A:ARG:HE	39	0.1
(1,1621)	1:70:A:ILE:HG21	1:74:A:LEU:HD11	36	0.1
(1,1621)	1:70:A:ILE:HG21	1:74:A:LEU:HD12	36	0.1
(1,1621)	1:70:A:ILE:HG21	1:74:A:LEU:HD13	36	0.1
(1,1621)	1:70:A:ILE:HG22	1:74:A:LEU:HD11	36	0.1
(1,1621)	1:70:A:ILE:HG22	1:74:A:LEU:HD12	36	0.1
(1,1621)	1:70:A:ILE:HG22	1:74:A:LEU:HD13	36	0.1
(1,1621)	1:70:A:ILE:HG23	1:74:A:LEU:HD11	36	0.1
(1,1621)	1:70:A:ILE:HG23	1:74:A:LEU:HD12	36	0.1
(1,1621)	1:70:A:ILE:HG23	1:74:A:LEU:HD13	36	0.1
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	4	0.1
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	4	0.1
(1,1592)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	4	0.1
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	25	0.1
(1,1520)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	34	0.1
(1,1452)	1:44:A:MET:HE1	1:47:A:LEU:HA	21	0.1
(1,1452)	1:44:A:MET:HE2	1:47:A:LEU:HA	21	0.1
(1,1452)	1:44:A:MET:HE3	1:47:A:LEU:HA	21	0.1
(1,1414)	1:34:A:VAL:HG21	1:47:A:LEU:HA	34	0.1
(1,1414)	1:34:A:VAL:HG22	1:47:A:LEU:HA	34	0.1
(1,1414)	1:34:A:VAL:HG23	1:47:A:LEU:HA	34	0.1
(1,1366)	1:25:A:ILE:HG21	1:43:A:ILE:HA	24	0.1
(1,1366)	1:25:A:ILE:HG22	1:43:A:ILE:HA	24	0.1
(1,1366)	1:25:A:ILE:HG23	1:43:A:ILE:HA	24	0.1
(1,1347)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	36	0.1
(1,1340)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	12	0.1
(1,1340)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	12	0.1
(1,1340)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	12	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	2	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	2	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	37	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	37	0.1
(1,1296)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	37	0.1
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	32	0.1
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	32	0.1
(1,1249)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	32	0.1
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	32	0.1
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	32	0.1
(1,1249)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	32	0.1
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	32	0.1
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	32	0.1
(1,1249)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	32	0.1
(1,1223)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	25	0.1
(1,1217)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	17	0.1
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE1	31	0.1
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE2	31	0.1
(1,1152)	1:4:A:GLY:HA2	1:6:A:MET:HE3	31	0.1
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE1	31	0.1
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE2	31	0.1
(1,1152)	1:4:A:GLY:HA3	1:6:A:MET:HE3	31	0.1
(1,1117)	1:77:A:GLN:HB3	1:77:A:GLN:H	8	0.1
(1,1117)	1:77:A:GLN:HB3	1:77:A:GLN:H	31	0.1
(1,1070)	1:71:A:LEU:HB3	1:72:A:HIS:H	32	0.1
(1,1063)	1:71:A:LEU:HB3	1:71:A:LEU:H	28	0.1
(1,1044)	1:69:A:ASP:H	1:67:A:LYS:HG3	18	0.1
(1,997)	1:62:A:GLU:H	1:65:A:LYS:H	18	0.1
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD2	13	0.1
(1,989)	1:61:A:CYS:H	1:63:A:LYS:HD3	13	0.1
(1,963)	1:58:A:ARG:HD2	1:58:A:ARG:H	30	0.1
(1,962)	1:58:A:ARG:HG3	1:58:A:ARG:H	37	0.1
(1,905)	1:53:A:TRP:HZ3	1:74:A:LEU:H	32	0.1
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD11	35	0.1
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD12	35	0.1
(1,886)	1:51:A:HIS:H	1:54:A:LEU:HD13	35	0.1
(1,850)	1:46:A:GLN:HB2	1:46:A:GLN:HE21	18	0.1
(1,850)	1:46:A:GLN:HB3	1:46:A:GLN:HE21	18	0.1
(1,846)	1:46:A:GLN:HA	1:46:A:GLN:HE22	9	0.1
(1,834)	1:44:A:MET:HG2	1:47:A:LEU:H	38	0.1
(1,834)	1:44:A:MET:HG3	1:47:A:LEU:H	38	0.1
(1,827)	1:43:A:ILE:HA	1:45:A:ASN:H	21	0.1
(1,818)	1:41:A:ASP:HB3	1:43:A:ILE:H	25	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	9	0.1
(1,817)	1:41:A:ASP:HB2	1:43:A:ILE:H	24	0.1
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG2	28	0.1
(1,816)	1:41:A:ASP:H	1:42:A:PRO:HG3	28	0.1
(1,760)	1:29:A:GLU:HB3	1:30:A:GLN:H	7	0.1
(1,678)	1:19:A:GLN:H	1:22:A:ILE:HB	34	0.1
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	17	0.1
(1,612)	1:15:A:ASN:HB3	1:16:A:GLN:H	19	0.1
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	20	0.1
(1,591)	1:14:A:TRP:HE1	1:54:A:LEU:HB2	24	0.1
(1,569)	1:13:A:GLU:HB2	1:15:A:ASN:H	3	0.1
(1,560)	1:12:A:ASP:H	1:16:A:GLN:HE22	14	0.1
(1,544)	1:10:A:THR:H	1:13:A:GLU:HB3	29	0.1
(1,531)	1:9:A:PHE:HB3	1:58:A:ARG:HE	39	0.1
(1,474)	1:70:A:ILE:HG21	1:74:A:LEU:HD11	36	0.1
(1,474)	1:70:A:ILE:HG21	1:74:A:LEU:HD12	36	0.1
(1,474)	1:70:A:ILE:HG21	1:74:A:LEU:HD13	36	0.1
(1,474)	1:70:A:ILE:HG22	1:74:A:LEU:HD11	36	0.1
(1,474)	1:70:A:ILE:HG22	1:74:A:LEU:HD12	36	0.1
(1,474)	1:70:A:ILE:HG22	1:74:A:LEU:HD13	36	0.1
(1,474)	1:70:A:ILE:HG23	1:74:A:LEU:HD11	36	0.1
(1,474)	1:70:A:ILE:HG23	1:74:A:LEU:HD12	36	0.1
(1,474)	1:70:A:ILE:HG23	1:74:A:LEU:HD13	36	0.1
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG21	4	0.1
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG22	4	0.1
(1,445)	1:64:A:TRP:HH2	1:70:A:ILE:HG23	4	0.1
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	25	0.1
(1,373)	1:53:A:TRP:HZ2	1:78:A:TRP:HE3	34	0.1
(1,305)	1:44:A:MET:HE1	1:47:A:LEU:HA	21	0.1
(1,305)	1:44:A:MET:HE2	1:47:A:LEU:HA	21	0.1
(1,305)	1:44:A:MET:HE3	1:47:A:LEU:HA	21	0.1
(1,267)	1:34:A:VAL:HG21	1:47:A:LEU:HA	34	0.1
(1,267)	1:34:A:VAL:HG22	1:47:A:LEU:HA	34	0.1
(1,267)	1:34:A:VAL:HG23	1:47:A:LEU:HA	34	0.1
(1,219)	1:25:A:ILE:HG21	1:43:A:ILE:HA	24	0.1
(1,219)	1:25:A:ILE:HG22	1:43:A:ILE:HA	24	0.1
(1,219)	1:25:A:ILE:HG23	1:43:A:ILE:HA	24	0.1
(1,200)	1:24:A:GLY:HA3	1:27:A:GLU:HG3	36	0.1
(1,193)	1:22:A:ILE:HD11	1:51:A:HIS:HD2	12	0.1
(1,193)	1:22:A:ILE:HD12	1:51:A:HIS:HD2	12	0.1
(1,193)	1:22:A:ILE:HD13	1:51:A:HIS:HD2	12	0.1
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	2	0.1
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	2	0.1
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD11	37	0.1
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD12	37	0.1
(1,149)	1:21:A:PHE:HB2	1:50:A:LEU:HD13	37	0.1
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD11	32	0.1
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD12	32	0.1
(1,102)	1:17:A:LEU:HD11	1:54:A:LEU:HD13	32	0.1
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD11	32	0.1
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD12	32	0.1
(1,102)	1:17:A:LEU:HD12	1:54:A:LEU:HD13	32	0.1
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD11	32	0.1
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD12	32	0.1
(1,102)	1:17:A:LEU:HD13	1:54:A:LEU:HD13	32	0.1
(1,76)	1:14:A:TRP:HZ2	1:55:A:ASP:HA	25	0.1
(1,70)	1:14:A:TRP:HZ2	1:54:A:LEU:HB2	17	0.1
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE1	31	0.1
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE2	31	0.1
(1,5)	1:4:A:GLY:HA2	1:6:A:MET:HE3	31	0.1
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE1	31	0.1
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE2	31	0.1
(1,5)	1:4:A:GLY:HA3	1:6:A:MET:HE3	31	0.1

10 Dihedral-angle violation analysis ⓘ

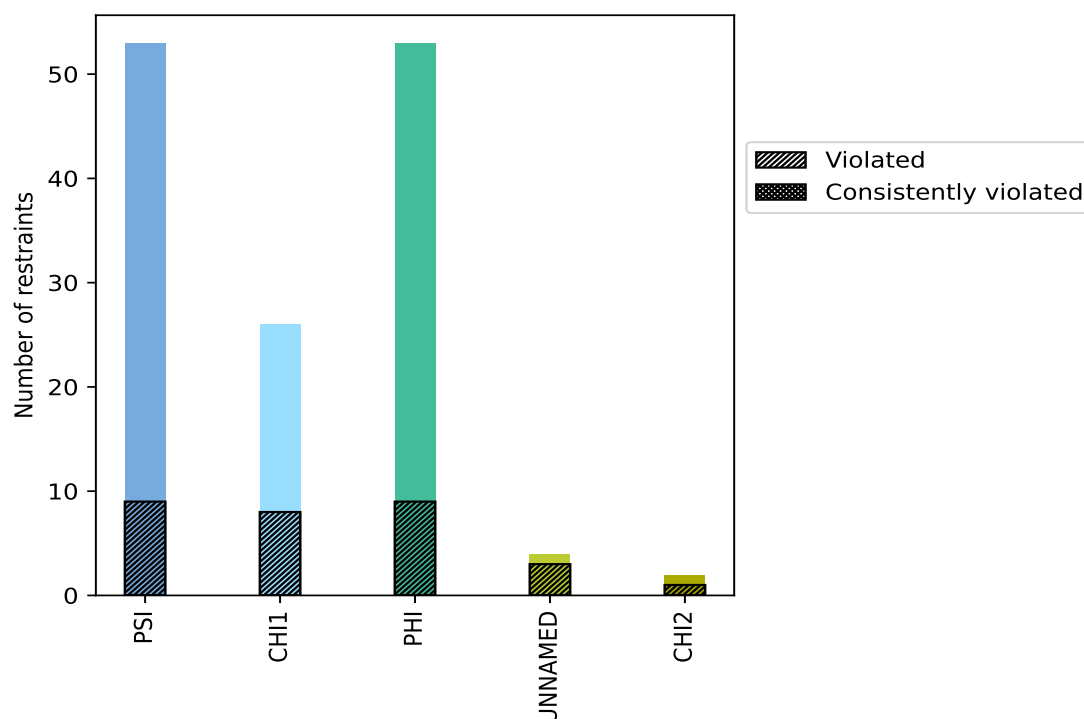
10.1 Summary of dihedral-angle violations ⓘ

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	53	38.4	9	17.0	6.5	0	0.0	0.0
CHI1	26	18.8	8	30.8	5.8	0	0.0	0.0
PHI	53	38.4	9	17.0	6.5	0	0.0	0.0
UNNAMED	4	2.9	3	75.0	2.2	0	0.0	0.0
CHI2	2	1.4	1	50.0	0.7	0	0.0	0.0
Total	138	100.0	30	21.7	21.7	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ



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

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

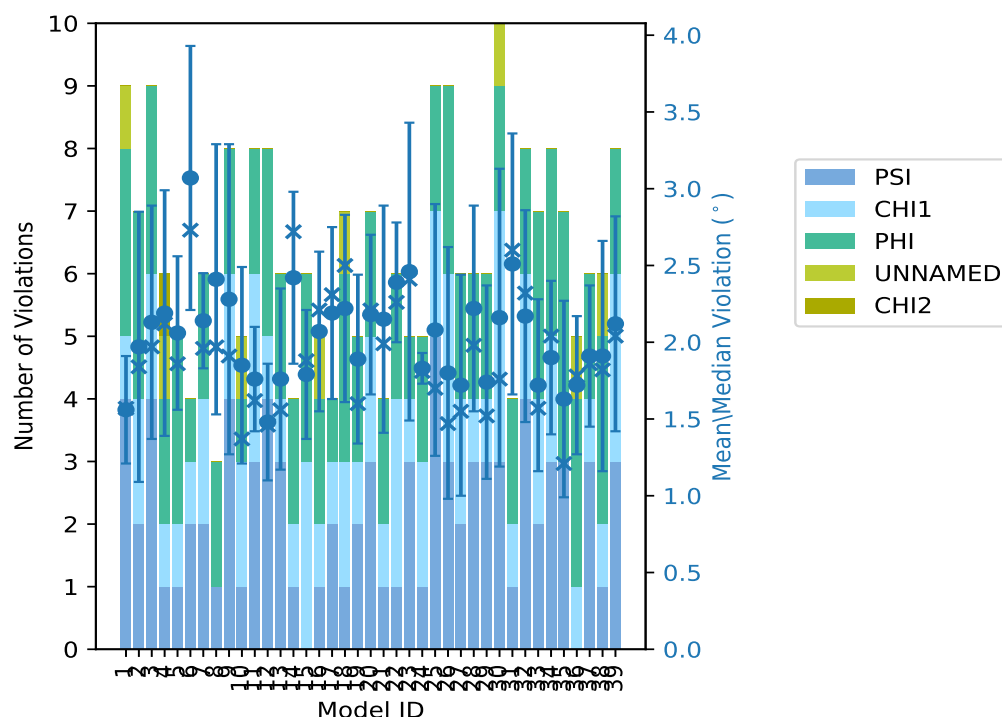
Model ID	Number of violations						Mean (°)	Max (°)	SD (°)	Median
	PSI	CHI1	PHI	UNNAMED	CHI2	Total				
1	4	1	3	1	0	9	1.56	2.29	0.35	1.57
2	2	2	3	0	0	7	1.97	3.75	0.88	1.84
3	4	2	3	0	0	9	2.13	3.42	0.76	1.97
4	1	1	2	1	1	6	2.19	3.26	0.8	2.12
5	1	1	3	0	0	5	2.06	2.7	0.5	1.86
6	2	1	1	0	0	4	3.07	4.52	0.86	2.73
7	2	2	2	0	0	6	2.14	2.65	0.31	1.96
8	1	0	2	0	0	3	2.41	3.63	0.88	1.97
9	4	2	2	0	0	8	2.28	4.05	1.01	1.91
10	1	2	1	1	0	5	1.85	2.75	0.64	1.37
11	3	3	2	0	0	8	1.76	2.25	0.34	1.62
12	4	1	3	0	0	8	1.48	1.99	0.38	1.46
13	3	1	2	0	0	6	1.76	2.57	0.59	1.56
14	1	1	2	0	0	4	2.42	2.81	0.56	2.72
15	0	3	3	0	0	6	1.79	2.34	0.42	1.88
16	1	1	2	1	0	5	2.07	2.77	0.52	2.21
17	2	1	1	0	0	4	2.19	2.76	0.56	2.31
18	1	2	3	1	0	7	2.22	2.83	0.61	2.5
19	2	1	2	0	0	5	1.89	2.58	0.55	1.6
20	3	2	2	0	0	7	2.18	2.76	0.52	2.21
21	1	1	2	0	0	4	2.15	3.26	0.74	1.99
22	1	3	2	0	0	6	2.39	3.13	0.39	2.26
23	3	1	1	0	0	5	2.46	4.13	0.97	2.41
24	1	2	2	0	0	5	1.83	1.97	0.1	1.81
25	5	2	2	0	0	9	2.08	3.91	0.82	1.7
26	3	3	3	0	0	9	1.8	2.97	0.82	1.47
27	2	2	2	0	0	6	1.72	3.22	0.72	1.55
28	3	1	2	0	0	6	2.22	3.3	0.67	1.98
29	3	1	2	0	0	6	1.74	2.85	0.63	1.52
30	3	4	2	1	0	10	2.16	4.13	0.97	1.76
31	1	1	2	0	0	4	2.51	3.62	0.85	2.6
32	4	2	2	0	0	8	2.17	3.14	0.69	2.32
33	2	2	3	0	0	7	1.72	2.72	0.56	1.57
34	3	2	3	0	0	8	1.9	2.57	0.5	2.04
35	3	0	4	0	0	7	1.63	2.8	0.64	1.21
36	0	1	3	1	0	5	1.72	2.47	0.45	1.78
37	3	1	2	0	0	6	1.91	2.65	0.46	1.86
38	1	1	3	1	0	6	1.91	3.36	0.75	1.82

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Model ID	Number of violations						Mean (°)	Max (°)	SD (°)	Median
	PSI	CHI1	PHI	UNNAMED	CHI2	Total				
39	3	3	2	0	0	8	2.12	3.24	0.7	2.04

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints						Fraction of the ensemble	
PSI	CHI1	PHI	UNNAMED	CHI2	Total	Count ¹	%
3	3	2	1	1	10	1	2.6
1	2	3	1	0	7	2	5.1
0	0	1	0	0	1	3	7.7
0	0	1	0	0	1	4	10.3
0	0	0	1	0	1	5	12.8

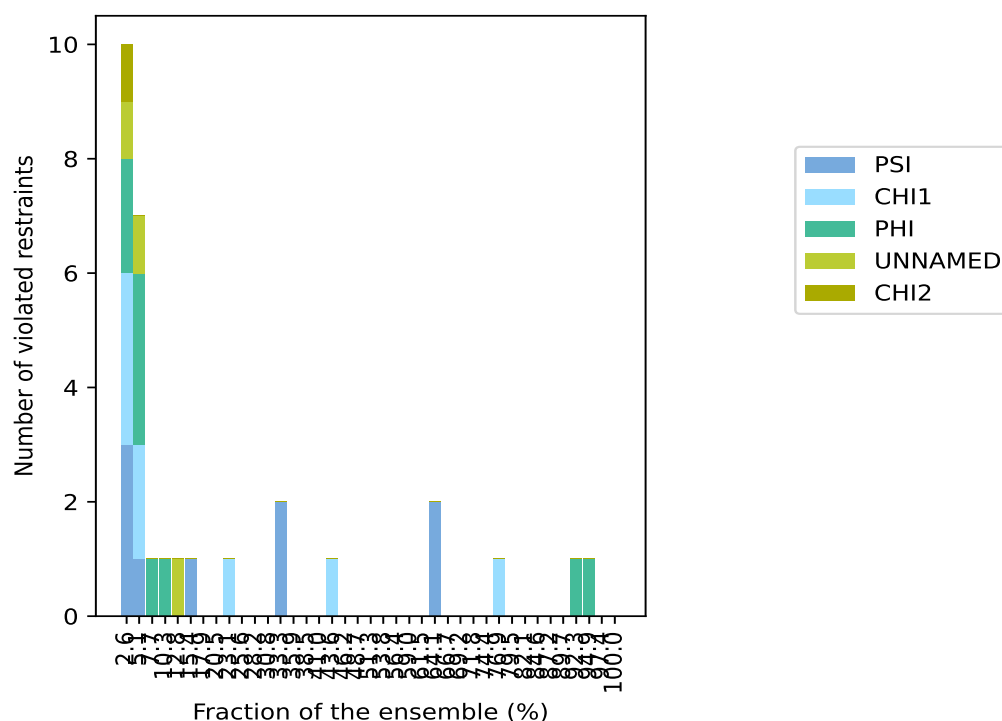
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PSI	Number of violated restraints					Fraction of the ensemble	
	CHI1	PHI	UNNAMED	CHI2	Total	Count ¹	%
1	0	0	0	0	1	6	15.4
0	0	0	0	0	0	7	17.9
0	0	0	0	0	0	8	20.5
0	1	0	0	0	1	9	23.1
0	0	0	0	0	0	10	25.6
0	0	0	0	0	0	11	28.2
0	0	0	0	0	0	12	30.8
2	0	0	0	0	2	13	33.3
0	0	0	0	0	0	14	35.9
0	0	0	0	0	0	15	38.5
0	0	0	0	0	0	16	41.0
0	1	0	0	0	1	17	43.6
0	0	0	0	0	0	18	46.2
0	0	0	0	0	0	19	48.7
0	0	0	0	0	0	20	51.3
0	0	0	0	0	0	21	53.8
0	0	0	0	0	0	22	56.4
0	0	0	0	0	0	23	59.0
0	0	0	0	0	0	24	61.5
2	0	0	0	0	2	25	64.1
0	0	0	0	0	0	26	66.7
0	0	0	0	0	0	27	69.2
0	0	0	0	0	0	28	71.8
0	0	0	0	0	0	29	74.4
0	1	0	0	0	1	30	76.9
0	0	0	0	0	0	31	79.5
0	0	0	0	0	0	32	82.1
0	0	0	0	0	0	33	84.6
0	0	0	0	0	0	34	87.2
0	0	0	0	0	0	35	89.7
0	0	1	0	0	1	36	92.3
0	0	1	0	0	1	37	94.9
0	0	0	0	0	0	38	97.4
0	0	0	0	0	0	39	100.0

¹ Number of models with violations

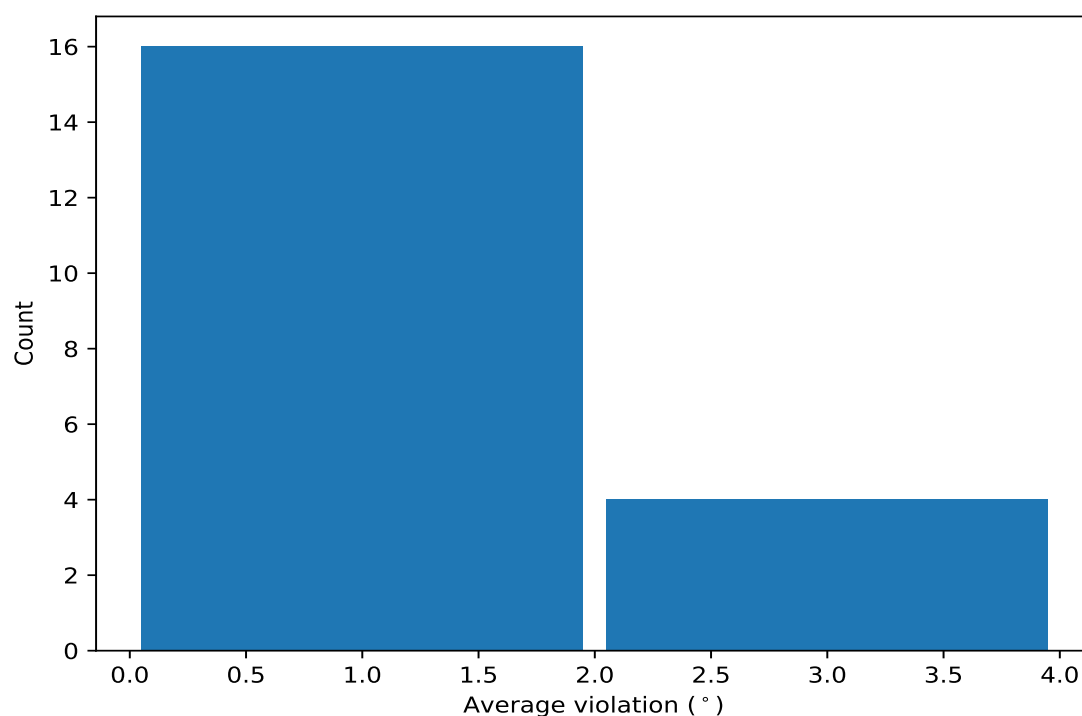
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

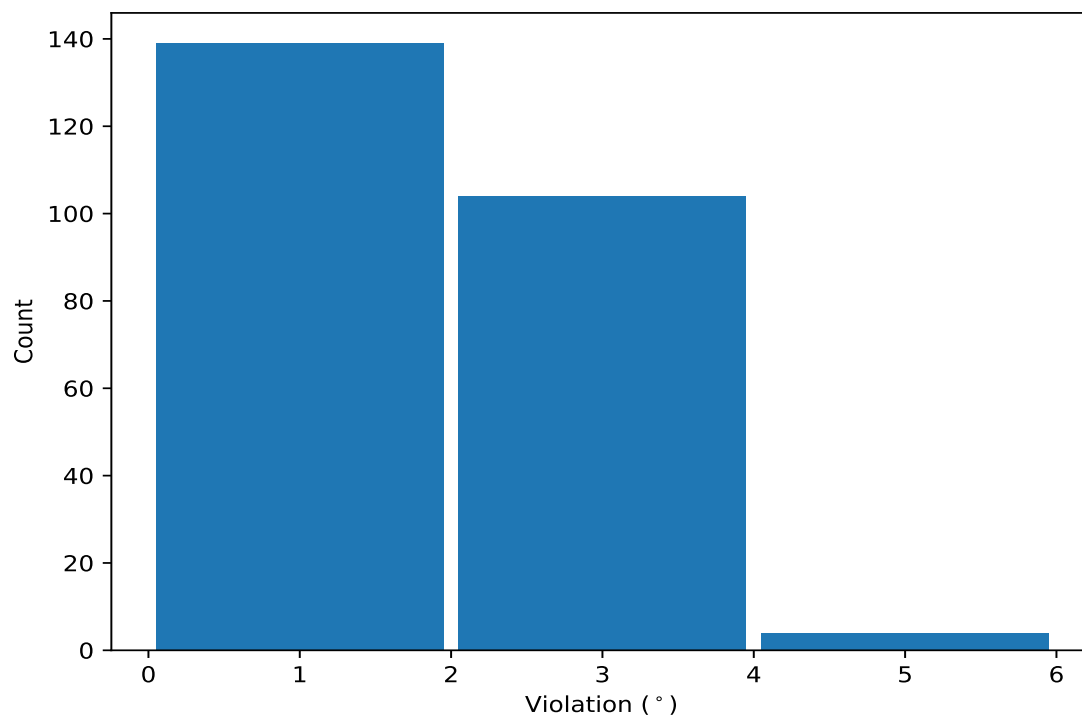
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	37	2.2	0.61	2.06
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	36	1.98	0.59	2.04
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	30	2.69	0.78	2.61
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	25	1.97	0.62	1.81
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	25	1.89	0.62	1.64
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	17	2.37	0.73	2.21
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	13	1.78	0.6	1.73
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	13	1.74	0.57	1.52
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	9	1.95	0.69	1.82
(1,88)	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1:55:A:ASP:N	6	1.55	0.56	1.32
(1,135)	1:54:A:LEU:CA	1:54:A:LEU:CB	1:54:A:LEU:CG	1:54:A:LEU:CD2	5	1.65	0.5	1.49
(1,21)	1:29:A:GLU:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	4	1.16	0.24	1.04
(1,28)	1:42:A:PRO:C	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	3	1.55	0.57	1.18
(1,124)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:CB	1:71:A:LEU:CG	2	2.55	1.12	2.55
(1,58)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:GLU:N	2	1.64	0.05	1.64
(1,137)	1:26:A:LEU:CA	1:26:A:LEU:CB	1:26:A:LEU:CG	1:26:A:LEU:CD2	2	1.57	0.11	1.57
(1,35)	1:53:A:TRP:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	2	1.23	0.18	1.23
(1,39)	1:58:A:ARG:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	2	1.18	0.07	1.18
(1,30)	1:48:A:ASP:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	2	1.14	0.04	1.14
(1,123)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:CB	1:66:A:SER:OG	2	1.02	0.02	1.02

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	6	4.52
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	30	4.13
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	23	4.13
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	9	4.05
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	25	3.91
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	2	3.75
(1,124)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:CB	1:71:A:LEU:CG	9	3.67
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	8	3.63
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	31	3.62
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	30	3.53
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	3	3.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	38	3.36
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	3	3.34
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	28	3.3
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	4	3.26
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	21	3.26
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	39	3.24
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	27	3.22
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	32	3.14
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	22	3.13
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	4	3.12
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	39	3.0
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	26	2.97
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	26	2.94
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	28	2.91
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	32	2.9
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	26	2.88
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	29	2.85
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	18	2.83
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	14	2.81
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	35	2.8
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	16	2.77
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	17	2.76
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	18	2.76
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	20	2.76
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	14	2.76
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	10	2.75
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	23	2.75
(1,88)	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1:55:A:ASP:N	6	2.74
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	20	2.73
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	33	2.72
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	6	2.72
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	25	2.7
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	9	2.7
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	5	2.7
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	17	2.69
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	31	2.68
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	14	2.67
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	25	2.67
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	20	2.67
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	7	2.65
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	37	2.65
(1,135)	1:54:A:LEU:CA	1:54:A:LEU:CB	1:54:A:LEU:CG	1:54:A:LEU:CD2	18	2.62
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	5	2.62
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	32	2.6
(1,122)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:CB	1:61:A:CYS:SG	22	2.6
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	30	2.58
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	19	2.58
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	13	2.57
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	34	2.57
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	13	2.54
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	3	2.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	10	2.52
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	2	2.52
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	30	2.52
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	19	2.51
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	31	2.51
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	7	2.5
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	18	2.5
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	36	2.47
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	16	2.44
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	23	2.41
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	22	2.41
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	21	2.38
(1,28)	1:42:A:PRO:C	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	35	2.36
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	33	2.35
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	15	2.34
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	32	2.34
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	39	2.31
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	34	2.31
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	6	2.3
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	1	2.29
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	32	2.29
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	11	2.25
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	29	2.23
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	34	2.23
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	18	2.22
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	34	2.21
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	20	2.21
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	16	2.21
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	37	2.2
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	11	2.19
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	4	2.19
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	28	2.18
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	37	2.13
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	38	2.13
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	39	2.12
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	22	2.11
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	11	2.09
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	2	2.09
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	22	2.07
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	4	2.06
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	9	2.06
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	25	2.05
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	15	2.02
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	38	2.01
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	22	2.0
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	7	2.0
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	12	1.99
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	3	1.97
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	8	1.97
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	39	1.97
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	3	1.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	24	1.97
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	15	1.94
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	20	1.93
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	17	1.93
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	7	1.92
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	24	1.91
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	7	1.91
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	39	1.9
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	1	1.89
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	7	1.87
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	34	1.87
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	12	1.87
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	5	1.86
(1,134)	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	1:74:A:LEU:CD2	36	1.85
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	2	1.84
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	30	1.83
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	15	1.82
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	24	1.81
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	27	1.79
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	36	1.78
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	12	1.78
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	28	1.78
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	29	1.77
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	9	1.76
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	12	1.75
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	24	1.73
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	3	1.73
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	13	1.73
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	35	1.72
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	24	1.72
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	1	1.71
(1,115)	1:21:A:PHE:N	1:21:A:PHE:CA	1:21:A:PHE:CB	1:21:A:PHE:CG	34	1.7
(1,58)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:GLU:N	33	1.7
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	25	1.7
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	30	1.69
(1,137)	1:26:A:LEU:CA	1:26:A:LEU:CB	1:26:A:LEU:CG	1:26:A:LEU:CD2	30	1.68
(1,88)	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1:55:A:ASP:N	28	1.67
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	3	1.66
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	11	1.65
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	26	1.64
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	38	1.64
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	23	1.63
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	30	1.62
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	8	1.62
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	27	1.61
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	15	1.61
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	19	1.6
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	21	1.6
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	37	1.59
(1,58)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:GLU:N	25	1.59
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	25	1.58

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	11	1.58
(1,54)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:PHE:N	11	1.58
(1,21)	1:29:A:GLU:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	5	1.58
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1	1.58
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	37	1.58
(1,135)	1:54:A:LEU:CA	1:54:A:LEU:CB	1:54:A:LEU:CG	1:54:A:LEU:CD2	1	1.57
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	20	1.57
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	32	1.57
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	33	1.57
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	5	1.56
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	19	1.54
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	32	1.52
(1,135)	1:54:A:LEU:CA	1:54:A:LEU:CB	1:54:A:LEU:CG	1:54:A:LEU:CD2	4	1.49
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	16	1.49
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	27	1.49
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	11	1.48
(1,130)	1:25:A:ILE:N	1:25:A:ILE:CA	1:25:A:ILE:CB	1:25:A:ILE:CG1	26	1.47
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	28	1.47
(1,137)	1:26:A:LEU:CA	1:26:A:LEU:CB	1:26:A:LEU:CG	1:26:A:LEU:CD2	16	1.46
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	14	1.46
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	3	1.45
(1,124)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:CB	1:71:A:LEU:CG	1	1.43
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	20	1.42
(1,35)	1:53:A:TRP:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	18	1.41
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	9	1.4
(1,67)	1:21:A:PHE:N	1:21:A:PHE:CA	1:21:A:PHE:C	1:22:A:ILE:N	17	1.4
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	13	1.39
(1,88)	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1:55:A:ASP:N	39	1.39
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	23	1.39
(1,126)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:CB	1:74:A:LEU:CG	10	1.37
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	21	1.36
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	33	1.36
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	9	1.36
(1,135)	1:54:A:LEU:CA	1:54:A:LEU:CB	1:54:A:LEU:CG	1:54:A:LEU:CD2	10	1.32
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	2	1.32
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	33	1.32
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	10	1.31
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	37	1.3
(1,125)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:CB	1:73:A:LYS:CG	11	1.28
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	29	1.26
(1,88)	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1:55:A:ASP:N	9	1.26
(1,39)	1:58:A:ARG:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	36	1.26
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	25	1.26
(1,121)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:CB	1:60:A:MET:CG	36	1.25
(1,135)	1:54:A:LEU:CA	1:54:A:LEU:CB	1:54:A:LEU:CG	1:54:A:LEU:CD2	38	1.24
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	25	1.24
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	31	1.24
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	19	1.23
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	1	1.22
(1,93)	1:60:A:MET:N	1:60:A:MET:CA	1:60:A:MET:C	1:61:A:CYS:N	35	1.21
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	18	1.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	35	1.2
(1,8)	1:14:A:TRP:C	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	2	1.2
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	27	1.19
(1,30)	1:48:A:ASP:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1	1.19
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	12	1.18
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	13	1.18
(1,28)	1:42:A:PRO:C	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	34	1.18
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	13	1.17
(1,88)	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1:55:A:ASP:N	29	1.15
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1	1.15
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	29	1.15
(1,95)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LYS:N	34	1.12
(1,39)	1:58:A:ARG:C	1:59:A:ASP:N	1:59:A:ASP:CA	1:59:A:ASP:C	26	1.11
(1,32)	1:50:A:LEU:C	1:51:A:HIS:N	1:51:A:HIS:CA	1:51:A:HIS:C	12	1.11
(1,28)	1:42:A:PRO:C	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	3	1.11
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	35	1.1
(1,30)	1:48:A:ASP:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	26	1.1
(1,88)	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1:55:A:ASP:N	12	1.09
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	26	1.06
(1,31)	1:49:A:LEU:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	12	1.06
(1,21)	1:29:A:GLU:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	38	1.06
(1,133)	1:22:A:ILE:CA	1:22:A:ILE:CB	1:22:A:ILE:CG1	1:22:A:ILE:CD1	4	1.05
(1,91)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:ASP:N	30	1.05
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	2	1.05
(1,123)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:CB	1:66:A:SER:OG	26	1.04
(1,35)	1:53:A:TRP:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	35	1.04
(1,15)	1:21:A:PHE:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	27	1.03
(1,94)	1:61:A:CYS:N	1:61:A:CYS:CA	1:61:A:CYS:C	1:62:A:GLU:N	32	1.01
(1,84)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:HIS:N	39	1.01
(1,21)	1:29:A:GLU:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	33	1.01
(1,123)	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:CB	1:66:A:SER:OG	30	1.0
(1,21)	1:29:A:GLU:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	15	1.0