



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 AM UTC

PDB ID : 2LX0 / pdb_00002lx0
BMRB ID : 18655
Title : Arced helix (ArcH) NMR structure of the reovirus p14 fusion-associated small transmembrane (FAST) protein transmembrane domain (TMD) in dodecyl phosphocholine (DPC) micelles
Authors : Sarker, M.; Key, T.; Duncan, R.; Rainey, J.K.
Deposited on : 2012-08-10

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

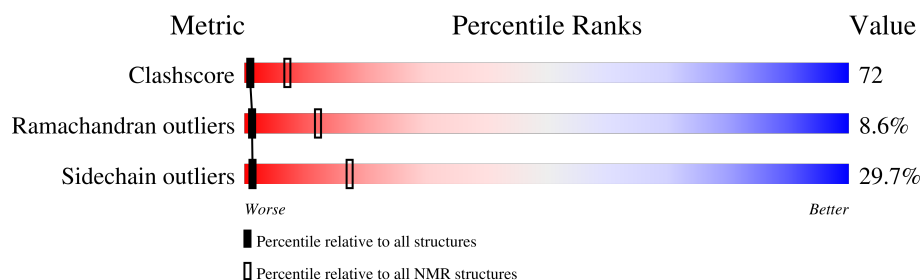
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 57%.

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	32	

2 Ensemble composition and analysis

This entry contains 50 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:31 (28)	0.38	10

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 7 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 10, 11, 13, 20, 22, 23, 25, 28, 32, 33, 34, 36, 37, 40, 47
2	4, 9, 15, 21, 24, 27, 38, 43, 44
3	5, 7, 8, 12, 14, 17, 39, 50
4	19, 29, 30, 31
5	35, 41
6	16, 18
7	42, 48
Single-model clusters	26; 45; 46; 49

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 567 atoms, of which 294 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Membrane fusion protein p14.

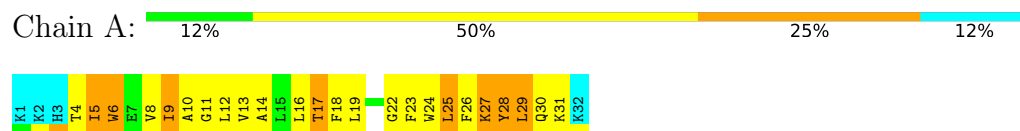
Mol	Chain	Residues	Atoms					Trace
1	A	32	Total	C	H	N	O	0
			567	192	294	42	39	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Membrane fusion protein p14

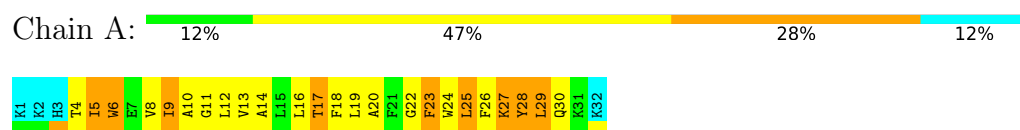


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

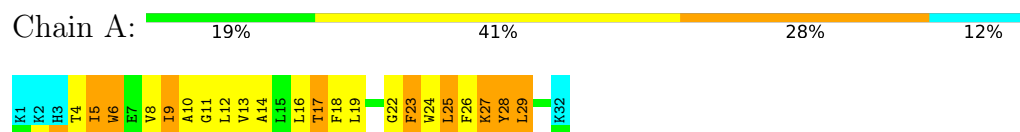
4.2.1 Score per residue for model 1

- Molecule 1: Membrane fusion protein p14



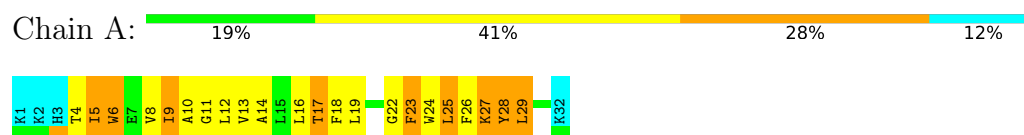
4.2.2 Score per residue for model 2

- Molecule 1: Membrane fusion protein p14



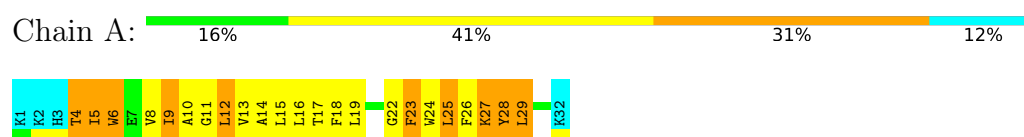
4.2.3 Score per residue for model 3

- Molecule 1: Membrane fusion protein p14



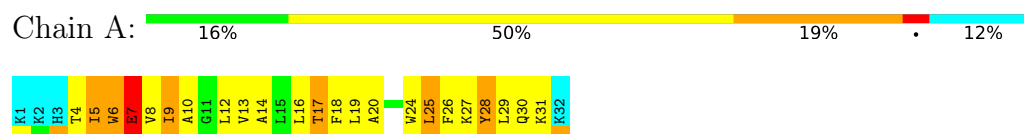
4.2.4 Score per residue for model 4

- Molecule 1: Membrane fusion protein p14



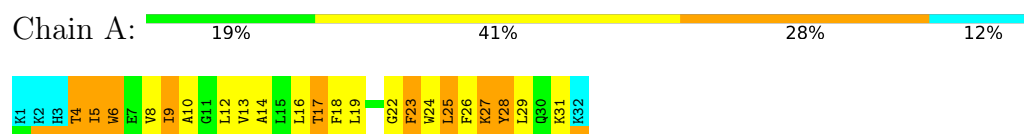
4.2.5 Score per residue for model 5

- Molecule 1: Membrane fusion protein p14



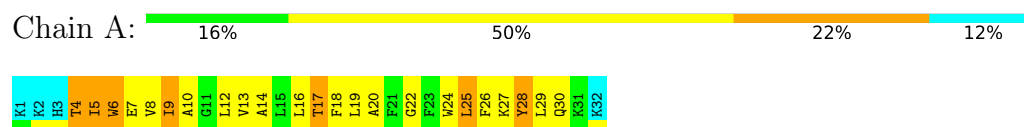
4.2.6 Score per residue for model 6

- Molecule 1: Membrane fusion protein p14



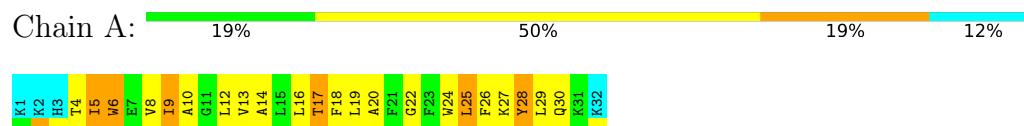
4.2.7 Score per residue for model 7

- Molecule 1: Membrane fusion protein p14



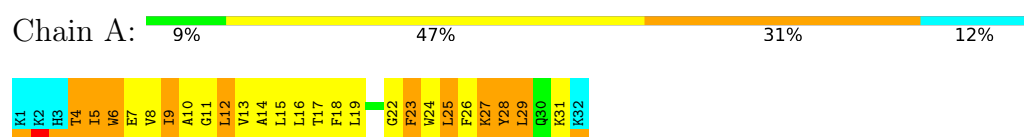
4.2.8 Score per residue for model 8

- Molecule 1: Membrane fusion protein p14



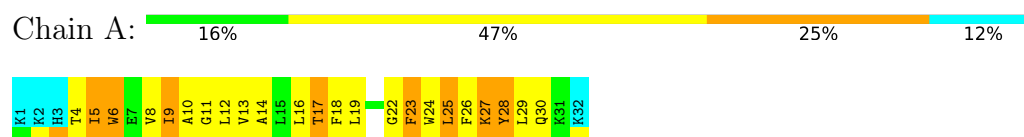
4.2.9 Score per residue for model 9

- Molecule 1: Membrane fusion protein p14



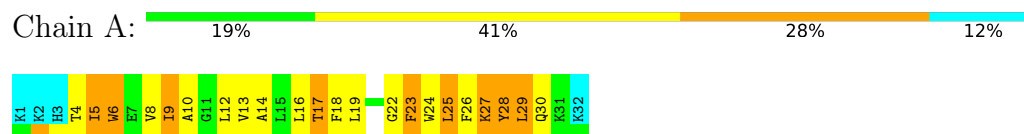
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Membrane fusion protein p14



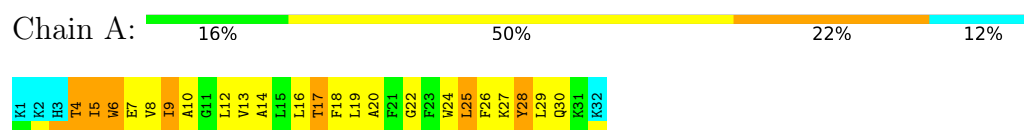
4.2.11 Score per residue for model 11

- Molecule 1: Membrane fusion protein p14



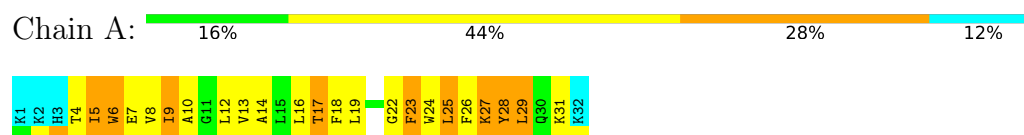
4.2.12 Score per residue for model 12

- Molecule 1: Membrane fusion protein p14



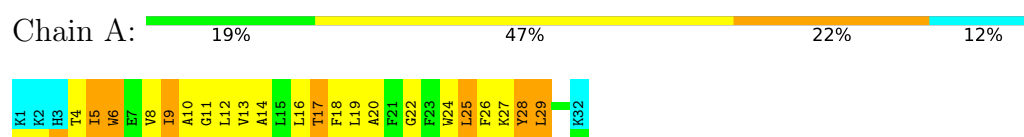
4.2.13 Score per residue for model 13

- Molecule 1: Membrane fusion protein p14



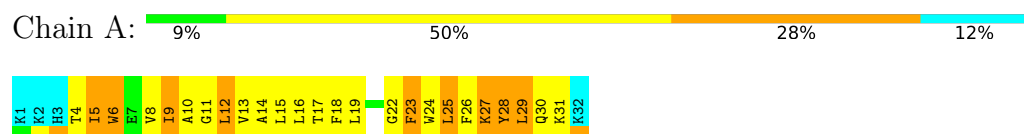
4.2.14 Score per residue for model 14

- Molecule 1: Membrane fusion protein p14



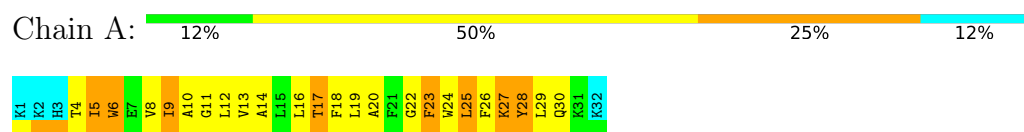
4.2.15 Score per residue for model 15

- Molecule 1: Membrane fusion protein p14



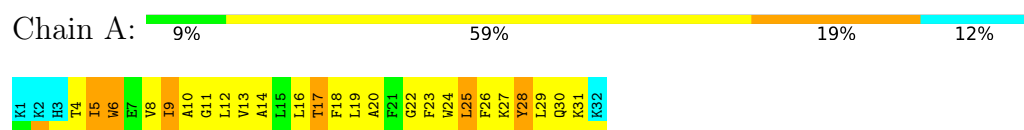
4.2.16 Score per residue for model 16

- Molecule 1: Membrane fusion protein p14



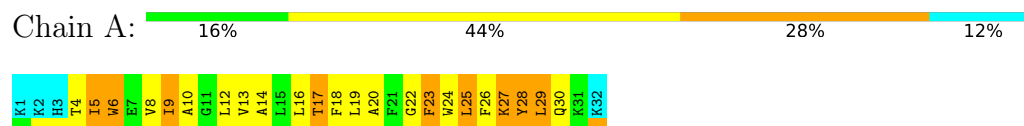
4.2.17 Score per residue for model 17

- Molecule 1: Membrane fusion protein p14



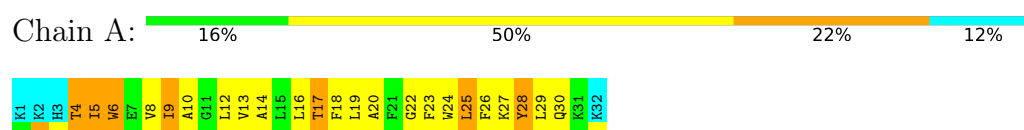
4.2.18 Score per residue for model 18

- Molecule 1: Membrane fusion protein p14



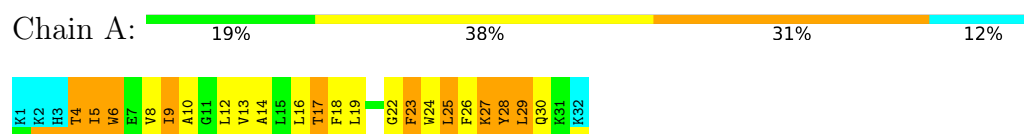
4.2.19 Score per residue for model 19

- Molecule 1: Membrane fusion protein p14



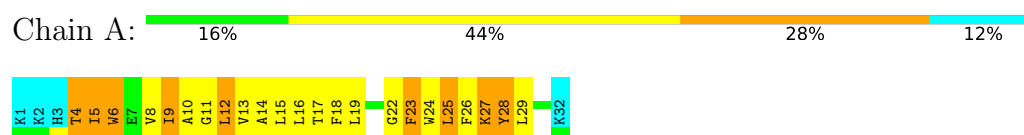
4.2.20 Score per residue for model 20

- Molecule 1: Membrane fusion protein p14



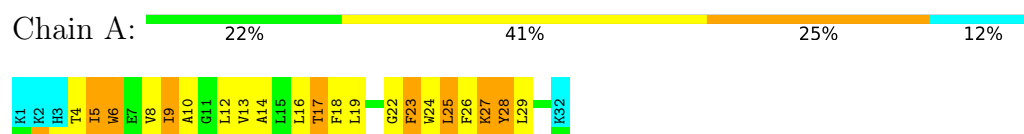
4.2.21 Score per residue for model 21

- Molecule 1: Membrane fusion protein p14



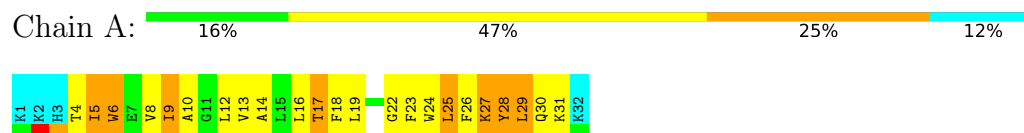
4.2.22 Score per residue for model 22

- Molecule 1: Membrane fusion protein p14



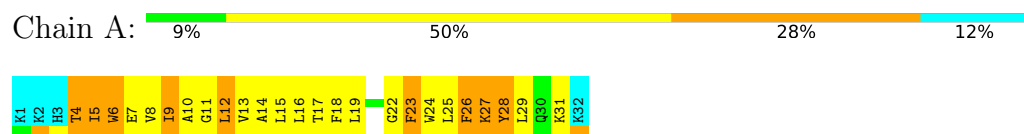
4.2.23 Score per residue for model 23

- Molecule 1: Membrane fusion protein p14



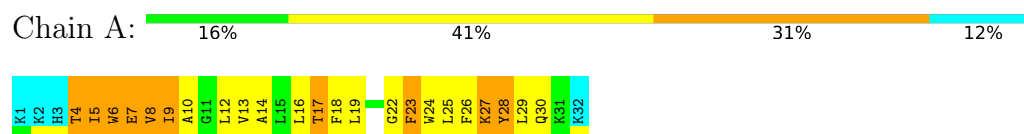
4.2.24 Score per residue for model 24

- Molecule 1: Membrane fusion protein p14



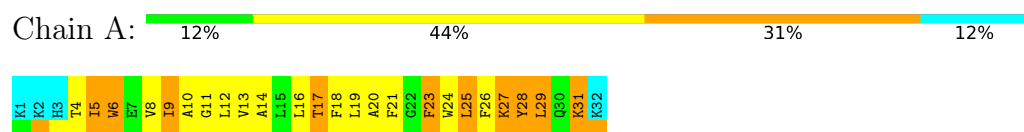
4.2.25 Score per residue for model 25

- Molecule 1: Membrane fusion protein p14



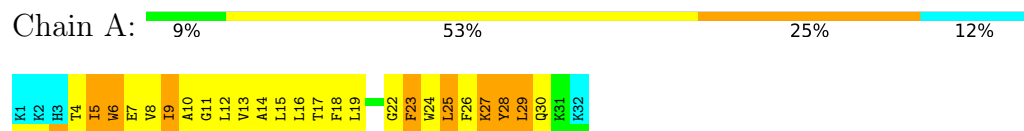
4.2.26 Score per residue for model 26

- Molecule 1: Membrane fusion protein p14



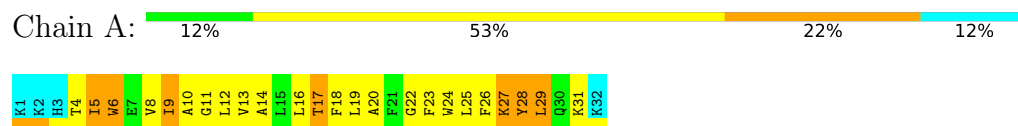
4.2.27 Score per residue for model 27

- Molecule 1: Membrane fusion protein p14



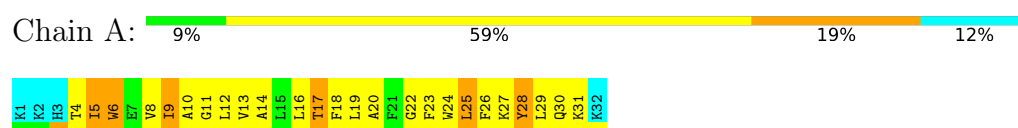
4.2.28 Score per residue for model 28

- Molecule 1: Membrane fusion protein p14



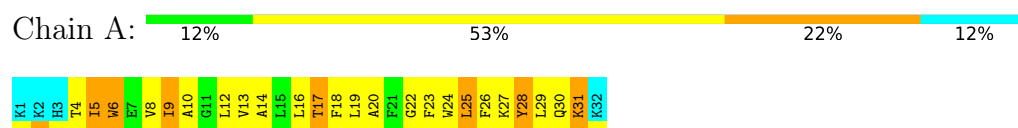
4.2.29 Score per residue for model 29

- Molecule 1: Membrane fusion protein p14



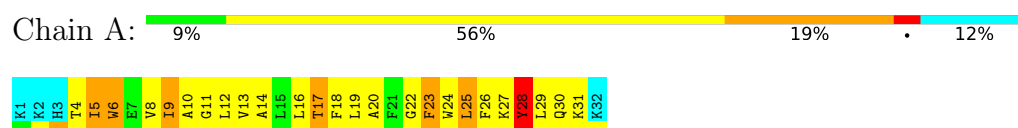
4.2.30 Score per residue for model 30

- Molecule 1: Membrane fusion protein p14



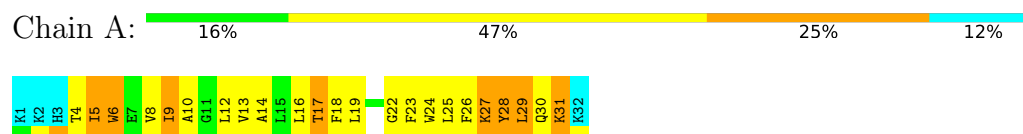
4.2.31 Score per residue for model 31

- Molecule 1: Membrane fusion protein p14



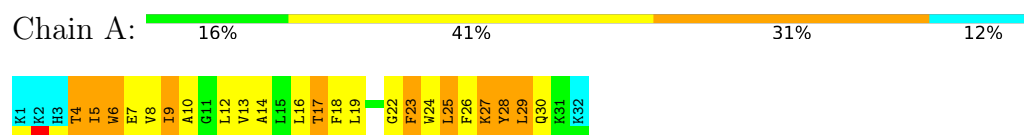
4.2.32 Score per residue for model 32

- Molecule 1: Membrane fusion protein p14



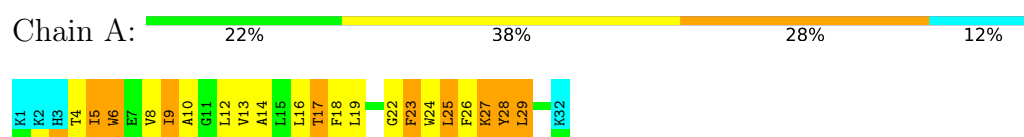
4.2.33 Score per residue for model 33

- Molecule 1: Membrane fusion protein p14



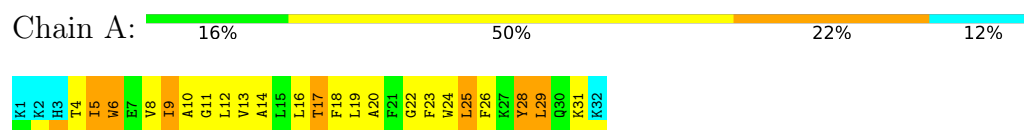
4.2.34 Score per residue for model 34

- Molecule 1: Membrane fusion protein p14



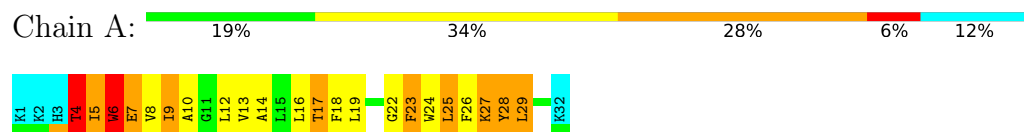
4.2.35 Score per residue for model 35

- Molecule 1: Membrane fusion protein p14



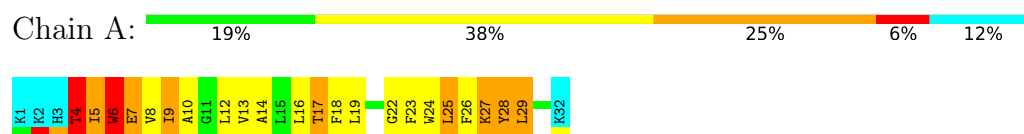
4.2.36 Score per residue for model 36

- Molecule 1: Membrane fusion protein p14



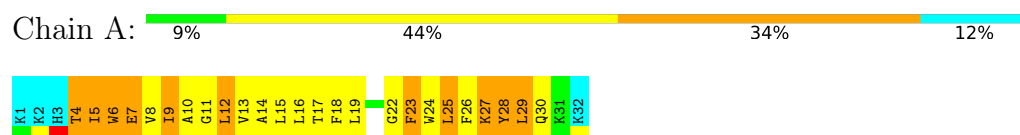
4.2.37 Score per residue for model 37

- Molecule 1: Membrane fusion protein p14



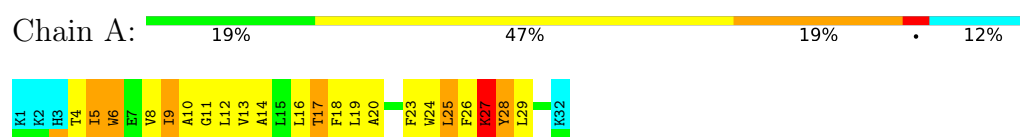
4.2.38 Score per residue for model 38

- Molecule 1: Membrane fusion protein p14



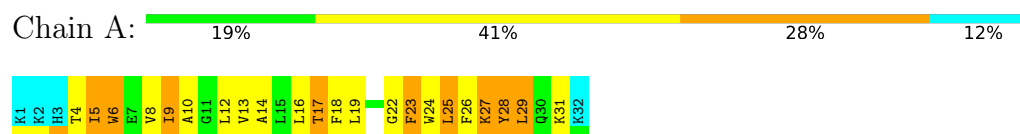
4.2.39 Score per residue for model 39

- Molecule 1: Membrane fusion protein p14



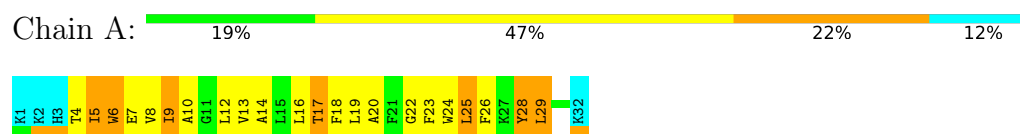
4.2.40 Score per residue for model 40

- Molecule 1: Membrane fusion protein p14



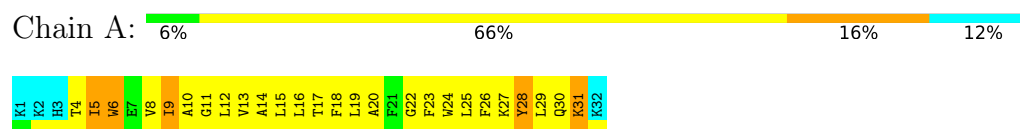
4.2.41 Score per residue for model 41

- Molecule 1: Membrane fusion protein p14



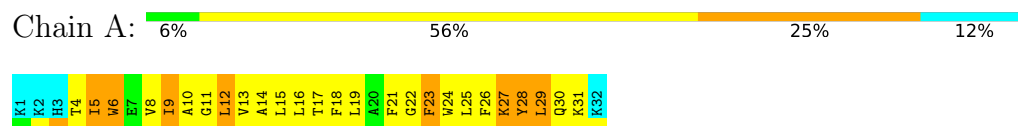
4.2.42 Score per residue for model 42

- Molecule 1: Membrane fusion protein p14



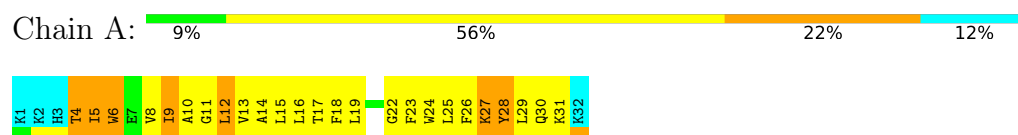
4.2.43 Score per residue for model 43

- Molecule 1: Membrane fusion protein p14



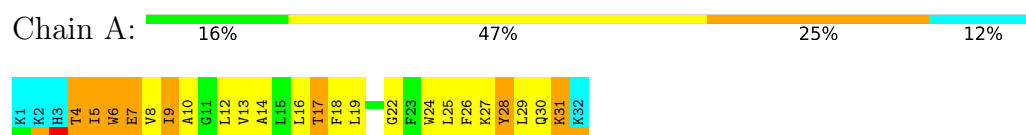
4.2.44 Score per residue for model 44

- Molecule 1: Membrane fusion protein p14



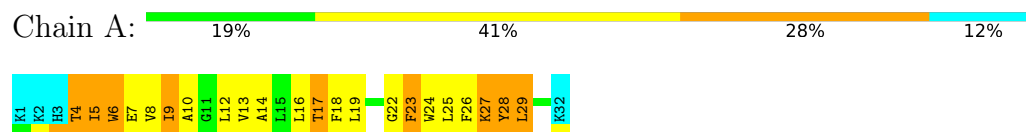
4.2.45 Score per residue for model 45

- Molecule 1: Membrane fusion protein p14



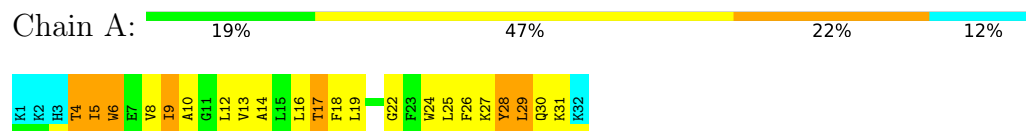
4.2.46 Score per residue for model 46

- Molecule 1: Membrane fusion protein p14



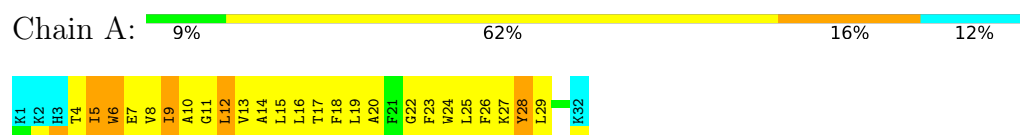
4.2.47 Score per residue for model 47

- Molecule 1: Membrane fusion protein p14



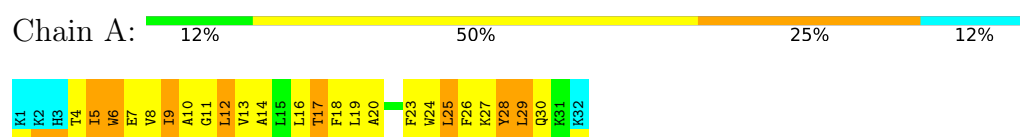
4.2.48 Score per residue for model 48

- Molecule 1: Membrane fusion protein p14



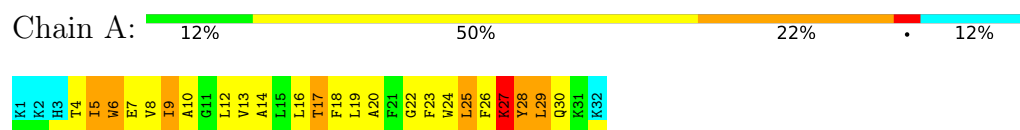
4.2.49 Score per residue for model 49

- Molecule 1: Membrane fusion protein p14



4.2.50 Score per residue for model 50

- Molecule 1: Membrane fusion protein p14



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.18
X-PLOR NIH	refinement	2.18

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	287
Number of shifts mapped to atoms	286
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	57%

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	0.49±0.01	0±0/244 (0.0± 0.0%)	1.05±0.03	0±0/333 (0.0± 0.1%)
All	All	0.49	0/12200 (0.0%)	1.05	3/16650 (0.0%)

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	26	PHE	CA-CB-CG	-5.16	108.64	113.80	24	2
1	A	23	PHE	CA-CB-CG	-5.06	108.74	113.80	46	1

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	235	246	246	35±3
All	All	11750	12300	12300	1739

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 72.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:GLY:O	1:A:15:LEU:HD12	0.67	1.90	42	11
1:A:29:LEU:C	1:A:29:LEU:HD12	0.65	2.17	47	2
1:A:29:LEU:HD12	1:A:29:LEU:O	0.64	1.92	43	2
1:A:24:TRP:CZ2	1:A:28:TYR:CD2	0.62	2.88	46	20
1:A:24:TRP:CZ2	1:A:28:TYR:CE2	0.62	2.87	12	16
1:A:4:THR:HG23	1:A:5:ILE:N	0.61	2.09	19	46
1:A:24:TRP:CE2	1:A:28:TYR:CD2	0.59	2.90	14	19
1:A:6:TRP:O	1:A:10:ALA:N	0.58	2.36	20	50
1:A:4:THR:HG23	1:A:5:ILE:H	0.58	1.59	11	44
1:A:29:LEU:O	1:A:29:LEU:HD23	0.57	2.00	7	25
1:A:26:PHE:O	1:A:30:GLN:N	0.56	2.38	49	17
1:A:26:PHE:C	1:A:28:TYR:H	0.55	2.08	16	48
1:A:22:GLY:O	1:A:26:PHE:CD2	0.55	2.60	16	17
1:A:10:ALA:C	1:A:12:LEU:N	0.55	2.65	18	50
1:A:24:TRP:O	1:A:25:LEU:C	0.55	2.50	33	50
1:A:10:ALA:O	1:A:14:ALA:N	0.54	2.40	49	50
1:A:14:ALA:O	1:A:18:PHE:N	0.54	2.40	40	50
1:A:13:VAL:O	1:A:16:LEU:N	0.54	2.40	49	50
1:A:28:TYR:C	1:A:28:TYR:CD1	0.54	2.85	47	6
1:A:19:LEU:HD22	1:A:19:LEU:N	0.54	2.17	39	4
1:A:4:THR:HG23	1:A:6:TRP:H	0.54	1.62	19	13
1:A:13:VAL:O	1:A:17:THR:N	0.54	2.41	14	50
1:A:19:LEU:N	1:A:19:LEU:CD2	0.54	2.71	46	48
1:A:19:LEU:N	1:A:19:LEU:HD22	0.53	2.19	46	44
1:A:4:THR:OG1	1:A:5:ILE:N	0.53	2.41	36	50
1:A:9:ILE:O	1:A:13:VAL:N	0.53	2.42	37	50
1:A:26:PHE:O	1:A:28:TYR:N	0.53	2.42	44	41
1:A:6:TRP:C	1:A:8:VAL:N	0.52	2.67	25	49
1:A:28:TYR:CD1	1:A:28:TYR:C	0.52	2.86	19	29
1:A:23:PHE:O	1:A:23:PHE:CG	0.52	2.63	46	4
1:A:23:PHE:CG	1:A:23:PHE:O	0.52	2.62	42	2
1:A:9:ILE:O	1:A:13:VAL:HG23	0.52	2.04	27	41
1:A:26:PHE:C	1:A:28:TYR:N	0.52	2.67	44	45
1:A:24:TRP:O	1:A:27:LYS:N	0.51	2.42	46	1
1:A:6:TRP:O	1:A:8:VAL:N	0.51	2.43	25	21
1:A:29:LEU:C	1:A:29:LEU:CD1	0.51	2.83	47	2
1:A:10:ALA:O	1:A:13:VAL:N	0.50	2.45	41	50
1:A:17:THR:O	1:A:20:ALA:N	0.50	2.44	12	17
1:A:5:ILE:O	1:A:8:VAL:N	0.50	2.44	24	46
1:A:19:LEU:CD1	1:A:19:LEU:N	0.50	2.74	40	1
1:A:4:THR:CG2	1:A:5:ILE:N	0.50	2.74	19	16
1:A:27:LYS:CD	1:A:27:LYS:N	0.50	2.75	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:O	1:A:29:LEU:HD13	0.49	2.08	40	2
1:A:30:GLN:CG	1:A:30:GLN:O	0.49	2.60	44	5
1:A:24:TRP:NE1	1:A:28:TYR:CG	0.48	2.81	17	1
1:A:4:THR:CG2	1:A:5:ILE:H	0.48	2.20	29	42
1:A:19:LEU:N	1:A:19:LEU:HD12	0.48	2.24	40	1
1:A:22:GLY:C	1:A:24:TRP:N	0.48	2.69	40	28
1:A:12:LEU:O	1:A:16:LEU:CD1	0.48	2.62	26	46
1:A:23:PHE:O	1:A:27:LYS:CG	0.48	2.62	15	26
1:A:6:TRP:C	1:A:8:VAL:H	0.47	2.17	29	27
1:A:6:TRP:O	1:A:11:GLY:N	0.47	2.47	27	19
1:A:12:LEU:O	1:A:16:LEU:HD12	0.47	2.09	17	33
1:A:10:ALA:C	1:A:12:LEU:H	0.47	2.18	49	50
1:A:25:LEU:O	1:A:29:LEU:N	0.47	2.43	34	4
1:A:5:ILE:O	1:A:6:TRP:C	0.47	2.58	37	30
1:A:7:GLU:N	1:A:7:GLU:CD	0.46	2.73	25	1
1:A:7:GLU:N	1:A:7:GLU:OE1	0.45	2.50	5	1
1:A:26:PHE:O	1:A:30:GLN:CB	0.45	2.64	49	1
1:A:30:GLN:O	1:A:30:GLN:CG	0.45	2.64	19	8
1:A:28:TYR:O	1:A:28:TYR:CD1	0.45	2.70	21	4
1:A:10:ALA:O	1:A:12:LEU:N	0.44	2.51	27	50
1:A:6:TRP:CG	1:A:10:ALA:CB	0.44	3.00	4	43
1:A:24:TRP:O	1:A:28:TYR:N	0.44	2.49	49	1
1:A:13:VAL:O	1:A:14:ALA:C	0.44	2.61	40	49
1:A:25:LEU:O	1:A:29:LEU:CB	0.44	2.66	33	10
1:A:22:GLY:O	1:A:23:PHE:C	0.43	2.60	18	5
1:A:17:THR:O	1:A:18:PHE:C	0.43	2.61	33	21
1:A:18:PHE:O	1:A:22:GLY:N	0.43	2.47	25	6
1:A:19:LEU:O	1:A:20:ALA:C	0.43	2.61	18	5
1:A:24:TRP:NE1	1:A:28:TYR:CB	0.43	2.82	17	1
1:A:27:LYS:CD	1:A:27:LYS:H	0.42	2.25	50	1
1:A:22:GLY:C	1:A:24:TRP:H	0.42	2.23	50	2
1:A:9:ILE:O	1:A:13:VAL:CG2	0.42	2.68	27	1
1:A:21:PHE:O	1:A:22:GLY:C	0.42	2.63	43	1
1:A:28:TYR:CG	1:A:29:LEU:N	0.42	2.86	2	6
1:A:21:PHE:CD1	1:A:21:PHE:N	0.41	2.89	26	1
1:A:28:TYR:CD1	1:A:28:TYR:O	0.41	2.74	49	1
1:A:17:THR:HG22	1:A:18:PHE:N	0.41	2.31	28	2
1:A:29:LEU:HD23	1:A:29:LEU:C	0.41	2.41	24	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	28/32 (88%)	17±1 (62±4%)	8±1 (29±4%)	2±1 (9±4%)	1	12
All	All	1400/1600 (88%)	869 (62%)	410 (29%)	121 (9%)	1	12

All 6 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	27	LYS	46
1	A	25	LEU	39
1	A	4	THR	18
1	A	7	GLU	15
1	A	6	TRP	2
1	A	28	TYR	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	23/27 (85%)	16±1 (70±3%)	7±1 (30±3%)	1	17
All	All	1150/1350 (85%)	809 (70%)	341 (30%)	1	17

All 13 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	5	ILE	50
1	A	6	TRP	50
1	A	9	ILE	50
1	A	28	TYR	50

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Mol	Chain	Res	Type	Models (Total)
1	A	17	THR	39
1	A	29	LEU	39
1	A	23	PHE	32
1	A	31	LYS	11
1	A	12	LEU	10
1	A	7	GLU	4
1	A	27	LYS	3
1	A	4	THR	2
1	A	8	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 57% for the well-defined parts and 56% 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	287
Number of shifts mapped to atoms	286
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	HIS	HD1	11.126	0.003	1

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 57%, i.e. 244 atoms were assigned a chemical shift out of a possible 427. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	66/142 (46%)	58/58 (100%)	0/56 (0%)	8/28 (29%)
Sidechain	142/212 (67%)	142/143 (99%)	0/66 (0%)	0/3 (0%)
Aromatic	36/73 (49%)	36/36 (100%)	0/35 (0%)	0/2 (0%)
Overall	244/427 (57%)	236/237 (100%)	0/157 (0%)	8/33 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 56%, i.e. 278 atoms were assigned a chemical shift out of a possible 496. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	71/162 (44%)	63/66 (95%)	0/64 (0%)	8/32 (25%)
Sidechain	168/254 (66%)	168/169 (99%)	0/79 (0%)	0/6 (0%)
Aromatic	39/80 (49%)	39/40 (98%)	0/37 (0%)	0/3 (0%)
Overall	278/496 (56%)	270/275 (98%)	0/180 (0%)	8/41 (20%)

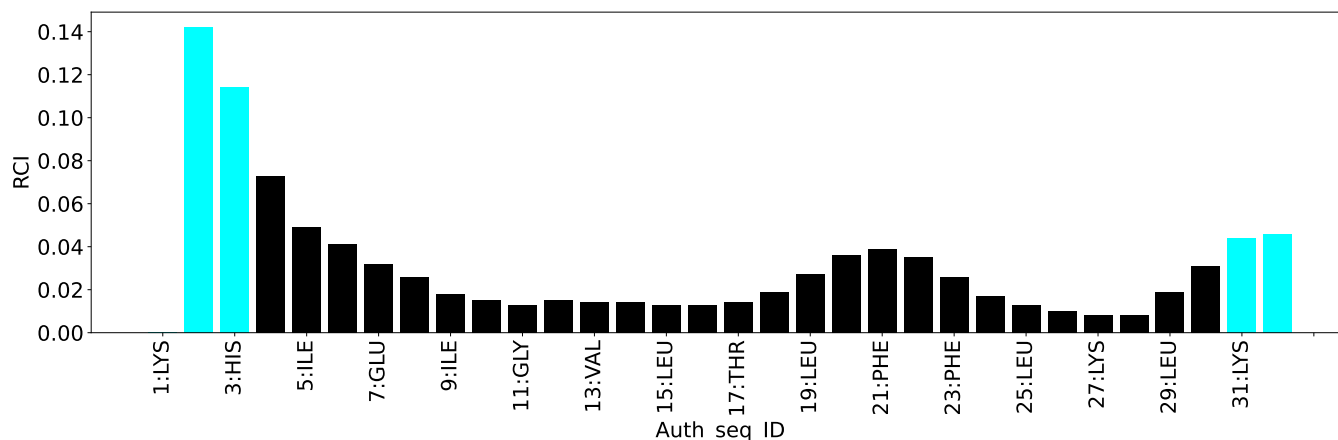
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1887
Intra-residue ($ i-j =0$)	739
Sequential ($ i-j =1$)	496
Medium range ($ i-j >1$ and $ i-j <5$)	621
Long range ($ i-j \geq 5$)	11
Inter-chain	0
Hydrogen bond restraints	20
Disulfide bond restraints	0
Total dihedral-angle restraints	38
Number of unmapped restraints	0
Number of restraints per residue	60.2
Number of long range restraints per residue ¹	0.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	9.8	0.2
0.2-0.5 (Medium)	15.0	0.5
>0.5 (Large)	16.6	1.99

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)	1.0	8.84
10.0-20.0 (Medium)	0.2	14.19
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

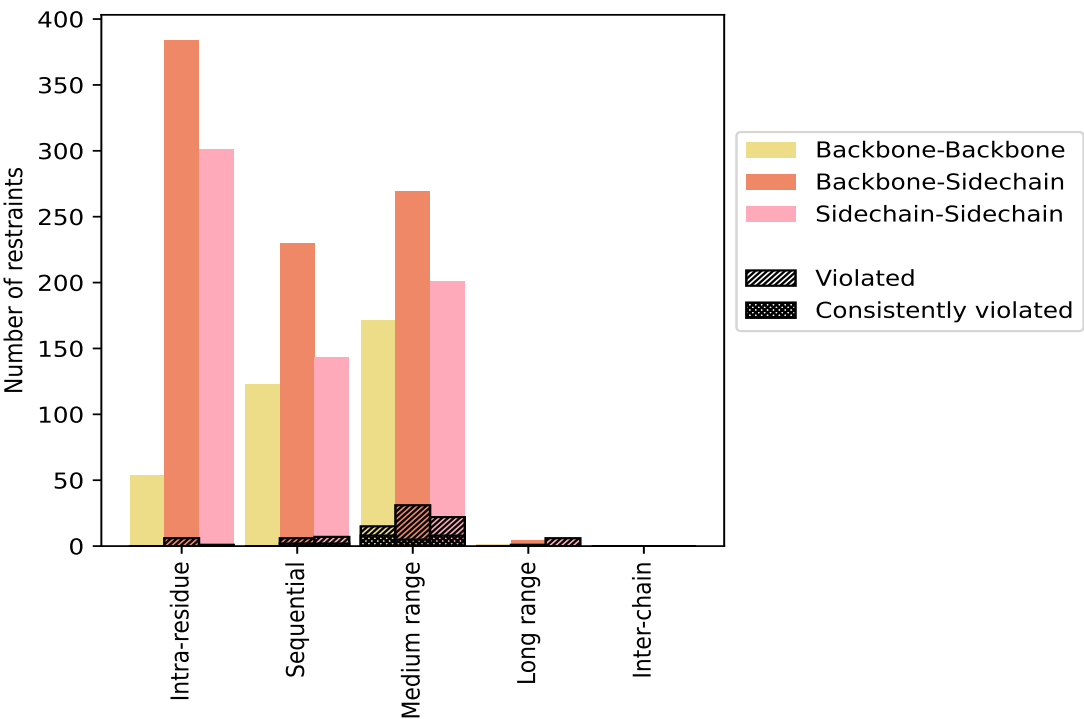
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	739	39.2	7	0.9	0.4	0	0.0	0.0
Backbone-Backbone	54	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	384	20.3	6	1.6	0.3	0	0.0	0.0
Sidechain-Sidechain	301	16.0	1	0.3	0.1	0	0.0	0.0
Sequential ($i-j =1$)	496	26.3	13	2.6	0.7	4	0.8	0.2
Backbone-Backbone	123	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	230	12.2	6	2.6	0.3	2	0.9	0.1
Sidechain-Sidechain	143	7.6	7	4.9	0.4	2	1.4	0.1
Medium range ($i-j >1$ & $i-j <5$)	621	32.9	59	9.5	3.1	21	3.4	1.1
Backbone-Backbone	171	9.1	15	8.8	0.8	8	4.7	0.4
Backbone-Sidechain	249	13.2	22	8.8	1.2	5	2.0	0.3
Sidechain-Sidechain	201	10.7	22	10.9	1.2	8	4.0	0.4
Long range ($i-j \geq 5$)	11	0.6	7	63.6	0.4	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	0.2	1	25.0	0.1	0	0.0	0.0
Sidechain-Sidechain	6	0.3	6	100.0	0.3	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	20	1.1	9	45.0	0.5	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1887	100.0	95	5.0	5.0	25	1.3	1.3
Backbone-Backbone	349	18.5	15	4.3	0.8	8	2.3	0.4
Backbone-Sidechain	887	47.0	44	5.0	2.3	7	0.8	0.4
Sidechain-Sidechain	651	34.5	36	5.5	1.9	10	1.5	0.5

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	15	22	6	0	43	0.59	1.84	0.42	0.42
2	0	13	24	6	0	43	0.58	1.84	0.43	0.44
3	0	13	20	6	0	39	0.56	1.94	0.39	0.45
4	0	15	21	0	0	36	0.64	1.76	0.43	0.47
5	0	13	24	6	0	43	0.55	1.98	0.39	0.41
6	1	13	26	2	0	42	0.55	1.8	0.43	0.38
7	0	13	28	2	0	43	0.51	1.78	0.39	0.38
8	0	13	26	0	0	39	0.54	1.81	0.38	0.41
9	0	15	25	2	0	42	0.59	1.75	0.43	0.49
10	1	15	22	6	0	44	0.55	1.96	0.45	0.38

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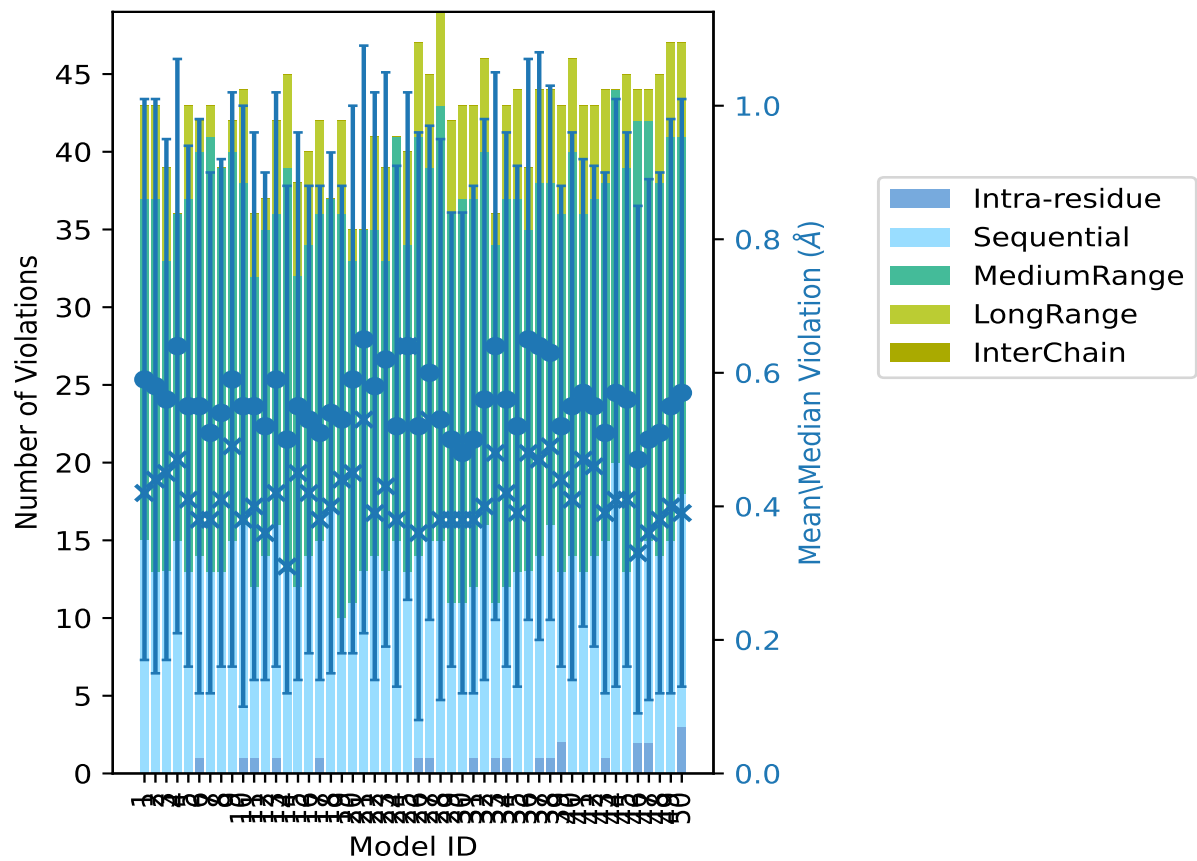
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	11	20	4	0	36	0.55	1.82	0.41	0.4
12	0	14	21	2	0	37	0.52	1.8	0.38	0.36
13	1	15	20	6	0	42	0.59	1.73	0.43	0.42
14	0	13	26	6	0	45	0.5	1.9	0.38	0.31
15	0	12	20	6	0	38	0.55	1.99	0.41	0.45
16	0	14	20	6	0	40	0.53	1.68	0.35	0.42
17	1	14	21	6	0	42	0.51	1.86	0.37	0.38
18	0	17	20	0	0	37	0.54	1.78	0.39	0.4
19	0	10	26	6	0	42	0.53	1.92	0.35	0.44
20	0	11	22	2	0	35	0.59	1.91	0.41	0.45
21	0	13	22	0	0	35	0.65	1.93	0.44	0.53
22	0	14	21	6	0	41	0.58	1.82	0.44	0.39
23	0	13	20	6	0	39	0.62	1.93	0.43	0.43
24	0	15	26	0	0	41	0.52	1.84	0.39	0.38
25	0	13	21	6	0	40	0.64	1.54	0.38	0.64
26	1	13	27	6	0	47	0.52	1.8	0.44	0.36
27	1	14	24	6	0	45	0.6	1.58	0.37	0.53
28	0	15	28	6	0	49	0.53	1.81	0.42	0.38
29	0	11	25	6	0	42	0.5	1.69	0.34	0.38
30	0	11	26	6	0	43	0.48	1.86	0.36	0.38
31	1	11	25	6	0	43	0.5	1.97	0.38	0.38
32	0	16	24	6	0	46	0.56	1.84	0.42	0.4
33	1	10	23	2	0	36	0.64	1.77	0.41	0.48
34	1	11	25	6	0	43	0.56	1.85	0.4	0.42
35	0	13	24	7	0	44	0.52	1.89	0.39	0.39
36	0	13	22	4	0	39	0.65	1.7	0.42	0.48
37	1	13	24	6	0	44	0.64	1.86	0.44	0.47
38	1	15	22	6	0	44	0.63	1.7	0.4	0.49
39	2	11	23	7	0	43	0.52	1.9	0.36	0.44
40	0	14	26	6	0	46	0.55	1.85	0.41	0.41
41	0	13	23	7	0	43	0.57	1.81	0.35	0.47
42	0	14	23	6	0	43	0.55	1.88	0.36	0.46
43	1	14	23	6	0	44	0.51	1.88	0.39	0.39
44	0	20	24	0	0	44	0.57	1.95	0.44	0.41
45	0	13	26	6	0	45	0.56	1.85	0.4	0.41
46	2	12	28	2	0	44	0.47	1.75	0.38	0.33
47	2	13	27	2	0	44	0.5	1.87	0.39	0.36
48	0	14	24	7	0	45	0.51	1.97	0.39	0.38
49	0	15	26	6	0	47	0.55	1.82	0.43	0.4
50	3	15	23	6	0	47	0.57	1.8	0.44	0.39

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 ⓘ



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 ⓘ

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, 1781(IR:732, SQ:483, MR:562, LR:4, 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	%
3	3	10	0	0	16	1	2.0
0	3	4	0	0	7	2	4.0
3	0	1	0	0	4	3	6.0
0	0	3	1	0	4	4	8.0

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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	2	0	0	2	5	10.0
0	0	1	0	0	1	6	12.0
0	0	4	0	0	4	7	14.0
0	0	2	0	0	2	8	16.0
0	0	0	0	0	0	9	18.0
1	0	0	0	0	1	10	20.0
0	0	2	0	0	2	11	22.0
0	1	0	0	0	1	12	24.0
0	0	0	0	0	0	13	26.0
0	0	0	0	0	0	14	28.0
0	0	1	0	0	1	15	30.0
0	0	0	0	0	0	16	32.0
0	0	0	0	0	0	17	34.0
0	0	0	0	0	0	18	36.0
0	0	0	0	0	0	19	38.0
0	0	0	0	0	0	20	40.0
0	0	0	0	0	0	21	42.0
0	0	0	0	0	0	22	44.0
0	0	0	0	0	0	23	46.0
0	0	0	0	0	0	24	48.0
0	0	0	0	0	0	25	50.0
0	0	1	0	0	1	26	52.0
0	0	0	0	0	0	27	54.0
0	0	0	0	0	0	28	56.0
0	0	4	0	0	4	29	58.0
0	2	0	0	0	2	30	60.0
0	0	1	0	0	1	31	62.0
0	0	0	0	0	0	32	64.0
0	0	0	0	0	0	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	0	0	0	35	70.0
0	0	0	4	0	4	36	72.0
0	0	0	0	0	0	37	74.0
0	0	0	0	0	0	38	76.0
0	0	0	0	0	0	39	78.0
0	0	0	0	0	0	40	80.0
0	0	0	0	0	0	41	82.0
0	0	0	2	0	2	42	84.0
0	0	0	0	0	0	43	86.0
0	0	0	0	0	0	44	88.0
0	0	0	0	0	0	45	90.0

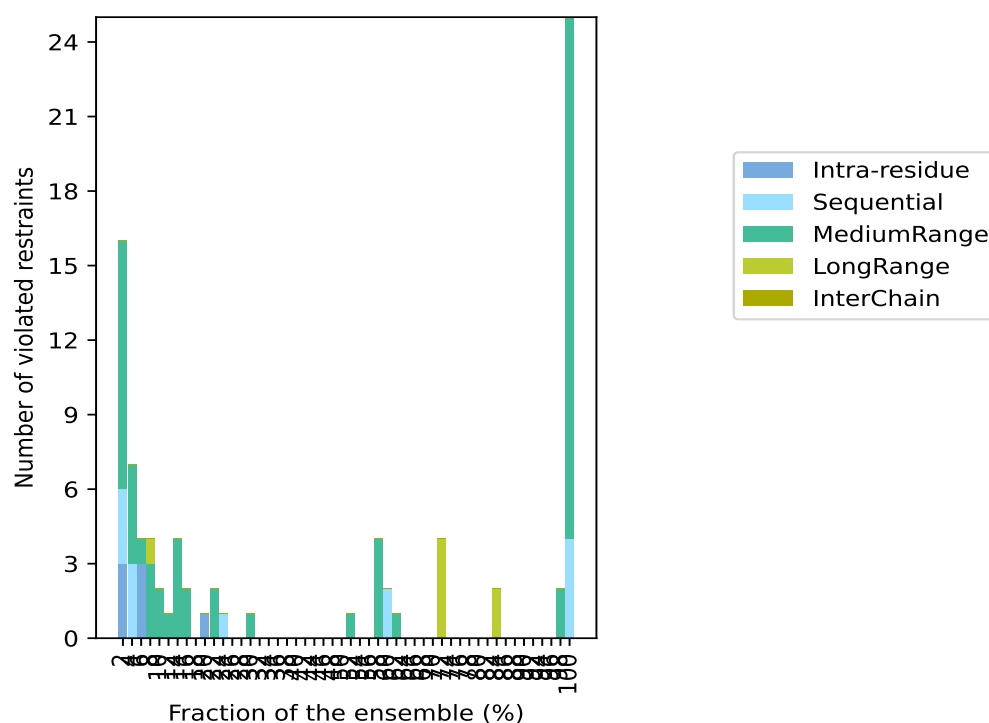
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	46	92.0
0	0	0	0	0	0	47	94.0
0	0	0	0	0	0	48	96.0
0	0	2	0	0	2	49	98.0
0	4	21	0	0	25	50	100.0

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

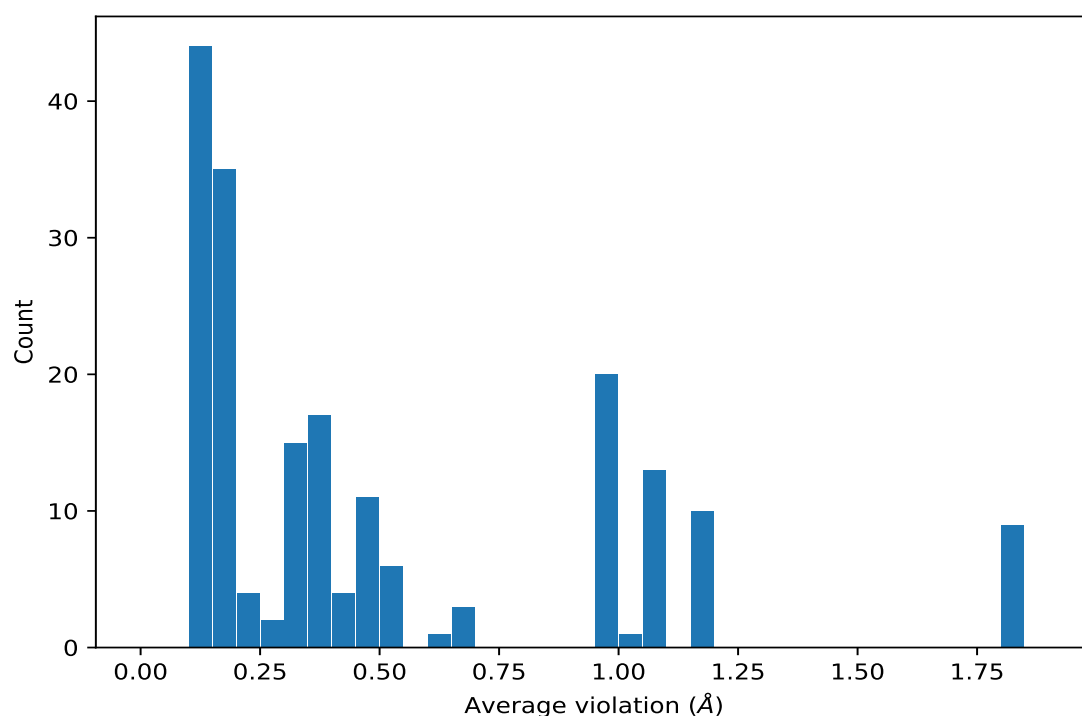
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG22	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG21	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG23	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG21	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG23	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG21	50	1.83	0.1	1.84
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG23	50	1.83	0.1	1.84
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	50	1.08	0.06	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	50	1.08	0.06	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	50	1.08	0.06	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD12	50	1.08	0.06	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	50	1.08	0.06	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	50	1.08	0.06	1.08
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	50	1.08	0.06	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	50	1.08	0.06	1.08
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	50	1.08	0.06	1.08
(1,1753)	1:15:A:LEU:HD12	1:16:A:LEU:H	50	1.08	0.06	1.08
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	50	1.08	0.06	1.08
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	50	1.08	0.06	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	50	1.08	0.03	1.08
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	50	0.97	0.04	0.96
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	50	0.97	0.04	0.96
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	50	0.97	0.04	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	50	0.97	0.04	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	50	0.97	0.04	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	50	0.97	0.04	0.96
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	50	0.97	0.18	1.02
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	50	0.97	0.18	1.02
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	50	0.97	0.18	1.02
(1,1842)	1:29:A:LEU:HD21	1:27:A:LYS:H	50	0.97	0.18	1.02
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	50	0.97	0.18	1.02
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	50	0.97	0.18	1.02
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	50	0.97	0.18	1.02
(1,1844)	1:27:A:LYS:H	1:29:A:LEU:HD21	50	0.97	0.18	1.02
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	50	0.95	0.02	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	50	0.95	0.02	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	50	0.95	0.02	0.95
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	50	0.95	0.02	0.95
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	50	0.95	0.02	0.95
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	50	0.95	0.02	0.95
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	50	0.66	0.05	0.66
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	50	0.66	0.05	0.66
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	50	0.66	0.05	0.66
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	50	0.54	0.15	0.51
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	50	0.54	0.15	0.51
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	50	0.54	0.15	0.51
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	50	0.54	0.15	0.51
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	50	0.54	0.15	0.51
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	50	0.54	0.15	0.51
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	50	0.46	0.05	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	50	0.46	0.05	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	50	0.45	0.12	0.43
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	50	0.45	0.12	0.43
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	50	0.45	0.12	0.43
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	50	0.39	0.03	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	50	0.39	0.03	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	50	0.38	0.03	0.37
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	50	0.38	0.03	0.37
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	50	0.38	0.03	0.37
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	50	0.29	0.0	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	50	0.29	0.0	0.29
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	50	0.18	0.01	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	50	0.18	0.01	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	50	0.18	0.01	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	50	0.18	0.01	0.17
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	49	0.41	0.06	0.39
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	49	0.41	0.06	0.39
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	49	0.41	0.06	0.39
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	49	0.41	0.06	0.39
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	44	1.01	0.27	1.12
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	42	0.45	0.23	0.5
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	42	0.45	0.23	0.5
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	42	0.45	0.23	0.5
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	42	0.45	0.23	0.5
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	42	0.45	0.23	0.5
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	42	0.45	0.23	0.5
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	41	0.6	0.16	0.62
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	36	0.39	0.29	0.27
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	36	0.39	0.29	0.27
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	36	0.39	0.29	0.27
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	36	0.39	0.29	0.27
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	36	0.39	0.29	0.27
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	36	0.39	0.29	0.27
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	36	0.39	0.29	0.27
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	36	0.39	0.29	0.27
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	36	0.39	0.29	0.27
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	36	0.39	0.29	0.27
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	36	0.39	0.29	0.27
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	36	0.39	0.29	0.27
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	31	0.32	0.06	0.31
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	31	0.32	0.06	0.31
(1,1711)	1:29:A:LEU:HD11	1:28:A:TYR:HE2	31	0.32	0.06	0.31
(1,1711)	1:25:A:LEU:HD22	1:28:A:TYR:HE2	31	0.32	0.06	0.31
(1,1711)	1:25:A:LEU:HD23	1:28:A:TYR:HE2	31	0.32	0.06	0.31
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	30	1.19	0.36	1.34
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	30	1.19	0.36	1.34
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ1	30	1.19	0.36	1.34
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ3	30	1.19	0.36	1.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE2	30	1.19	0.36	1.34
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	30	1.19	0.36	1.34
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	30	1.19	0.36	1.34
(1,1867)	1:27:A:LYS:HZ1	1:24:A:TRP:H	30	1.19	0.36	1.34
(1,1867)	1:27:A:LYS:HZ3	1:24:A:TRP:H	30	1.19	0.36	1.34
(1,1867)	1:23:A:PHE:HE2	1:24:A:TRP:H	30	1.19	0.36	1.34
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	29	0.21	0.08	0.19
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	29	0.21	0.08	0.19
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	29	0.21	0.08	0.19
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	29	0.21	0.08	0.19
(1,1745)	1:25:A:LEU:HD22	1:24:A:TRP:HE3	29	0.17	0.03	0.16
(1,1745)	1:25:A:LEU:HD11	1:24:A:TRP:HE3	29	0.17	0.03	0.16
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	29	0.17	0.03	0.16
(1,1745)	1:25:A:LEU:HD21	1:24:A:TRP:HE3	29	0.17	0.03	0.16
(1,1745)	1:25:A:LEU:HD23	1:24:A:TRP:HE3	29	0.17	0.03	0.16
(1,1745)	1:25:A:LEU:HD12	1:24:A:TRP:HE3	29	0.17	0.03	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD22	29	0.17	0.03	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD11	29	0.17	0.03	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	29	0.17	0.03	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD21	29	0.17	0.03	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD23	29	0.17	0.03	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD12	29	0.17	0.03	0.16
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	26	0.13	0.02	0.13
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	18	0.34	0.1	0.34
(1,1789)	1:17:A:THR:HB	1:16:A:LEU:H	15	0.16	0.03	0.16
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	15	0.16	0.03	0.16
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	12	0.15	0.02	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	12	0.15	0.02	0.14
(1,1722)	1:25:A:LEU:HD12	1:21:A:PHE:HD2	11	0.34	0.23	0.24
(1,1722)	1:25:A:LEU:HD11	1:21:A:PHE:HD2	11	0.34	0.23	0.24
(1,1722)	1:25:A:LEU:HD13	1:21:A:PHE:HD2	11	0.34	0.23	0.24
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD12	11	0.34	0.23	0.24
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD11	11	0.34	0.23	0.24
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD13	11	0.34	0.23	0.24
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	10	0.11	0.03	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	10	0.11	0.03	0.1
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	8	0.16	0.05	0.16
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	8	0.11	0.01	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	8	0.11	0.01	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	8	0.11	0.01	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	8	0.11	0.01	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	8	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	8	0.11	0.01	0.11
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	8	0.11	0.01	0.11
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	8	0.11	0.01	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	8	0.11	0.01	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	8	0.11	0.01	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	8	0.11	0.01	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	8	0.11	0.01	0.11
(1,1807)	1:24:A:TRP:HA	1:27:A:LYS:HG3	7	0.16	0.04	0.17
(1,1807)	1:26:A:PHE:HA	1:27:A:LYS:HG3	7	0.16	0.04	0.17
(1,1809)	1:27:A:LYS:HG3	1:24:A:TRP:HA	7	0.16	0.04	0.17
(1,1809)	1:27:A:LYS:HG3	1:26:A:PHE:HA	7	0.16	0.04	0.17
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	7	0.13	0.02	0.13
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	7	0.13	0.02	0.13
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	7	0.12	0.02	0.12
(1,1850)	1:27:A:LYS:HG3	1:30:A:GLN:HB3	6	0.19	0.09	0.16
(1,1849)	1:27:A:LYS:H	1:23:A:PHE:HD1	5	0.17	0.07	0.13
(1,1849)	1:27:A:LYS:H	1:23:A:PHE:HD2	5	0.17	0.07	0.13
(1,1852)	1:23:A:PHE:HD1	1:27:A:LYS:H	5	0.17	0.07	0.13
(1,1852)	1:23:A:PHE:HD2	1:27:A:LYS:H	5	0.17	0.07	0.13
(1,1841)	1:8:A:VAL:HG21	1:6:A:TRP:H	4	0.3	0.02	0.3
(1,1841)	1:8:A:VAL:HG22	1:6:A:TRP:H	4	0.3	0.02	0.3
(1,1799)	1:27:A:LYS:HG3	1:23:A:PHE:HD1	4	0.19	0.03	0.2
(1,1834)	1:23:A:PHE:HD1	1:27:A:LYS:HG3	4	0.19	0.03	0.2
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD2	4	0.12	0.01	0.12
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD3	4	0.12	0.01	0.12
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD2	4	0.12	0.01	0.12
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD3	4	0.12	0.01	0.12
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE1	3	0.13	0.02	0.12
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE2	3	0.13	0.02	0.12
(1,405)	1:23:A:PHE:HE1	1:23:A:PHE:H	3	0.13	0.02	0.12
(1,405)	1:23:A:PHE:HE2	1:23:A:PHE:H	3	0.13	0.02	0.12
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD1	3	0.12	0.02	0.12
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD2	3	0.12	0.02	0.12
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD1	3	0.12	0.02	0.12
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD2	3	0.12	0.02	0.12
(2,17)	1:22:A:GLY:O	1:26:A:PHE:H	3	0.11	0.01	0.11
(1,98)	1:6:A:TRP:HD1	1:6:A:TRP:HE3	3	0.1	0.0	0.1
(1,1823)	1:20:A:ALA:H	1:21:A:PHE:HD2	2	0.34	0.08	0.34
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ1	2	0.15	0.04	0.15
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ2	2	0.15	0.04	0.15
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ3	2	0.15	0.04	0.15
(1,1623)	1:23:A:PHE:HA	1:19:A:LEU:HA	2	0.12	0.01	0.12

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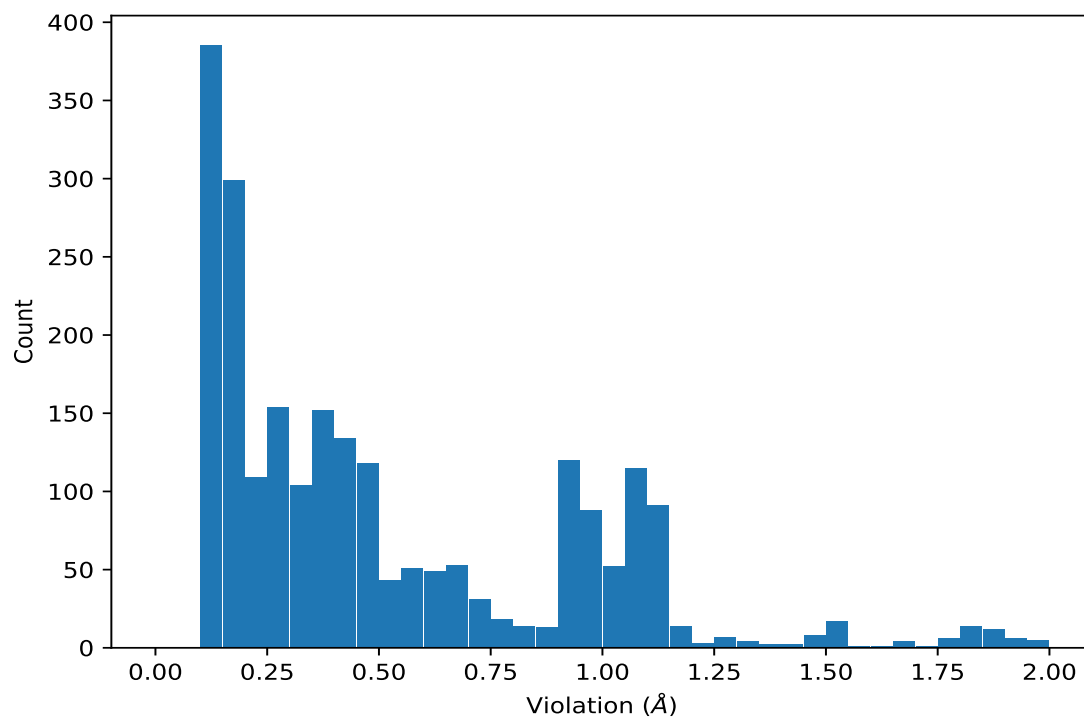
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1179)	1:5:A:ILE:H	1:3:A:HIS:HE1	2	0.12	0.02	0.12
(1,1079)	1:27:A:LYS:HG2	1:26:A:PHE:HD1	2	0.11	0.01	0.11
(1,1079)	1:27:A:LYS:HG2	1:26:A:PHE:HD2	2	0.11	0.01	0.11
(1,1079)	1:27:A:LYS:HG3	1:26:A:PHE:HD1	2	0.11	0.01	0.11
(1,1079)	1:27:A:LYS:HG3	1:26:A:PHE:HD2	2	0.11	0.01	0.11
(1,1085)	1:26:A:PHE:HD1	1:27:A:LYS:HG2	2	0.11	0.01	0.11
(1,1085)	1:26:A:PHE:HD1	1:27:A:LYS:HG3	2	0.11	0.01	0.11
(1,1085)	1:26:A:PHE:HD2	1:27:A:LYS:HG2	2	0.11	0.01	0.11
(1,1085)	1:26:A:PHE:HD2	1:27:A:LYS:HG3	2	0.11	0.01	0.11
(1,1286)	1:7:A:GLU:HB2	1:4:A:THR:H	2	0.11	0.01	0.11
(1,1286)	1:7:A:GLU:HB3	1:4:A:THR:H	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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)
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG21	15	1.99
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG23	5	1.98
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG23	31	1.97
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG22	48	1.97
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	10	1.96
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG22	44	1.95
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG22	3	1.94
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	21	1.93
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG21	23	1.93
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG23	19	1.92
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG21	20	1.91
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	14	1.9
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	39	1.9
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG21	35	1.89
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG22	42	1.88
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	43	1.88
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	47	1.87
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG22	17	1.86
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG21	30	1.86
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG23	37	1.86
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG23	34	1.85
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	40	1.85
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG23	45	1.85
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	1	1.84
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	2	1.84
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	24	1.84
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG21	32	1.84
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	11	1.82
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG23	22	1.82
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG22	49	1.82
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG21	8	1.81
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG23	28	1.81
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG21	41	1.81
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	6	1.8
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	12	1.8
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG21	26	1.8
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	50	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	7	1.78
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG21	18	1.78
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG21	33	1.77
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG21	4	1.76
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG23	9	1.75
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG22	46	1.75
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG22	13	1.73
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG21	36	1.7
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG23	38	1.7
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG21	29	1.69
(1,1730)	1:9:A:ILE:HD11	1:5:A:ILE:HG23	16	1.68
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	50	1.62
(1,1730)	1:9:A:ILE:HD13	1:5:A:ILE:HG23	27	1.58
(1,1730)	1:9:A:ILE:HD12	1:5:A:ILE:HG21	25	1.54
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	13	1.51
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	23	1.51
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	26	1.51
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	13	1.51
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	23	1.51
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	26	1.51
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	1	1.5
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	2	1.5
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	10	1.5
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	22	1.5
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	49	1.5
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	1	1.5
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	2	1.5
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	10	1.5
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	22	1.5
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	49	1.5
(1,1867)	1:27:A:LYS:HZ3	1:24:A:TRP:H	9	1.48
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	25	1.48
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ3	9	1.48
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	25	1.48
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	21	1.46
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	40	1.46
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	21	1.46
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	40	1.46
(1,1867)	1:27:A:LYS:HZ1	1:24:A:TRP:H	4	1.45
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ1	4	1.45
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	44	1.36
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	44	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	28	1.34
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	32	1.34
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	28	1.34
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	32	1.34
(1,1867)	1:27:A:LYS:HZ3	1:24:A:TRP:H	6	1.29
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ3	6	1.29
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	37	1.28
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	37	1.28
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	50	1.27
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	50	1.27
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	35	1.25
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	41	1.22
(1,1867)	1:27:A:LYS:HZ3	1:24:A:TRP:H	27	1.21
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ3	27	1.21
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	44	1.19
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	33	1.19
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	33	1.19
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	34	1.18
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	34	1.18
(1,1753)	1:15:A:LEU:HD12	1:16:A:LEU:H	5	1.18
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD12	5	1.18
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	50	1.17
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	48	1.17
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	35	1.17
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	35	1.17
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	36	1.16
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	28	1.16
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	28	1.16
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	3	1.15
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	42	1.15
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	14	1.15
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	14	1.15
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	36	1.15
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	36	1.15
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	36	1.15
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	36	1.15
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	7	1.15
(1,1753)	1:15:A:LEU:HD12	1:16:A:LEU:H	45	1.15
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	49	1.15
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	50	1.15
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	7	1.15
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD12	45	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	49	1.15
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	50	1.15
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	11	1.14
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	20	1.14
(1,1753)	1:15:A:LEU:HD12	1:16:A:LEU:H	13	1.14
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	18	1.14
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	20	1.14
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	25	1.14
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	30	1.14
(1,1753)	1:15:A:LEU:HD12	1:16:A:LEU:H	32	1.14
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD12	13	1.14
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	18	1.14
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	20	1.14
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	25	1.14
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	30	1.14
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD12	32	1.14
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	4	1.13
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	23	1.13
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	26	1.13
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	37	1.13
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	38	1.13
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	37	1.13
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	37	1.13
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	37	1.13
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	37	1.13
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	2	1.13
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	6	1.13
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	34	1.13
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	36	1.13
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	37	1.13
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	47	1.13
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	2	1.13
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	6	1.13
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	34	1.13
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	36	1.13
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	37	1.13
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	47	1.13
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	1	1.12
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	2	1.12
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	9	1.12
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	10	1.12
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	13	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	27	1.12
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	28	1.12
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	46	1.12
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	7	1.12
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	7	1.12
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	33	1.12
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	41	1.12
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	46	1.12
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	33	1.12
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	41	1.12
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	46	1.12
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	6	1.11
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	8	1.11
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	28	1.11
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	8	1.11
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	28	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	4	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	8	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	11	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	24	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	30	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	36	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	37	1.11
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	40	1.11
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	29	1.11
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	29	1.11
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	15	1.1
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	32	1.1
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	33	1.1
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	27	1.1
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	27	1.1
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	18	1.1
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	21	1.1
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	22	1.1
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	44	1.1
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	24	1.09
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	26	1.09
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	33	1.09
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	26	1.09
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	33	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	7	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	9	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	23	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	31	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	33	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	34	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	38	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	42	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	43	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	46	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	48	1.09
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	49	1.09
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	26	1.09
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	26	1.09
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	34	1.08
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	5	1.08
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	9	1.08
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	32	1.08
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	5	1.08
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	9	1.08
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	32	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	1	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	5	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	10	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	12	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	14	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	15	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	28	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	32	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	35	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	45	1.08
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	50	1.08
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	1	1.08
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	14	1.08
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	27	1.08
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	44	1.08
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	48	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	1	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	14	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	27	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	44	1.08
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	48	1.08
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	21	1.07
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	4	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	10	1.07
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	11	1.07
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	13	1.07
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	17	1.07
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	37	1.07
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	38	1.07
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	4	1.07
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	10	1.07
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	11	1.07
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	13	1.07
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	17	1.07
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	37	1.07
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	38	1.07
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	38	1.07
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	38	1.07
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	38	1.07
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	2	1.07
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	3	1.07
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	13	1.07
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	19	1.07
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	26	1.07
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	39	1.07
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	47	1.07
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	38	1.07
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	9	1.07
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	22	1.07
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	42	1.07
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	9	1.07
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	22	1.07
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	42	1.07
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	37	1.07
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	37	1.07
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	22	1.06
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	25	1.06
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	2	1.06
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	3	1.06
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	36	1.06
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	2	1.06
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	3	1.06
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	36	1.06
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	45	1.06
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	45	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	45	1.06
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	6	1.06
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	20	1.06
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	45	1.06
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	4	1.06
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	15	1.06
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	38	1.06
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	43	1.06
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	4	1.06
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	15	1.06
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	38	1.06
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	43	1.06
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	36	1.06
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	36	1.06
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	38	1.05
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	38	1.05
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	20	1.05
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	44	1.05
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	20	1.05
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	44	1.05
(1,1753)	1:15:A:LEU:HD11	1:16:A:LEU:H	21	1.05
(1,1753)	1:15:A:LEU:HD13	1:16:A:LEU:H	24	1.05
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD11	21	1.05
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD13	24	1.05
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	40	1.04
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	17	1.04
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	10	1.04
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	11	1.04
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	31	1.04
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	10	1.04
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	11	1.04
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	31	1.04
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	1	1.03
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	1	1.03
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	16	1.03
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	39	1.03
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	39	1.03
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	12	1.03
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	45	1.03
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	46	1.03
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	12	1.03
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	45	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	46	1.03
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	49	1.02
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	15	1.02
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	31	1.02
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	15	1.02
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	31	1.02
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	29	1.02
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	41	1.02
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	3	1.02
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	16	1.02
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	3	1.02
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	16	1.02
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	38	1.02
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	38	1.02
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	6	1.01
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	21	1.01
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	6	1.01
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	21	1.01
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	9	1.01
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	33	1.01
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	50	1.01
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	9	1.01
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	33	1.01
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	50	1.01
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	12	1.0
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	12	1.0
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	19	1.0
(1,1753)	1:15:A:LEU:HD22	1:16:A:LEU:H	23	1.0
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	19	1.0
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD22	23	1.0
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	8	1.0
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	47	1.0
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	8	1.0
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	47	1.0
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	22	0.99
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	49	0.99
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	22	0.99
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	49	0.99
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	5	0.99
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	7	0.99
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	13	0.99
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	18	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	24	0.99
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	5	0.99
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	7	0.99
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	13	0.99
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	18	0.99
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	24	0.99
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	23	0.98
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	23	0.98
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	4	0.98
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	50	0.98
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	4	0.98
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	50	0.98
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	17	0.98
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	17	0.98
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	4	0.98
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	11	0.98
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	21	0.98
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	30	0.98
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	4	0.98
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	11	0.98
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	21	0.98
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	30	0.98
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	50	0.98
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	50	0.98
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	40	0.97
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	40	0.97
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	8	0.97
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	15	0.97
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	21	0.97
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	24	0.97
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	43	0.97
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	44	0.97
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	48	0.97
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	8	0.97
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	15	0.97
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	21	0.97
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	24	0.97
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	43	0.97
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	44	0.97
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	48	0.97
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	44	0.97
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	44	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	39	0.96
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	39	0.96
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	7	0.96
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	9	0.96
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	10	0.96
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	11	0.96
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	14	0.96
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	22	0.96
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	28	0.96
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	30	0.96
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	33	0.96
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	34	0.96
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	40	0.96
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	49	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	7	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	9	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	10	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	11	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	14	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	22	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	28	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	30	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	33	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	34	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	40	0.96
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	49	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	10	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	20	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	22	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	34	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	40	0.96
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	41	0.96
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	10	0.96
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	20	0.96
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	22	0.96
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	34	0.96
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	40	0.96
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	41	0.96
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	27	0.95
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	2	0.95
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	3	0.95
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	6	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	18	0.95
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	26	0.95
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	31	0.95
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	32	0.95
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	35	0.95
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	39	0.95
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	42	0.95
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	46	0.95
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	47	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	2	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	3	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	6	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	18	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	26	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	31	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	32	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	35	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	39	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	42	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	46	0.95
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	47	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	1	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	2	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	6	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	19	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	23	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	28	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	29	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	31	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	32	0.95
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	35	0.95
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	1	0.95
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	2	0.95
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	6	0.95
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	19	0.95
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	23	0.95
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	28	0.95
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	29	0.95
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	31	0.95
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	32	0.95
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	35	0.95
(1,1827)	1:9:A:ILE:HG13	1:6:A:TRP:HE3	25	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	1	0.94
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	12	0.94
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	13	0.94
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	20	0.94
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	23	0.94
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	1	0.94
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	12	0.94
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	13	0.94
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	20	0.94
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	23	0.94
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	8	0.94
(1,1753)	1:15:A:LEU:HD21	1:16:A:LEU:H	12	0.94
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	8	0.94
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD21	12	0.94
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	3	0.94
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	14	0.94
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	26	0.94
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	43	0.94
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	49	0.94
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	3	0.94
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	14	0.94
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	26	0.94
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	43	0.94
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	49	0.94
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	39	0.93
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	34	0.93
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	34	0.93
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	5	0.93
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	19	0.93
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	5	0.93
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	19	0.93
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	15	0.93
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	16	0.93
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	17	0.93
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	48	0.93
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	15	0.93
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	16	0.93
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	17	0.93
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	48	0.93
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	24	0.92
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	45	0.92
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	24	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	45	0.92
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	16	0.92
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	29	0.92
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	36	0.92
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	37	0.92
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	38	0.92
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	16	0.92
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	29	0.92
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	36	0.92
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	37	0.92
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	38	0.92
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB3	39	0.92
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	42	0.92
(1,1727)	1:10:A:ALA:HB3	1:9:A:ILE:HG12	39	0.92
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	42	0.92
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	43	0.91
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	43	0.91
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	25	0.91
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	25	0.91
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	17	0.91
(1,1788)	1:5:A:ILE:HD12	1:9:A:ILE:HG13	25	0.91
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	17	0.91
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD12	25	0.91
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB1	27	0.91
(1,1727)	1:10:A:ALA:HB1	1:9:A:ILE:HG12	27	0.91
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	5	0.9
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	27	0.9
(1,1788)	1:5:A:ILE:HD11	1:9:A:ILE:HG13	41	0.9
(1,1788)	1:5:A:ILE:HD13	1:9:A:ILE:HG13	45	0.9
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	27	0.9
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD11	41	0.9
(1,1762)	1:9:A:ILE:HG13	1:5:A:ILE:HD13	45	0.9
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	47	0.89
(1,1753)	1:15:A:LEU:HD23	1:16:A:LEU:H	40	0.89
(1,1746)	1:16:A:LEU:H	1:15:A:LEU:HD23	40	0.89
(1,1739)	1:9:A:ILE:HG12	1:10:A:ALA:HB2	25	0.89
(1,1727)	1:10:A:ALA:HB2	1:9:A:ILE:HG12	25	0.89
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	35	0.87
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	35	0.87
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	16	0.86
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	18	0.86
(1,1844)	1:27:A:LYS:H	1:29:A:LEU:HD21	43	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	16	0.86
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	18	0.86
(1,1842)	1:29:A:LEU:HD21	1:27:A:LYS:H	43	0.86
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	43	0.85
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	43	0.85
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	37	0.84
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	41	0.83
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	41	0.83
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	36	0.83
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	16	0.82
(1,1867)	1:23:A:PHE:HE1	1:24:A:TRP:H	18	0.82
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	16	0.82
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE1	18	0.82
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD12	27	0.81
(1,1722)	1:25:A:LEU:HD12	1:21:A:PHE:HD2	27	0.81
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	38	0.8
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	45	0.8
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	48	0.79
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	48	0.79
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	35	0.78
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	25	0.78
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	25	0.78
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	32	0.77
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	32	0.77
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	41	0.76
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	29	0.76
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	29	0.76
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	25	0.76
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	25	0.76
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	25	0.76
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	25	0.76
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	38	0.76
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	28	0.76
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	28	0.76
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	44	0.75
(1,1844)	1:27:A:LYS:H	1:29:A:LEU:HD21	47	0.74
(1,1842)	1:29:A:LEU:HD21	1:27:A:LYS:H	47	0.74
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	27	0.73
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	27	0.73
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	4	0.73
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	43	0.73
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	44	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	47	0.73
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	47	0.73
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	42	0.72
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	48	0.72
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	16	0.72
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	16	0.72
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	42	0.72
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	42	0.72
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	9	0.72
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	21	0.72
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	24	0.72
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	5	0.71
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	17	0.71
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	19	0.71
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	47	0.71
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	5	0.71
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	17	0.71
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	19	0.71
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	47	0.71
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	49	0.71
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD12	49	0.71
(1,1722)	1:25:A:LEU:HD12	1:21:A:PHE:HD2	49	0.71
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	14	0.71
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	14	0.71
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	28	0.7
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	13	0.7
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	42	0.7
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	13	0.7
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	42	0.7
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	29	0.7
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	29	0.7
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	42	0.7
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	48	0.7
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	45	0.7
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	45	0.7
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	1	0.69
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	11	0.69
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	15	0.69
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	32	0.69
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	34	0.69
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	8	0.69
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	40	0.68
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	40	0.68
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	32	0.67
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	41	0.67
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	41	0.67
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD22	19	0.67
(1,1842)	1:25:A:LEU:HD22	1:27:A:LYS:H	19	0.67
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	2	0.67
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	6	0.67
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	14	0.67
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	23	0.67
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	25	0.67
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	47	0.67
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	7	0.67
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	44	0.67
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	7	0.67
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	44	0.67
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	23	0.66
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	23	0.66
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	19	0.66
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	19	0.66
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	19	0.66
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	19	0.66
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	16	0.66
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	18	0.66
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	19	0.66
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	20	0.66
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	29	0.66
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	35	0.66
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	36	0.65
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	7	0.65
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	13	0.65
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	22	0.65
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	36	0.65
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	37	0.65
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	3	0.64
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	11	0.64
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	20	0.64
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	5	0.64
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	10	0.64
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	40	0.64
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	48	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	48	0.64
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	4	0.63
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	6	0.63
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	9	0.63
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	23	0.63
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	24	0.63
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	37	0.63
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	38	0.63
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	8	0.63
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	26	0.63
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	27	0.63
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	33	0.63
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	1	0.62
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	2	0.62
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	10	0.62
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	13	0.62
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	15	0.62
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	26	0.62
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	27	0.62
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	31	0.62
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	31	0.62
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	30	0.62
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	41	0.62
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	46	0.62
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	40	0.62
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	40	0.62
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	25	0.61
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	34	0.61
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	8	0.61
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	14	0.61
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	33	0.61
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	50	0.61
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	33	0.61
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	50	0.61
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	3	0.61
(1,1779)	1:12:A:LEU:HD21	1:9:A:ILE:H	28	0.61
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	31	0.61
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	39	0.61
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	22	0.61
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	39	0.61
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	22	0.61
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	39	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	46	0.6
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	42	0.6
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	48	0.6
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	1	0.6
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	1	0.6
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD23	30	0.6
(1,1842)	1:25:A:LEU:HD23	1:27:A:LYS:H	30	0.6
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	41	0.6
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	42	0.6
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	48	0.6
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	41	0.6
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	41	0.6
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	41	0.6
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	12	0.6
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	45	0.6
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	21	0.6
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	35	0.6
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	21	0.6
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	35	0.6
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	21	0.59
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	22	0.59
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	33	0.59
(1,1867)	1:23:A:PHE:HE2	1:24:A:TRP:H	50	0.59
(1,1858)	1:24:A:TRP:H	1:23:A:PHE:HE2	50	0.59
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	46	0.59
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	46	0.59
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	40	0.58
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	26	0.58
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	30	0.58
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	30	0.58
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	26	0.58
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	17	0.58
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	17	0.58
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	46	0.57
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	27	0.57
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	27	0.57
(1,1779)	1:12:A:LEU:HD23	1:9:A:ILE:H	50	0.57
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	15	0.57
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	41	0.57
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	15	0.57
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	41	0.57
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	49	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	3	0.56
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	3	0.56
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	49	0.56
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	47	0.55
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	49	0.55
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	7	0.55
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	7	0.55
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	12	0.55
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	12	0.55
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD12	24	0.54
(1,1722)	1:25:A:LEU:HD12	1:21:A:PHE:HD2	24	0.54
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	42	0.54
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	42	0.54
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	9	0.53
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	27	0.53
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	9	0.53
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	27	0.53
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	27	0.53
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	27	0.53
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	21	0.53
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	21	0.53
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	16	0.53
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	16	0.53
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	43	0.52
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	43	0.52
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	5	0.52
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	34	0.52
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	5	0.52
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	34	0.52
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	24	0.51
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	24	0.51
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	4	0.51
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	15	0.51
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	24	0.51
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	38	0.51
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	4	0.51
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	15	0.51
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	24	0.51
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	38	0.51
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	7	0.5
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	9	0.5
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	9	0.5
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	20	0.5
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	9	0.5
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	40	0.5
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	44	0.5
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	9	0.5
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	40	0.5
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	44	0.5
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	26	0.5
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	26	0.5
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	39	0.49
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	19	0.49
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	44	0.49
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	47	0.49
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	31	0.49
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	34	0.49
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	19	0.49
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	31	0.49
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	34	0.49
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	44	0.49
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	47	0.49
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	42	0.49
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	48	0.49
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	42	0.49
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	48	0.49
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	1	0.49
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	11	0.49
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	20	0.49
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	1	0.49
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	11	0.49
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	20	0.49
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	5	0.48
(1,1867)	1:27:A:LYS:HZ3	1:24:A:TRP:H	30	0.48
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	16	0.48
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	18	0.48
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	46	0.48
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	39	0.48
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ3	30	0.48
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	39	0.48
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	16	0.48
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	18	0.48
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	46	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	1:12:A:LEU:HD22	1:9:A:ILE:H	17	0.48
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	15	0.48
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	48	0.48
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	36	0.48
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	3	0.48
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	9	0.48
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	25	0.48
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	33	0.48
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	36	0.48
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	3	0.48
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	9	0.48
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	25	0.48
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	33	0.48
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	36	0.48
(1,1867)	1:27:A:LYS:HZ2	1:24:A:TRP:H	29	0.47
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	32	0.47
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	39	0.47
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	41	0.47
(1,1858)	1:24:A:TRP:H	1:27:A:LYS:HZ2	29	0.47
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	32	0.47
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	39	0.47
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	41	0.47
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	37	0.47
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	28	0.47
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	28	0.47
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	2	0.47
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	4	0.47
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	10	0.47
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	13	0.47
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	37	0.47
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	38	0.47
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	2	0.47
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	4	0.47
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	10	0.47
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	13	0.47
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	37	0.47
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	38	0.47
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	4	0.46
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	17	0.46
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	31	0.46
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	35	0.46
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	38	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	50	0.46
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	2	0.46
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	2	0.46
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	4	0.46
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	17	0.46
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	31	0.46
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	35	0.46
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	38	0.46
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	50	0.46
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	42	0.46
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	43	0.46
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	6	0.46
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	6	0.46
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	45	0.45
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	30	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	2	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	3	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	5	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	15	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	19	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	29	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	30	0.45
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	32	0.45
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	32	0.45
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	2	0.45
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	3	0.45
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	5	0.45
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	15	0.45
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	19	0.45
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	29	0.45
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	30	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	1	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	3	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	6	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	14	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	20	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	23	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	31	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	35	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	39	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	40	0.45
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	49	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1764)	1:18:A:PHE:H	1:19:A:LEU:HA	27	0.45
(1,1755)	1:19:A:LEU:HA	1:18:A:PHE:H	27	0.45
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	6	0.44
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	7	0.44
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	11	0.44
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	12	0.44
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	13	0.44
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	14	0.44
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	36	0.44
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	37	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	6	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	7	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	11	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	12	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	13	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	14	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	36	0.44
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	37	0.44
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	14	0.44
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	27	0.44
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	39	0.44
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	14	0.44
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	27	0.44
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	39	0.44
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	2	0.44
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	10	0.44
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	26	0.44
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	28	0.44
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	34	0.44
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	27	0.44
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	38	0.44
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	45	0.44
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	8	0.44
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	8	0.44
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	18	0.44
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	18	0.44
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	19	0.43
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	29	0.43
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	31	0.43
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	39	0.43
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	10	0.43
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	23	0.43
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	28	0.43
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	33	0.43
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	10	0.43
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	20	0.43
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	23	0.43
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	28	0.43
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	33	0.43
(1,1823)	1:20:A:ALA:H	1:21:A:PHE:HD2	49	0.43
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	22	0.43
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	32	0.43
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	44	0.43
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	7	0.43
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	7	0.43
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	1	0.42
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	8	0.42
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	34	0.42
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	45	0.42
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	1	0.42
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	8	0.42
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	34	0.42
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	45	0.42
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	16	0.42
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	17	0.42
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	28	0.42
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	16	0.42
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	17	0.42
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	28	0.42
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	7	0.42
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	21	0.42
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	25	0.42
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	14	0.42
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	14	0.42
(1,1711)	1:29:A:LEU:HD11	1:28:A:TYR:HE2	8	0.42
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	43	0.41
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	5	0.41
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	43	0.41
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	5	0.41
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	5	0.41
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	5	0.41
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	23	0.41
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	35	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	40	0.41
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	42	0.41
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	23	0.41
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	35	0.41
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	40	0.41
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	42	0.41
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	4	0.41
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	8	0.41
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	11	0.41
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	24	0.41
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	30	0.41
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	12	0.41
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	31	0.41
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	35	0.41
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	41	0.41
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	12	0.41
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	31	0.41
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	35	0.41
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	41	0.41
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	45	0.41
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	22	0.4
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	22	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	1	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	11	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	18	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	19	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	20	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	29	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	32	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	43	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	48	0.4
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	49	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	1	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	11	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	18	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	19	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	20	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	29	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	32	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	43	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	48	0.4
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	49	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	47	0.4
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	13	0.4
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	16	0.4
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	33	0.4
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	5	0.4
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	50	0.4
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	5	0.4
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	50	0.4
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	49	0.4
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	49	0.4
(2,9)	1:17:A:THR:O	1:21:A:PHE:H	26	0.39
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	21	0.39
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	42	0.39
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	21	0.39
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	42	0.39
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	42	0.39
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	42	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	2	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	3	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	8	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	15	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	22	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	34	0.39
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	44	0.39
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	2	0.39
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	3	0.39
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	8	0.39
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	15	0.39
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	22	0.39
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	34	0.39
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	44	0.39
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	5	0.39
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	9	0.39
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	13	0.39
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	18	0.39
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	19	0.39
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	33	0.39
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	50	0.39
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	4	0.39
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	29	0.39
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	41	0.39
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	17	0.39
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	19	0.39
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	22	0.39
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	30	0.39
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	39	0.39
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	46	0.39
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	10	0.39
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	17	0.39
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	19	0.39
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	22	0.39
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	30	0.39
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	39	0.39
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	46	0.39
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	42	0.38
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	48	0.38
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	25	0.38
(1,1861)	1:18:A:PHE:HE2	1:19:A:LEU:H	40	0.38
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	25	0.38
(1,1836)	1:19:A:LEU:H	1:18:A:PHE:HE2	40	0.38
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	6	0.38
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	10	0.38
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	21	0.38
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	24	0.38
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	30	0.38
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	31	0.38
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	6	0.38
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	10	0.38
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	21	0.38
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	24	0.38
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	30	0.38
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	31	0.38
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	17	0.38
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	8	0.38
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	9	0.38
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	15	0.38
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	19	0.38
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	26	0.38
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	28	0.38
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	43	0.38
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	44	0.38
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	48	0.38
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	49	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	50	0.38
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	23	0.38
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	29	0.38
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	34	0.38
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	23	0.38
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	29	0.38
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	34	0.38
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	27	0.38
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	5	0.38
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	7	0.38
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	42	0.38
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	27	0.38
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	7	0.37
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	25	0.37
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	46	0.37
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	47	0.37
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	7	0.37
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	25	0.37
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	46	0.37
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	47	0.37
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	35	0.37
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	41	0.37
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	35	0.37
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	41	0.37
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	16	0.37
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	2	0.37
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	7	0.37
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	10	0.37
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	11	0.37
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	12	0.37
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	17	0.37
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	18	0.37
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	21	0.37
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	22	0.37
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	24	0.37
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	30	0.37
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	31	0.37
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	32	0.37
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	34	0.37
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	35	0.37
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	39	0.37
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	40	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	46	0.37
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	6	0.37
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	32	0.37
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	6	0.37
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	32	0.37
(1,1850)	1:27:A:LYS:HG3	1:30:A:GLN:HB3	18	0.36
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	23	0.36
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	40	0.36
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	23	0.36
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	40	0.36
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	23	0.36
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	40	0.36
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	23	0.36
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	40	0.36
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	4	0.36
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	5	0.36
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	26	0.36
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	36	0.36
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	41	0.36
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	4	0.36
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	5	0.36
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	26	0.36
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	36	0.36
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	41	0.36
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	12	0.36
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	46	0.36
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	1	0.36
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	3	0.36
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	14	0.36
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	23	0.36
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	42	0.36
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	47	0.36
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	1	0.36
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	45	0.36
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	1	0.36
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	45	0.36
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	43	0.35
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	9	0.35
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	33	0.35
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	37	0.35
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	38	0.35
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	45	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	50	0.35
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	9	0.35
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	33	0.35
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	37	0.35
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	38	0.35
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	45	0.35
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	50	0.35
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	50	0.35
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	50	0.35
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG22	29	0.35
(1,1771)	1:8:A:VAL:HG21	1:5:A:ILE:HB	6	0.35
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	13	0.35
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	25	0.35
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	36	0.35
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	37	0.35
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	13	0.35
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	25	0.35
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	36	0.35
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	37	0.35
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	25	0.35
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	35	0.35
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	41	0.35
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	12	0.34
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	50	0.34
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	13	0.34
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	13	0.34
(1,1771)	1:8:A:VAL:HG23	1:5:A:ILE:HB	5	0.34
(1,1771)	1:8:A:VAL:HG22	1:5:A:ILE:HB	20	0.34
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	11	0.34
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	18	0.34
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	33	0.34
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	11	0.34
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	18	0.34
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	33	0.34
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	19	0.34
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	24	0.34
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	19	0.34
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	35	0.33
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	41	0.33
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	17	0.33
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	17	0.33
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	17	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	17	0.33
(1,1803)	1:12:A:LEU:HA	1:9:A:ILE:HA	12	0.33
(1,1801)	1:9:A:ILE:HA	1:12:A:LEU:HA	12	0.33
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG21	27	0.33
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	41	0.33
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	2	0.33
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	16	0.33
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	20	0.33
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	2	0.33
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	16	0.33
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	20	0.33
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD11	44	0.33
(1,1722)	1:25:A:LEU:HD11	1:21:A:PHE:HD2	44	0.33
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	29	0.33
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	23	0.33
(1,1711)	1:25:A:LEU:HD22	1:28:A:TYR:HE2	43	0.33
(1,1711)	1:25:A:LEU:HD23	1:28:A:TYR:HE2	47	0.33
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	29	0.33
(1,1841)	1:8:A:VAL:HG21	1:6:A:TRP:H	37	0.32
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	1	0.32
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	3	0.32
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	1	0.32
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	3	0.32
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	1	0.32
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	3	0.32
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	1	0.32
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	3	0.32
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	3	0.32
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	3	0.32
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	31	0.32
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	1	0.32
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	31	0.32
(1,1841)	1:8:A:VAL:HG22	1:6:A:TRP:H	36	0.31
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	29	0.31
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	39	0.31
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	29	0.31
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	39	0.31
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	29	0.31
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	39	0.31
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	29	0.31
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	39	0.31
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	47	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	47	0.31
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD13	30	0.31
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	2	0.31
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	3	0.31
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	4	0.31
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	6	0.31
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	9	0.31
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	14	0.31
(1,1711)	1:29:A:LEU:HD11	1:28:A:TYR:HE2	36	0.31
(1,1711)	1:29:A:LEU:HD11	1:28:A:TYR:HE2	37	0.31
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	38	0.31
(1,1711)	1:29:A:LEU:HD11	1:28:A:TYR:HE2	48	0.31
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	49	0.31
(1,1708)	1:25:A:LEU:HD13	1:26:A:PHE:HZ	30	0.31
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	8	0.3
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	14	0.3
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	20	0.3
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	27	0.3
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	39	0.3
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	41	0.3
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	14	0.3
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	20	0.3
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	27	0.3
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	39	0.3
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	41	0.3
(1,1791)	1:26:A:PHE:HA	1:29:A:LEU:H	46	0.3
(1,1764)	1:18:A:PHE:H	1:16:A:LEU:HA	49	0.3
(1,1755)	1:16:A:LEU:HA	1:18:A:PHE:H	49	0.3
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	22	0.3
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	39	0.3
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	8	0.29
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	14	0.29
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	46	0.29
(1,1852)	1:23:A:PHE:HD1	1:27:A:LYS:H	46	0.29
(1,1849)	1:27:A:LYS:H	1:23:A:PHE:HD1	46	0.29
(1,1841)	1:8:A:VAL:HG22	1:6:A:TRP:H	38	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	1	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	2	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	3	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	4	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	5	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	7	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	8	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	10	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	11	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	12	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	13	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	15	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	16	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	17	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	18	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	19	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	21	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	22	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	23	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	24	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	25	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	26	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	28	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	29	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	30	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	31	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	32	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	33	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	34	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	35	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	36	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	37	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	40	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	43	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	44	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	45	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	46	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	47	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	48	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	49	0.29
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	50	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	1	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	2	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	3	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	4	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	5	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	7	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	8	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	10	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	11	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	12	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	13	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	15	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	16	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	17	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	18	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	19	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	21	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	22	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	23	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	24	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	25	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	26	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	28	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	29	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	30	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	31	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	32	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	33	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	34	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	35	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	36	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	37	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	40	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	43	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	44	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	45	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	46	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	47	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	48	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	49	0.29
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	50	0.29
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	8	0.29
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	8	0.29
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	18	0.29
(1,1711)	1:29:A:LEU:HD12	1:28:A:TYR:HE2	21	0.29
(1,1841)	1:8:A:VAL:HG21	1:6:A:TRP:H	45	0.28
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	31	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	9	0.28
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	38	0.28
(1,1833)	1:11:A:GLY:H	1:12:A:LEU:HA	42	0.28
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	31	0.28
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	31	0.28
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	9	0.28
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	38	0.28
(1,1825)	1:12:A:LEU:HA	1:11:A:GLY:H	42	0.28
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	31	0.28
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	7	0.28
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	12	0.28
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	17	0.28
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	48	0.28
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	7	0.28
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	12	0.28
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	17	0.28
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	48	0.28
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD12	32	0.28
(1,1722)	1:25:A:LEU:HD12	1:21:A:PHE:HD2	32	0.28
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD11	24	0.28
(1,1708)	1:25:A:LEU:HD11	1:26:A:PHE:HZ	24	0.28
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	14	0.27
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	14	0.27
(2,19)	1:23:A:PHE:O	1:27:A:LYS:H	17	0.26
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	2	0.26
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	16	0.26
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	2	0.26
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	16	0.26
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	2	0.26
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	16	0.26
(1,1823)	1:20:A:ALA:H	1:21:A:PHE:HD2	27	0.26
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	2	0.26
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	16	0.26
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	5	0.26
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	42	0.26
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	5	0.26
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	42	0.26
(1,1080)	1:27:A:LYS:H	1:26:A:PHE:HD1	46	0.26
(1,1080)	1:27:A:LYS:H	1:26:A:PHE:HD2	46	0.26
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	46	0.25
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	46	0.25
(1,1850)	1:27:A:LYS:HG3	1:30:A:GLN:HB3	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	5	0.24
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	12	0.24
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	12	0.24
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	30	0.24
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	30	0.24
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	30	0.24
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	30	0.24
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	39	0.24
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	39	0.24
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD11	43	0.24
(1,1745)	1:25:A:LEU:HD11	1:24:A:TRP:HE3	43	0.24
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD11	28	0.24
(1,1722)	1:25:A:LEU:HD11	1:21:A:PHE:HD2	28	0.24
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	7	0.23
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	28	0.23
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	28	0.23
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	13	0.23
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	14	0.23
(1,1834)	1:23:A:PHE:HD1	1:27:A:LYS:HG3	45	0.23
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	13	0.23
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	14	0.23
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	13	0.23
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	14	0.23
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	13	0.23
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	14	0.23
(1,1799)	1:27:A:LYS:HG3	1:23:A:PHE:HD1	45	0.23
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD22	12	0.23
(1,1745)	1:25:A:LEU:HD22	1:24:A:TRP:HE3	12	0.23
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	14	0.22
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	22	0.22
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	22	0.22
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	34	0.22
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	48	0.22
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	34	0.22
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	48	0.22
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	34	0.22
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	48	0.22
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	34	0.22
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	48	0.22
(1,1809)	1:27:A:LYS:HG3	1:24:A:TRP:HA	47	0.22
(1,1807)	1:24:A:TRP:HA	1:27:A:LYS:HG3	47	0.22
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	24	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	31	0.22
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	24	0.22
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	31	0.22
(1,1772)	1:5:A:ILE:HG13	1:8:A:VAL:HG23	25	0.22
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	12	0.21
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	26	0.21
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	35	0.21
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	26	0.21
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	35	0.21
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	26	0.21
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	35	0.21
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	26	0.21
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	35	0.21
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	36	0.21
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	37	0.21
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	38	0.21
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	36	0.21
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	37	0.21
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	38	0.21
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	36	0.21
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	37	0.21
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	38	0.21
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	36	0.21
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	37	0.21
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	38	0.21
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD23	8	0.21
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	14	0.21
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD21	28	0.21
(1,1745)	1:25:A:LEU:HD23	1:24:A:TRP:HE3	8	0.21
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	14	0.21
(1,1745)	1:25:A:LEU:HD21	1:24:A:TRP:HE3	28	0.21
(1,1715)	1:26:A:PHE:HZ	1:25:A:LEU:HD12	23	0.21
(1,1708)	1:25:A:LEU:HD12	1:26:A:PHE:HZ	23	0.21
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	7	0.2
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	17	0.2
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	26	0.2
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	26	0.2
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	10	0.2
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	15	0.2
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	28	0.2
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	32	0.2
(1,1834)	1:23:A:PHE:HD1	1:27:A:LYS:HG3	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	10	0.2
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	15	0.2
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	28	0.2
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	32	0.2
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	10	0.2
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	15	0.2
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	28	0.2
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	32	0.2
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	10	0.2
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	15	0.2
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	28	0.2
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	32	0.2
(1,1809)	1:27:A:LYS:HG3	1:24:A:TRP:HA	14	0.2
(1,1807)	1:24:A:TRP:HA	1:27:A:LYS:HG3	14	0.2
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	45	0.2
(1,1799)	1:27:A:LYS:HG3	1:23:A:PHE:HD1	14	0.2
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	9	0.2
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	45	0.2
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	45	0.2
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	45	0.2
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD22	1	0.2
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD12	35	0.2
(1,1745)	1:25:A:LEU:HD22	1:24:A:TRP:HE3	1	0.2
(1,1745)	1:25:A:LEU:HD12	1:24:A:TRP:HE3	35	0.2
(1,1711)	1:29:A:LEU:HD11	1:28:A:TYR:HE2	46	0.2
(2,13)	1:19:A:LEU:O	1:23:A:PHE:H	28	0.19
(1,1852)	1:23:A:PHE:HD1	1:27:A:LYS:H	5	0.19
(1,1849)	1:27:A:LYS:H	1:23:A:PHE:HD1	5	0.19
(1,1839)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	22	0.19
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	43	0.19
(1,1839)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	49	0.19
(1,1834)	1:23:A:PHE:HD1	1:27:A:LYS:HG3	8	0.19
(1,1832)	1:8:A:VAL:HG21	1:3:A:HIS:HB3	22	0.19
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	43	0.19
(1,1832)	1:8:A:VAL:HG23	1:3:A:HIS:HB3	49	0.19
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	22	0.19
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	43	0.19
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	49	0.19
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG21	22	0.19
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	43	0.19
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG23	49	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	7	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	8	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	9	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	12	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	13	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	24	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	25	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	33	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	41	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	46	0.19
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	50	0.19
(1,1799)	1:27:A:LYS:HG3	1:23:A:PHE:HD1	8	0.19
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	19	0.19
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	30	0.19
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	19	0.19
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	30	0.19
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	4	0.19
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	43	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	4	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	7	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	8	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	9	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	12	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	13	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	24	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	25	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	33	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	41	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	46	0.19
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	50	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	4	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	7	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	8	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	9	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	12	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	13	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	24	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	25	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	33	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	41	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	46	0.19
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	50	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	4	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	7	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	8	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	9	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	12	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	13	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	24	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	25	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	33	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	41	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	46	0.19
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	50	0.19
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	17	0.19
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	17	0.19
(1,1530)	1:29:A:LEU:H	1:32:A:LYS:HB2	34	0.19
(1,1530)	1:29:A:LEU:H	1:32:A:LYS:HB3	34	0.19
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	28	0.19
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	28	0.19
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	50	0.19
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	50	0.19
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ1	49	0.19
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ2	49	0.19
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ3	49	0.19
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	33	0.19
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	33	0.19
(2,20)	1:23:A:PHE:O	1:27:A:LYS:N	45	0.18
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	14	0.18
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	14	0.18
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	5	0.18
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	11	0.18
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	19	0.18
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	21	0.18
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	30	0.18
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	44	0.18
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	29	0.18
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	45	0.18
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	29	0.18
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	45	0.18
(1,1789)	1:17:A:THR:HB	1:16:A:LEU:H	44	0.18
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	5	0.18
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	11	0.18
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	21	0.18
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	30	0.18
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	44	0.18
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	5	0.18
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	11	0.18
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	19	0.18
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	21	0.18
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	30	0.18
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	44	0.18
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	5	0.18
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	11	0.18
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	19	0.18
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	21	0.18
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	30	0.18
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	44	0.18
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD21	18	0.18
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	41	0.18
(1,1745)	1:25:A:LEU:HD21	1:24:A:TRP:HE3	18	0.18
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	41	0.18
(1,1711)	1:29:A:LEU:HD11	1:28:A:TYR:HE2	30	0.18
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	30	0.17
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	15	0.17
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	35	0.17
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	15	0.17
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	35	0.17
(1,1850)	1:27:A:LYS:HG3	1:30:A:GLN:HB3	43	0.17
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	11	0.17
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	13	0.17
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	20	0.17
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	33	0.17
(1,1809)	1:27:A:LYS:HG3	1:24:A:TRP:HA	7	0.17
(1,1809)	1:27:A:LYS:HG3	1:24:A:TRP:HA	8	0.17
(1,1807)	1:24:A:TRP:HA	1:27:A:LYS:HG3	7	0.17
(1,1807)	1:24:A:TRP:HA	1:27:A:LYS:HG3	8	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	1	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	2	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	3	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	6	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	10	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	14	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	15	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	17	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	18	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	20	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	22	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	23	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	26	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	27	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	28	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	29	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	31	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	32	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	34	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	35	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	39	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	40	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	42	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	43	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	47	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	48	0.17
(1,1800)	1:5:A:ILE:HA	1:8:A:VAL:HA	49	0.17
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	28	0.17
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	28	0.17
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	24	0.17
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	38	0.17
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	40	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	1	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	2	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	3	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	6	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	10	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	14	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	15	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	16	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	17	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	18	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	20	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	22	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	23	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	26	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	27	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	28	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	29	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	31	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	32	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	34	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	35	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	39	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	40	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	42	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	43	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	47	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	48	0.17
(1,1776)	1:8:A:VAL:HA	1:5:A:ILE:HA	49	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	1	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	2	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	3	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	6	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	10	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	14	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	15	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	16	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	17	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	18	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	20	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	22	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	23	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	26	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	27	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	28	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	29	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	31	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	32	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	34	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	35	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	39	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	40	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	42	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	43	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	47	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	48	0.17
(1,1775)	1:8:A:VAL:HA	1:5:A:ILE:HA	49	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	1	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	2	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	6	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	10	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	14	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	15	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	16	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	17	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	18	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	20	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	22	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	23	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	26	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	27	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	28	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	29	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	31	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	32	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	34	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	35	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	39	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	40	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	42	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	43	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	47	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	48	0.17
(1,1774)	1:8:A:VAL:HA	1:5:A:ILE:HA	49	0.17
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD12	37	0.17
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD23	45	0.17
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD11	47	0.17
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD21	50	0.17
(1,1745)	1:25:A:LEU:HD12	1:24:A:TRP:HE3	37	0.17
(1,1745)	1:25:A:LEU:HD23	1:24:A:TRP:HE3	45	0.17
(1,1745)	1:25:A:LEU:HD11	1:24:A:TRP:HE3	47	0.17
(1,1745)	1:25:A:LEU:HD21	1:24:A:TRP:HE3	50	0.17
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD11	6	0.17
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD11	34	0.17
(1,1722)	1:25:A:LEU:HD11	1:21:A:PHE:HD2	6	0.17
(1,1722)	1:25:A:LEU:HD11	1:21:A:PHE:HD2	34	0.17
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	44	0.17
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	44	0.17
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	32	0.17
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	32	0.17
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	29	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	31	0.16
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	39	0.16
(2,10)	1:17:A:THR:O	1:21:A:PHE:N	26	0.16
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	48	0.16
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	48	0.16
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	10	0.16
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	26	0.16
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	27	0.16
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	18	0.16
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	47	0.16
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	18	0.16
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	47	0.16
(1,1789)	1:17:A:THR:HB	1:16:A:LEU:H	48	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD11	2	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	6	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD22	7	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD22	32	0.16
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD21	44	0.16
(1,1745)	1:25:A:LEU:HD11	1:24:A:TRP:HE3	2	0.16
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	6	0.16
(1,1745)	1:25:A:LEU:HD22	1:24:A:TRP:HE3	7	0.16
(1,1745)	1:25:A:LEU:HD22	1:24:A:TRP:HE3	32	0.16
(1,1745)	1:25:A:LEU:HD21	1:24:A:TRP:HE3	44	0.16
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD13	22	0.16
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD13	26	0.16
(1,1722)	1:25:A:LEU:HD13	1:21:A:PHE:HD2	22	0.16
(1,1722)	1:25:A:LEU:HD13	1:21:A:PHE:HD2	26	0.16
(1,1711)	1:29:A:LEU:HD13	1:28:A:TYR:HE2	29	0.16
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	31	0.16
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	31	0.16
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	19	0.15
(2,7)	1:14:A:ALA:O	1:18:A:PHE:H	26	0.15
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	6	0.15
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG21	10	0.15
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	38	0.15
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	43	0.15
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG23	49	0.15
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	6	0.15
(1,1854)	1:8:A:VAL:HG21	1:3:A:HIS:HD2	10	0.15
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	38	0.15
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	43	0.15
(1,1854)	1:8:A:VAL:HG23	1:3:A:HIS:HD2	49	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1850)	1:27:A:LYS:HG3	1:30:A:GLN:HB3	44	0.15
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	50	0.15
(1,1834)	1:23:A:PHE:HD1	1:27:A:LYS:HG3	7	0.15
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	50	0.15
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	50	0.15
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	50	0.15
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	49	0.15
(1,1799)	1:27:A:LYS:HG3	1:23:A:PHE:HD1	7	0.15
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	15	0.15
(1,1789)	1:17:A:THR:HB	1:16:A:LEU:H	42	0.15
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	9	0.15
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	10	0.15
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	38	0.15
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	9	0.15
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	10	0.15
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	38	0.15
(1,1742)	1:21:A:PHE:HD2	1:25:A:LEU:HD11	10	0.15
(1,1722)	1:25:A:LEU:HD11	1:21:A:PHE:HD2	10	0.15
(1,1529)	1:29:A:LEU:HA	1:32:A:LYS:HG2	24	0.15
(1,1529)	1:29:A:LEU:HA	1:32:A:LYS:HG3	24	0.15
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD1	43	0.15
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD2	43	0.15
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD1	43	0.15
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD2	43	0.15
(1,1282)	1:30:A:GLN:HB2	1:32:A:LYS:HE2	33	0.15
(1,1282)	1:30:A:GLN:HB2	1:32:A:LYS:HE3	33	0.15
(1,1282)	1:30:A:GLN:HB3	1:32:A:LYS:HE2	33	0.15
(1,1282)	1:30:A:GLN:HB3	1:32:A:LYS:HE3	33	0.15
(1,405)	1:23:A:PHE:HE1	1:23:A:PHE:H	50	0.15
(1,405)	1:23:A:PHE:HE2	1:23:A:PHE:H	50	0.15
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE1	50	0.15
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE2	50	0.15
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	45	0.14
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	45	0.14
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	49	0.14
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	1	0.14
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	16	0.14
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	26	0.14
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	40	0.14
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	1	0.14
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	16	0.14
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	26	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	40	0.14
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD11	4	0.14
(1,1745)	1:25:A:LEU:HD11	1:24:A:TRP:HE3	4	0.14
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	26	0.14
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	26	0.14
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	31	0.14
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	31	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	10	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	10	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	11	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	11	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	13	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	13	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	20	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	20	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	44	0.14
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	44	0.14
(2,17)	1:22:A:GLY:O	1:26:A:PHE:H	35	0.13
(1,1852)	1:23:A:PHE:HD2	1:27:A:LYS:H	29	0.13
(1,1850)	1:27:A:LYS:HG3	1:30:A:GLN:HB3	32	0.13
(1,1849)	1:27:A:LYS:H	1:23:A:PHE:HD2	29	0.13
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	1	0.13
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	2	0.13
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	3	0.13
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	4	0.13
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	36	0.13
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	37	0.13
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	38	0.13
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	27	0.13
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	43	0.13
(1,1798)	1:20:A:ALA:H	1:22:A:GLY:HA3	46	0.13
(1,1790)	1:22:A:GLY:HA3	1:20:A:ALA:H	46	0.13
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	21	0.13
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	28	0.13
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD13	3	0.13
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD21	5	0.13
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD12	13	0.13
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD12	36	0.13
(1,1745)	1:25:A:LEU:HD13	1:24:A:TRP:HE3	3	0.13
(1,1745)	1:25:A:LEU:HD21	1:24:A:TRP:HE3	5	0.13
(1,1745)	1:25:A:LEU:HD12	1:24:A:TRP:HE3	13	0.13
(1,1745)	1:25:A:LEU:HD12	1:24:A:TRP:HE3	36	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD2	35	0.13
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD3	35	0.13
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD2	35	0.13
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD3	35	0.13
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD2	48	0.13
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD3	48	0.13
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD2	48	0.13
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD3	48	0.13
(1,1623)	1:23:A:PHE:HA	1:19:A:LEU:HA	28	0.13
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	48	0.13
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	48	0.13
(1,1179)	1:5:A:ILE:H	1:3:A:HIS:HE1	27	0.13
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	26	0.13
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	26	0.13
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	27	0.13
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	27	0.13
(1,395)	1:23:A:PHE:H	1:23:A:PHE:HD1	50	0.13
(1,395)	1:23:A:PHE:H	1:23:A:PHE:HD2	50	0.13
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	42	0.12
(1,1852)	1:23:A:PHE:HD2	1:27:A:LYS:H	19	0.12
(1,1852)	1:23:A:PHE:HD2	1:27:A:LYS:H	30	0.12
(1,1849)	1:27:A:LYS:H	1:23:A:PHE:HD2	19	0.12
(1,1849)	1:27:A:LYS:H	1:23:A:PHE:HD2	30	0.12
(1,1839)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	11	0.12
(1,1832)	1:8:A:VAL:HG22	1:3:A:HIS:HB3	11	0.12
(1,1830)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	11	0.12
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	6	0.12
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	9	0.12
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	34	0.12
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	35	0.12
(1,1818)	1:3:A:HIS:HB3	1:8:A:VAL:HG22	11	0.12
(1,1809)	1:27:A:LYS:HG3	1:26:A:PHE:HA	12	0.12
(1,1809)	1:27:A:LYS:HG3	1:24:A:TRP:HA	45	0.12
(1,1807)	1:26:A:PHE:HA	1:27:A:LYS:HG3	12	0.12
(1,1807)	1:24:A:TRP:HA	1:27:A:LYS:HG3	45	0.12
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	42	0.12
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	9	0.12
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	9	0.12
(1,1789)	1:17:A:THR:HB	1:14:A:ALA:H	46	0.12
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD12	24	0.12
(1,1745)	1:25:A:LEU:HD12	1:24:A:TRP:HE3	24	0.12
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD2	41	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD3	41	0.12
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD2	41	0.12
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD3	41	0.12
(1,1623)	1:23:A:PHE:HA	1:19:A:LEU:HA	40	0.12
(1,1622)	1:21:A:PHE:HA	1:17:A:THR:HA	49	0.12
(1,1605)	1:18:A:PHE:HA	1:14:A:ALA:HB1	26	0.12
(1,1605)	1:18:A:PHE:HA	1:14:A:ALA:HB2	26	0.12
(1,1605)	1:18:A:PHE:HA	1:14:A:ALA:HB3	26	0.12
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD1	47	0.12
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD2	47	0.12
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD1	47	0.12
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD2	47	0.12
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	6	0.12
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	6	0.12
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	6	0.12
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	6	0.12
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	6	0.12
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	6	0.12
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	20	0.12
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	20	0.12
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	20	0.12
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	20	0.12
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	20	0.12
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	20	0.12
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	47	0.12
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	47	0.12
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	47	0.12
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	47	0.12
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	47	0.12
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	47	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	6	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	6	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	6	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	6	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	6	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	6	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	20	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	20	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	20	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	20	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	20	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	47	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	47	0.12
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	47	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	47	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	47	0.12
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	47	0.12
(1,1286)	1:7:A:GLU:HB2	1:4:A:THR:H	37	0.12
(1,1286)	1:7:A:GLU:HB3	1:4:A:THR:H	37	0.12
(1,1264)	1:28:A:TYR:HD1	1:30:A:GLN:H	40	0.12
(1,1264)	1:28:A:TYR:HD2	1:30:A:GLN:H	40	0.12
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD1	34	0.12
(1,1135)	1:29:A:LEU:HG	1:28:A:TYR:HD2	34	0.12
(1,1085)	1:26:A:PHE:HD1	1:27:A:LYS:HG2	18	0.12
(1,1085)	1:26:A:PHE:HD1	1:27:A:LYS:HG3	18	0.12
(1,1085)	1:26:A:PHE:HD2	1:27:A:LYS:HG2	18	0.12
(1,1085)	1:26:A:PHE:HD2	1:27:A:LYS:HG3	18	0.12
(1,1079)	1:27:A:LYS:HG2	1:26:A:PHE:HD1	18	0.12
(1,1079)	1:27:A:LYS:HG2	1:26:A:PHE:HD2	18	0.12
(1,1079)	1:27:A:LYS:HG3	1:26:A:PHE:HD1	18	0.12
(1,1079)	1:27:A:LYS:HG3	1:26:A:PHE:HD2	18	0.12
(1,959)	1:18:A:PHE:HE1	1:19:A:LEU:HD11	40	0.12
(1,959)	1:18:A:PHE:HE1	1:19:A:LEU:HD12	40	0.12
(1,959)	1:18:A:PHE:HE1	1:19:A:LEU:HD13	40	0.12
(1,959)	1:18:A:PHE:HE1	1:19:A:LEU:HD21	40	0.12
(1,959)	1:18:A:PHE:HE1	1:19:A:LEU:HD22	40	0.12
(1,959)	1:18:A:PHE:HE1	1:19:A:LEU:HD23	40	0.12
(1,959)	1:18:A:PHE:HE2	1:19:A:LEU:HD11	40	0.12
(1,959)	1:18:A:PHE:HE2	1:19:A:LEU:HD12	40	0.12
(1,959)	1:18:A:PHE:HE2	1:19:A:LEU:HD13	40	0.12
(1,959)	1:18:A:PHE:HE2	1:19:A:LEU:HD21	40	0.12
(1,959)	1:18:A:PHE:HE2	1:19:A:LEU:HD22	40	0.12
(1,959)	1:18:A:PHE:HE2	1:19:A:LEU:HD23	40	0.12
(1,955)	1:19:A:LEU:HD11	1:18:A:PHE:HE1	40	0.12
(1,955)	1:19:A:LEU:HD11	1:18:A:PHE:HE2	40	0.12
(1,955)	1:19:A:LEU:HD12	1:18:A:PHE:HE1	40	0.12
(1,955)	1:19:A:LEU:HD12	1:18:A:PHE:HE2	40	0.12
(1,955)	1:19:A:LEU:HD13	1:18:A:PHE:HE1	40	0.12
(1,955)	1:19:A:LEU:HD13	1:18:A:PHE:HE2	40	0.12
(1,955)	1:19:A:LEU:HD21	1:18:A:PHE:HE1	40	0.12
(1,955)	1:19:A:LEU:HD21	1:18:A:PHE:HE2	40	0.12
(1,955)	1:19:A:LEU:HD22	1:18:A:PHE:HE1	40	0.12
(1,955)	1:19:A:LEU:HD22	1:18:A:PHE:HE2	40	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:19:A:LEU:HD23	1:18:A:PHE:HE1	40	0.12
(1,955)	1:19:A:LEU:HD23	1:18:A:PHE:HE2	40	0.12
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	17	0.12
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	17	0.12
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	34	0.12
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	34	0.12
(1,405)	1:23:A:PHE:HE1	1:23:A:PHE:H	46	0.12
(1,405)	1:23:A:PHE:HE2	1:23:A:PHE:H	46	0.12
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE1	46	0.12
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE2	46	0.12
(2,17)	1:22:A:GLY:O	1:26:A:PHE:H	41	0.11
(2,14)	1:19:A:LEU:O	1:23:A:PHE:N	48	0.11
(1,1860)	1:3:A:HIS:HD2	1:8:A:VAL:HG22	37	0.11
(1,1854)	1:8:A:VAL:HG22	1:3:A:HIS:HD2	37	0.11
(1,1850)	1:27:A:LYS:HG3	1:30:A:GLN:HB3	28	0.11
(1,1844)	1:27:A:LYS:H	1:25:A:LEU:HD21	46	0.11
(1,1842)	1:25:A:LEU:HD21	1:27:A:LYS:H	46	0.11
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	24	0.11
(1,1809)	1:27:A:LYS:HG3	1:26:A:PHE:HA	17	0.11
(1,1807)	1:26:A:PHE:HA	1:27:A:LYS:HG3	17	0.11
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	44	0.11
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	48	0.11
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	25	0.11
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	25	0.11
(1,1789)	1:17:A:THR:HB	1:16:A:LEU:H	22	0.11
(1,1789)	1:17:A:THR:HB	1:16:A:LEU:H	32	0.11
(1,1763)	1:24:A:TRP:HE3	1:25:A:LEU:HD11	16	0.11
(1,1745)	1:25:A:LEU:HD11	1:24:A:TRP:HE3	16	0.11
(1,1674)	1:29:A:LEU:H	1:25:A:LEU:HG	49	0.11
(1,1672)	1:25:A:LEU:HG	1:29:A:LEU:H	49	0.11
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	9	0.11
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	9	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	9	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	9	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	9	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	9	0.11
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	21	0.11
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	21	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	21	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	21	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	21	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	21	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	44	0.11
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	44	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	44	0.11
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	44	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	44	0.11
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	44	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	9	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	9	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	9	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	9	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	9	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	9	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	21	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	21	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	21	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	21	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	21	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	21	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	44	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	44	0.11
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	44	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	44	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	44	0.11
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	44	0.11
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	30	0.11
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	30	0.11
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	42	0.11
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	42	0.11
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ1	47	0.11
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ2	47	0.11
(1,1126)	1:28:A:TYR:H	1:27:A:LYS:HZ3	47	0.11
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	43	0.11
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	43	0.11
(1,405)	1:23:A:PHE:HE1	1:23:A:PHE:H	39	0.11
(1,405)	1:23:A:PHE:HE2	1:23:A:PHE:H	39	0.11
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE1	39	0.11
(1,404)	1:23:A:PHE:H	1:23:A:PHE:HE2	39	0.11
(2,17)	1:22:A:GLY:O	1:26:A:PHE:H	48	0.1
(2,8)	1:14:A:ALA:O	1:18:A:PHE:N	40	0.1
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	15	0.1
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	23	0.1
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	28	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	31	0.1
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	32	0.1
(1,1821)	1:25:A:LEU:HG	1:28:A:TYR:HE2	50	0.1
(1,1802)	1:9:A:ILE:HA	1:12:A:LEU:HG	15	0.1
(1,1798)	1:19:A:LEU:H	1:22:A:GLY:HA3	2	0.1
(1,1790)	1:22:A:GLY:HA3	1:19:A:LEU:H	2	0.1
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD2	39	0.1
(1,1701)	1:22:A:GLY:HA2	1:27:A:LYS:HD3	39	0.1
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD2	39	0.1
(1,1701)	1:22:A:GLY:HA3	1:27:A:LYS:HD3	39	0.1
(1,1610)	1:19:A:LEU:HG	1:15:A:LEU:HG	40	0.1
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD1	46	0.1
(1,1504)	1:29:A:LEU:HB2	1:26:A:PHE:HD2	46	0.1
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD1	46	0.1
(1,1504)	1:29:A:LEU:HB3	1:26:A:PHE:HD2	46	0.1
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	7	0.1
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	7	0.1
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	7	0.1
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	7	0.1
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	7	0.1
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	7	0.1
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB2	24	0.1
(1,1353)	1:10:A:ALA:HB1	1:7:A:GLU:HB3	24	0.1
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB2	24	0.1
(1,1353)	1:10:A:ALA:HB2	1:7:A:GLU:HB3	24	0.1
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB2	24	0.1
(1,1353)	1:10:A:ALA:HB3	1:7:A:GLU:HB3	24	0.1
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	7	0.1
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	7	0.1
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	7	0.1
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	7	0.1
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	7	0.1
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	7	0.1
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB1	24	0.1
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB2	24	0.1
(1,1352)	1:7:A:GLU:HB2	1:10:A:ALA:HB3	24	0.1
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB1	24	0.1
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB2	24	0.1
(1,1352)	1:7:A:GLU:HB3	1:10:A:ALA:HB3	24	0.1
(1,1286)	1:7:A:GLU:HB2	1:4:A:THR:H	36	0.1
(1,1286)	1:7:A:GLU:HB3	1:4:A:THR:H	36	0.1
(1,1273)	1:31:A:LYS:HD2	1:29:A:LEU:HA	32	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:31:A:LYS:HD3	1:29:A:LEU:HA	32	0.1
(1,1179)	1:5:A:ILE:H	1:3:A:HIS:HE1	19	0.1
(1,1085)	1:26:A:PHE:HD1	1:27:A:LYS:HG2	44	0.1
(1,1085)	1:26:A:PHE:HD1	1:27:A:LYS:HG3	44	0.1
(1,1085)	1:26:A:PHE:HD2	1:27:A:LYS:HG2	44	0.1
(1,1085)	1:26:A:PHE:HD2	1:27:A:LYS:HG3	44	0.1
(1,1079)	1:27:A:LYS:HG2	1:26:A:PHE:HD1	44	0.1
(1,1079)	1:27:A:LYS:HG2	1:26:A:PHE:HD2	44	0.1
(1,1079)	1:27:A:LYS:HG3	1:26:A:PHE:HD1	44	0.1
(1,1079)	1:27:A:LYS:HG3	1:26:A:PHE:HD2	44	0.1
(1,602)	1:29:A:LEU:HD11	1:29:A:LEU:HA	47	0.1
(1,602)	1:29:A:LEU:HD12	1:29:A:LEU:HA	47	0.1
(1,602)	1:29:A:LEU:HD13	1:29:A:LEU:HA	47	0.1
(1,602)	1:29:A:LEU:HD21	1:29:A:LEU:HA	47	0.1
(1,602)	1:29:A:LEU:HD22	1:29:A:LEU:HA	47	0.1
(1,602)	1:29:A:LEU:HD23	1:29:A:LEU:HA	47	0.1
(1,601)	1:29:A:LEU:HA	1:29:A:LEU:HD11	47	0.1
(1,601)	1:29:A:LEU:HA	1:29:A:LEU:HD12	47	0.1
(1,601)	1:29:A:LEU:HA	1:29:A:LEU:HD13	47	0.1
(1,601)	1:29:A:LEU:HA	1:29:A:LEU:HD21	47	0.1
(1,601)	1:29:A:LEU:HA	1:29:A:LEU:HD22	47	0.1
(1,601)	1:29:A:LEU:HA	1:29:A:LEU:HD23	47	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	10	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	10	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	11	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	11	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	13	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	13	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	26	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	26	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	27	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	27	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD1	31	0.1
(1,575)	1:28:A:TYR:HA	1:28:A:TYR:HD2	31	0.1
(1,98)	1:6:A:TRP:HD1	1:6:A:TRP:HE3	6	0.1
(1,98)	1:6:A:TRP:HD1	1:6:A:TRP:HE3	37	0.1
(1,98)	1:6:A:TRP:HD1	1:6:A:TRP:HE3	38	0.1

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

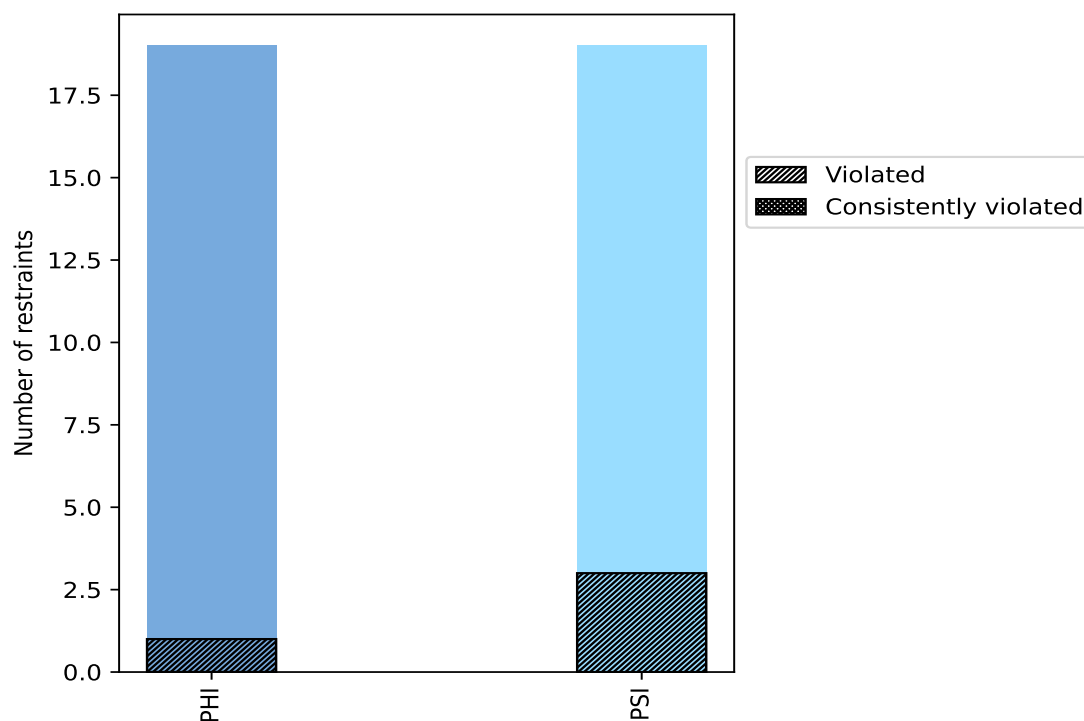
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	19	50.0	1	5.3	2.6	0	0.0	0.0
PSI	19	50.0	3	15.8	7.9	0	0.0	0.0
Total	38	100.0	4	10.5	10.5	0	0.0	0.0

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

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



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

10.2 Dihedral-angle violation statistics for each model [i](#)

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.

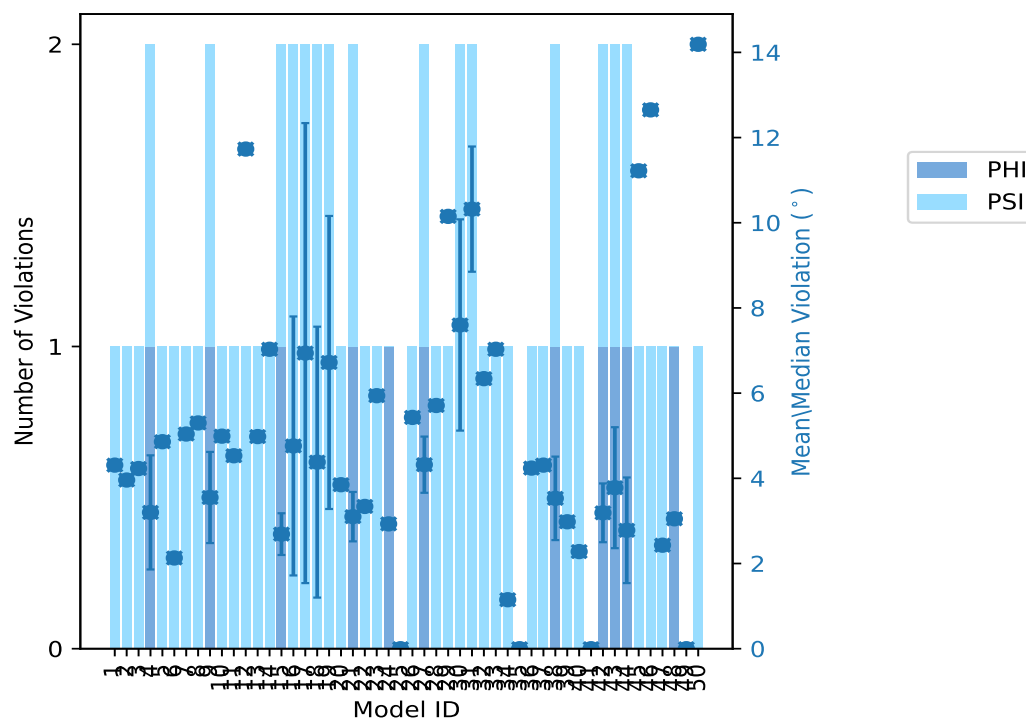
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	4.31	4.31	0.0	4.31
2	0	1	1	3.96	3.96	0.0	3.96
3	0	1	1	4.23	4.23	0.0	4.23
4	1	1	2	3.2	4.54	1.34	3.2
5	0	1	1	4.86	4.86	0.0	4.86
6	0	1	1	2.13	2.13	0.0	2.13
7	0	1	1	5.04	5.04	0.0	5.04
8	0	1	1	5.3	5.3	0.0	5.3
9	1	1	2	3.55	4.62	1.07	3.55
10	0	1	1	4.99	4.99	0.0	4.99
11	0	1	1	4.53	4.53	0.0	4.53
12	0	1	1	11.73	11.73	0.0	11.73
13	0	1	1	4.98	4.98	0.0	4.98
14	0	1	1	7.03	7.03	0.0	7.03
15	1	1	2	2.69	3.18	0.49	2.69
16	0	2	2	4.76	7.8	3.04	4.76
17	0	2	2	6.94	12.34	5.4	6.94
18	0	2	2	4.38	7.57	3.18	4.38
19	0	2	2	6.72	10.16	3.44	6.72
20	0	1	1	3.85	3.85	0.0	3.85
21	1	1	2	3.1	3.69	0.58	3.1
22	0	1	1	3.34	3.34	0.0	3.34
23	0	1	1	5.94	5.94	0.0	5.94
24	1	0	1	2.93	2.93	0.0	2.93
25	0	0	0	0.0	0.0	0.0	0.0
26	0	1	1	5.43	5.43	0.0	5.43
27	1	1	2	4.32	4.98	0.66	4.32
28	0	1	1	5.71	5.71	0.0	5.71
29	0	1	1	10.15	10.15	0.0	10.15
30	0	2	2	7.6	10.09	2.48	7.6
31	0	2	2	10.32	11.79	1.47	10.32
32	0	1	1	6.34	6.34	0.0	6.34
33	0	1	1	7.03	7.03	0.0	7.03
34	0	1	1	1.15	1.15	0.0	1.15
35	0	0	0	0.0	0.0	0.0	0.0
36	0	1	1	4.24	4.24	0.0	4.24
37	0	1	1	4.31	4.31	0.0	4.31
38	1	1	2	3.53	4.51	0.98	3.53

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	0	1	1	2.98	2.98	0.0	2.98
40	0	1	1	2.28	2.28	0.0	2.28
41	0	0	0	0.0	0.0	0.0	0.0
42	1	1	2	3.19	3.88	0.69	3.19
43	1	1	2	3.78	5.2	1.42	3.78
44	1	1	2	2.78	4.02	1.24	2.78
45	0	1	1	11.22	11.22	0.0	11.22
46	0	1	1	12.65	12.65	0.0	12.65
47	0	1	1	2.43	2.43	0.0	2.43
48	1	0	1	3.05	3.05	0.0	3.05
49	0	0	0	0.0	0.0	0.0	0.0
50	0	1	1	14.19	14.19	0.0	14.19

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	
PHI	PSI	Total	Count ¹	%
0	0	0	1	2.0
0	0	0	2	4.0
0	0	0	3	6.0
0	0	0	4	8.0
0	0	0	5	10.0
0	1	1	6	12.0
0	0	0	7	14.0
0	0	0	8	16.0
0	0	0	9	18.0
0	1	1	10	20.0
1	0	1	11	22.0
0	0	0	12	24.0
0	0	0	13	26.0
0	0	0	14	28.0
0	0	0	15	30.0
0	0	0	16	32.0
0	0	0	17	34.0
0	0	0	18	36.0
0	0	0	19	38.0
0	0	0	20	40.0
0	0	0	21	42.0
0	0	0	22	44.0
0	0	0	23	46.0
0	0	0	24	48.0
0	0	0	25	50.0
0	0	0	26	52.0
0	0	0	27	54.0
0	0	0	28	56.0
0	0	0	29	58.0
0	0	0	30	60.0
0	0	0	31	62.0
0	0	0	32	64.0
0	0	0	33	66.0
0	1	1	34	68.0
0	0	0	35	70.0
0	0	0	36	72.0
0	0	0	37	74.0

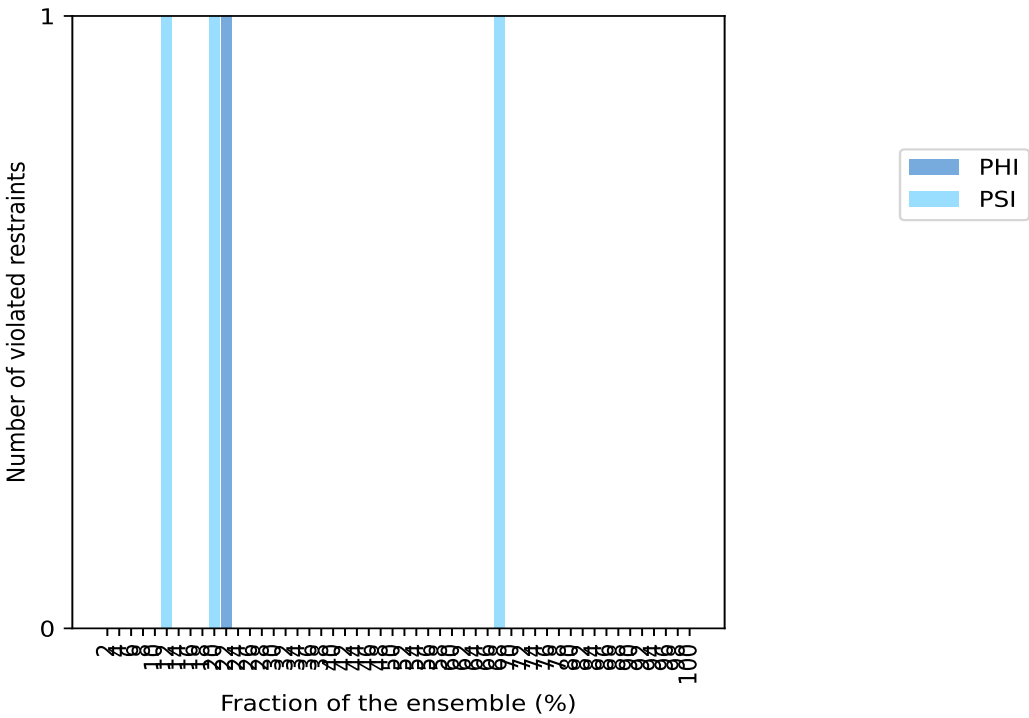
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	38	76.0
0	0	0	39	78.0
0	0	0	40	80.0
0	0	0	41	82.0
0	0	0	42	84.0
0	0	0	43	86.0
0	0	0	44	88.0
0	0	0	45	90.0
0	0	0	46	92.0
0	0	0	47	94.0
0	0	0	48	96.0
0	0	0	49	98.0
0	0	0	50	100.0

¹ Number of models with violations

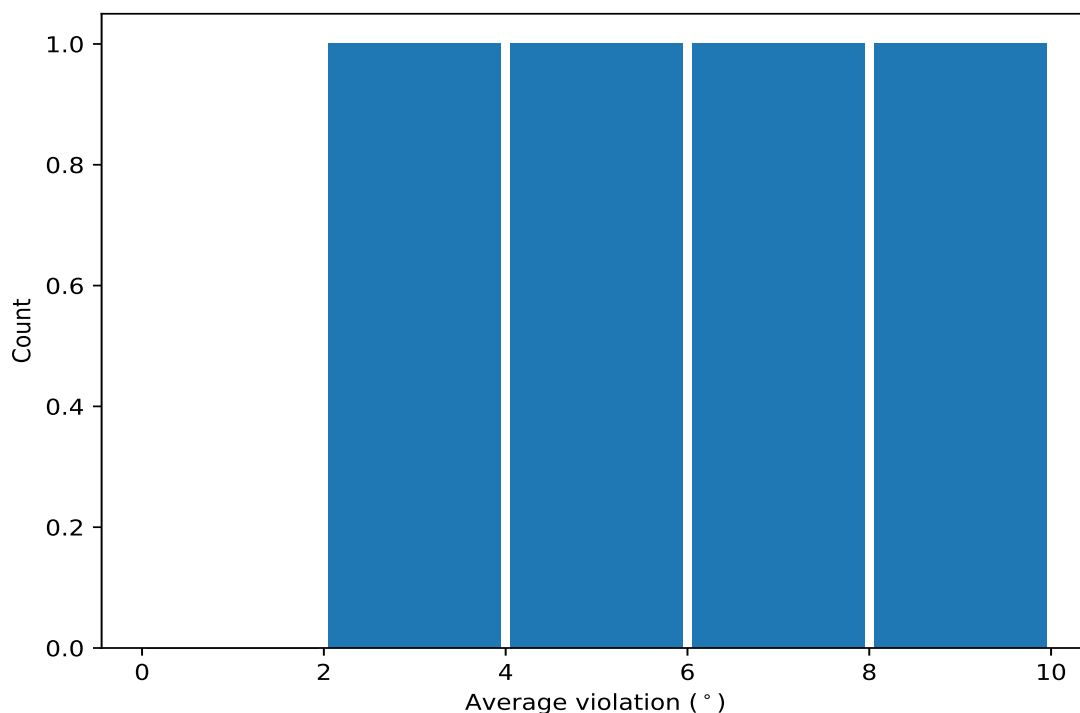
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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.

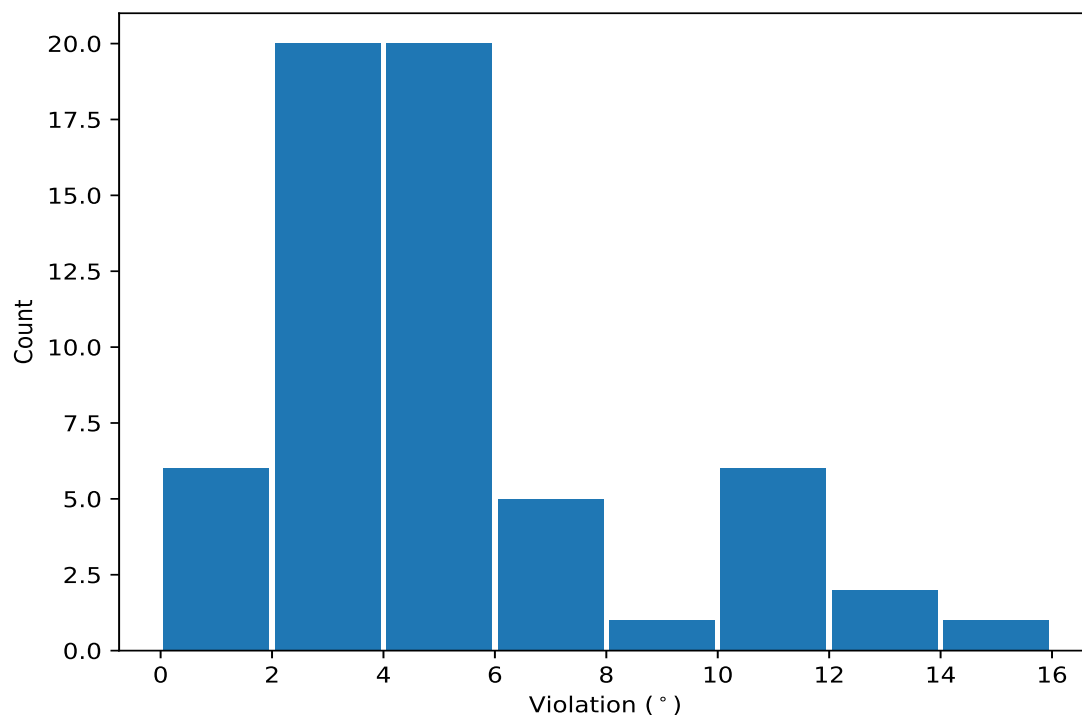
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	34	4.61	2.16	4.52
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	11	2.51	0.55	2.5
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	10	7.49	4.58	8.17
(1,30)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:TRP:N	6	9.1	1.1	9.46

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 (°)
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	50	14.19
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	46	12.65
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	17	12.34
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	31	11.79
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	12	11.73
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	45	11.22
(1,30)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:TRP:N	19	10.16
(1,30)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:TRP:N	29	10.15
(1,30)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:TRP:N	30	10.09
(1,30)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:TRP:N	31	8.84
(1,30)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:TRP:N	16	7.8
(1,30)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:TRP:N	18	7.57
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	14	7.03
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	33	7.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	32	6.34
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	23	5.94
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	28	5.71
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	26	5.43
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	8	5.3
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	43	5.2
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	30	5.12
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	7	5.04
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	10	4.99
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	13	4.98
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	27	4.98
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	5	4.86
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	9	4.62
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	4	4.54
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	11	4.53
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	38	4.51
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	1	4.31
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	37	4.31
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	36	4.24
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	3	4.23
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	44	4.02
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	2	3.96
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	42	3.88
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	20	3.85
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	21	3.69
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	27	3.66
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	22	3.34
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	19	3.27
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	15	3.18
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	48	3.05
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	39	2.98
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	24	2.93
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	38	2.55
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	21	2.52
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	42	2.5
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	9	2.48
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	47	2.43
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	43	2.37
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	40	2.28
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	15	2.2
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	6	2.13
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	4	1.85
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	16	1.71
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	17	1.53
(1,17)	1:16:A:LEU:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	44	1.53
(1,38)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:TYR:N	18	1.2
(1,36)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:LYS:N	34	1.15