



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:42 PM UTC

PDB ID : 5JOJ / pdb_00005joj
BMRB ID : 30071
Title : Calcium-loaded EF-hand domain of L-plastin
Authors : Ishida, H.; Jensen, K.V.; Woodman, G.W.; Hyndman, M.E.; Vogel, H.J.
Deposited on : 2016-05-02

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

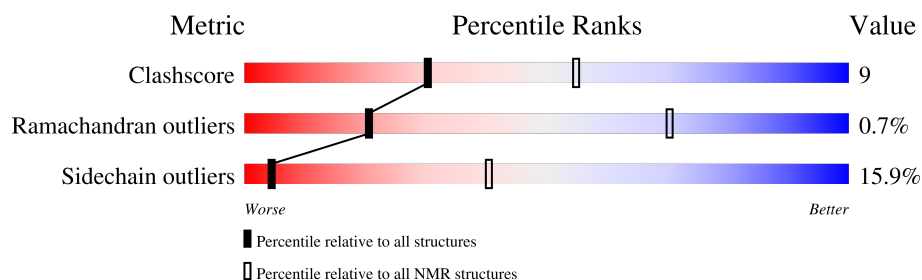
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 36%.

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	97	69% 21% • 9%

2 Ensemble composition and analysis

This entry contains 30 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:5-A:80, A:84-A:95 (88)	0.42	14

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 5 clusters and 8 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1527 atoms, of which 758 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Plastin-2.

Mol	Chain	Residues	Atoms						Trace
1	A	97	Total	C	H	N	O	S	0
			1525	482	758	131	149	5	

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

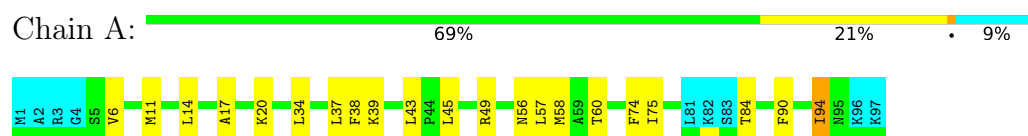
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

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: Plastin-2

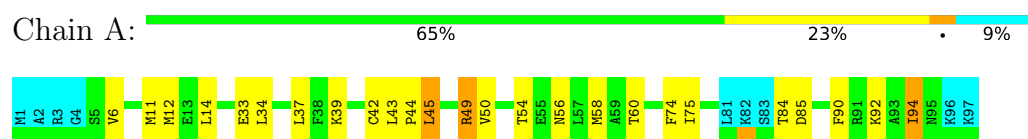


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

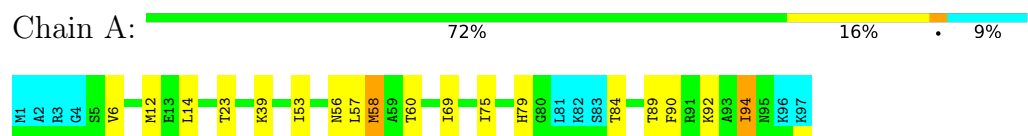
4.2.1 Score per residue for model 1

- Molecule 1: Plastin-2



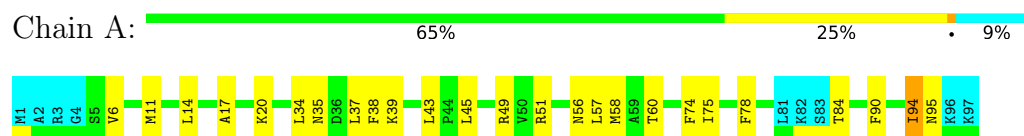
4.2.2 Score per residue for model 2

- Molecule 1: Plastin-2



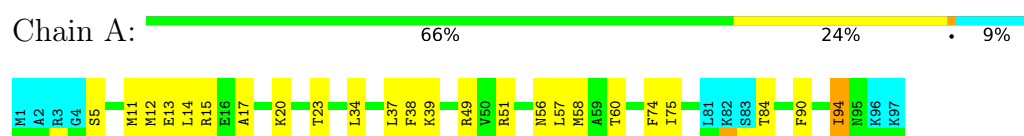
4.2.3 Score per residue for model 3

- Molecule 1: Plastin-2



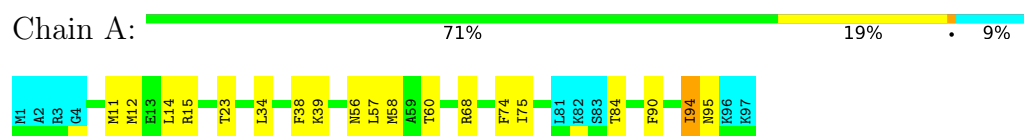
4.2.4 Score per residue for model 4

- Molecule 1: Plastin-2



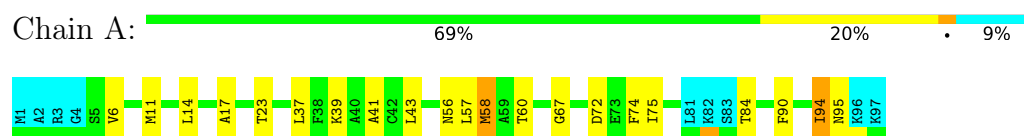
4.2.5 Score per residue for model 5

- Molecule 1: Plastin-2



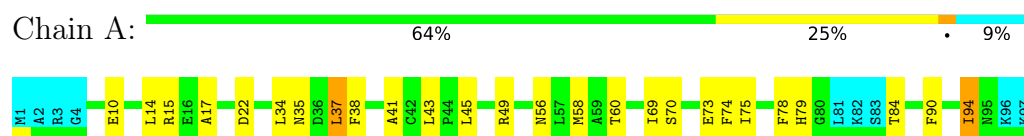
4.2.6 Score per residue for model 6

- Molecule 1: Plastin-2



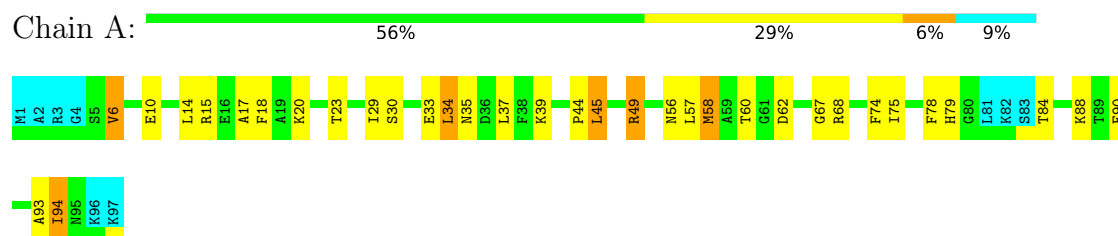
4.2.7 Score per residue for model 7

- Molecule 1: Plastin-2



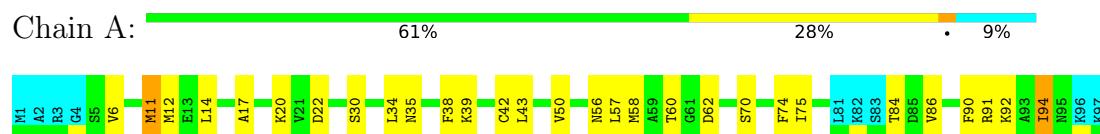
4.2.8 Score per residue for model 8

- Molecule 1: Plastin-2



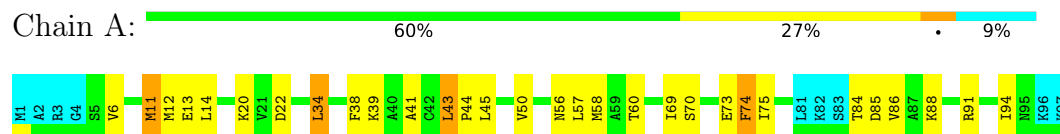
4.2.9 Score per residue for model 9

- Molecule 1: Plastin-2



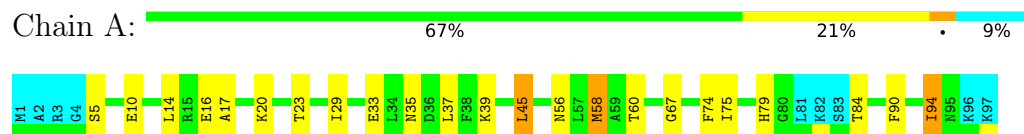
4.2.10 Score per residue for model 10

- Molecule 1: Plastin-2



4.2.11 Score per residue for model 11

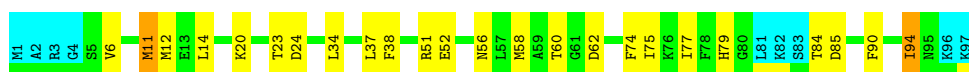
- Molecule 1: Plastin-2



4.2.12 Score per residue for model 12

- Molecule 1: Plastin-2





4.2.13 Score per residue for model 13

- Molecule 1: Plastin-2

Chain A: 68% 21% 9%



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Plastin-2

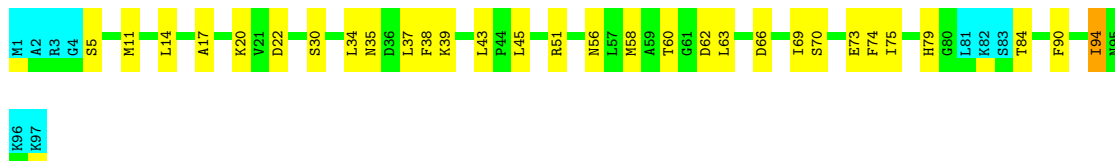
Chain A: 71% 16% 9%



4.2.15 Score per residue for model 15

- Molecule 1: Plastin-2

Chain A: 60% 30% 9%



4.2.16 Score per residue for model 16

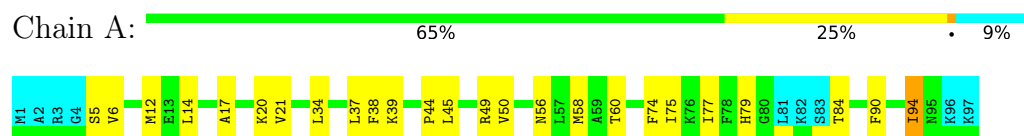
- Molecule 1: Plastin-2

Chain A: 64% 26% 9%



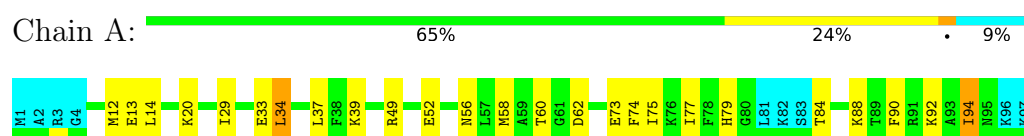
4.2.17 Score per residue for model 17

- Molecule 1: Plastin-2



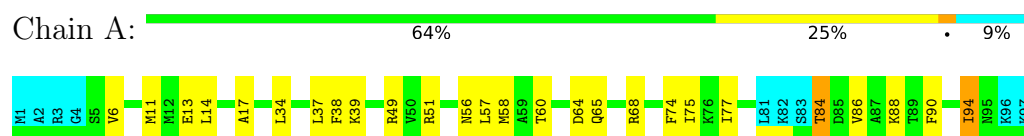
4.2.18 Score per residue for model 18

- Molecule 1: Plastin-2



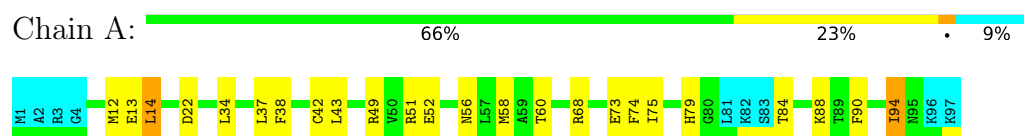
4.2.19 Score per residue for model 19

- Molecule 1: Plastin-2



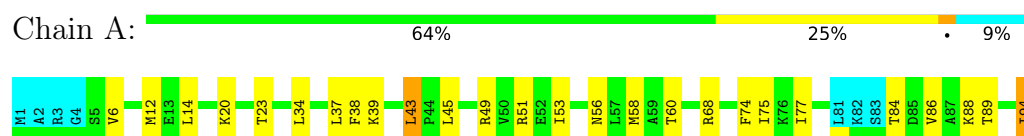
4.2.20 Score per residue for model 20

- Molecule 1: Plastin-2



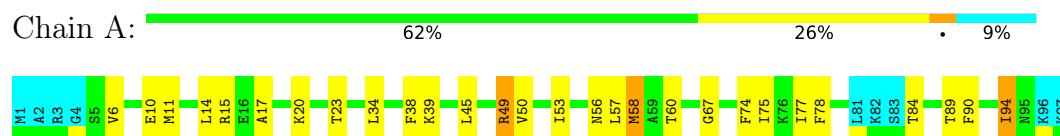
4.2.21 Score per residue for model 21

- Molecule 1: Plastin-2



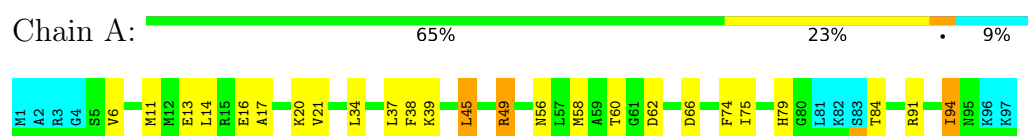
4.2.22 Score per residue for model 22

- Molecule 1: Plastin-2



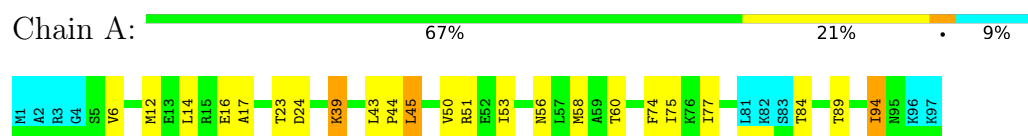
4.2.23 Score per residue for model 23

- Molecule 1: Plastin-2



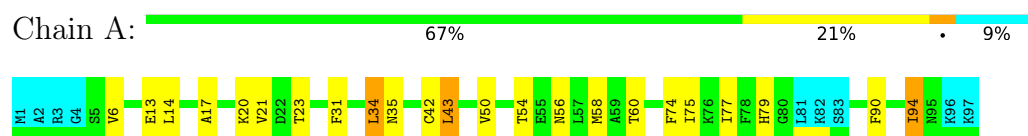
4.2.24 Score per residue for model 24

- Molecule 1: Plastin-2



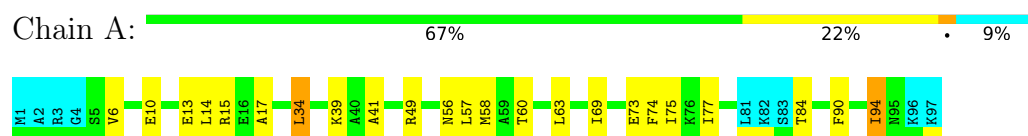
4.2.25 Score per residue for model 25

- Molecule 1: Plastin-2



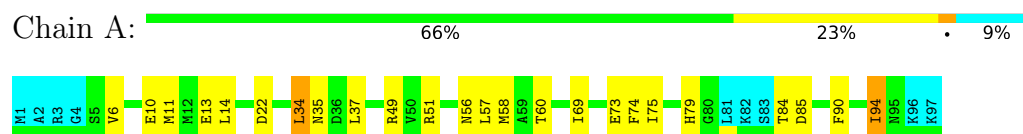
4.2.26 Score per residue for model 26

- Molecule 1: Plastin-2



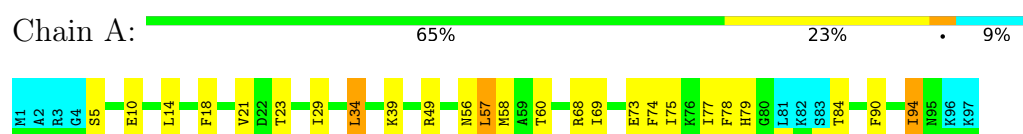
4.2.27 Score per residue for model 27

- Molecule 1: Plastin-2



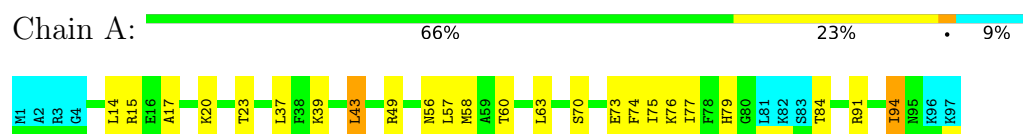
4.2.28 Score per residue for model 28

- Molecule 1: Plastin-2



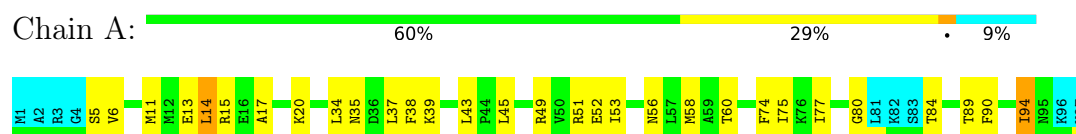
4.2.29 Score per residue for model 29

- Molecule 1: Plastin-2



4.2.30 Score per residue for model 30

- Molecule 1: Plastin-2



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 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
CYANA	refinement	
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	473
Number of shifts mapped to atoms	473
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	36%

6 Model quality

6.1 Standard geometry

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	698	673	673	12±3
All	All	21000	20190	20190	369

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:HD13	1:A:75:ILE:HG23	0.76	1.55	2	27
1:A:43:LEU:HD11	1:A:45:LEU:HD12	0.76	1.57	15	3
1:A:34:LEU:HD21	1:A:57:LEU:HD23	0.75	1.58	9	7
1:A:14:LEU:HD23	1:A:75:ILE:HG23	0.73	1.59	20	2
1:A:56:ASN:O	1:A:60:THR:HG22	0.69	1.87	24	30
1:A:37:LEU:CD2	1:A:94:ILE:HD12	0.68	2.19	30	10
1:A:34:LEU:HD22	1:A:38:PHE:CZ	0.68	2.23	16	13
1:A:17:ALA:HB1	1:A:94:ILE:HG21	0.67	1.65	17	18
1:A:37:LEU:CD1	1:A:94:ILE:HD12	0.66	2.21	7	1
1:A:11:MET:HE1	1:A:75:ILE:HD13	0.65	1.66	5	1
1:A:90:PHE:CZ	1:A:94:ILE:HD13	0.64	2.27	16	24
1:A:43:LEU:HD13	1:A:43:LEU:N	0.63	2.08	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PRO:O	1:A:45:LEU:HD22	0.62	1.94	10	1
1:A:11:MET:HE2	1:A:75:ILE:HD13	0.62	1.71	9	3
1:A:44:PRO:O	1:A:45:LEU:HD12	0.61	1.95	8	4
1:A:34:LEU:HD21	1:A:57:LEU:CD2	0.61	2.25	22	2
1:A:14:LEU:CD1	1:A:75:ILE:HG23	0.60	2.27	7	19
1:A:21:VAL:CG2	1:A:94:ILE:HD11	0.59	2.28	23	4
1:A:14:LEU:CD2	1:A:75:ILE:HG23	0.58	2.28	20	2
1:A:90:PHE:CE2	1:A:94:ILE:HD13	0.58	2.33	30	12
1:A:45:LEU:HD13	1:A:49:ARG:HB3	0.57	1.75	23	1
1:A:58:MET:HE1	1:A:67:GLY:O	0.57	1.98	11	2
1:A:43:LEU:CD1	1:A:45:LEU:HD12	0.57	2.29	3	3
1:A:14:LEU:HD23	1:A:75:ILE:HG12	0.57	1.77	16	2
1:A:63:LEU:HD13	1:A:73:GLU:HG2	0.56	1.75	29	1
1:A:11:MET:HE1	1:A:75:ILE:CD1	0.56	2.31	5	1
1:A:53:ILE:HD12	1:A:89:THR:HG21	0.54	1.78	2	6
1:A:14:LEU:HD13	1:A:75:ILE:HG12	0.54	1.79	6	18
1:A:37:LEU:O	1:A:37:LEU:HD12	0.54	2.03	30	3
1:A:42:CYS:C	1:A:43:LEU:HD22	0.54	2.27	1	4
1:A:37:LEU:HD22	1:A:94:ILE:HD12	0.53	1.80	30	5
1:A:34:LEU:HD22	1:A:58:MET:HG2	0.53	1.78	14	3
1:A:45:LEU:O	1:A:45:LEU:HD23	0.53	2.03	11	1
1:A:75:ILE:HG22	1:A:79:HIS:CD2	0.53	2.39	18	1
1:A:90:PHE:CE1	1:A:94:ILE:HD13	0.53	2.39	26	6
1:A:11:MET:HE2	1:A:15:ARG:HD3	0.53	1.81	5	1
1:A:50:VAL:O	1:A:54:THR:HG22	0.52	2.04	25	2
1:A:34:LEU:HD22	1:A:58:MET:SD	0.52	2.44	28	6
1:A:6:VAL:HG21	1:A:75:ILE:HG21	0.52	1.82	2	12
1:A:34:LEU:HD12	1:A:58:MET:SD	0.52	2.45	4	11
1:A:6:VAL:HG11	1:A:75:ILE:CG2	0.52	2.35	27	2
1:A:14:LEU:HD13	1:A:75:ILE:CG2	0.52	2.33	18	6
1:A:63:LEU:HD23	1:A:73:GLU:HG2	0.51	1.79	15	2
1:A:21:VAL:HG23	1:A:94:ILE:HD11	0.51	1.82	23	1
1:A:29:ILE:HG21	1:A:34:LEU:HD13	0.51	1.83	18	1
1:A:34:LEU:HD11	1:A:74:PHE:CZ	0.51	2.40	14	2
1:A:37:LEU:HD21	1:A:94:ILE:HD12	0.51	1.82	29	3
1:A:14:LEU:HD21	1:A:78:PHE:CD2	0.51	2.41	7	3
1:A:58:MET:HE1	1:A:67:GLY:C	0.50	2.31	6	2
1:A:44:PRO:C	1:A:45:LEU:HD22	0.50	2.31	10	1
1:A:11:MET:HE3	1:A:11:MET:O	0.49	2.07	23	1
1:A:34:LEU:HD21	1:A:57:LEU:CG	0.49	2.37	22	1
1:A:11:MET:HA	1:A:14:LEU:HD12	0.49	1.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ALA:CB	1:A:94:ILE:HG21	0.49	2.37	30	4
1:A:18:PHE:HA	1:A:29:ILE:HD11	0.49	1.84	28	2
1:A:6:VAL:HG12	1:A:10:GLU:HG2	0.49	1.84	27	2
1:A:39:LYS:HD2	1:A:50:VAL:HG21	0.48	1.84	24	1
1:A:39:LYS:HE3	1:A:50:VAL:HG21	0.48	1.85	24	1
1:A:84:THR:OG1	1:A:86:VAL:HG22	0.48	2.09	19	1
1:A:14:LEU:HD21	1:A:78:PHE:CD1	0.48	2.43	28	2
1:A:37:LEU:HD12	1:A:94:ILE:HD12	0.47	1.85	7	1
1:A:34:LEU:HD21	1:A:57:LEU:HD13	0.47	1.87	28	1
1:A:41:ALA:HB1	1:A:43:LEU:HD23	0.47	1.87	6	1
1:A:57:LEU:HD13	1:A:86:VAL:CG2	0.46	2.40	10	2
1:A:41:ALA:CB	1:A:43:LEU:HD23	0.46	2.40	6	1
1:A:38:PHE:CB	1:A:50:VAL:HG23	0.46	2.41	9	4
1:A:29:ILE:CG2	1:A:34:LEU:HD13	0.46	2.39	18	1
1:A:43:LEU:HD12	1:A:43:LEU:O	0.46	2.11	21	2
1:A:37:LEU:HD11	1:A:93:ALA:O	0.46	2.11	8	1
1:A:45:LEU:HD22	1:A:49:ARG:HG3	0.45	1.88	22	1
1:A:45:LEU:HD23	1:A:49:ARG:HB3	0.45	1.88	8	3
1:A:21:VAL:HG21	1:A:94:ILE:HD11	0.45	1.87	28	1
1:A:37:LEU:HD13	1:A:37:LEU:C	0.45	2.37	17	7
1:A:69:ILE:HG23	1:A:73:GLU:HB3	0.45	1.89	27	6
1:A:43:LEU:N	1:A:43:LEU:CD1	0.44	2.79	25	1
1:A:34:LEU:HD21	1:A:57:LEU:HG	0.44	1.89	22	1
1:A:37:LEU:HD11	1:A:94:ILE:HD12	0.44	1.86	7	1
1:A:45:LEU:O	1:A:45:LEU:HD12	0.44	2.13	7	1
1:A:43:LEU:HD22	1:A:44:PRO:HD2	0.44	1.89	13	1
1:A:37:LEU:O	1:A:37:LEU:HD13	0.44	2.13	20	1
1:A:43:LEU:HD13	1:A:45:LEU:HB2	0.43	1.90	21	1
1:A:53:ILE:HA	1:A:86:VAL:HG12	0.43	1.90	21	1
1:A:38:PHE:HB3	1:A:50:VAL:HG23	0.43	1.89	9	1
1:A:38:PHE:HB2	1:A:50:VAL:HG23	0.42	1.91	10	1
1:A:34:LEU:HD11	1:A:74:PHE:HZ	0.42	1.71	14	1
1:A:58:MET:HE2	1:A:69:ILE:HG13	0.42	1.90	2	1
1:A:29:ILE:HG23	1:A:33:GLU:HG3	0.42	1.91	11	1
1:A:41:ALA:O	1:A:43:LEU:HD12	0.42	2.14	10	1
1:A:37:LEU:HD13	1:A:37:LEU:O	0.42	2.14	3	1
1:A:37:LEU:HD23	1:A:38:PHE:CD1	0.41	2.50	23	1
1:A:14:LEU:HD12	1:A:75:ILE:HA	0.41	1.93	30	1
1:A:73:GLU:O	1:A:77:ILE:HD13	0.41	2.16	18	1
1:A:14:LEU:HD23	1:A:75:ILE:CG2	0.41	2.39	20	1
1:A:6:VAL:HG11	1:A:11:MET:SD	0.41	2.56	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:PHE:N	1:A:58:MET:HE2	0.40	2.31	25	1
1:A:43:LEU:HD13	1:A:44:PRO:N	0.40	2.31	13	1
1:A:41:ALA:HB1	1:A:43:LEU:HD13	0.40	1.92	7	1
1:A:43:LEU:O	1:A:43:LEU:HD22	0.40	2.17	25	1
1:A:6:VAL:HG11	1:A:75:ILE:HG23	0.40	1.92	27	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	88/97 (91%)	77±5 (88±6%)	9±2 (11±2%)	1±1 (1±1%)	20	70
All	All	2610/2910 (90%)	2313 (89%)	279 (11%)	18 (1%)	20	70

All 4 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	5	SER	7
1	A	22	ASP	5
1	A	6	VAL	5
1	A	42	CYS	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	75/82 (91%)	63±3 (84±4%)	12±3 (16±4%)	4	40
All	All	2250/2460 (91%)	1892 (84%)	358 (16%)	4	40

All 44 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	94	ILE	30
1	A	74	PHE	29
1	A	84	THR	27
1	A	39	LYS	25
1	A	49	ARG	18
1	A	20	LYS	17
1	A	23	THR	15
1	A	12	MET	13
1	A	79	HIS	13
1	A	58	MET	11
1	A	11	MET	11
1	A	51	ARG	11
1	A	35	ASN	10
1	A	13	GLU	10
1	A	34	LEU	9
1	A	57	LEU	8
1	A	15	ARG	8
1	A	68	ARG	7
1	A	62	ASP	7
1	A	88	LYS	7
1	A	43	LEU	7
1	A	52	GLU	6
1	A	45	LEU	5
1	A	85	ASP	5
1	A	92	LYS	5
1	A	10	GLU	5
1	A	70	SER	5
1	A	91	ARG	4
1	A	33	GLU	3
1	A	95	ASN	3
1	A	30	SER	3
1	A	16	GLU	3
1	A	66	ASP	3
1	A	24	ASP	2
1	A	77	ILE	2
1	A	76	LYS	2
1	A	14	LEU	2
1	A	72	ASP	1
1	A	37	LEU	1
1	A	6	VAL	1
1	A	64	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	65	GLN	1
1	A	22	ASP	1
1	A	73	GLU	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 36% for the well-defined parts and 36% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *lpl-ef-h5.str*

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	473
Number of shifts mapped to atoms	473
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	97	-0.40 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	90	0.32 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	97	-0.49 ± 0.12	None needed (< 0.5 ppm)
^{15}N	95	0.37 ± 0.41	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 36%, i.e. 430 atoms were assigned a chemical shift out of a possible 1189. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	348/442 (79%)	86/180 (48%)	176/176 (100%)	86/86 (100%)
Sidechain	82/652 (13%)	0/420 (0%)	82/206 (40%)	0/26 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/95 (0%)	0/47 (0%)	0/47 (0%)	0/1 (0%)
Overall	430/1189 (36%)	86/647 (13%)	258/429 (60%)	86/113 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 473 atoms were assigned a chemical shift out of a possible 1322. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	383/488 (78%)	94/199 (47%)	194/194 (100%)	95/95 (100%)
Sidechain	90/739 (12%)	0/476 (0%)	90/231 (39%)	0/32 (0%)
Aromatic	0/95 (0%)	0/47 (0%)	0/47 (0%)	0/1 (0%)
Overall	473/1322 (36%)	94/722 (13%)	284/472 (60%)	95/128 (74%)

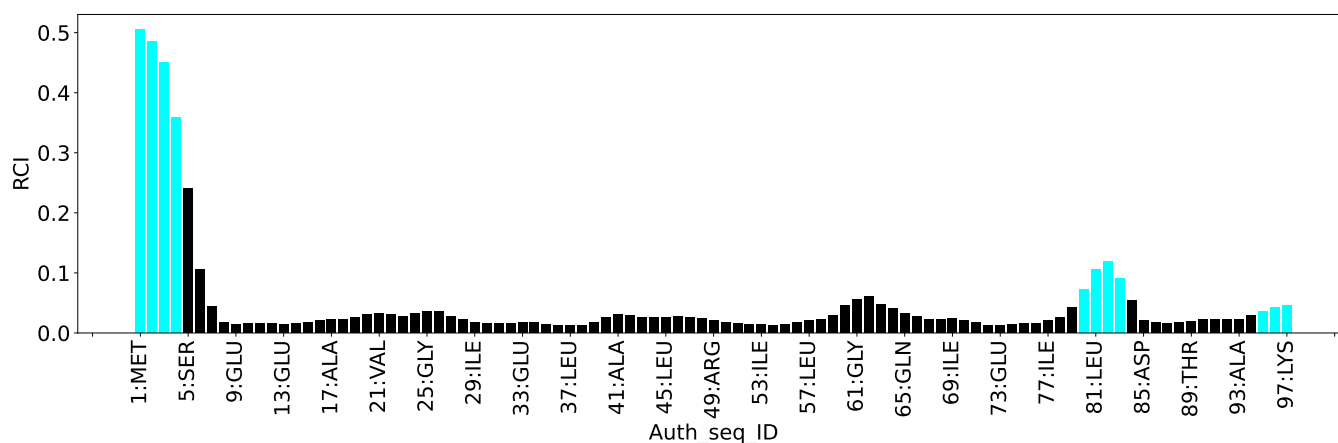
7.1.4 Statistically unusual chemical shifts [i](#)

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	1746
Intra-residue ($ i-j =0$)	359
Sequential ($ i-j =1$)	354
Medium range ($ i-j >1$ and $ i-j <5$)	485
Long range ($ i-j \geq 5$)	476
Inter-chain	0
Hydrogen bond restraints	72
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	0
Number of restraints per residue	19.2
Number of long range restraints per residue ¹	4.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	12.2	0.2
0.2-0.5 (Medium)	3.3	0.5
>0.5 (Large)	2.5	1.62

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)	2.1	3.39
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

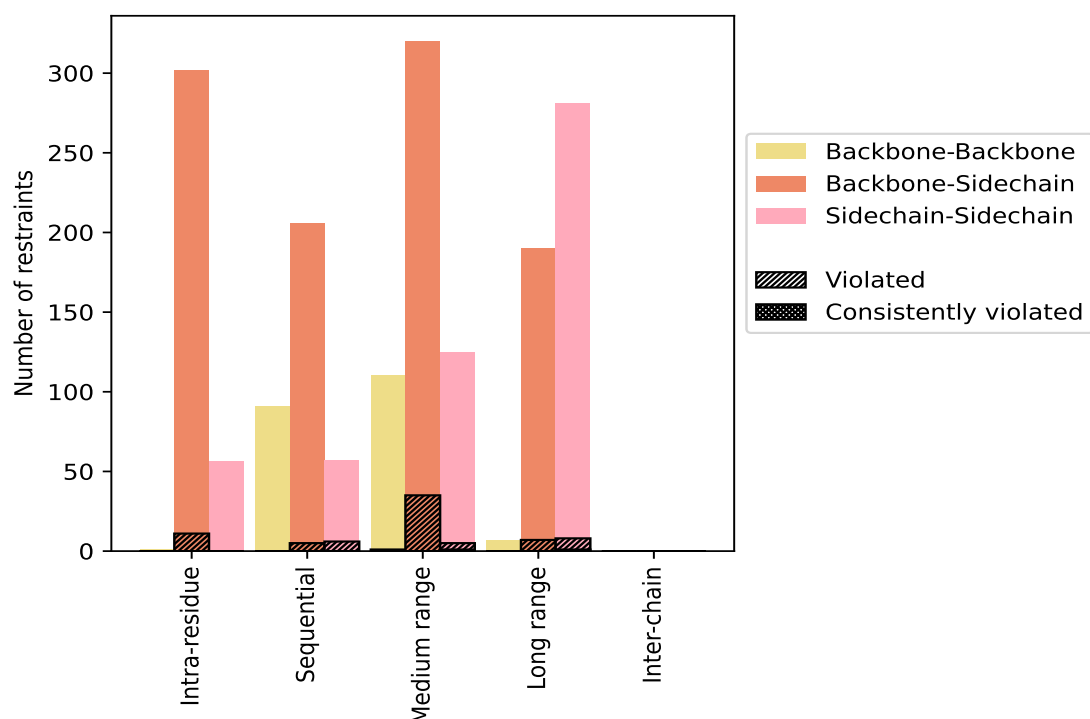
9.1 Summary of distance violations [i](#)

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)	359	20.6	11	3.1	0.6	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	302	17.3	11	3.6	0.6	0	0.0	0.0
Sidechain-Sidechain	56	3.2	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	354	20.3	11	3.1	0.6	0	0.0	0.0
Backbone-Backbone	91	5.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	206	11.8	5	2.4	0.3	0	0.0	0.0
Sidechain-Sidechain	57	3.3	6	10.5	0.3	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	485	27.8	23	4.7	1.3	1	0.2	0.1
Backbone-Backbone	110	6.3	1	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	250	14.3	17	6.8	1.0	0	0.0	0.0
Sidechain-Sidechain	125	7.2	5	4.0	0.3	1	0.8	0.1
Long range (i-j ≥5)	476	27.3	15	3.2	0.9	1	0.2	0.1
Backbone-Backbone	7	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	188	10.8	7	3.7	0.4	0	0.0	0.0
Sidechain-Sidechain	281	16.1	8	2.8	0.5	1	0.4	0.1
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	72	4.1	18	25.0	1.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1746	100.0	78	4.5	4.5	2	0.1	0.1
Backbone-Backbone	209	12.0	1	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	1018	58.3	58	5.7	3.3	0	0.0	0.0
Sidechain-Sidechain	519	29.7	19	3.7	1.1	2	0.4	0.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	3	3	6	1	0	13	0.38	1.5	0.42	0.17
2	1	2	5	3	0	11	0.39	1.49	0.43	0.17
3	2	1	13	4	0	20	0.28	1.43	0.33	0.15
4	1	1	11	4	0	17	0.28	1.62	0.39	0.13
5	2	3	9	2	0	16	0.33	1.51	0.38	0.16
6	2	1	14	4	0	21	0.28	1.48	0.33	0.13
7	3	1	12	5	0	21	0.28	1.28	0.31	0.14
8	3	2	12	5	0	22	0.26	1.37	0.32	0.15
9	2	4	5	2	0	13	0.37	1.52	0.42	0.17
10	2	5	7	4	0	18	0.21	1.02	0.21	0.14

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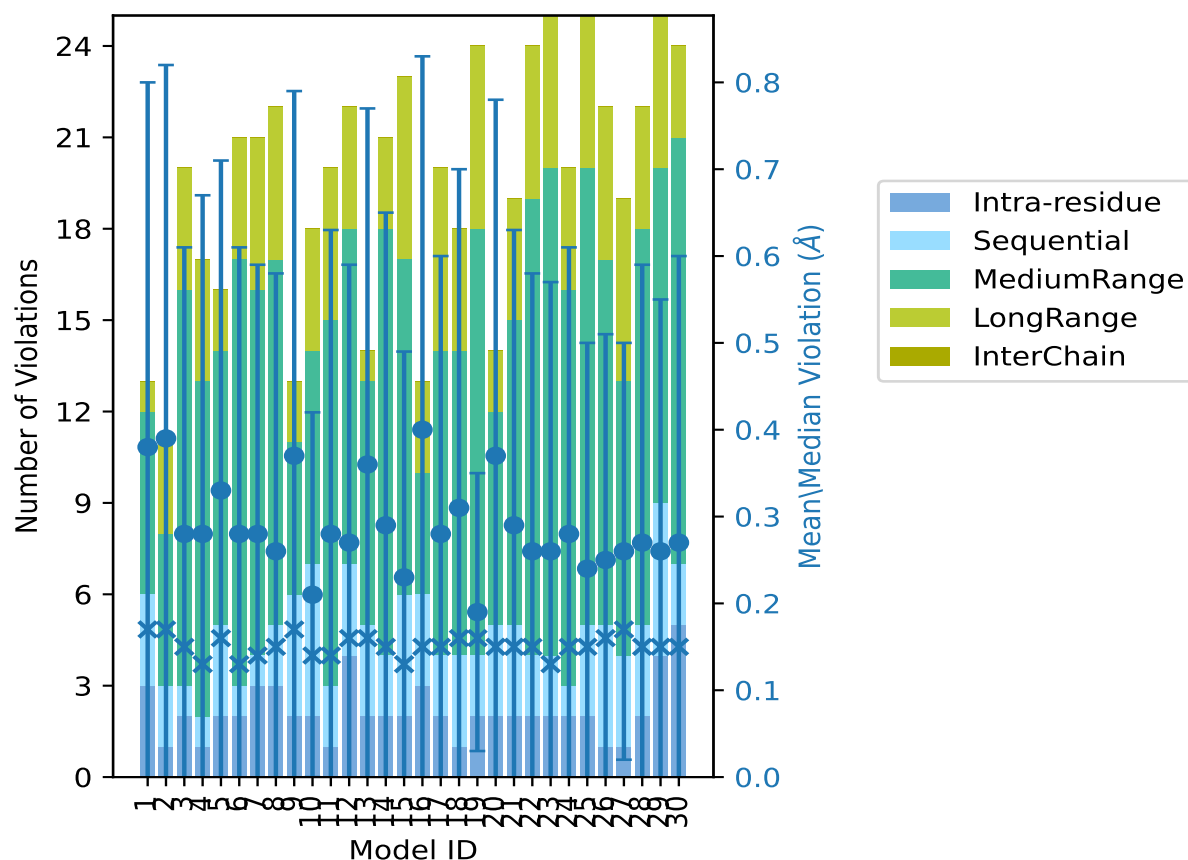
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	2	12	5	0	20	0.28	1.44	0.35	0.14
12	4	3	11	4	0	22	0.27	1.46	0.32	0.16
13	2	3	8	1	0	14	0.36	1.49	0.41	0.16
14	2	2	14	3	0	21	0.29	1.53	0.36	0.15
15	2	4	11	6	0	23	0.23	1.08	0.26	0.13
16	3	3	4	3	0	13	0.4	1.48	0.43	0.15
17	2	2	10	6	0	20	0.28	1.35	0.32	0.15
18	1	3	10	4	0	18	0.31	1.61	0.39	0.16
19	2	2	14	6	0	24	0.19	0.89	0.16	0.16
20	2	3	7	2	0	14	0.37	1.52	0.41	0.15
21	2	3	10	4	0	19	0.29	1.52	0.34	0.15
22	2	2	15	5	0	24	0.26	1.47	0.32	0.15
23	2	2	16	5	0	25	0.26	1.41	0.31	0.13
24	2	1	13	4	0	20	0.28	1.46	0.33	0.15
25	2	3	15	5	0	25	0.24	1.28	0.26	0.15
26	1	4	12	5	0	22	0.25	1.05	0.26	0.16
27	1	3	9	6	0	19	0.26	1.08	0.24	0.17
28	2	3	13	4	0	22	0.27	1.51	0.32	0.15
29	4	5	11	5	0	25	0.26	1.42	0.29	0.15
30	5	2	14	3	0	24	0.27	1.52	0.33	0.15

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1614(IR:348, SQ:343, MR:462, LR:461, 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	%
6	2	5	4	0	17	1	3.3
1	1	4	2	0	8	2	6.7
1	3	1	0	0	5	3	10.0
0	0	3	3	0	6	4	13.3
0	0	1	0	0	1	5	16.7
0	2	1	0	0	3	6	20.0

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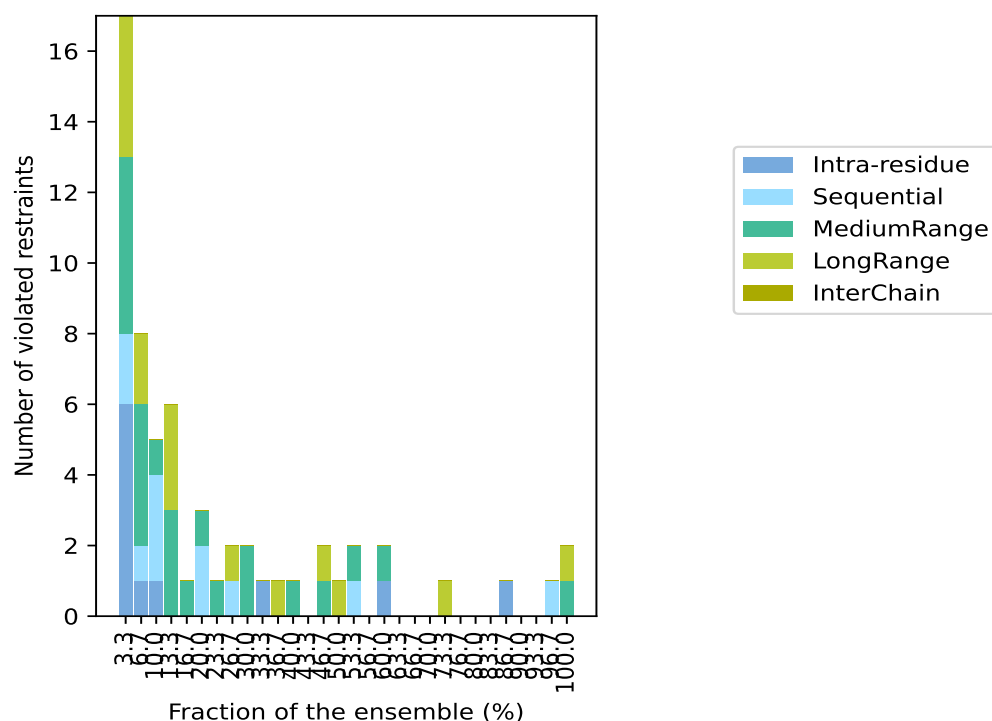
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	0	0	1	7	23.3
0	1	0	1	0	2	8	26.7
0	0	2	0	0	2	9	30.0
1	0	0	0	0	1	10	33.3
0	0	0	1	0	1	11	36.7
0	0	1	0	0	1	12	40.0
0	0	0	0	0	0	13	43.3
0	0	1	1	0	2	14	46.7
0	0	0	1	0	1	15	50.0
0	1	1	0	0	2	16	53.3
0	0	0	0	0	0	17	56.7
1	0	1	0	0	2	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	1	0	1	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
1	0	0	0	0	1	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	1	0	0	0	1	29	96.7
0	0	1	1	0	2	30	100.0

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

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

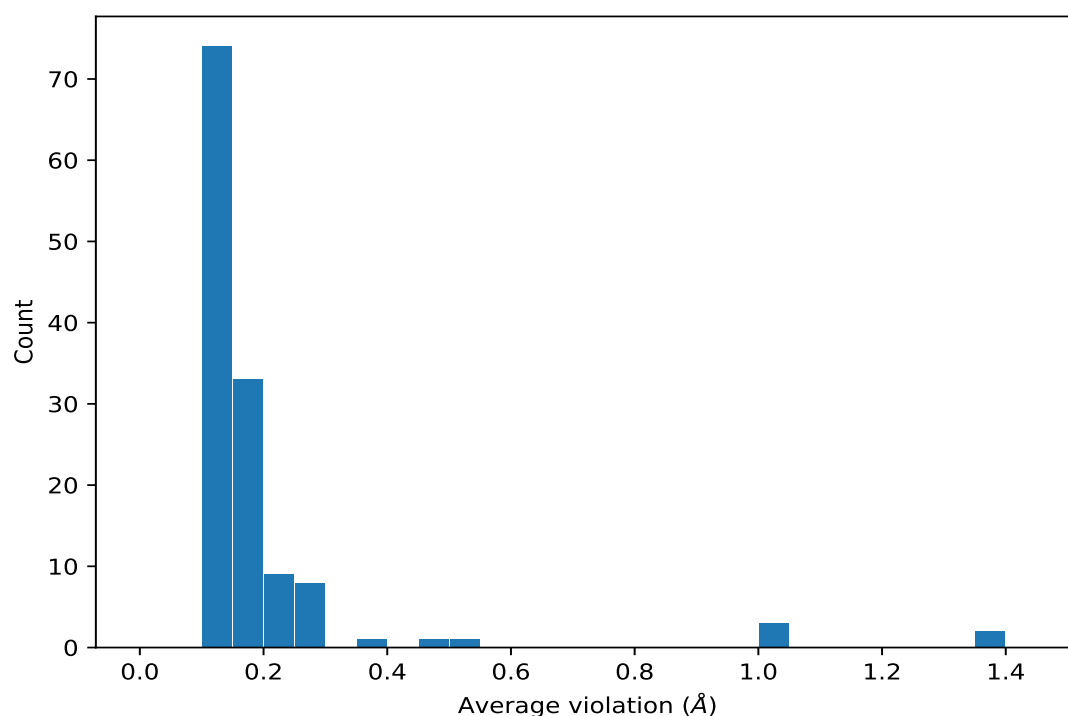
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	30	1.01	0.1	1.04
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	30	1.01	0.1	1.04
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	30	1.01	0.1	1.04
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	30	0.35	0.04	0.34
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	29	1.37	0.29	1.47
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	29	1.37	0.29	1.47
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	28	0.15	0.02	0.14
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	26	0.5	0.09	0.52
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	23	0.13	0.02	0.13
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	23	0.12	0.02	0.12
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	22	0.15	0.03	0.16
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	22	0.15	0.03	0.16
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	19	0.24	0.02	0.23
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	19	0.22	0.02	0.22
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	19	0.18	0.02	0.18
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	18	0.13	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	18	0.13	0.02	0.15
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	18	0.11	0.01	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	18	0.11	0.01	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	18	0.11	0.01	0.11
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	16	0.15	0.02	0.15
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	16	0.15	0.02	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	16	0.13	0.02	0.13
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	16	0.13	0.02	0.13
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	15	0.12	0.01	0.12
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	15	0.11	0.01	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	15	0.11	0.01	0.11
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	14	0.12	0.01	0.12
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	14	0.12	0.02	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	14	0.12	0.02	0.11
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	12	0.2	0.04	0.2
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	12	0.13	0.03	0.12
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	11	0.12	0.04	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	11	0.12	0.04	0.11
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	10	0.19	0.01	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	10	0.19	0.01	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	10	0.19	0.01	0.19
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	9	0.19	0.1	0.14
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	9	0.13	0.01	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	9	0.13	0.01	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	9	0.13	0.01	0.13
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	8	0.14	0.02	0.14
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	8	0.14	0.02	0.14
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	8	0.11	0.01	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	8	0.11	0.01	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	8	0.11	0.01	0.11
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	7	0.13	0.02	0.14
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	7	0.13	0.02	0.14
(1,105)	1:94:A:ILE:HB	1:95:A:ASN:HB2	6	0.17	0.04	0.19
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG11	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG12	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG13	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG21	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG22	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG23	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG11	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG12	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG13	6	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG21	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG22	6	0.15	0.02	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG23	6	0.15	0.02	0.16
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD1	6	0.11	0.01	0.11
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD2	6	0.11	0.01	0.11
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG2	5	0.14	0.02	0.14
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG3	5	0.14	0.02	0.14
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG2	5	0.14	0.02	0.14
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG3	5	0.14	0.02	0.14
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG2	5	0.14	0.02	0.14
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG3	5	0.14	0.02	0.14
(1,1383)	1:50:A:VAL:HG11	1:52:A:GLU:H	4	0.18	0.01	0.18
(1,1383)	1:50:A:VAL:HG12	1:52:A:GLU:H	4	0.18	0.01	0.18
(1,1383)	1:50:A:VAL:HG13	1:52:A:GLU:H	4	0.18	0.01	0.18
(1,1383)	1:50:A:VAL:HG21	1:52:A:GLU:H	4	0.18	0.01	0.18
(1,1383)	1:50:A:VAL:HG22	1:52:A:GLU:H	4	0.18	0.01	0.18
(1,1383)	1:50:A:VAL:HG23	1:52:A:GLU:H	4	0.18	0.01	0.18
(1,830)	1:84:A:THR:HB	1:86:A:VAL:H	4	0.18	0.03	0.18
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE1	4	0.13	0.02	0.13
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE2	4	0.13	0.02	0.13
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE1	4	0.13	0.02	0.13
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE2	4	0.13	0.02	0.13
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE1	4	0.13	0.02	0.13
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE2	4	0.13	0.02	0.13
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD11	4	0.12	0.03	0.12
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD12	4	0.12	0.03	0.12
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD13	4	0.12	0.03	0.12
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD11	4	0.12	0.01	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD12	4	0.12	0.01	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD13	4	0.12	0.01	0.13
(1,159)	1:37:A:LEU:HD21	1:90:A:PHE:HA	4	0.11	0.01	0.11
(1,159)	1:37:A:LEU:HD22	1:90:A:PHE:HA	4	0.11	0.01	0.11
(1,159)	1:37:A:LEU:HD23	1:90:A:PHE:HA	4	0.11	0.01	0.11
(1,416)	1:14:A:LEU:H	1:14:A:LEU:HG	3	0.48	0.23	0.64
(1,1571)	1:88:A:LYS:HB2	1:89:A:THR:HA	3	0.26	0.06	0.22
(1,1571)	1:88:A:LYS:HB3	1:89:A:THR:HA	3	0.26	0.06	0.22
(1,483)	1:23:A:THR:HB	1:24:A:ASP:H	3	0.17	0.0	0.17
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB2	3	0.16	0.02	0.16
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB3	3	0.16	0.02	0.16
(1,762)	1:69:A:ILE:HA	1:73:A:GLU:H	3	0.12	0.02	0.11
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG11	2	0.26	0.03	0.26
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG12	2	0.26	0.03	0.26

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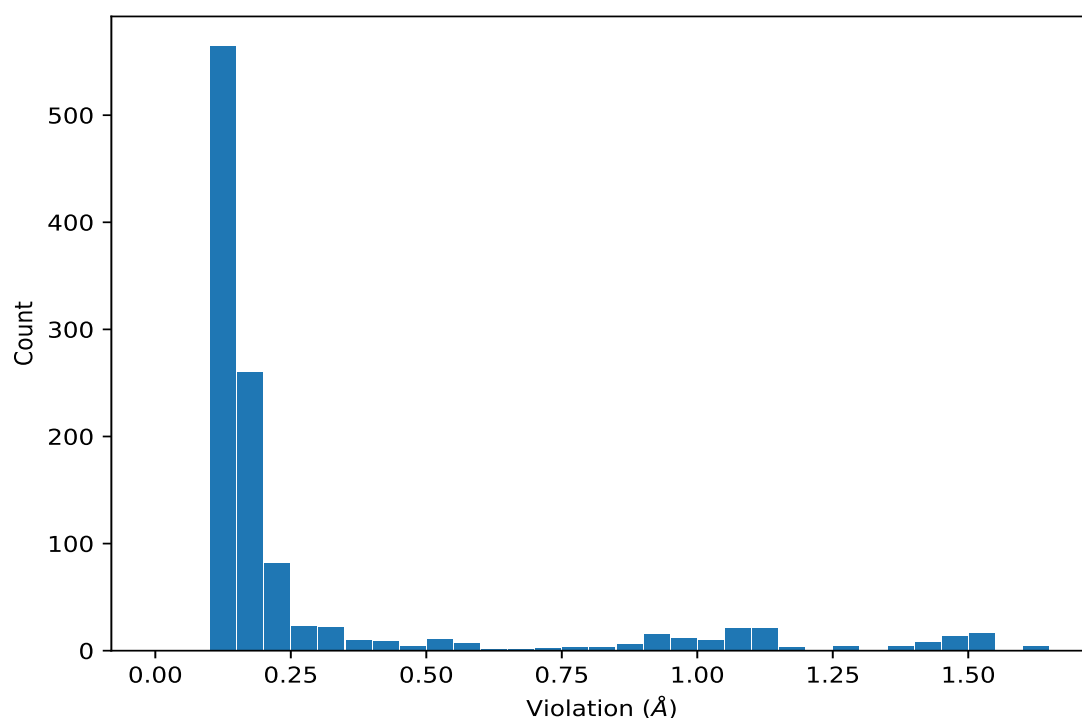
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG13	2	0.26	0.03	0.26
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG21	2	0.26	0.03	0.26
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG22	2	0.26	0.03	0.26
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG23	2	0.26	0.03	0.26
(4,59)	1:80:A:GLY:H	1:76:A:LYS:O	2	0.21	0.09	0.21
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG21	2	0.2	0.06	0.2
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG22	2	0.2	0.06	0.2
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG23	2	0.2	0.06	0.2
(1,1555)	1:85:A:ASP:HA	1:88:A:LYS:HB2	2	0.2	0.0	0.2
(1,1555)	1:85:A:ASP:HA	1:88:A:LYS:HB3	2	0.2	0.0	0.2
(1,1035)	1:46:A:PRO:HA	1:48:A:TYR:HE1	2	0.14	0.02	0.14
(1,1035)	1:46:A:PRO:HA	1:48:A:TYR:HE2	2	0.14	0.02	0.14
(1,1343)	1:45:A:LEU:H	1:45:A:LEU:HB2	2	0.12	0.02	0.12
(1,1343)	1:45:A:LEU:H	1:45:A:LEU:HB3	2	0.12	0.02	0.12
(1,1368)	1:48:A:TYR:HE1	1:49:A:ARG:HG2	2	0.12	0.02	0.12
(1,1368)	1:48:A:TYR:HE1	1:49:A:ARG:HG3	2	0.12	0.02	0.12
(1,1368)	1:48:A:TYR:HE2	1:49:A:ARG:HG2	2	0.12	0.02	0.12
(1,1368)	1:48:A:TYR:HE2	1:49:A:ARG:HG3	2	0.12	0.02	0.12
(1,1349)	1:45:A:LEU:HD11	1:48:A:TYR:HE1	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD11	1:48:A:TYR:HE2	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD12	1:48:A:TYR:HE1	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD12	1:48:A:TYR:HE2	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD13	1:48:A:TYR:HE1	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD13	1:48:A:TYR:HE2	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD21	1:48:A:TYR:HE1	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD21	1:48:A:TYR:HE2	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD22	1:48:A:TYR:HE1	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD22	1:48:A:TYR:HE2	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD23	1:48:A:TYR:HE1	2	0.12	0.01	0.12
(1,1349)	1:45:A:LEU:HD23	1:48:A:TYR:HE2	2	0.12	0.01	0.12
(1,962)	1:38:A:PHE:HD1	1:57:A:LEU:HB3	2	0.12	0.0	0.12
(1,962)	1:38:A:PHE:HD2	1:57:A:LEU:HB3	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	4	1.62
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	4	1.62
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	18	1.61
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	18	1.61
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	14	1.53
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	14	1.53
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	9	1.52
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	9	1.52
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	20	1.52
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	20	1.52
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	21	1.52
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	21	1.52
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	30	1.52
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	30	1.52
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	5	1.51
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	5	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	28	1.51
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	28	1.51
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	1	1.5
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	1	1.5
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	2	1.49
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	2	1.49
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	13	1.49
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	13	1.49
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	6	1.48
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	6	1.48
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	16	1.48
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	16	1.48
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	22	1.47
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	22	1.47
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	12	1.46
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	12	1.46
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	24	1.46
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	24	1.46
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	11	1.44
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	11	1.44
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	3	1.43
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	3	1.43
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	29	1.42
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	29	1.42
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	23	1.41
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	23	1.41
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	8	1.37
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	8	1.37
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	17	1.35
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	17	1.35
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	7	1.28
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	7	1.28
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	25	1.28
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	25	1.28
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	14	1.16
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	14	1.16
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	14	1.16
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	11	1.13
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	11	1.13
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	11	1.13
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	1	1.12
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	1	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	1	1.12
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	8	1.12
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	8	1.12
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	8	1.12
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	16	1.11
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	16	1.11
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	16	1.11
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	7	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	7	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	7	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	18	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	18	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	18	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	23	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	23	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	23	1.1
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	13	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	13	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	13	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	15	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	15	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	15	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	27	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	27	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	27	1.08
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	9	1.07
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	9	1.07
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	9	1.07
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	20	1.06
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	20	1.06
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	20	1.06
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	30	1.06
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	30	1.06
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	30	1.06
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	26	1.05
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	26	1.05
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	26	1.05
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	15	1.04
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	15	1.04
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	17	1.03
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	17	1.03
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	17	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	26	1.02
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	26	1.02
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	10	1.02
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	10	1.02
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	10	1.02
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	22	0.99
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	22	0.99
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	22	0.99
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	5	0.98
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	5	0.98
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	5	0.98
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	6	0.96
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	6	0.96
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	6	0.96
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	3	0.95
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	3	0.95
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	3	0.95
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	4	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	4	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	4	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	12	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	12	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	12	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	28	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	28	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	28	0.94
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	2	0.93
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	2	0.93
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	2	0.93
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	29	0.9
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	29	0.9
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	29	0.9
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	19	0.89
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	19	0.89
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	19	0.89
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	24	0.89
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	24	0.89
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	24	0.89
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	21	0.83
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	21	0.83
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	21	0.83
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG21	25	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG22	25	0.78
(1,933)	1:56:A:ASN:HD21	1:60:A:THR:HG23	25	0.78
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	27	0.72
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	27	0.72
(1,416)	1:14:A:LEU:H	1:14:A:LEU:HG	16	0.65
(1,416)	1:14:A:LEU:H	1:14:A:LEU:HG	20	0.64
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	13	0.59
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	22	0.59
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	9	0.57
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	16	0.57
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	1	0.56
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	2	0.55
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	21	0.55
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	5	0.54
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	14	0.54
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	3	0.53
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	30	0.53
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	6	0.52
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	12	0.52
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	24	0.52
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	23	0.51
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	29	0.51
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	7	0.5
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	28	0.5
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	11	0.49
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	17	0.47
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	20	0.47
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	25	0.47
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	24	0.43
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	4	0.42
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	13	0.42
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	6	0.42
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	8	0.41
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	9	0.41
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	14	0.41
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	18	0.41
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	21	0.4
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	5	0.38
(1,476)	1:23:A:THR:H	1:23:A:THR:HG21	26	0.38
(1,476)	1:23:A:THR:H	1:23:A:THR:HG22	26	0.38
(1,476)	1:23:A:THR:H	1:23:A:THR:HG23	26	0.38
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	27	0.36
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	1	0.36
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	10	0.36
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	23	0.35
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	30	0.35
(1,1571)	1:88:A:LYS:HB2	1:89:A:THR:HA	27	0.34
(1,1571)	1:88:A:LYS:HB3	1:89:A:THR:HA	27	0.34
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	10	0.34
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	16	0.34
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	22	0.34
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	29	0.34
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	2	0.33
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	3	0.33
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	6	0.33
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	8	0.33
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	11	0.33
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	19	0.33
(1,1133)	1:9:A:GLU:H	1:9:A:GLU:HG2	12	0.32
(1,1133)	1:9:A:GLU:H	1:9:A:GLU:HG3	12	0.32
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	7	0.32
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	15	0.32
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	25	0.32
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	20	0.31
(4,59)	1:80:A:GLY:H	1:76:A:LYS:O	18	0.3
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	12	0.3
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	26	0.3
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	28	0.3
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG11	28	0.29
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG12	28	0.29
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG13	28	0.29
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG21	28	0.29
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG22	28	0.29
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG23	28	0.29
(1,957)	1:18:A:PHE:HE2	1:75:A:ILE:HG21	27	0.29
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	11	0.28
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	6	0.27
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	23	0.27
(1,1009)	1:14:A:LEU:HG	1:79:A:HIS:HD2	18	0.27
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	19	0.26
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	27	0.26
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	29	0.26
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG21	27	0.26
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG22	27	0.26
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG23	27	0.26
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	29	0.25
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	30	0.25
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	15	0.25
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	25	0.25
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	19	0.25
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	19	0.24
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	2	0.24
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	3	0.23
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	6	0.23
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	17	0.23
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	23	0.23
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	3	0.23
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	7	0.23
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	8	0.23
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	17	0.23
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG11	13	0.23
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG12	13	0.23
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG13	13	0.23
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG21	13	0.23
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG22	13	0.23
(1,1355)	1:46:A:PRO:HA	1:50:A:VAL:HG23	13	0.23
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	30	0.23
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	30	0.23
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	30	0.23
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	1	0.23
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	7	0.22
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	15	0.22
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	22	0.22
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	4	0.22
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	14	0.22
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	22	0.22
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	28	0.22
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	30	0.22
(1,1571)	1:88:A:LYS:HB2	1:89:A:THR:HA	5	0.22
(1,1571)	1:88:A:LYS:HB3	1:89:A:THR:HA	5	0.22
(1,1548)	1:81:A:LEU:HA	1:81:A:LEU:HD11	22	0.22
(1,1548)	1:81:A:LEU:HA	1:81:A:LEU:HD12	22	0.22
(1,1548)	1:81:A:LEU:HA	1:81:A:LEU:HD13	22	0.22
(1,1548)	1:81:A:LEU:HA	1:81:A:LEU:HD21	22	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:81:A:LEU:HA	1:81:A:LEU:HD22	22	0.22
(1,1548)	1:81:A:LEU:HA	1:81:A:LEU:HD23	22	0.22
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	12	0.22
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	5	0.22
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	25	0.21
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	29	0.21
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	30	0.21
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	8	0.21
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	11	0.21
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	25	0.21
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	26	0.21
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	27	0.21
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	24	0.21
(1,1571)	1:88:A:LYS:HB2	1:89:A:THR:HA	26	0.21
(1,1571)	1:88:A:LYS:HB3	1:89:A:THR:HA	26	0.21
(1,830)	1:84:A:THR:HB	1:86:A:VAL:H	19	0.21
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	13	0.21
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	21	0.21
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	8	0.21
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	8	0.21
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	8	0.21
(1,105)	1:94:A:ILE:HB	1:95:A:ASN:HB2	29	0.21
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	3	0.2
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	7	0.2
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	6	0.2
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	19	0.2
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	23	0.2
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	28	0.2
(4,11)	1:17:A:ALA:H	1:13:A:GLU:O	26	0.2
(1,1555)	1:85:A:ASP:HA	1:88:A:LYS:HB2	5	0.2
(1,1555)	1:85:A:ASP:HA	1:88:A:LYS:HB3	5	0.2
(1,1555)	1:85:A:ASP:HA	1:88:A:LYS:HB2	26	0.2
(1,1555)	1:85:A:ASP:HA	1:88:A:LYS:HB3	26	0.2
(1,830)	1:84:A:THR:HB	1:86:A:VAL:H	24	0.2
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	27	0.2
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	27	0.2
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	29	0.2
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	29	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	12	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	12	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	12	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	15	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	15	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	29	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	29	0.2
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	29	0.2
(1,105)	1:94:A:ILE:HB	1:95:A:ASN:HB2	9	0.2
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	24	0.19
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	3	0.19
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	17	0.19
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	26	0.19
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	26	0.19
(1,1383)	1:50:A:VAL:HG11	1:52:A:GLU:H	3	0.19
(1,1383)	1:50:A:VAL:HG12	1:52:A:GLU:H	3	0.19
(1,1383)	1:50:A:VAL:HG13	1:52:A:GLU:H	3	0.19
(1,1383)	1:50:A:VAL:HG21	1:52:A:GLU:H	3	0.19
(1,1383)	1:50:A:VAL:HG22	1:52:A:GLU:H	3	0.19
(1,1383)	1:50:A:VAL:HG23	1:52:A:GLU:H	3	0.19
(1,1383)	1:50:A:VAL:HG11	1:52:A:GLU:H	24	0.19
(1,1383)	1:50:A:VAL:HG12	1:52:A:GLU:H	24	0.19
(1,1383)	1:50:A:VAL:HG13	1:52:A:GLU:H	24	0.19
(1,1383)	1:50:A:VAL:HG21	1:52:A:GLU:H	24	0.19
(1,1383)	1:50:A:VAL:HG22	1:52:A:GLU:H	24	0.19
(1,1383)	1:50:A:VAL:HG23	1:52:A:GLU:H	24	0.19
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	23	0.19
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	23	0.19
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	9	0.19
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	12	0.19
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	18	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	1	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	1	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	1	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	19	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	19	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	19	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	21	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	21	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	21	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	30	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	30	0.19
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	30	0.19
(1,105)	1:94:A:ILE:HB	1:95:A:ASN:HB2	10	0.19
(1,105)	1:94:A:ILE:HB	1:95:A:ASN:HB2	23	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	12	0.18
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	22	0.18
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	23	0.18
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	13	0.18
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	7	0.18
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	11	0.18
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	22	0.18
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	14	0.18
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	18	0.18
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	18	0.18
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	12	0.18
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	12	0.18
(1,1501)	1:64:A:ASP:HB2	1:65:A:GLN:HE21	10	0.18
(1,1501)	1:64:A:ASP:HB3	1:65:A:GLN:HE21	10	0.18
(1,1383)	1:50:A:VAL:HG11	1:52:A:GLU:H	7	0.18
(1,1383)	1:50:A:VAL:HG12	1:52:A:GLU:H	7	0.18
(1,1383)	1:50:A:VAL:HG13	1:52:A:GLU:H	7	0.18
(1,1383)	1:50:A:VAL:HG21	1:52:A:GLU:H	7	0.18
(1,1383)	1:50:A:VAL:HG22	1:52:A:GLU:H	7	0.18
(1,1383)	1:50:A:VAL:HG23	1:52:A:GLU:H	7	0.18
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB2	25	0.18
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB3	25	0.18
(1,1037)	1:65:A:GLN:HA	1:65:A:GLN:HE21	19	0.18
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	22	0.18
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	22	0.18
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	12	0.18
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	12	0.18
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	18	0.17
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	21	0.17
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	8	0.17
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	15	0.17
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	25	0.17
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	26	0.17
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	27	0.17
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	4	0.17
(4,15)	1:19:A:ALA:H	1:15:A:ARG:O	24	0.17
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	2	0.17
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	2	0.17
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	16	0.17
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	16	0.17
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	28	0.17
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	28	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:50:A:VAL:HG11	1:52:A:GLU:H	25	0.17
(1,1383)	1:50:A:VAL:HG12	1:52:A:GLU:H	25	0.17
(1,1383)	1:50:A:VAL:HG13	1:52:A:GLU:H	25	0.17
(1,1383)	1:50:A:VAL:HG21	1:52:A:GLU:H	25	0.17
(1,1383)	1:50:A:VAL:HG22	1:52:A:GLU:H	25	0.17
(1,1383)	1:50:A:VAL:HG23	1:52:A:GLU:H	25	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG11	5	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG12	5	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG13	5	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG21	5	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG22	5	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG23	5	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG11	5	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG12	5	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG13	5	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG21	5	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG22	5	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG23	5	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG11	9	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG12	9	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG13	9	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG21	9	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG22	9	0.17
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG23	9	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG11	9	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG12	9	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG13	9	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG21	9	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG22	9	0.17
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG23	9	0.17
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	17	0.17
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	17	0.17
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	24	0.17
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	24	0.17
(1,483)	1:23:A:THR:HB	1:24:A:ASP:H	1	0.17
(1,483)	1:23:A:THR:HB	1:24:A:ASP:H	20	0.17
(1,483)	1:23:A:THR:HB	1:24:A:ASP:H	30	0.17
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	4	0.17
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	4	0.17
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	4	0.17
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	19	0.16
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	14	0.16
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	28	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG11	14	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG12	14	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG13	14	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG21	14	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG22	14	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG23	14	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG11	14	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG12	14	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG13	14	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG21	14	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG22	14	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG23	14	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG11	19	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG12	19	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG13	19	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG21	19	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG22	19	0.16
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG23	19	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG11	19	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG12	19	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG13	19	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG21	19	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG22	19	0.16
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG23	19	0.16
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB2	21	0.16
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB3	21	0.16
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG2	22	0.16
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG3	22	0.16
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG2	22	0.16
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG3	22	0.16
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG2	22	0.16
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG3	22	0.16
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	6	0.16
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	6	0.16
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	19	0.16
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	19	0.16
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	25	0.16
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	25	0.16
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	8	0.16
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	11	0.16
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	11	0.16
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	14	0.16
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	14	0.16
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	25	0.16
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	25	0.16
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	26	0.16
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	26	0.16
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD21	18	0.16
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD22	18	0.16
(1,157)	1:37:A:LEU:HA	1:37:A:LEU:HD23	18	0.16
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE1	10	0.16
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE2	10	0.16
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE1	10	0.16
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE2	10	0.16
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE1	10	0.16
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE2	10	0.16
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD11	21	0.16
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD12	21	0.16
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD13	21	0.16
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	19	0.15
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	30	0.15
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	17	0.15
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	29	0.15
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	1	0.15
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	5	0.15
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	21	0.15
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	26	0.15
(4,29)	1:51:A:ARG:H	1:47:A:GLY:O	14	0.15
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	28	0.15
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	28	0.15
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	8	0.15
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	8	0.15
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	9	0.15
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	9	0.15
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	12	0.15
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	12	0.15
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	29	0.15
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	29	0.15
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	10	0.15
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	10	0.15
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	28	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	28	0.15
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	29	0.15
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	29	0.15
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG2	3	0.15
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG3	3	0.15
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG2	3	0.15
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG3	3	0.15
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG2	3	0.15
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG3	3	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	8	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	8	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	17	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	17	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	22	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	22	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	27	0.15
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	27	0.15
(1,1035)	1:46:A:PRO:HA	1:48:A:TYR:HE1	19	0.15
(1,1035)	1:46:A:PRO:HA	1:48:A:TYR:HE2	19	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	5	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	5	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	9	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	9	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	12	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	12	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	14	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	14	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	15	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	15	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	16	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	16	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	17	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	17	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	29	0.15
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	29	0.15
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	26	0.15
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	26	0.15
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	28	0.15
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	28	0.15
(1,830)	1:84:A:THR:HB	1:86:A:VAL:H	21	0.15
(1,830)	1:84:A:THR:HB	1:86:A:VAL:H	25	0.15
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	4	0.15
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	15	0.15
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	15	0.15
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	30	0.15
(1,416)	1:14:A:LEU:H	1:14:A:LEU:HG	30	0.15
(1,220)	1:75:A:ILE:HG21	1:79:A:HIS:HA	18	0.15
(1,220)	1:75:A:ILE:HG22	1:79:A:HIS:HA	18	0.15
(1,220)	1:75:A:ILE:HG23	1:79:A:HIS:HA	18	0.15
(1,165)	1:37:A:LEU:HA	1:37:A:LEU:HD11	7	0.15
(1,165)	1:37:A:LEU:HA	1:37:A:LEU:HD12	7	0.15
(1,165)	1:37:A:LEU:HA	1:37:A:LEU:HD13	7	0.15
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG21	8	0.15
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG22	8	0.15
(1,133)	1:6:A:VAL:HA	1:75:A:ILE:HG23	8	0.15
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	5	0.14
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	23	0.14
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	11	0.14
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	12	0.14
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	17	0.14
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	23	0.14
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	28	0.14
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	4	0.14
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	14	0.14
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	1	0.14
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	1	0.14
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	20	0.14
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	20	0.14
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	21	0.14
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	21	0.14
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	22	0.14
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	22	0.14
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG11	15	0.14
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG12	15	0.14
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG13	15	0.14
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG21	15	0.14
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG22	15	0.14
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG23	15	0.14
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG11	15	0.14
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG12	15	0.14
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG13	15	0.14
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG21	15	0.14
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG22	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG23	15	0.14
(1,1368)	1:48:A:TYR:HE1	1:49:A:ARG:HG2	10	0.14
(1,1368)	1:48:A:TYR:HE1	1:49:A:ARG:HG3	10	0.14
(1,1368)	1:48:A:TYR:HE2	1:49:A:ARG:HG2	10	0.14
(1,1368)	1:48:A:TYR:HE2	1:49:A:ARG:HG3	10	0.14
(1,1343)	1:45:A:LEU:H	1:45:A:LEU:HB2	7	0.14
(1,1343)	1:45:A:LEU:H	1:45:A:LEU:HB3	7	0.14
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB2	29	0.14
(1,1330)	1:42:A:CYS:H	1:43:A:LEU:HB3	29	0.14
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG2	7	0.14
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG3	7	0.14
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG2	7	0.14
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG3	7	0.14
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG2	7	0.14
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG3	7	0.14
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	25	0.14
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	25	0.14
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	7	0.14
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	17	0.14
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	28	0.14
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	29	0.14
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	29	0.14
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	10	0.14
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	10	0.14
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	25	0.14
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	25	0.14
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	29	0.14
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	29	0.14
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	3	0.14
(1,809)	1:77:A:ILE:HD11	1:79:A:HIS:H	18	0.14
(1,809)	1:77:A:ILE:HD12	1:79:A:HIS:H	18	0.14
(1,809)	1:77:A:ILE:HD13	1:79:A:HIS:H	18	0.14
(1,762)	1:69:A:ILE:HA	1:73:A:GLU:H	20	0.14
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	3	0.14
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	3	0.14
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	6	0.14
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	6	0.14
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	7	0.14
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	7	0.14
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	16	0.14
(1,420)	1:14:A:LEU:H	1:18:A:PHE:HZ	20	0.14
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	21	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	21	0.14
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	30	0.14
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	30	0.14
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE1	22	0.14
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE2	22	0.14
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE1	22	0.14
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE2	22	0.14
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE1	22	0.14
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE2	22	0.14
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	11	0.14
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	11	0.14
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	11	0.14
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	12	0.14
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	12	0.14
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	12	0.14
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD11	7	0.14
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD12	7	0.14
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD13	7	0.14
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	1	0.13
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	3	0.13
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	6	0.13
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	7	0.13
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	8	0.13
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	28	0.13
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	11	0.13
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	15	0.13
(4,39)	1:56:A:ASN:H	1:52:A:GLU:O	14	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	2	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	4	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	6	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	8	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	10	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	13	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	18	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	27	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	29	0.13
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	30	0.13
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	21	0.13
(4,33)	1:53:A:ILE:H	1:49:A:ARG:O	14	0.13
(4,16)	1:19:A:ALA:N	1:15:A:ARG:O	24	0.13
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	11	0.13
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	25	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	27	0.13
(3,60)	1:80:A:GLY:N	1:76:A:LYS:O	18	0.13
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	11	0.13
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	11	0.13
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	13	0.13
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	13	0.13
(1,1595)	1:96:A:LYS:HB2	1:97:A:LYS:H	15	0.13
(1,1595)	1:96:A:LYS:HB3	1:97:A:LYS:H	15	0.13
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	19	0.13
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	19	0.13
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	25	0.13
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	25	0.13
(1,1349)	1:45:A:LEU:HD11	1:48:A:TYR:HE1	7	0.13
(1,1349)	1:45:A:LEU:HD11	1:48:A:TYR:HE2	7	0.13
(1,1349)	1:45:A:LEU:HD12	1:48:A:TYR:HE1	7	0.13
(1,1349)	1:45:A:LEU:HD12	1:48:A:TYR:HE2	7	0.13
(1,1349)	1:45:A:LEU:HD13	1:48:A:TYR:HE1	7	0.13
(1,1349)	1:45:A:LEU:HD13	1:48:A:TYR:HE2	7	0.13
(1,1349)	1:45:A:LEU:HD21	1:48:A:TYR:HE1	7	0.13
(1,1349)	1:45:A:LEU:HD21	1:48:A:TYR:HE2	7	0.13
(1,1349)	1:45:A:LEU:HD22	1:48:A:TYR:HE1	7	0.13
(1,1349)	1:45:A:LEU:HD22	1:48:A:TYR:HE2	7	0.13
(1,1349)	1:45:A:LEU:HD23	1:48:A:TYR:HE1	7	0.13
(1,1349)	1:45:A:LEU:HD23	1:48:A:TYR:HE2	7	0.13
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	3	0.13
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	3	0.13
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	30	0.13
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	30	0.13
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	15	0.13
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	23	0.13
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	25	0.13
(1,1054)	1:77:A:ILE:HG21	1:78:A:PHE:HZ	18	0.13
(1,1054)	1:77:A:ILE:HG22	1:78:A:PHE:HZ	18	0.13
(1,1054)	1:77:A:ILE:HG23	1:78:A:PHE:HZ	18	0.13
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	13	0.13
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	13	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD11	5	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD12	5	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD13	5	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD11	21	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD12	21	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD13	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD11	30	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD12	30	0.13
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD13	30	0.13
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	7	0.13
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	7	0.13
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	28	0.13
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	28	0.13
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	23	0.13
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	23	0.13
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	23	0.13
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	19	0.13
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	19	0.13
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	28	0.13
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	28	0.13
(1,159)	1:37:A:LEU:HD21	1:90:A:PHE:HA	25	0.13
(1,159)	1:37:A:LEU:HD22	1:90:A:PHE:HA	25	0.13
(1,159)	1:37:A:LEU:HD23	1:90:A:PHE:HA	25	0.13
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	1	0.13
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	1	0.13
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	8	0.13
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	8	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	6	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	6	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	6	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	15	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	15	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	15	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	22	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	22	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	22	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	29	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	29	0.13
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	29	0.13
(4,63)	1:90:A:PHE:H	1:86:A:VAL:O	5	0.12
(4,59)	1:80:A:GLY:H	1:76:A:LYS:O	23	0.12
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	13	0.12
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	22	0.12
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	25	0.12
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	26	0.12
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	24	0.12
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	9	0.12
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:55:A:GLU:H	1:51:A:ARG:O	22	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	1	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	4	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	10	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	11	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	15	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	22	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	23	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	26	0.12
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	27	0.12
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	3	0.12
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	7	0.12
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	15	0.12
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	19	0.12
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	23	0.12
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	26	0.12
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG2	23	0.12
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG3	23	0.12
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG2	23	0.12
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG3	23	0.12
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG2	23	0.12
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG3	23	0.12
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	15	0.12
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	15	0.12
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	23	0.12
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	23	0.12
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	29	0.12
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	29	0.12
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	8	0.12
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	11	0.12
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	22	0.12
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	26	0.12
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	27	0.12
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	8	0.12
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	8	0.12
(1,1035)	1:46:A:PRO:HA	1:48:A:TYR:HE1	23	0.12
(1,1035)	1:46:A:PRO:HA	1:48:A:TYR:HE2	23	0.12
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	24	0.12
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	24	0.12
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	28	0.12
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	28	0.12
(1,962)	1:38:A:PHE:HD1	1:57:A:LEU:HB3	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,962)	1:38:A:PHE:HD2	1:57:A:LEU:HB3	19	0.12
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	20	0.12
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	12	0.12
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	12	0.12
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	15	0.12
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	15	0.12
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	29	0.12
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	29	0.12
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	3	0.12
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	3	0.12
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	3	0.12
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	10	0.12
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	10	0.12
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	10	0.12
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	15	0.12
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	15	0.12
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	15	0.12
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	24	0.12
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	24	0.12
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	24	0.12
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	26	0.12
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	26	0.12
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	26	0.12
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	16	0.12
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	16	0.12
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	30	0.12
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	30	0.12
(1,372)	1:29:A:ILE:HG21	1:58:A:MET:HE1	21	0.12
(1,372)	1:29:A:ILE:HG21	1:58:A:MET:HE2	21	0.12
(1,372)	1:29:A:ILE:HG21	1:58:A:MET:HE3	21	0.12
(1,372)	1:29:A:ILE:HG22	1:58:A:MET:HE1	21	0.12
(1,372)	1:29:A:ILE:HG22	1:58:A:MET:HE2	21	0.12
(1,372)	1:29:A:ILE:HG22	1:58:A:MET:HE3	21	0.12
(1,372)	1:29:A:ILE:HG23	1:58:A:MET:HE1	21	0.12
(1,372)	1:29:A:ILE:HG23	1:58:A:MET:HE2	21	0.12
(1,372)	1:29:A:ILE:HG23	1:58:A:MET:HE3	21	0.12
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD1	4	0.12
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD2	4	0.12
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD1	14	0.12
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD2	14	0.12
(1,315)	1:46:A:PRO:HA	1:49:A:ARG:HB2	10	0.12
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	11	0.12
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	11	0.12
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	17	0.12
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	17	0.12
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	17	0.12
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE1	18	0.12
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE2	18	0.12
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE1	18	0.12
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE2	18	0.12
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE1	18	0.12
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE2	18	0.12
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	8	0.12
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	8	0.12
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	8	0.12
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	17	0.12
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	17	0.12
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	17	0.12
(4,67)	1:92:A:LYS:H	1:88:A:LYS:O	5	0.11
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	4	0.11
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	10	0.11
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	14	0.11
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	24	0.11
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	8	0.11
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	25	0.11
(4,41)	1:57:A:LEU:H	1:53:A:ILE:O	14	0.11
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	12	0.11
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	16	0.11
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	17	0.11
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	18	0.11
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	20	0.11
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	30	0.11
(4,31)	1:52:A:GLU:H	1:48:A:TYR:O	15	0.11
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	6	0.11
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	22	0.11
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	29	0.11
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	30	0.11
(1,1574)	1:88:A:LYS:HD2	1:89:A:THR:HA	27	0.11
(1,1574)	1:88:A:LYS:HD3	1:89:A:THR:HA	27	0.11
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	26	0.11
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	26	0.11
(1,1532)	1:77:A:ILE:HA	1:81:A:LEU:HB2	22	0.11
(1,1532)	1:77:A:ILE:HA	1:81:A:LEU:HB3	22	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG11	10	0.11
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG12	10	0.11
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG13	10	0.11
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG21	10	0.11
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG22	10	0.11
(1,1376)	1:49:A:ARG:HD2	1:50:A:VAL:HG23	10	0.11
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG11	10	0.11
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG12	10	0.11
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG13	10	0.11
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG21	10	0.11
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG22	10	0.11
(1,1376)	1:49:A:ARG:HD3	1:50:A:VAL:HG23	10	0.11
(1,1368)	1:48:A:TYR:HE1	1:49:A:ARG:HG2	15	0.11
(1,1368)	1:48:A:TYR:HE1	1:49:A:ARG:HG3	15	0.11
(1,1368)	1:48:A:TYR:HE2	1:49:A:ARG:HG2	15	0.11
(1,1368)	1:48:A:TYR:HE2	1:49:A:ARG:HG3	15	0.11
(1,1349)	1:45:A:LEU:HD11	1:48:A:TYR:HE1	14	0.11
(1,1349)	1:45:A:LEU:HD11	1:48:A:TYR:HE2	14	0.11
(1,1349)	1:45:A:LEU:HD12	1:48:A:TYR:HE1	14	0.11
(1,1349)	1:45:A:LEU:HD12	1:48:A:TYR:HE2	14	0.11
(1,1349)	1:45:A:LEU:HD13	1:48:A:TYR:HE1	14	0.11
(1,1349)	1:45:A:LEU:HD13	1:48:A:TYR:HE2	14	0.11
(1,1349)	1:45:A:LEU:HD21	1:48:A:TYR:HE1	14	0.11
(1,1349)	1:45:A:LEU:HD21	1:48:A:TYR:HE2	14	0.11
(1,1349)	1:45:A:LEU:HD22	1:48:A:TYR:HE1	14	0.11
(1,1349)	1:45:A:LEU:HD22	1:48:A:TYR:HE2	14	0.11
(1,1349)	1:45:A:LEU:HD23	1:48:A:TYR:HE1	14	0.11
(1,1349)	1:45:A:LEU:HD23	1:48:A:TYR:HE2	14	0.11
(1,1343)	1:45:A:LEU:H	1:45:A:LEU:HB2	23	0.11
(1,1343)	1:45:A:LEU:H	1:45:A:LEU:HB3	23	0.11
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG2	6	0.11
(1,1238)	1:29:A:ILE:HD11	1:33:A:GLU:HG3	6	0.11
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG2	6	0.11
(1,1238)	1:29:A:ILE:HD12	1:33:A:GLU:HG3	6	0.11
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG2	6	0.11
(1,1238)	1:29:A:ILE:HD13	1:33:A:GLU:HG3	6	0.11
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	14	0.11
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	14	0.11
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	24	0.11
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	24	0.11
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	3	0.11
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:18:A:PHE:HZ	1:75:A:ILE:HD11	19	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	17	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	17	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	18	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	18	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	21	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	21	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	22	0.11
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	22	0.11
(1,1043)	1:14:A:LEU:HA	1:78:A:PHE:HE1	15	0.11
(1,1043)	1:14:A:LEU:HA	1:78:A:PHE:HE2	15	0.11
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	1	0.11
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	1	0.11
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	8	0.11
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	8	0.11
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	13	0.11
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	13	0.11
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	21	0.11
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	21	0.11
(1,962)	1:38:A:PHE:HD1	1:57:A:LEU:HB3	4	0.11
(1,962)	1:38:A:PHE:HD2	1:57:A:LEU:HB3	4	0.11
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	14	0.11
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	18	0.11
(1,762)	1:69:A:ILE:HA	1:73:A:GLU:H	12	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	2	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	2	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	3	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	3	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	11	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	11	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	17	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	17	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	19	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	19	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	20	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	20	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	23	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	23	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	25	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	25	0.11
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	26	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	26	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:18:A:PHE:HE1	1:72:A:ASP:H	27	0.11
(1,751)	1:18:A:PHE:HE2	1:72:A:ASP:H	27	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	6	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	6	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	6	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	7	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	7	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	7	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	9	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	9	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	9	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	11	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	11	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	11	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	12	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	12	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	12	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	17	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	17	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	17	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	28	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	28	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	28	0.11
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	30	0.11
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	30	0.11
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	30	0.11
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD1	22	0.11
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD2	22	0.11
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD1	23	0.11
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD2	23	0.11
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD1	24	0.11
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD2	24	0.11
(1,159)	1:37:A:LEU:HD21	1:90:A:PHE:HA	5	0.11
(1,159)	1:37:A:LEU:HD22	1:90:A:PHE:HA	5	0.11
(1,159)	1:37:A:LEU:HD23	1:90:A:PHE:HA	5	0.11
(1,136)	1:5:A:SER:HA	1:75:A:ILE:HG21	16	0.11
(1,136)	1:5:A:SER:HA	1:75:A:ILE:HG22	16	0.11
(1,136)	1:5:A:SER:HA	1:75:A:ILE:HG23	16	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	14	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	14	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	14	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	15	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	15	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	24	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	24	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	24	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	29	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	29	0.11
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	29	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	4	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	4	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	5	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	5	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	19	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	19	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	23	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	23	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	28	0.11
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	28	0.11
(1,105)	1:94:A:ILE:HB	1:95:A:ASN:HB2	16	0.11
(1,105)	1:94:A:ILE:HB	1:95:A:ASN:HB2	17	0.11
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE1	9	0.11
(1,59)	1:29:A:ILE:HG21	1:38:A:PHE:HE2	9	0.11
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE1	9	0.11
(1,59)	1:29:A:ILE:HG22	1:38:A:PHE:HE2	9	0.11
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE1	9	0.11
(1,59)	1:29:A:ILE:HG23	1:38:A:PHE:HE2	9	0.11
(1,23)	1:14:A:LEU:HA	1:14:A:LEU:HG	30	0.11
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	2	0.1
(4,55)	1:78:A:PHE:H	1:74:A:PHE:O	20	0.1
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	4	0.1
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	19	0.1
(4,53)	1:77:A:ILE:H	1:73:A:GLU:O	28	0.1
(4,43)	1:58:A:MET:H	1:54:A:THR:O	13	0.1
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	6	0.1
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	8	0.1
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	9	0.1
(4,35)	1:54:A:THR:H	1:50:A:VAL:O	29	0.1
(4,13)	1:18:A:PHE:H	1:14:A:LEU:O	8	0.1
(4,1)	1:12:A:MET:H	1:8:A:ASP:O	12	0.1
(1,1559)	1:85:A:ASP:HB2	1:86:A:VAL:HB	13	0.1
(1,1559)	1:85:A:ASP:HB3	1:86:A:VAL:HB	13	0.1
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	7	0.1
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB2	11	0.1
(1,1142)	1:12:A:MET:HA	1:15:A:ARG:HB3	11	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	6	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	6	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	10	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	10	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	12	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	12	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE1	27	0.1
(1,1065)	1:14:A:LEU:HG	1:90:A:PHE:HE2	27	0.1
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	3	0.1
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	3	0.1
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	6	0.1
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	6	0.1
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE1	30	0.1
(1,997)	1:48:A:TYR:HA	1:48:A:TYR:HE2	30	0.1
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD1	2	0.1
(1,967)	1:34:A:LEU:HA	1:38:A:PHE:HD2	2	0.1
(1,936)	1:52:A:GLU:HA	1:56:A:ASN:HD22	11	0.1
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD11	24	0.1
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD12	24	0.1
(1,864)	1:91:A:ARG:H	1:94:A:ILE:HD13	24	0.1
(1,762)	1:69:A:ILE:HA	1:73:A:GLU:H	21	0.1
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	4	0.1
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	4	0.1
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	4	0.1
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	22	0.1
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	22	0.1
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	22	0.1
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	25	0.1
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	25	0.1
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	25	0.1
(1,748)	1:69:A:ILE:HG21	1:72:A:ASP:H	27	0.1
(1,748)	1:69:A:ILE:HG22	1:72:A:ASP:H	27	0.1
(1,748)	1:69:A:ILE:HG23	1:72:A:ASP:H	27	0.1
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	10	0.1
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	10	0.1
(1,744)	1:18:A:PHE:HE1	1:71:A:PHE:H	12	0.1
(1,744)	1:18:A:PHE:HE2	1:71:A:PHE:H	12	0.1
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD1	19	0.1
(1,330)	1:15:A:ARG:HD2	1:18:A:PHE:HD2	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:81:A:LEU:HA	1:81:A:LEU:HD11	29	0.1
(1,195)	1:81:A:LEU:HA	1:81:A:LEU:HD12	29	0.1
(1,195)	1:81:A:LEU:HA	1:81:A:LEU:HD13	29	0.1
(1,159)	1:37:A:LEU:HD21	1:90:A:PHE:HA	24	0.1
(1,159)	1:37:A:LEU:HD22	1:90:A:PHE:HA	24	0.1
(1,159)	1:37:A:LEU:HD23	1:90:A:PHE:HA	24	0.1
(1,159)	1:37:A:LEU:HD21	1:90:A:PHE:HA	26	0.1
(1,159)	1:37:A:LEU:HD22	1:90:A:PHE:HA	26	0.1
(1,159)	1:37:A:LEU:HD23	1:90:A:PHE:HA	26	0.1
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	2	0.1
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	2	0.1
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	2	0.1
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD11	23	0.1
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD12	23	0.1
(1,127)	1:10:A:GLU:HG3	1:75:A:ILE:HD13	23	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	3	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	3	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	6	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	6	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	25	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	25	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE1	26	0.1
(1,123)	1:75:A:ILE:HA	1:78:A:PHE:HE2	26	0.1
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD21	25	0.1
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD22	25	0.1
(1,31)	1:10:A:GLU:HG3	1:14:A:LEU:HD23	25	0.1
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD11	4	0.1
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD12	4	0.1
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD13	4	0.1
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD11	19	0.1
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD12	19	0.1
(1,7)	1:37:A:LEU:HA	1:94:A:ILE:HD13	19	0.1

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

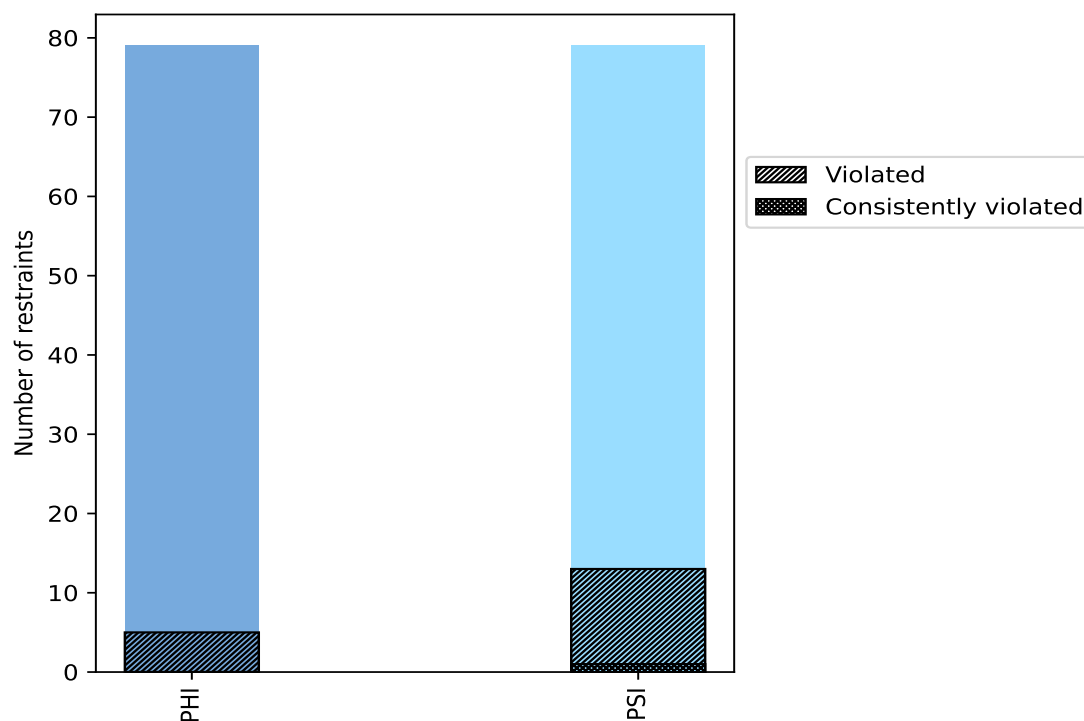
10.1 Summary of dihedral-angle violations [i](#)

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	79	50.0	5	6.3	3.2	0	0.0	0.0
PSI	79	50.0	13	16.5	8.2	1	1.3	0.6
Total	158	100.0	18	11.4	11.4	1	0.6	0.6

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

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



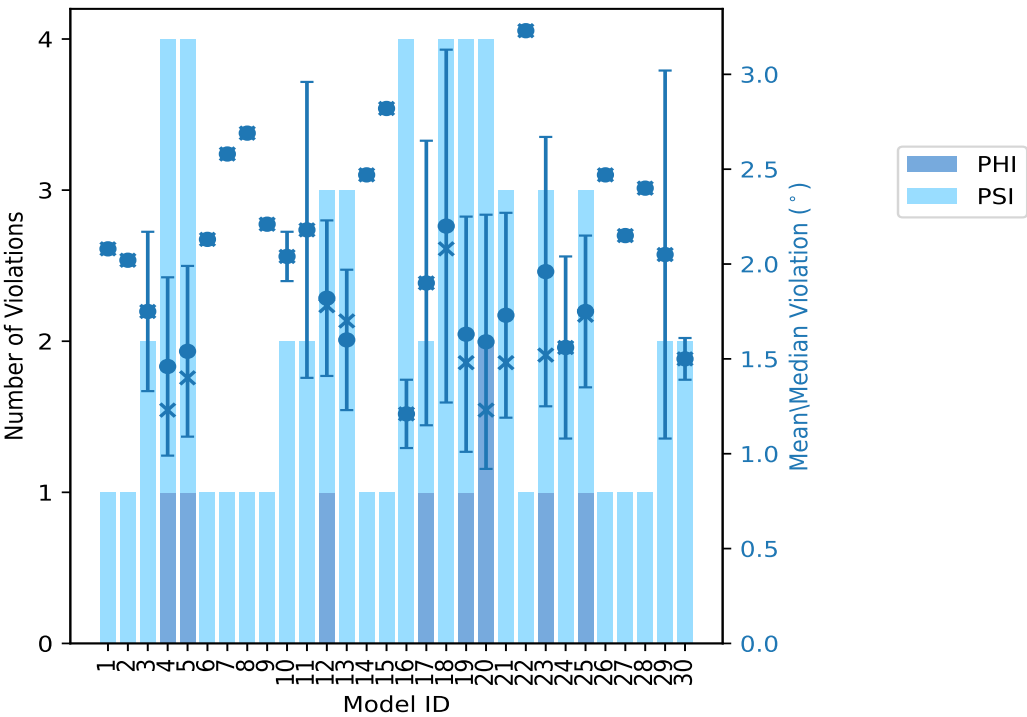
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	2.08	2.08	0.0	2.08
2	0	1	1	2.02	2.02	0.0	2.02
3	0	2	2	1.75	2.17	0.42	1.75
4	1	3	4	1.46	2.28	0.47	1.23
5	1	3	4	1.54	2.29	0.45	1.4
6	0	1	1	2.13	2.13	0.0	2.13
7	0	1	1	2.58	2.58	0.0	2.58
8	0	1	1	2.69	2.69	0.0	2.69
9	0	1	1	2.21	2.21	0.0	2.21
10	0	2	2	2.04	2.16	0.13	2.04
11	0	2	2	2.18	2.96	0.78	2.18
12	1	2	3	1.82	2.34	0.41	1.78
13	0	3	3	1.6	1.99	0.37	1.7
14	0	1	1	2.47	2.47	0.0	2.47
15	0	1	1	2.82	2.82	0.0	2.82
16	0	4	4	1.21	1.4	0.18	1.21
17	1	1	2	1.9	2.65	0.75	1.9
18	0	4	4	2.2	3.39	0.93	2.08
19	1	3	4	1.63	2.56	0.62	1.48
20	2	2	4	1.59	2.75	0.67	1.23
21	0	3	3	1.73	2.48	0.54	1.48
22	0	1	1	3.23	3.23	0.0	3.23
23	1	2	3	1.96	2.96	0.71	1.52
24	0	2	2	1.56	2.04	0.48	1.56
25	1	2	3	1.75	2.25	0.4	1.73
26	0	1	1	2.47	2.47	0.0	2.47
27	0	1	1	2.15	2.15	0.0	2.15
28	0	1	1	2.4	2.4	0.0	2.4
29	0	2	2	2.05	3.02	0.97	2.05
30	0	2	2	1.5	1.6	0.11	1.5

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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	%
3	6	9	1	3.3
1	1	2	2	6.7
0	2	2	3	10.0
1	3	4	4	13.3
0	0	0	5	16.7
0	0	0	6	20.0
0	0	0	7	23.3
0	0	0	8	26.7
0	0	0	9	30.0
0	0	0	10	33.3
0	0	0	11	36.7

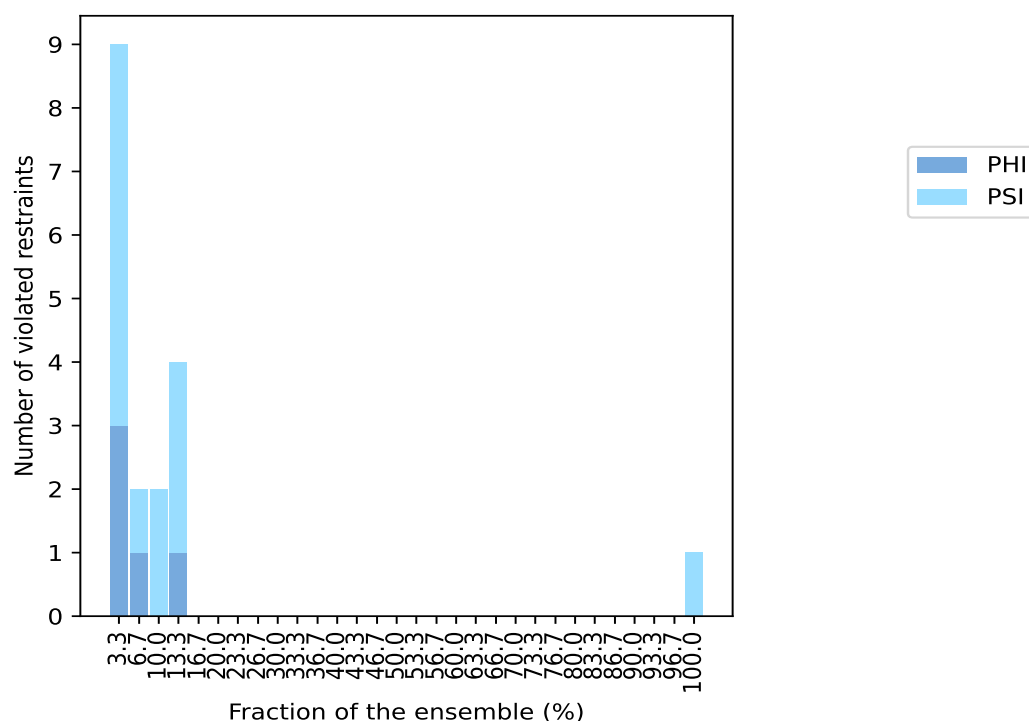
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	40.0
0	0	0	13	43.3
0	0	0	14	46.7
0	0	0	15	50.0
0	0	0	16	53.3
0	0	0	17	56.7
0	0	0	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
0	0	0	23	76.7
0	0	0	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
0	1	1	30	100.0

¹ Number of models with violations

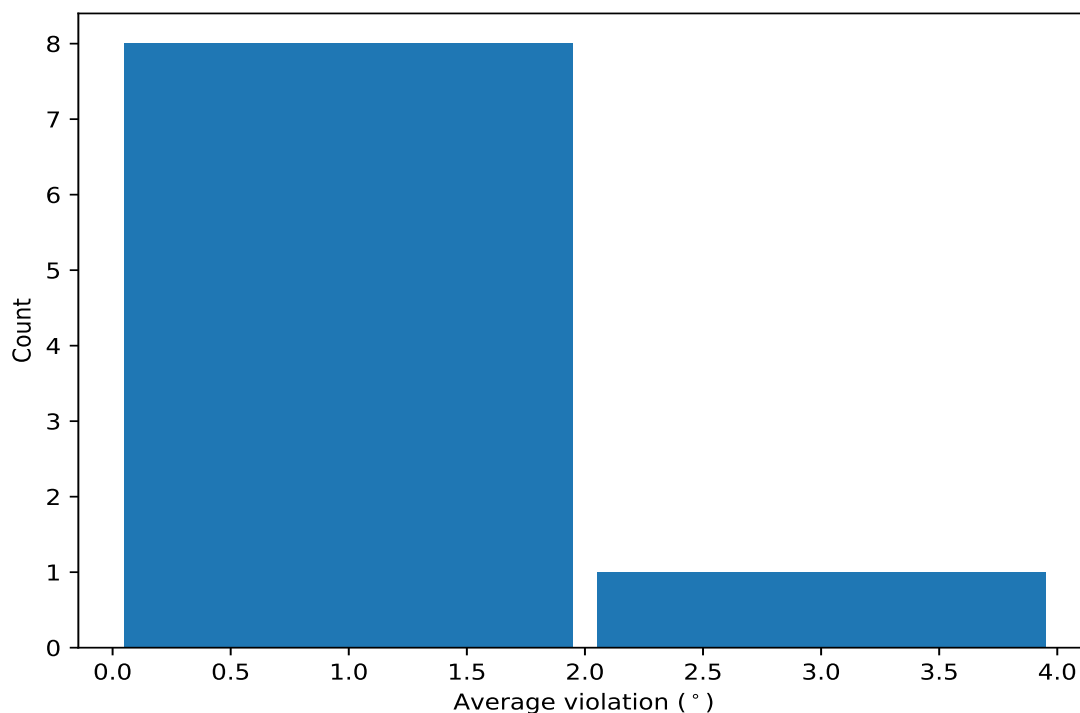
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

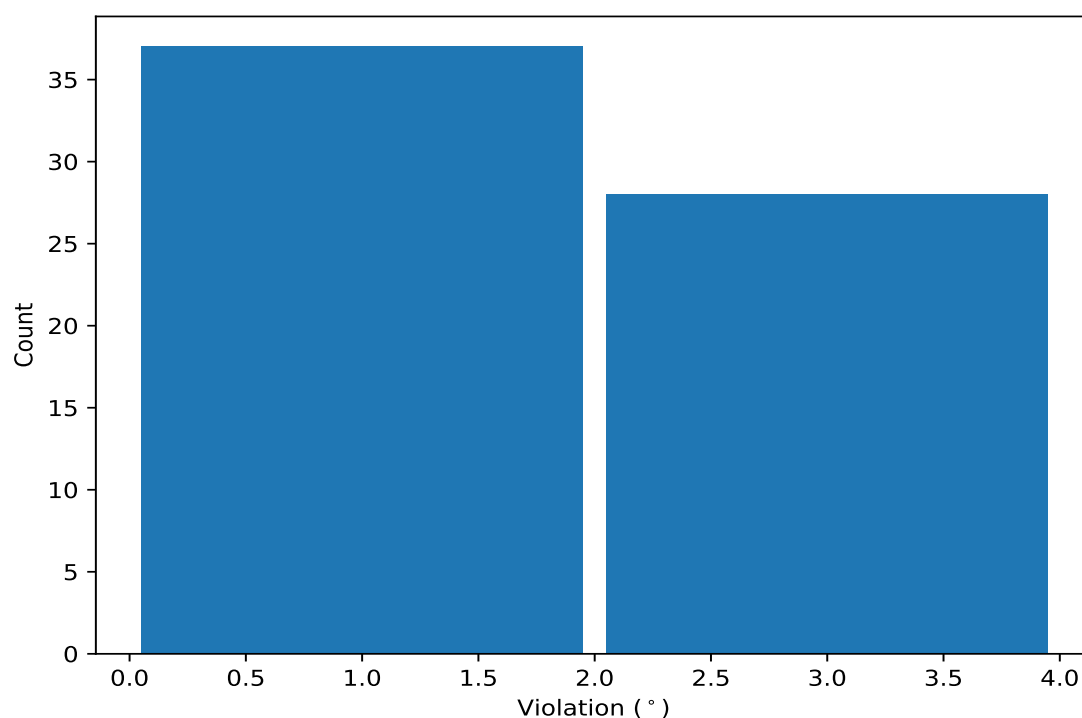
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	30	2.42	0.44	2.37
(1,73)	1:44:A:PRO:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	4	1.53	0.26	1.56
(1,10)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:MET:N	4	1.37	0.27	1.33
(1,154)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:ILE:N	4	1.3	0.07	1.28
(1,52)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLU:N	4	1.22	0.13	1.2
(1,148)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:ARG:N	3	1.5	0.34	1.52
(1,54)	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	1:34:A:LEU:N	3	1.15	0.14	1.11
(1,63)	1:37:A:LEU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	2	1.38	0.02	1.38
(1,78)	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	1:50:A:VAL:N	2	1.1	0.02	1.1

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 (°)
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	18	3.39
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	22	3.23
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	29	3.02
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	11	2.96
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	23	2.96
(1,134)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:GLY:N	18	2.84
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	15	2.82
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	20	2.75
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	8	2.69
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	17	2.65
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	7	2.58
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	19	2.56
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	21	2.48
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	14	2.47
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	26	2.47
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	28	2.4
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	12	2.34
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	5	2.29
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	4	2.28
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	25	2.25
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	9	2.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	3	2.17
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	10	2.16
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	27	2.15
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	6	2.13
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	1	2.08
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	24	2.04
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	2	2.02
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	13	1.99
(1,148)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:ARG:N	10	1.91
(1,73)	1:44:A:PRO:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	19	1.82
(1,10)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:MET:N	12	1.78
(1,73)	1:44:A:PRO:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	25	1.73
(1,68)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ALA:N	13	1.7
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	30	1.6
(1,148)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:ARG:N	23	1.52
(1,150)	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	1:92:A:LYS:N	21	1.48
(1,52)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLU:N	11	1.41
(1,154)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:ILE:N	16	1.4
(1,73)	1:44:A:PRO:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	5	1.4
(1,63)	1:37:A:LEU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	23	1.4
(1,122)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:PHE:N	16	1.39
(1,28)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:VAL:N	30	1.39
(1,10)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:MET:N	5	1.39
(1,63)	1:37:A:LEU:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	12	1.35
(1,54)	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	1:34:A:LEU:N	3	1.33
(1,154)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:ILE:N	18	1.31
(1,52)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLU:N	25	1.28
(1,10)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:MET:N	18	1.27
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:GLU:N	20	1.26
(1,154)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:ILE:N	4	1.25
(1,154)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:ILE:N	21	1.23
(1,103)	1:62:A:ASP:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	4	1.22
(1,109)	1:66:A:ASP:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	20	1.19
(1,73)	1:44:A:PRO:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	20	1.17
(1,33)	1:22:A:ASP:C	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	17	1.15
(1,78)	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	1:50:A:VAL:N	19	1.13
(1,54)	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	1:34:A:LEU:N	4	1.11
(1,52)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLU:N	13	1.11
(1,148)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:ARG:N	29	1.08
(1,78)	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	1:50:A:VAL:N	5	1.08
(1,52)	1:32:A:ASN:N	1:32:A:ASN:CA	1:32:A:ASN:C	1:33:A:GLU:N	24	1.08
(1,10)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:MET:N	16	1.03
(1,4)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:GLU:N	16	1.03
(1,54)	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	1:34:A:LEU:N	19	1.0