



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:19 PM UTC

PDB ID : 2LC0 / pdb_00002lc0
Title : Rv0020c_Nter structure
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Deposited on : 2011-04-11

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

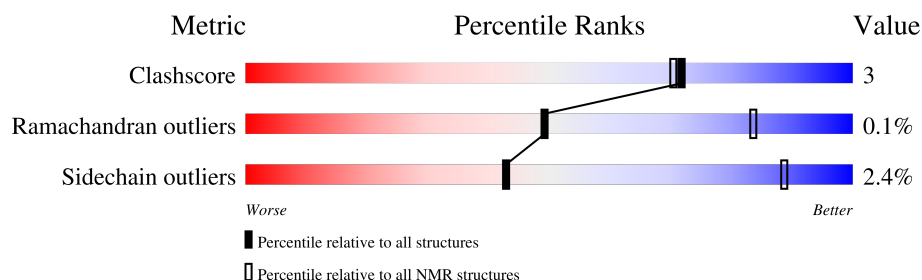
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	132	 67% 29%

2 Ensemble composition and analysis

This entry contains 30 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:34-A:127 (94)	0.97	3

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2063 atoms, of which 1021 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative uncharacterized protein TB39.8.

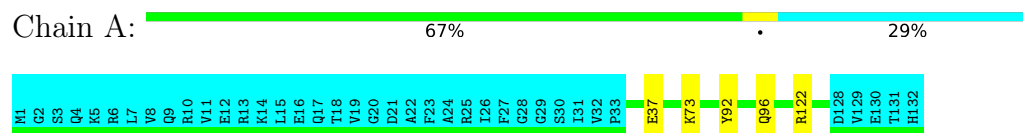
Mol	Chain	Residues	Atoms						Trace
1	A	132	Total	C	H	N	O	S	0
			2063	648	1021	191	202	1	

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: Putative uncharacterized protein TB39.8

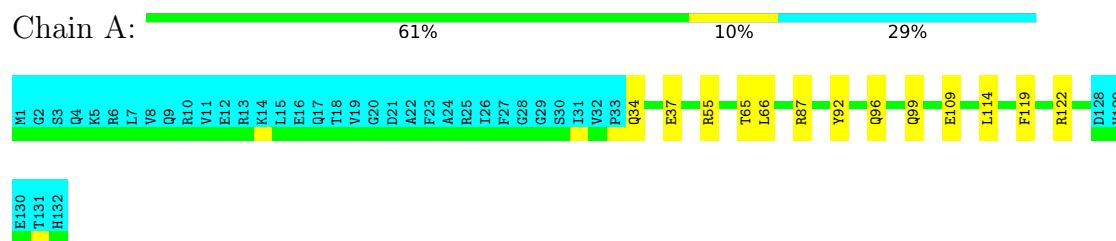


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

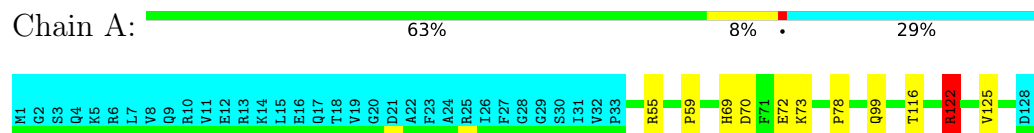
4.2.1 Score per residue for model 1

- Molecule 1: Putative uncharacterized protein TB39.8



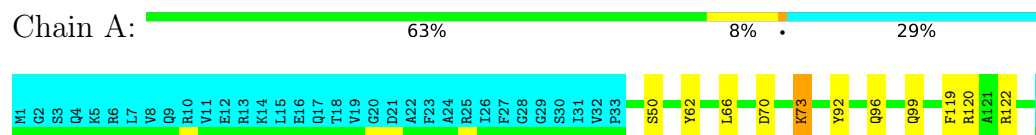
4.2.2 Score per residue for model 2

- Molecule 1: Putative uncharacterized protein TB39.8



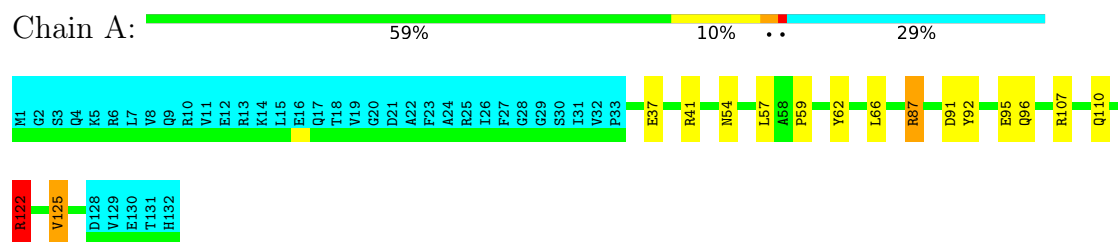
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Putative uncharacterized protein TB39.8



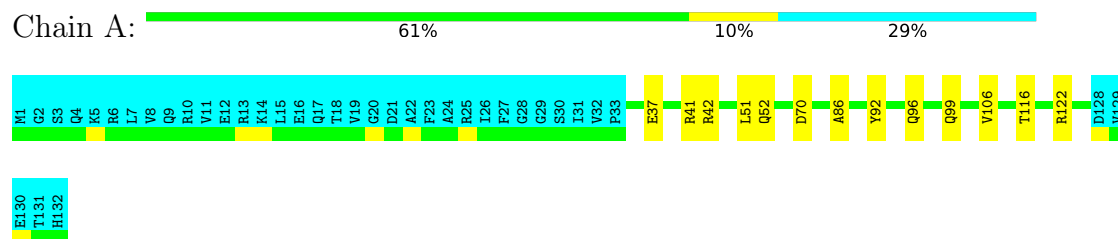
4.2.4 Score per residue for model 4

- Molecule 1: Putative uncharacterized protein TB39.8



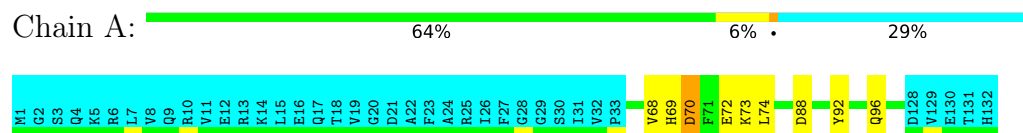
4.2.5 Score per residue for model 5

- Molecule 1: Putative uncharacterized protein TB39.8



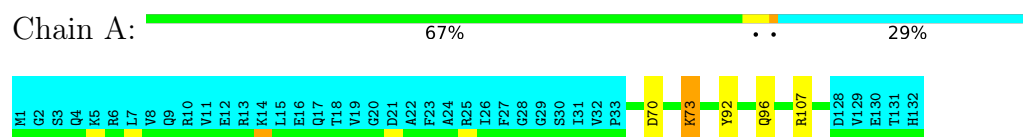
4.2.6 Score per residue for model 6

- Molecule 1: Putative uncharacterized protein TB39.8



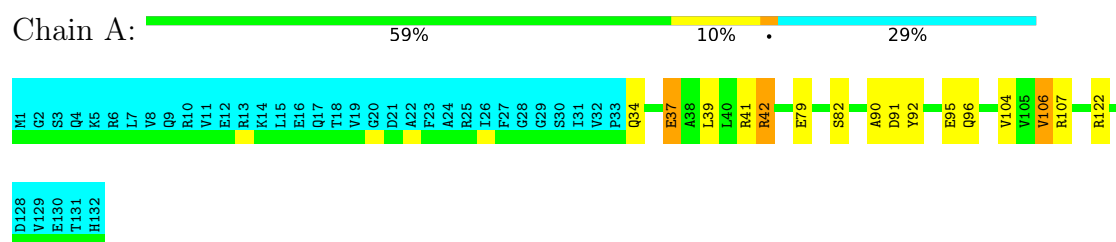
4.2.7 Score per residue for model 7

- Molecule 1: Putative uncharacterized protein TB39.8



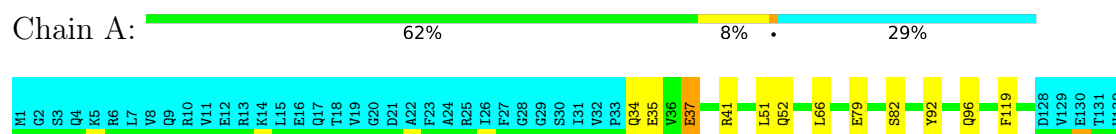
4.2.8 Score per residue for model 8

- Molecule 1: Putative uncharacterized protein TB39.8



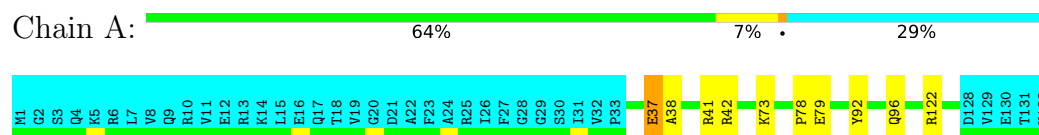
4.2.9 Score per residue for model 9

- Molecule 1: Putative uncharacterized protein TB39.8



4.2.10 Score per residue for model 10

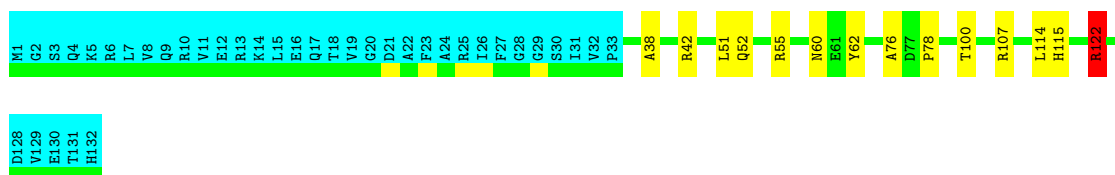
- Molecule 1: Putative uncharacterized protein TB39.8



4.2.11 Score per residue for model 11

- Molecule 1: Putative uncharacterized protein TB39.8

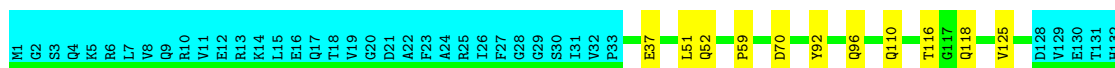




4.2.12 Score per residue for model 12

- Molecule 1: Putative uncharacterized protein TB39.8

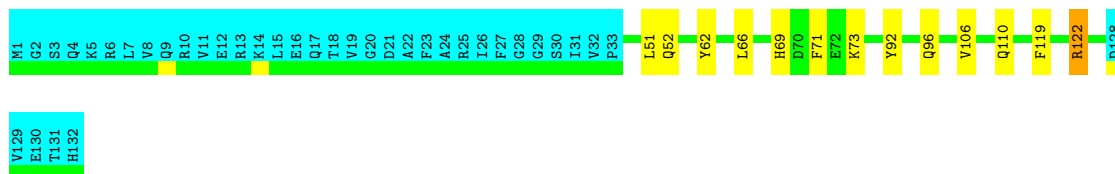
Chain A: 63% 8% 29%



4.2.13 Score per residue for model 13

- Molecule 1: Putative uncharacterized protein TB39.8

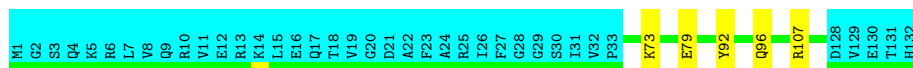
Chain A: 61% 9% 29%



4.2.14 Score per residue for model 14

- Molecule 1: Putative uncharacterized protein TB39.8

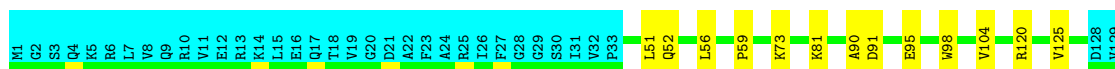
Chain A: 67% 1% 29%



4.2.15 Score per residue for model 15

- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 61% 10% 29%

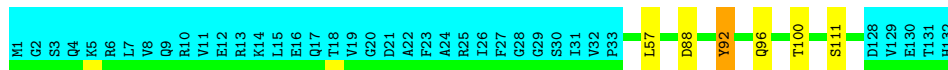




4.2.16 Score per residue for model 16

- Molecule 1: Putative uncharacterized protein TB39.8

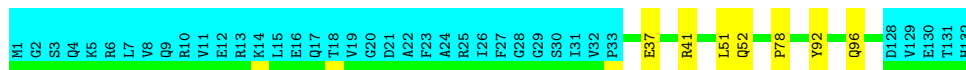
Chain A: 67% 29%



4.2.17 Score per residue for model 17

- Molecule 1: Putative uncharacterized protein TB39.8

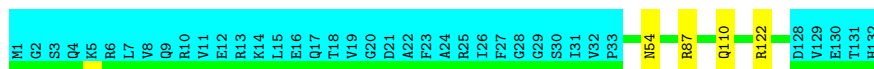
Chain A: 66% 5% 29%



4.2.18 Score per residue for model 18

- Molecule 1: Putative uncharacterized protein TB39.8

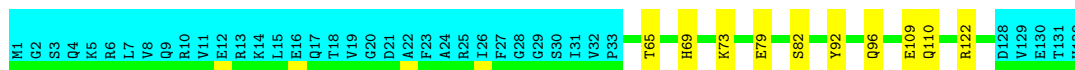
Chain A: 68% 29%



4.2.19 Score per residue for model 19

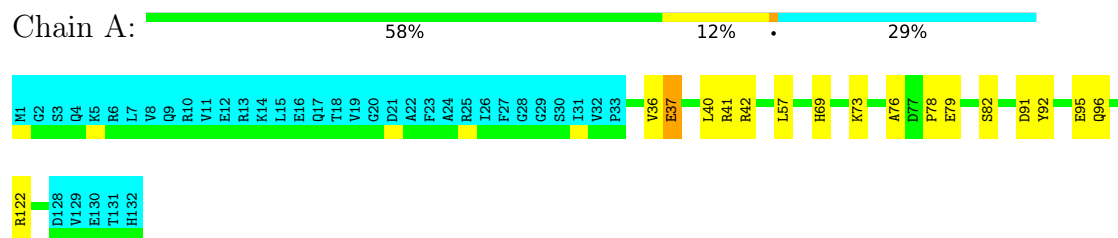
- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 64% 8% 29%



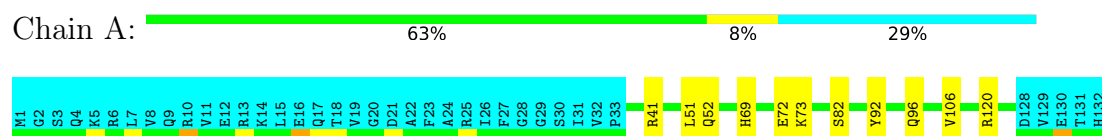
4.2.20 Score per residue for model 20

- Molecule 1: Putative uncharacterized protein TB39.8



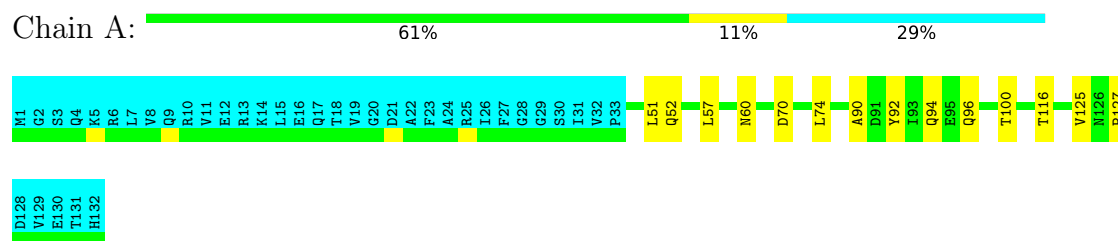
4.2.21 Score per residue for model 21

- Molecule 1: Putative uncharacterized protein TB39.8



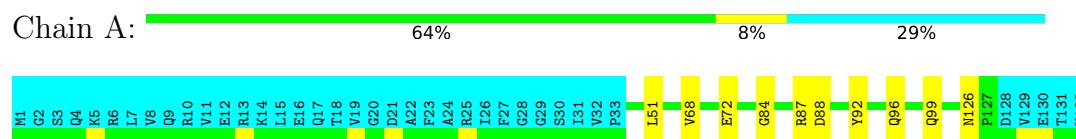
4.2.22 Score per residue for model 22

- Molecule 1: Putative uncharacterized protein TB39.8



4.2.23 Score per residue for model 23

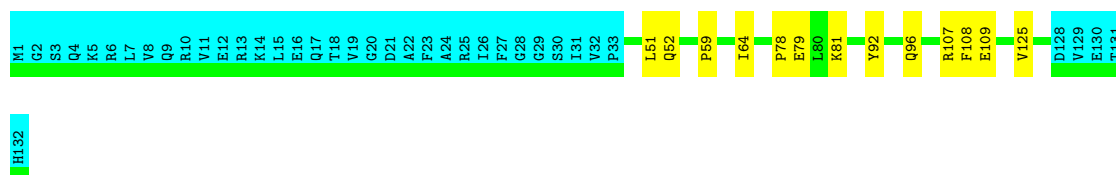
- Molecule 1: Putative uncharacterized protein TB39.8



4.2.24 Score per residue for model 24

- Molecule 1: Putative uncharacterized protein TB39.8

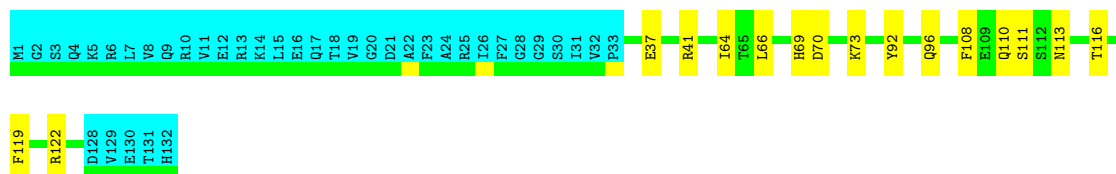




4.2.25 Score per residue for model 25

- Molecule 1: Putative uncharacterized protein TB39.8

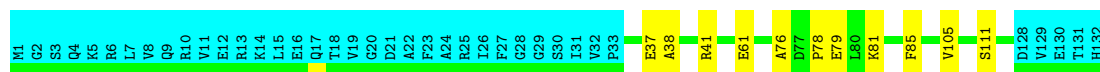
Chain A: 59% 12% 29%



4.2.26 Score per residue for model 26

- Molecule 1: Putative uncharacterized protein TB39.8

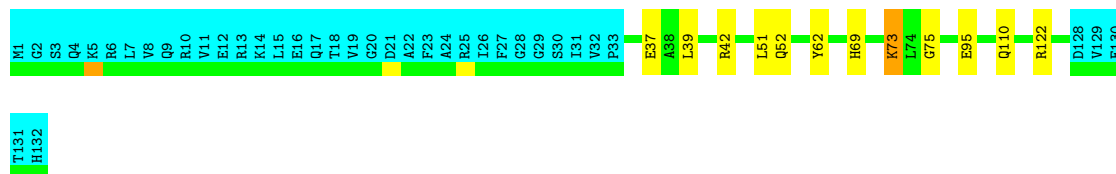
Chain A: 63% 8% 29%



4.2.27 Score per residue for model 27

- Molecule 1: Putative uncharacterized protein TB39.8

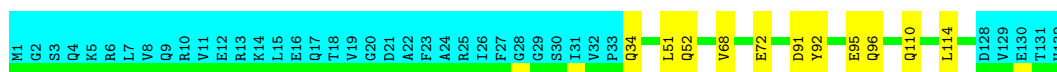
Chain A: 62% 8% 29%



4.2.28 Score per residue for model 28

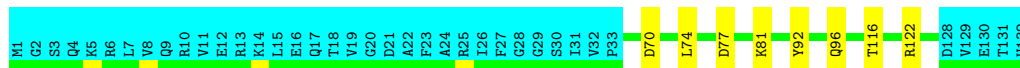
- Molecule 1: Putative uncharacterized protein TB39.8

Chain A: 63% 8% 29%



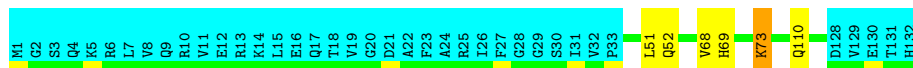
4.2.29 Score per residue for model 29

- Molecule 1: Putative uncharacterized protein TB39.8



4.2.30 Score per residue for model 30

- Molecule 1: Putative uncharacterized protein TB39.8



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

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	structure solution	2.1
CNS	refinement	1.2

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	1326
Number of shifts mapped to atoms	1326
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.05±0.04	1±1/757 (0.1± 0.1%)	0.92±0.03	0±1/1026 (0.0± 0.1%)
All	All	1.05	17/22710 (0.1%)	0.92	8/30780 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	122	ARG	C-N	-7.43	1.29	1.33	25	5
1	A	50	SER	C-N	-5.80	1.28	1.33	3	1
1	A	122	ARG	N-CA	-5.72	1.39	1.46	4	5
1	A	125	VAL	C-N	-5.39	1.28	1.33	4	1
1	A	106	VAL	N-CA	-5.32	1.40	1.46	8	1
1	A	120	ARG	C-N	-5.22	1.26	1.33	15	1
1	A	111	SER	N-CA	-5.11	1.40	1.46	16	2
1	A	110	GLN	C-N	-5.07	1.26	1.33	25	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	79	GLU	N-CA-C	5.22	117.38	111.11	24	2
1	A	75	GLY	N-CA-C	-5.20	105.05	114.46	27	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ASN	N-CA-C	-5.18	106.64	113.12	4	1
1	A	78	PRO	CA-C-N	5.16	128.56	120.82	2	2
1	A	78	PRO	C-N-CA	5.16	128.56	120.82	2	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	107	ARG	Sidechain	2
1	A	42	ARG	Sidechain	1
1	A	55	ARG	Sidechain	1

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	743	715	715	5±2
All	All	22290	21450	21450	147

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ASP:OD1	1:A:116:THR:HA	0.61	1.96	25	5
1:A:79:GLU:HA	1:A:82:SER:OG	0.59	1.97	20	3
1:A:84:GLY:O	1:A:87:ARG:HG2	0.56	2.00	23	1
1:A:81:LYS:HE3	1:A:85:PHE:CZ	0.56	2.35	26	1
1:A:37:GLU:O	1:A:41:ARG:HG3	0.56	2.01	8	5
1:A:37:GLU:O	1:A:41:ARG:HG2	0.52	2.04	4	3
1:A:92:TYR:O	1:A:96:GLN:HG2	0.52	2.05	19	23
1:A:69:HIS:O	1:A:73:LYS:HD3	0.51	2.05	6	2
1:A:76:ALA:O	1:A:78:PRO:HD3	0.51	2.05	20	2
1:A:70:ASP:OD2	1:A:116:THR:HA	0.51	2.05	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:SER:HB3	1:A:106:VAL:O	0.50	2.07	8	2
1:A:69:HIS:O	1:A:73:LYS:HG2	0.49	2.07	30	6
1:A:66:LEU:HD13	1:A:119:PHE:HB3	0.49	1.85	13	4
1:A:88:ASP:O	1:A:92:TYR:HB2	0.48	2.08	6	1
1:A:68:VAL:HA	1:A:110:GLN:HB2	0.48	1.85	30	1
1:A:62:TYR:HA	1:A:122:ARG:O	0.48	2.09	3	3
1:A:55:ARG:HG3	1:A:99:GLN:NE2	0.47	2.24	1	2
1:A:87:ARG:N	1:A:87:ARG:HD2	0.47	2.24	18	1
1:A:68:VAL:O	1:A:72:GLU:HG3	0.47	2.10	6	3
1:A:51:LEU:HD23	1:A:99:GLN:NE2	0.47	2.25	5	2
1:A:59:PRO:HA	1:A:125:VAL:HG22	0.46	1.86	12	4
1:A:70:ASP:O	1:A:74:LEU:HG	0.46	2.10	22	3
1:A:62:TYR:O	1:A:106:VAL:HA	0.46	2.10	13	1
1:A:59:PRO:HA	1:A:125:VAL:HB	0.46	1.88	4	1
1:A:51:LEU:HG	1:A:52:GLN:H	0.46	1.71	17	13
1:A:64:ILE:O	1:A:108:PHE:HA	0.46	2.10	24	2
1:A:70:ASP:HA	1:A:73:LYS:HE3	0.45	1.88	3	2
1:A:69:HIS:O	1:A:72:GLU:HG2	0.45	2.11	2	2
1:A:65:THR:HA	1:A:109:GLU:O	0.45	2.12	1	2
1:A:86:ALA:HB2	1:A:106:VAL:HG12	0.45	1.89	5	1
1:A:111:SER:HB3	1:A:113:ASN:OD1	0.45	2.11	25	1
1:A:70:ASP:HA	1:A:73:LYS:CE	0.45	2.42	3	2
1:A:66:LEU:O	1:A:110:GLN:HA	0.45	2.12	4	1
1:A:122:ARG:NE	1:A:122:ARG:HA	0.44	2.27	13	1
1:A:91:ASP:O	1:A:95:GLU:HG3	0.44	2.13	28	4
1:A:120:ARG:HA	1:A:120:ARG:NE	0.44	2.27	21	1
1:A:38:ALA:O	1:A:42:ARG:HG2	0.43	2.13	11	1
1:A:122:ARG:HE	1:A:122:ARG:HA	0.43	1.74	2	3
1:A:38:ALA:O	1:A:42:ARG:HG3	0.43	2.14	10	1
1:A:76:ALA:C	1:A:78:PRO:HD3	0.43	2.39	26	1
1:A:125:VAL:O	1:A:127:PRO:HD3	0.43	2.14	22	1
1:A:61:GLU:HA	1:A:105:VAL:O	0.42	2.14	26	1
1:A:71:PHE:CG	1:A:110:GLN:HB3	0.42	2.49	13	1
1:A:87:ARG:HD3	1:A:87:ARG:O	0.42	2.14	4	1
1:A:59:PRO:HB2	1:A:62:TYR:CZ	0.42	2.49	4	1
1:A:34:GLN:HA	1:A:37:GLU:CD	0.42	2.40	1	1
1:A:38:ALA:O	1:A:41:ARG:HG2	0.42	2.15	26	1
1:A:90:ALA:HB2	1:A:104:VAL:HG11	0.41	1.91	8	2
1:A:122:ARG:HD2	1:A:122:ARG:C	0.41	2.40	10	1
1:A:69:HIS:HB3	1:A:116:THR:OG1	0.41	2.16	2	1
1:A:60:ASN:HB3	1:A:100:THR:OG1	0.41	2.16	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ARG:HG3	1:A:88:ASP:N	0.41	2.31	23	1
1:A:70:ASP:CG	1:A:116:THR:HA	0.41	2.41	22	2
1:A:56:LEU:HB2	1:A:98:TRP:CD1	0.41	2.50	15	1
1:A:66:LEU:HG	1:A:119:PHE:CB	0.41	2.46	1	1
1:A:39:LEU:O	1:A:42:ARG:HB3	0.41	2.16	27	1
1:A:77:ASP:O	1:A:81:LYS:HG2	0.41	2.16	29	1
1:A:57:LEU:CD1	1:A:100:THR:HA	0.40	2.46	22	1
1:A:114:LEU:HD13	1:A:115:HIS:N	0.40	2.31	11	1
1:A:36:VAL:O	1:A:40:LEU:HG	0.40	2.16	20	1
1:A:57:LEU:HD22	1:A:100:THR:HA	0.40	1.92	16	1
1:A:37:GLU:HB3	1:A:85:PHE:CE1	0.40	2.51	26	1
1:A:91:ASP:O	1:A:95:GLU:HG2	0.40	2.16	15	1
1:A:90:ALA:O	1:A:94:GLN:HG2	0.40	2.16	22	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	94/132 (71%)	91±1 (97±1%)	3±1 (3±1%)	0±0 (0±0%)	49	83
All	All	2820/3960 (71%)	2741 (97%)	76 (3%)	3 (0%)	49	83

All 2 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	78	PRO	2
1	A	34	GLN	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	77/109 (71%)	75±2 (98±2%)	2±2 (2±2%)	43 89
All	All	2310/3270 (71%)	2255 (98%)	55 (2%)	43 89

All 23 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	73	LYS	7
1	A	122	ARG	6
1	A	37	GLU	6
1	A	110	GLN	5
1	A	107	ARG	4
1	A	42	ARG	3
1	A	79	GLU	3
1	A	87	ARG	2
1	A	114	LEU	2
1	A	57	LEU	2
1	A	34	GLN	2
1	A	81	LYS	2
1	A	120	ARG	1
1	A	70	ASP	1
1	A	39	LEU	1
1	A	35	GLU	1
1	A	118	GLN	1
1	A	88	ASP	1
1	A	92	TYR	1
1	A	54	ASN	1
1	A	41	ARG	1
1	A	109	GLU	1
1	A	95	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1326
Number of shifts mapped to atoms	1326
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	124	-0.13 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	102	-0.27 ± 0.04	None needed (< 0.5 ppm)
$^{13}\text{C}'$	116	-0.06 ± 0.10	None needed (< 0.5 ppm)
^{15}N	121	0.20 ± 0.19	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 78%, i.e. 996 atoms were assigned a chemical shift out of a possible 1279. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	460/473 (97%)	191/194 (98%)	181/188 (96%)	88/91 (97%)
Sidechain	498/713 (70%)	405/459 (88%)	77/219 (35%)	16/35 (46%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	38/93 (41%)	37/46 (80%)	0/44 (0%)	1/3 (33%)
Overall	996/1279 (78%)	633/699 (91%)	258/451 (57%)	105/129 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1325 atoms were assigned a chemical shift out of a possible 1811. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	621/665 (93%)	260/273 (95%)	240/264 (91%)	121/128 (95%)
Sidechain	658/1026 (64%)	538/661 (81%)	102/313 (33%)	18/52 (35%)
Aromatic	46/120 (38%)	45/60 (75%)	0/56 (0%)	1/4 (25%)
Overall	1325/1811 (73%)	843/994 (85%)	342/633 (54%)	140/184 (76%)

7.1.4 Statistically unusual chemical shifts [i](#)

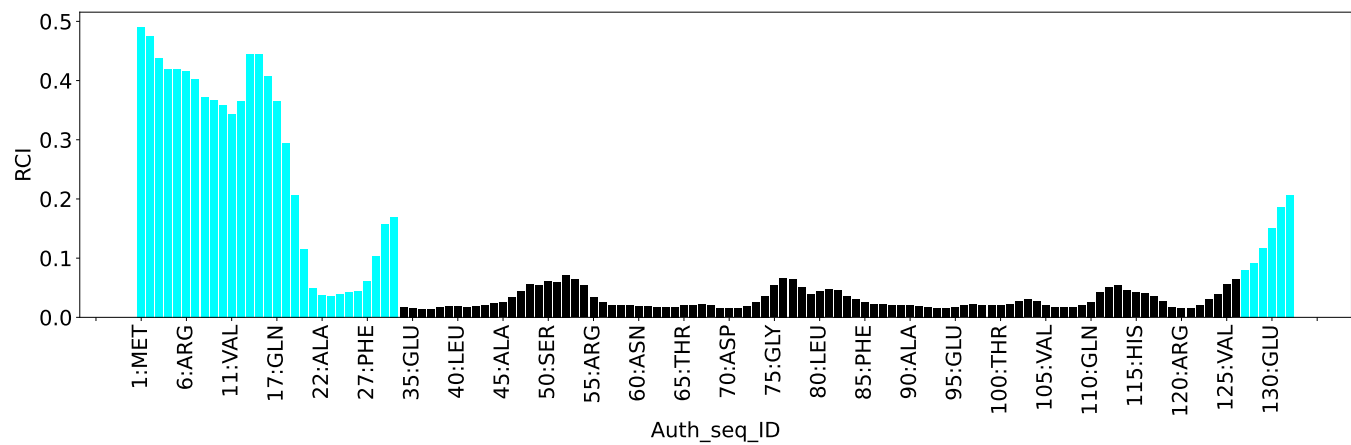
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	96	GLN	HB2	-0.11	0.80 – 3.29	-8.7
1	A	96	GLN	HG2	0.30	1.01 – 3.62	-7.7
1	A	96	GLN	HB3	0.43	0.71 – 3.33	-6.1

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	1589
Intra-residue ($ i-j =0$)	458
Sequential ($ i-j =1$)	483
Medium range ($ i-j >1$ and $ i-j <5$)	209
Long range ($ i-j \geq 5$)	347
Inter-chain	0
Hydrogen bond restraints	92
Disulfide bond restraints	0
Total dihedral-angle restraints	186
Number of unmapped restraints	0
Number of restraints per residue	13.4
Number of long range restraints per residue ¹	2.8

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)	2.8	0.2
0.2-0.5 (Medium)	0.4	0.29
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	4.8	5.93
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

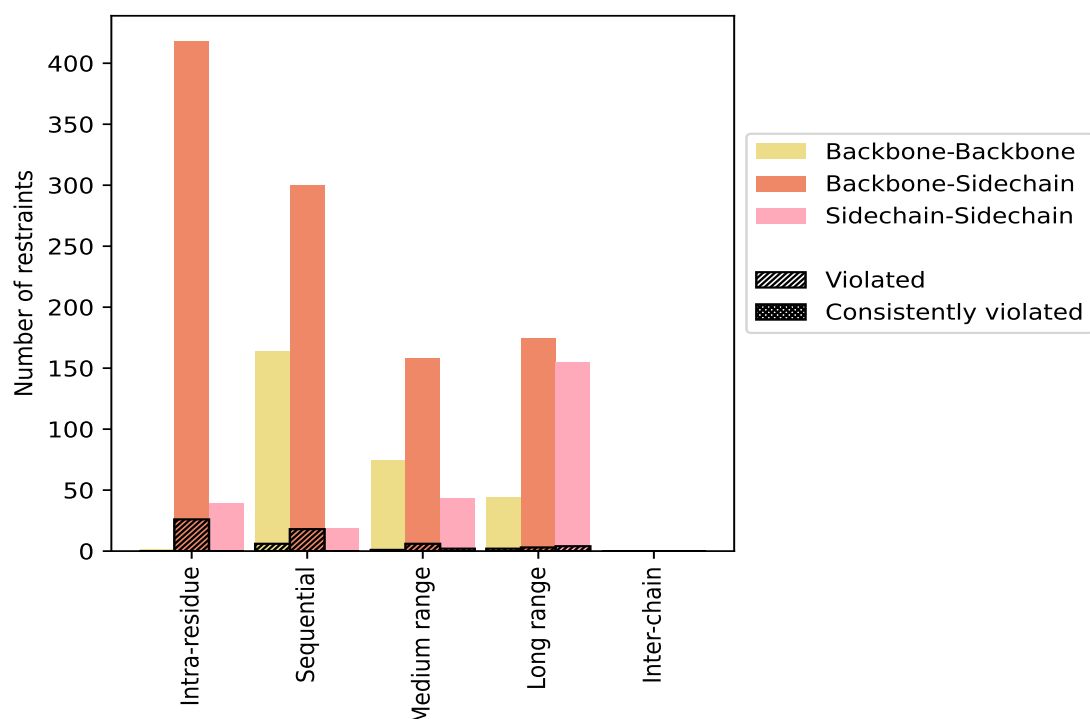
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	458	28.8	26	5.7	1.6	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	418	26.3	26	6.2	1.6	0	0.0	0.0
Sidechain-Sidechain	39	2.5	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	483	30.4	24	5.0	1.5	0	0.0	0.0
Backbone-Backbone	164	10.3	6	3.7	0.4	0	0.0	0.0
Backbone-Sidechain	300	18.9	18	6.0	1.1	0	0.0	0.0
Sidechain-Sidechain	19	1.2	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	209	13.2	9	4.3	0.6	0	0.0	0.0
Backbone-Backbone	74	4.7	1	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	92	5.8	6	6.5	0.4	0	0.0	0.0
Sidechain-Sidechain	43	2.7	2	4.7	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	347	21.8	9	2.6	0.6	0	0.0	0.0
Backbone-Backbone	44	2.8	2	4.5	0.1	0	0.0	0.0
Backbone-Sidechain	148	9.3	3	2.0	0.2	0	0.0	0.0
Sidechain-Sidechain	155	9.8	4	2.6	0.3	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	92	5.8	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1589	100.0	68	4.3	4.3	0	0.0	0.0
Backbone-Backbone	283	17.8	9	3.2	0.6	0	0.0	0.0
Backbone-Sidechain	1050	66.1	53	5.0	3.3	0	0.0	0.0
Sidechain-Sidechain	256	16.1	6	2.3	0.4	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	0	0	1	0	2	0.17	0.24	0.07	0.17
2	2	4	0	1	0	7	0.14	0.25	0.05	0.11
3	0	2	0	0	0	2	0.16	0.19	0.04	0.16
4	2	0	0	0	0	2	0.22	0.29	0.06	0.22
5	2	1	0	0	0	3	0.15	0.24	0.06	0.12
6	1	3	3	0	0	7	0.14	0.19	0.03	0.12
7	2	3	0	1	0	6	0.14	0.24	0.05	0.11
8	2	0	1	0	0	3	0.15	0.23	0.06	0.12
9	0	2	0	1	0	3	0.1	0.11	0.0	0.1
10	2	1	0	1	0	4	0.12	0.15	0.02	0.12

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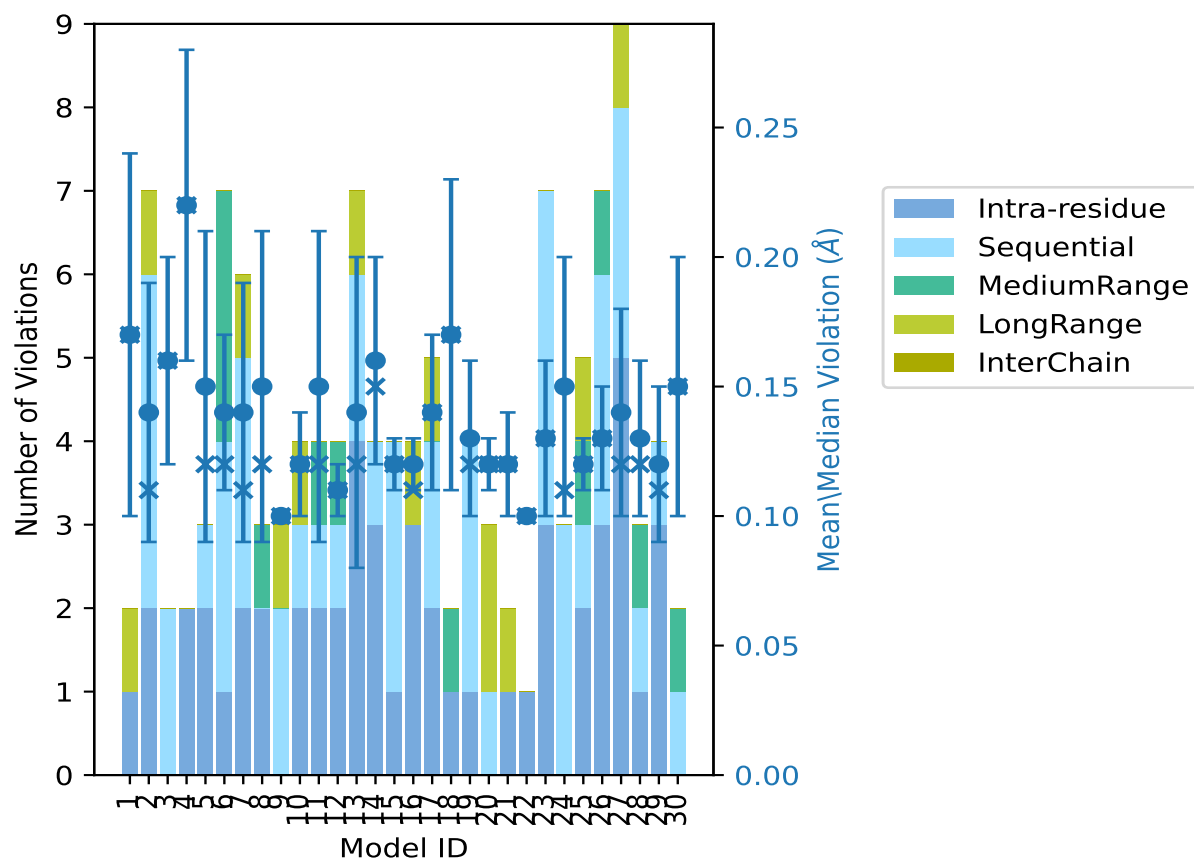
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	1	1	0	0	4	0.15	0.26	0.06	0.12
12	2	1	1	0	0	4	0.11	0.13	0.01	0.11
13	4	2	0	1	0	7	0.14	0.28	0.06	0.12
14	3	1	0	0	0	4	0.16	0.23	0.04	0.15
15	1	3	0	0	0	4	0.12	0.13	0.01	0.12
16	3	0	0	1	0	4	0.12	0.14	0.01	0.11
17	2	2	0	1	0	5	0.14	0.18	0.03	0.14
18	1	0	1	0	0	2	0.17	0.23	0.06	0.17
19	1	3	0	0	0	4	0.13	0.19	0.03	0.12
20	0	1	0	2	0	3	0.12	0.13	0.01	0.12
21	1	0	0	1	0	2	0.12	0.14	0.02	0.12
22	1	0	0	0	0	1	0.1	0.1	0.0	0.1
23	3	4	0	0	0	7	0.13	0.17	0.03	0.13
24	0	3	0	0	0	3	0.15	0.22	0.05	0.11
25	2	1	1	1	0	5	0.12	0.14	0.01	0.12
26	3	3	1	0	0	7	0.13	0.16	0.02	0.13
27	5	3	0	1	0	9	0.14	0.23	0.04	0.12
28	1	1	1	0	0	3	0.13	0.17	0.03	0.12
29	3	1	0	0	0	4	0.12	0.18	0.03	0.11
30	0	1	1	0	0	2	0.15	0.2	0.05	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, 1429(IR:432, SQ:459, MR:200, LR:338, 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	%
15	13	8	5	0	41	1	3.3
5	5	0	4	0	14	2	6.7
3	4	1	0	0	8	3	10.0
0	0	0	0	0	0	4	13.3
1	1	0	0	0	2	5	16.7
1	0	0	0	0	1	6	20.0

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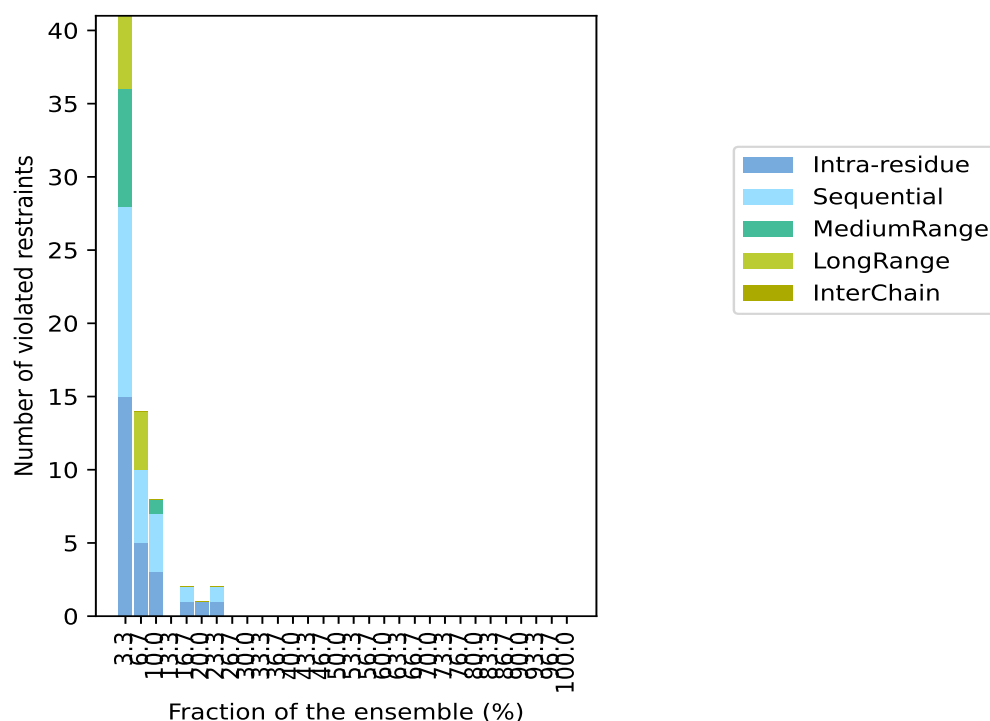
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	1	0	0	0	2	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	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	0	0	0	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
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	30	100.0

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

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

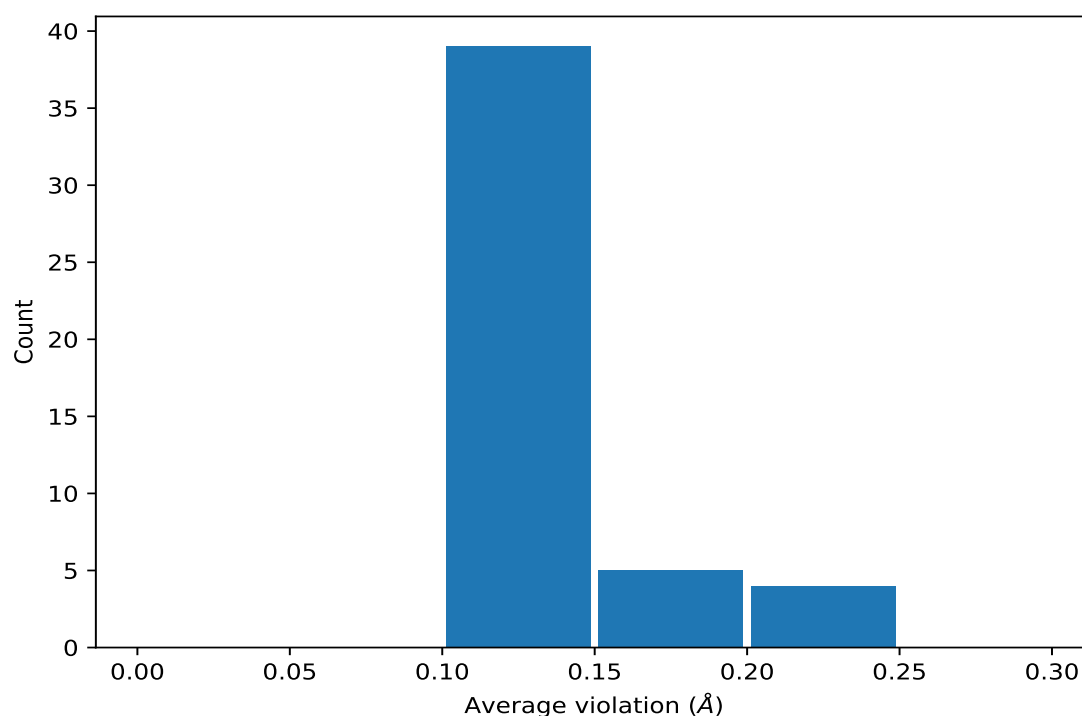
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	7	0.24	0.05	0.25
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	7	0.11	0.01	0.1
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG21	6	0.12	0.01	0.12
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG22	6	0.12	0.01	0.12
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG23	6	0.12	0.01	0.12
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.12	0.01	0.12
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG3	5	0.12	0.01	0.12
(2,393)	1:49:A:GLN:HG2	1:50:A:SER:H	5	0.11	0.02	0.1
(2,393)	1:49:A:GLN:HG3	1:50:A:SER:H	5	0.11	0.02	0.1
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG2	3	0.21	0.04	0.24
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG3	3	0.21	0.04	0.24
(2,82)	1:20:A:GLY:H	1:21:A:ASP:H	3	0.2	0.02	0.19
(2,70)	1:18:A:THR:H	1:18:A:THR:HG21	3	0.13	0.02	0.14
(2,70)	1:18:A:THR:H	1:18:A:THR:HG22	3	0.13	0.02	0.14
(2,70)	1:18:A:THR:H	1:18:A:THR:HG23	3	0.13	0.02	0.14
(2,765)	1:68:A:VAL:HB	1:71:A:PHE:H	3	0.13	0.01	0.13

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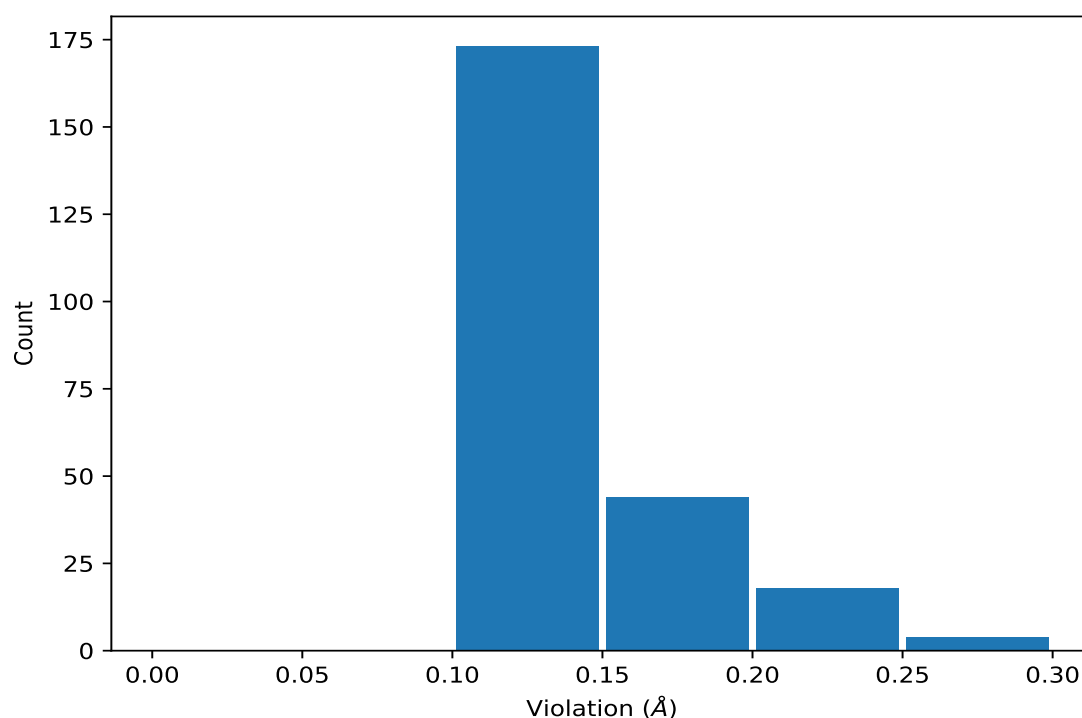
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,67)	1:18:A:THR:HB	1:19:A:VAL:H	3	0.13	0.01	0.13
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG2	3	0.12	0.02	0.13
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG3	3	0.12	0.02	0.13
(2,1494)	1:131:A:THR:HG21	1:132:A:HIS:H	3	0.12	0.0	0.12
(2,1494)	1:131:A:THR:HG22	1:132:A:HIS:H	3	0.12	0.0	0.12
(2,1494)	1:131:A:THR:HG23	1:132:A:HIS:H	3	0.12	0.0	0.12
(2,87)	1:21:A:ASP:H	1:22:A:ALA:H	3	0.11	0.01	0.11
(2,1132)	1:96:A:GLN:H	1:96:A:GLN:HG2	2	0.18	0.04	0.18
(2,910)	1:81:A:LYS:HA	1:81:A:LYS:HD2	2	0.18	0.0	0.18
(2,910)	1:81:A:LYS:HA	1:81:A:LYS:HD3	2	0.18	0.0	0.18
(2,1387)	1:120:A:ARG:HB2	1:121:A:ALA:H	2	0.17	0.05	0.17
(2,1387)	1:120:A:ARG:HB3	1:121:A:ALA:H	2	0.17	0.05	0.17
(2,969)	1:87:A:ARG:H	1:87:A:ARG:HD2	2	0.14	0.01	0.14
(2,385)	1:49:A:GLN:HE21	1:57:A:LEU:HB2	2	0.12	0.02	0.12
(2,385)	1:49:A:GLN:HE21	1:57:A:LEU:HB3	2	0.12	0.02	0.12
(2,385)	1:49:A:GLN:HE22	1:57:A:LEU:HB2	2	0.12	0.02	0.12
(2,385)	1:49:A:GLN:HE22	1:57:A:LEU:HB3	2	0.12	0.02	0.12
(2,1480)	1:129:A:VAL:H	1:130:A:GLU:H	2	0.12	0.02	0.12
(2,235)	1:41:A:ARG:HB2	1:92:A:TYR:HE1	2	0.12	0.01	0.12
(2,235)	1:41:A:ARG:HB2	1:92:A:TYR:HE2	2	0.12	0.01	0.12
(2,235)	1:41:A:ARG:HB3	1:92:A:TYR:HE1	2	0.12	0.01	0.12
(2,235)	1:41:A:ARG:HB3	1:92:A:TYR:HE2	2	0.12	0.01	0.12
(2,59)	1:17:A:GLN:HG3	1:18:A:THR:H	2	0.11	0.0	0.11
(2,1318)	1:113:A:ASN:H	1:113:A:ASN:HB3	2	0.11	0.01	0.11
(2,1482)	1:130:A:GLU:HB2	1:131:A:THR:H	2	0.11	0.0	0.11
(2,1482)	1:130:A:GLU:HB3	1:131:A:THR:H	2	0.11	0.0	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG21	2	0.11	0.0	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG22	2	0.11	0.0	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG23	2	0.11	0.0	0.11
(2,154)	1:28:A:GLY:H	1:29:A:GLY:H	2	0.11	0.0	0.11
(2,384)	1:49:A:GLN:HB2	1:57:A:LEU:H	2	0.11	0.0	0.11
(2,402)	1:49:A:GLN:H	1:56:A:LEU:HA	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	4	0.29
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	13	0.28
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	11	0.26
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	2	0.25
(2,1410)	1:122:A:ARG:H	1:122:A:ARG:HD2	1	0.24
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG2	5	0.24
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG3	5	0.24
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG2	7	0.24
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG3	7	0.24
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	8	0.23
(2,1132)	1:96:A:GLN:H	1:96:A:GLN:HG2	18	0.23
(2,241)	1:41:A:ARG:H	1:41:A:ARG:HG2	14	0.23
(2,241)	1:41:A:ARG:H	1:41:A:ARG:HG3	14	0.23
(2,82)	1:20:A:GLY:H	1:21:A:ASP:H	27	0.23
(2,1387)	1:120:A:ARG:HB2	1:121:A:ALA:H	24	0.22
(2,1387)	1:120:A:ARG:HB3	1:121:A:ALA:H	24	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1476)	1:129:A:VAL:HG11	1:131:A:THR:HB	30	0.2
(2,1476)	1:129:A:VAL:HG12	1:131:A:THR:HB	30	0.2
(2,1476)	1:129:A:VAL:HG13	1:131:A:THR:HB	30	0.2
(2,1476)	1:129:A:VAL:HG21	1:131:A:THR:HB	30	0.2
(2,1476)	1:129:A:VAL:HG22	1:131:A:THR:HB	30	0.2
(2,1476)	1:129:A:VAL:HG23	1:131:A:THR:HB	30	0.2
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	19	0.19
(2,1348)	1:115:A:HIS:H	1:118:A:GLN:HE22	6	0.19
(2,82)	1:20:A:GLY:H	1:21:A:ASP:H	3	0.19
(2,1365)	1:118:A:GLN:HG2	1:119:A:PHE:H	6	0.18
(2,1365)	1:118:A:GLN:HG3	1:119:A:PHE:H	6	0.18
(2,910)	1:81:A:LYS:HA	1:81:A:LYS:HD2	17	0.18
(2,910)	1:81:A:LYS:HA	1:81:A:LYS:HD3	17	0.18
(2,126)	1:25:A:ARG:H	1:25:A:ARG:HG2	29	0.18
(2,126)	1:25:A:ARG:H	1:25:A:ARG:HG3	29	0.18
(2,1291)	1:111:A:SER:HA	1:114:A:LEU:HB2	28	0.17
(2,1291)	1:111:A:SER:HA	1:114:A:LEU:HB3	28	0.17
(2,959)	1:87:A:ARG:HB2	1:88:A:ASP:H	23	0.17
(2,959)	1:87:A:ARG:HB3	1:88:A:ASP:H	23	0.17
(2,910)	1:81:A:LYS:HA	1:81:A:LYS:HD2	23	0.17
(2,910)	1:81:A:LYS:HA	1:81:A:LYS:HD3	23	0.17
(2,256)	1:42:A:ARG:H	1:42:A:ARG:HD3	14	0.17
(2,82)	1:20:A:GLY:H	1:21:A:ASP:H	2	0.17
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG2	17	0.16
(2,1106)	1:95:A:GLU:H	1:95:A:GLU:HG3	17	0.16
(2,1058)	1:93:A:ILE:HA	1:93:A:ILE:HG12	27	0.16
(2,841)	1:72:A:GLU:H	1:72:A:GLU:HG2	4	0.16
(2,841)	1:72:A:GLU:H	1:72:A:GLU:HG3	4	0.16
(2,180)	1:36:A:VAL:HG21	1:40:A:LEU:HD11	26	0.16
(2,180)	1:36:A:VAL:HG21	1:40:A:LEU:HD12	26	0.16
(2,180)	1:36:A:VAL:HG21	1:40:A:LEU:HD13	26	0.16
(2,180)	1:36:A:VAL:HG21	1:40:A:LEU:HD21	26	0.16
(2,180)	1:36:A:VAL:HG21	1:40:A:LEU:HD22	26	0.16
(2,180)	1:36:A:VAL:HG21	1:40:A:LEU:HD23	26	0.16
(2,180)	1:36:A:VAL:HG22	1:40:A:LEU:HD11	26	0.16
(2,180)	1:36:A:VAL:HG22	1:40:A:LEU:HD12	26	0.16
(2,180)	1:36:A:VAL:HG22	1:40:A:LEU:HD13	26	0.16
(2,180)	1:36:A:VAL:HG22	1:40:A:LEU:HD21	26	0.16
(2,180)	1:36:A:VAL:HG22	1:40:A:LEU:HD22	26	0.16
(2,180)	1:36:A:VAL:HG22	1:40:A:LEU:HD23	26	0.16
(2,180)	1:36:A:VAL:HG23	1:40:A:LEU:HD11	26	0.16
(2,180)	1:36:A:VAL:HG23	1:40:A:LEU:HD12	26	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:36:A:VAL:HG23	1:40:A:LEU:HD13	26	0.16
(2,180)	1:36:A:VAL:HG23	1:40:A:LEU:HD21	26	0.16
(2,180)	1:36:A:VAL:HG23	1:40:A:LEU:HD22	26	0.16
(2,180)	1:36:A:VAL:HG23	1:40:A:LEU:HD23	26	0.16
(2,70)	1:18:A:THR:H	1:18:A:THR:HG21	26	0.16
(2,70)	1:18:A:THR:H	1:18:A:THR:HG22	26	0.16
(2,70)	1:18:A:THR:H	1:18:A:THR:HG23	26	0.16
(2,1409)	1:122:A:ARG:H	1:122:A:ARG:HD3	10	0.15
(2,1480)	1:129:A:VAL:H	1:130:A:GLU:H	23	0.14
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG21	13	0.14
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG22	13	0.14
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG23	13	0.14
(2,1132)	1:96:A:GLN:H	1:96:A:GLN:HG2	27	0.14
(2,988)	1:89:A:LEU:HA	1:92:A:TYR:HE1	6	0.14
(2,988)	1:89:A:LEU:HA	1:92:A:TYR:HE2	6	0.14
(2,969)	1:87:A:ARG:H	1:87:A:ARG:HD2	2	0.14
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG2	13	0.14
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG3	13	0.14
(2,765)	1:68:A:VAL:HB	1:71:A:PHE:H	25	0.14
(2,475)	1:55:A:ARG:HG3	1:56:A:LEU:H	7	0.14
(2,393)	1:49:A:GLN:HG2	1:50:A:SER:H	17	0.14
(2,393)	1:49:A:GLN:HG3	1:50:A:SER:H	17	0.14
(2,385)	1:49:A:GLN:HE21	1:57:A:LEU:HB2	27	0.14
(2,385)	1:49:A:GLN:HE21	1:57:A:LEU:HB3	27	0.14
(2,385)	1:49:A:GLN:HE22	1:57:A:LEU:HB2	27	0.14
(2,385)	1:49:A:GLN:HE22	1:57:A:LEU:HB3	27	0.14
(2,70)	1:18:A:THR:H	1:18:A:THR:HG21	16	0.14
(2,70)	1:18:A:THR:H	1:18:A:THR:HG22	16	0.14
(2,70)	1:18:A:THR:H	1:18:A:THR:HG23	16	0.14
(2,67)	1:18:A:THR:HB	1:19:A:VAL:H	26	0.14
(2,29)	1:10:A:ARG:HA	1:10:A:ARG:HG2	21	0.14
(2,29)	1:10:A:ARG:HA	1:10:A:ARG:HG3	21	0.14
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG21	14	0.13
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG22	14	0.13
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG23	14	0.13
(2,969)	1:87:A:ARG:H	1:87:A:ARG:HD2	15	0.13
(2,949)	1:86:A:ALA:HB1	1:106:A:VAL:HG21	20	0.13
(2,949)	1:86:A:ALA:HB1	1:106:A:VAL:HG22	20	0.13
(2,949)	1:86:A:ALA:HB1	1:106:A:VAL:HG23	20	0.13
(2,949)	1:86:A:ALA:HB2	1:106:A:VAL:HG21	20	0.13
(2,949)	1:86:A:ALA:HB2	1:106:A:VAL:HG22	20	0.13
(2,949)	1:86:A:ALA:HB2	1:106:A:VAL:HG23	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,949)	1:86:A:ALA:HB3	1:106:A:VAL:HG21	20	0.13
(2,949)	1:86:A:ALA:HB3	1:106:A:VAL:HG22	20	0.13
(2,949)	1:86:A:ALA:HB3	1:106:A:VAL:HG23	20	0.13
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG2	26	0.13
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG3	26	0.13
(2,765)	1:68:A:VAL:HB	1:71:A:PHE:H	11	0.13
(2,235)	1:41:A:ARG:HB2	1:92:A:TYR:HE1	25	0.13
(2,235)	1:41:A:ARG:HB2	1:92:A:TYR:HE2	25	0.13
(2,235)	1:41:A:ARG:HB3	1:92:A:TYR:HE1	25	0.13
(2,235)	1:41:A:ARG:HB3	1:92:A:TYR:HE2	25	0.13
(2,67)	1:18:A:THR:HB	1:19:A:VAL:H	14	0.13
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	12	0.13
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG3	12	0.13
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	23	0.13
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG3	23	0.13
(2,1494)	1:131:A:THR:HG21	1:132:A:HIS:H	15	0.12
(2,1494)	1:131:A:THR:HG22	1:132:A:HIS:H	15	0.12
(2,1494)	1:131:A:THR:HG23	1:132:A:HIS:H	15	0.12
(2,1494)	1:131:A:THR:HG21	1:132:A:HIS:H	20	0.12
(2,1494)	1:131:A:THR:HG22	1:132:A:HIS:H	20	0.12
(2,1494)	1:131:A:THR:HG23	1:132:A:HIS:H	20	0.12
(2,1485)	1:130:A:GLU:HG2	1:131:A:THR:H	5	0.12
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG21	25	0.12
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG22	25	0.12
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG23	25	0.12
(2,1404)	1:122:A:ARG:HD3	1:123:A:GLY:H	28	0.12
(2,1387)	1:120:A:ARG:HB2	1:121:A:ALA:H	15	0.12
(2,1387)	1:120:A:ARG:HB3	1:121:A:ALA:H	15	0.12
(2,1318)	1:113:A:ASN:H	1:113:A:ASN:HB3	13	0.12
(2,1027)	1:91:A:ASP:H	1:92:A:TYR:HD1	6	0.12
(2,1027)	1:91:A:ASP:H	1:92:A:TYR:HD2	6	0.12
(2,765)	1:68:A:VAL:HB	1:71:A:PHE:H	6	0.12
(2,128)	1:25:A:ARG:H	1:25:A:ARG:HG2	29	0.12
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	3	0.12
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	27	0.12
(2,87)	1:21:A:ASP:H	1:22:A:ALA:H	19	0.12
(2,86)	1:21:A:ASP:H	1:21:A:ASP:HB2	27	0.12
(2,86)	1:21:A:ASP:H	1:21:A:ASP:HB3	27	0.12
(2,54)	1:17:A:GLN:HA	1:18:A:THR:H	19	0.12
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.12
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG3	8	0.12
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG3	10	0.12
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG21	16	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG22	16	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG23	16	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG21	26	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG22	26	0.11
(2,1496)	1:131:A:THR:H	1:131:A:THR:HG23	26	0.11
(2,1494)	1:131:A:THR:HG21	1:132:A:HIS:H	24	0.11
(2,1494)	1:131:A:THR:HG22	1:132:A:HIS:H	24	0.11
(2,1494)	1:131:A:THR:HG23	1:132:A:HIS:H	24	0.11
(2,1482)	1:130:A:GLU:HB2	1:131:A:THR:H	7	0.11
(2,1482)	1:130:A:GLU:HB3	1:131:A:THR:H	7	0.11
(2,1482)	1:130:A:GLU:HB2	1:131:A:THR:H	12	0.11
(2,1482)	1:130:A:GLU:HB3	1:131:A:THR:H	12	0.11
(2,1468)	1:128:A:ASP:H	1:129:A:VAL:HG11	6	0.11
(2,1468)	1:128:A:ASP:H	1:129:A:VAL:HG12	6	0.11
(2,1468)	1:128:A:ASP:H	1:129:A:VAL:HG13	6	0.11
(2,1468)	1:128:A:ASP:H	1:129:A:VAL:HG21	6	0.11
(2,1468)	1:128:A:ASP:H	1:129:A:VAL:HG22	6	0.11
(2,1468)	1:128:A:ASP:H	1:129:A:VAL:HG23	6	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG21	7	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG22	7	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG23	7	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG21	12	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG22	12	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG23	12	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG21	27	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG22	27	0.11
(2,1420)	1:124:A:THR:H	1:124:A:THR:HG23	27	0.11
(2,1340)	1:115:A:HIS:H	1:115:A:HIS:HB3	28	0.11
(2,1338)	1:115:A:HIS:HB3	1:116:A:THR:H	23	0.11
(2,1234)	1:107:A:ARG:HA	1:107:A:ARG:HD3	11	0.11
(2,1228)	1:106:A:VAL:H	1:106:A:VAL:HB	6	0.11
(2,1083)	1:94:A:GLN:HB3	1:96:A:GLN:H	18	0.11
(2,751)	1:66:A:LEU:HG	1:119:A:PHE:HB2	13	0.11
(2,589)	1:61:A:GLU:HG2	1:124:A:THR:H	10	0.11
(2,589)	1:61:A:GLU:HG3	1:124:A:THR:H	10	0.11
(2,402)	1:49:A:GLN:H	1:56:A:LEU:HA	7	0.11
(2,393)	1:49:A:GLN:HG2	1:50:A:SER:H	7	0.11
(2,393)	1:49:A:GLN:HG3	1:50:A:SER:H	7	0.11
(2,384)	1:49:A:GLN:HB2	1:57:A:LEU:H	9	0.11
(2,287)	1:43:A:GLU:H	1:89:A:LEU:HD11	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,287)	1:43:A:GLU:H	1:89:A:LEU:HD12	16	0.11
(2,287)	1:43:A:GLU:H	1:89:A:LEU:HD13	16	0.11
(2,287)	1:43:A:GLU:H	1:89:A:LEU:HD21	16	0.11
(2,287)	1:43:A:GLU:H	1:89:A:LEU:HD22	16	0.11
(2,287)	1:43:A:GLU:H	1:89:A:LEU:HD23	16	0.11
(2,235)	1:41:A:ARG:HB2	1:92:A:TYR:HE1	20	0.11
(2,235)	1:41:A:ARG:HB2	1:92:A:TYR:HE2	20	0.11
(2,235)	1:41:A:ARG:HB3	1:92:A:TYR:HE1	20	0.11
(2,235)	1:41:A:ARG:HB3	1:92:A:TYR:HE2	20	0.11
(2,154)	1:28:A:GLY:H	1:29:A:GLY:H	24	0.11
(2,87)	1:21:A:ASP:H	1:22:A:ALA:H	26	0.11
(2,67)	1:18:A:THR:HB	1:19:A:VAL:H	2	0.11
(2,59)	1:17:A:GLN:HG3	1:18:A:THR:H	15	0.11
(2,59)	1:17:A:GLN:HG3	1:18:A:THR:H	26	0.11
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	16	0.11
(2,6)	1:6:A:ARG:HA	1:6:A:ARG:HG3	16	0.11
(2,5)	1:5:A:LYS:H	1:5:A:LYS:HD2	25	0.11
(2,5)	1:5:A:LYS:H	1:5:A:LYS:HD3	25	0.11
(2,1480)	1:129:A:VAL:H	1:130:A:GLU:H	25	0.1
(2,1376)	1:119:A:PHE:HB2	1:120:A:ARG:HA	13	0.1
(2,1344)	1:115:A:HIS:H	1:118:A:GLN:HB3	8	0.1
(2,1318)	1:113:A:ASN:H	1:113:A:ASN:HB3	29	0.1
(2,1303)	1:111:A:SER:H	1:111:A:SER:HB3	23	0.1
(2,1281)	1:110:A:GLN:HG2	1:111:A:SER:H	27	0.1
(2,1281)	1:110:A:GLN:HG3	1:111:A:SER:H	27	0.1
(2,1130)	1:96:A:GLN:H	1:96:A:GLN:HG2	27	0.1
(2,1130)	1:96:A:GLN:H	1:96:A:GLN:HG3	27	0.1
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG2	5	0.1
(2,916)	1:81:A:LYS:H	1:81:A:LYS:HG3	5	0.1
(2,833)	1:72:A:GLU:HB3	1:73:A:LYS:H	13	0.1
(2,447)	1:52:A:GLN:HA	1:54:A:ASN:H	12	0.1
(2,406)	1:50:A:SER:HA	1:56:A:LEU:HA	2	0.1
(2,402)	1:49:A:GLN:H	1:56:A:LEU:HA	1	0.1
(2,393)	1:49:A:GLN:HG2	1:50:A:SER:H	11	0.1
(2,393)	1:49:A:GLN:HG3	1:50:A:SER:H	11	0.1
(2,393)	1:49:A:GLN:HG2	1:50:A:SER:H	23	0.1
(2,393)	1:49:A:GLN:HG3	1:50:A:SER:H	23	0.1
(2,393)	1:49:A:GLN:HG2	1:50:A:SER:H	30	0.1
(2,393)	1:49:A:GLN:HG3	1:50:A:SER:H	30	0.1
(2,385)	1:49:A:GLN:HE21	1:57:A:LEU:HB2	17	0.1
(2,385)	1:49:A:GLN:HE21	1:57:A:LEU:HB3	17	0.1
(2,385)	1:49:A:GLN:HE22	1:57:A:LEU:HB2	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,385)	1:49:A:GLN:HE22	1:57:A:LEU:HB3	17	0.1
(2,384)	1:49:A:GLN:HB2	1:57:A:LEU:H	21	0.1
(2,154)	1:28:A:GLY:H	1:29:A:GLY:H	2	0.1
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	2	0.1
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	9	0.1
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	10	0.1
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	19	0.1
(2,88)	1:22:A:ALA:HA	1:23:A:PHE:HB2	29	0.1
(2,87)	1:21:A:ASP:H	1:22:A:ALA:H	17	0.1
(2,83)	1:21:A:ASP:HA	1:22:A:ALA:H	9	0.1
(2,70)	1:18:A:THR:H	1:18:A:THR:HG21	22	0.1
(2,70)	1:18:A:THR:H	1:18:A:THR:HG22	22	0.1
(2,70)	1:18:A:THR:H	1:18:A:THR:HG23	22	0.1

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

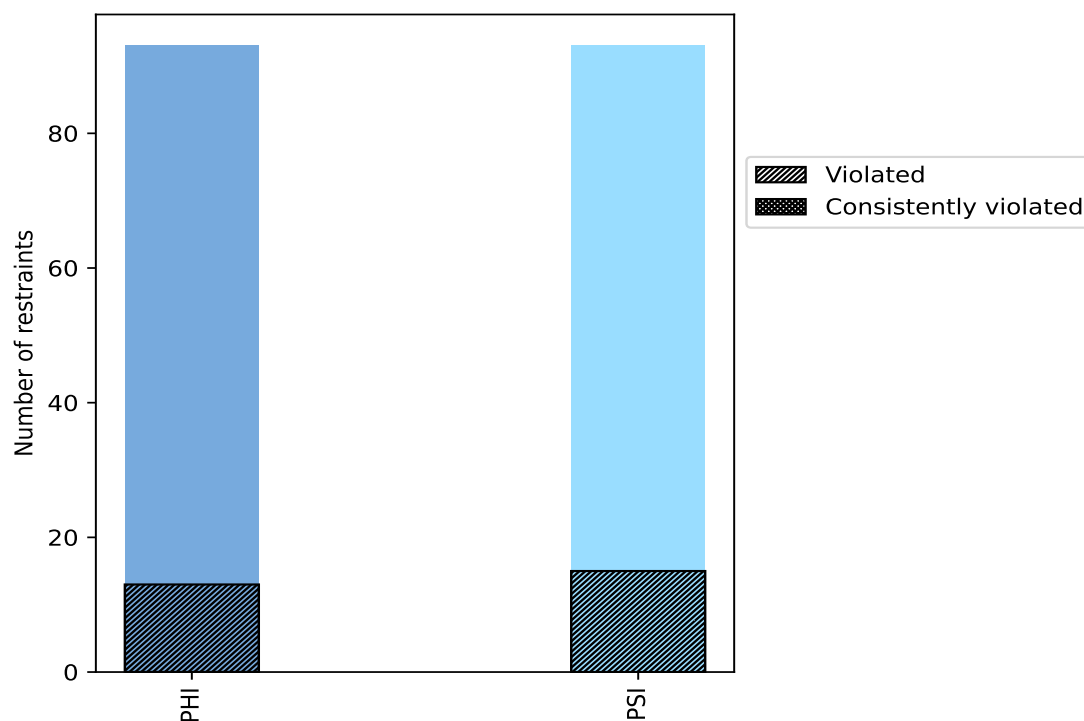
10.1 Summary of dihedral-angle violations [i](#)

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	93	50.0	13	14.0	7.0	0	0.0	0.0
PSI	93	50.0	15	16.1	8.1	0	0.0	0.0
Total	186	100.0	28	15.1	15.1	0	0.0	0.0

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

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



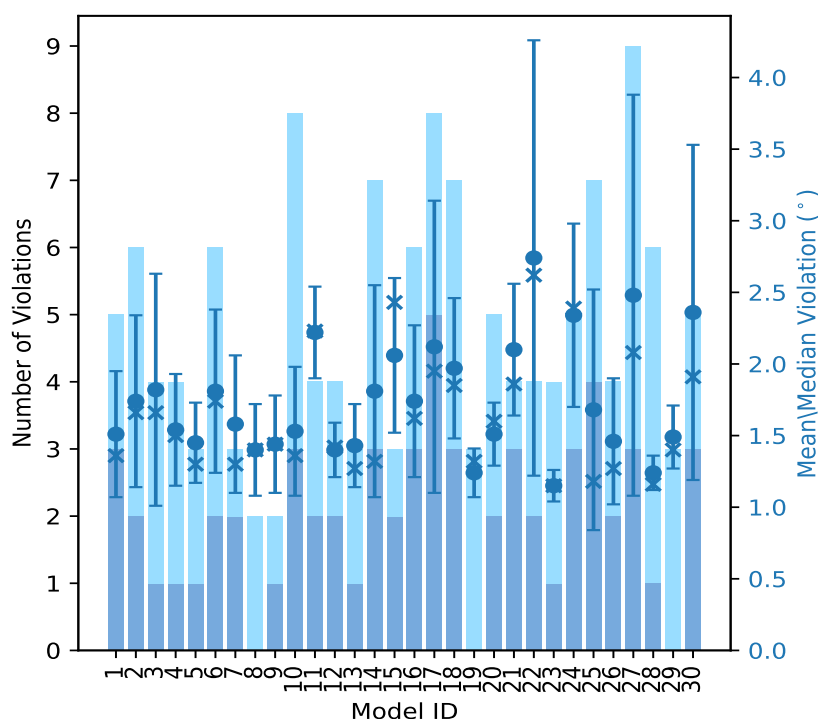
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	3	2	5	1.51	2.19	0.44	1.36
2	2	4	6	1.74	2.92	0.6	1.66
3	1	3	4	1.82	2.94	0.81	1.66
4	1	3	4	1.54	2.03	0.39	1.5
5	1	2	3	1.45	1.84	0.28	1.3
6	2	4	6	1.81	2.67	0.57	1.74
7	2	1	3	1.58	2.26	0.48	1.3
8	0	2	2	1.4	1.73	0.32	1.4
9	1	1	2	1.44	1.78	0.34	1.44
10	3	5	8	1.53	2.2	0.45	1.36
11	2	2	4	2.22	2.66	0.32	2.23
12	2	2	4	1.4	1.6	0.19	1.42
13	1	2	3	1.43	1.84	0.29	1.27
14	3	4	7	1.81	3.27	0.74	1.32
15	2	1	3	2.06	2.44	0.54	2.43
16	3	3	6	1.74	2.68	0.53	1.62
17	5	3	8	2.12	3.72	1.02	1.95
18	3	4	7	1.97	2.71	0.49	1.85
19	0	3	3	1.24	1.39	0.17	1.32
20	2	3	5	1.51	1.67	0.22	1.6
21	3	1	4	2.1	2.9	0.46	1.86
22	2	2	4	2.74	4.54	1.52	2.62
23	1	3	4	1.15	1.26	0.11	1.15
24	3	2	5	2.34	3.11	0.64	2.39
25	4	3	7	1.68	3.54	0.84	1.18
26	2	2	4	1.46	2.19	0.44	1.27
27	3	6	9	2.48	5.93	1.4	2.08
28	1	5	6	1.24	1.45	0.12	1.16
29	0	3	3	1.49	1.79	0.22	1.4
30	3	2	5	2.36	3.82	1.17	1.91

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
8	5	13	1	3.3
1	2	3	2	6.7
1	3	4	3	10.0
0	1	1	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	1	1	9	30.0
1	0	1	10	33.3
0	0	0	11	36.7

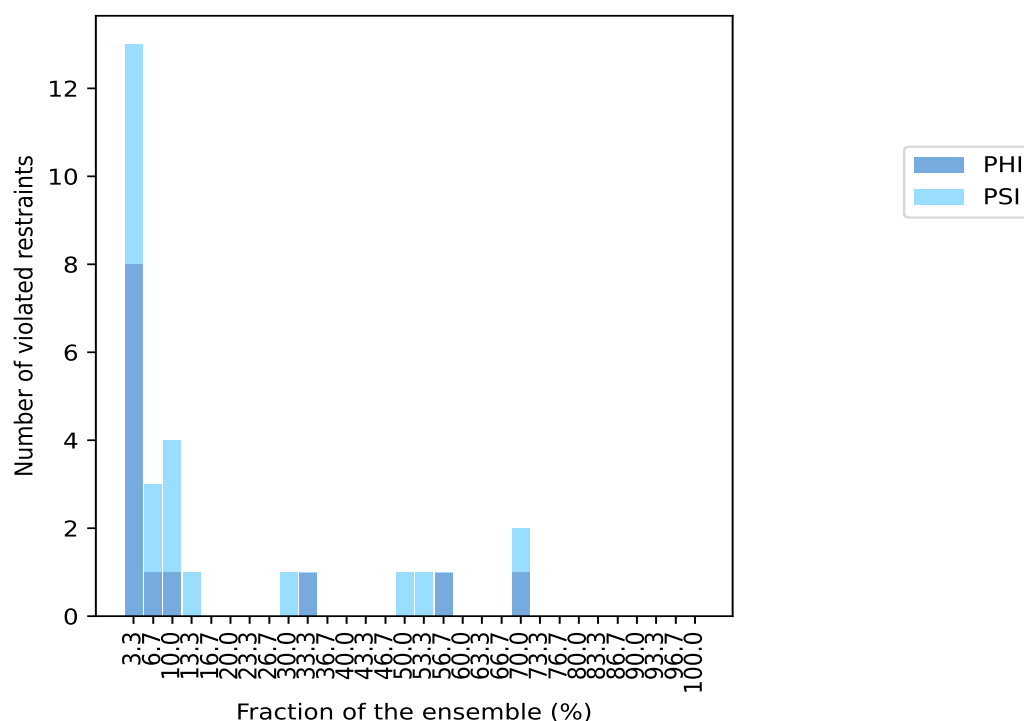
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	40.0
0	0	0	13	43.3
0	0	0	14	46.7
0	1	1	15	50.0
0	1	1	16	53.3
1	0	1	17	56.7
0	0	0	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
1	1	2	21	70.0
0	0	0	22	73.3
0	0	0	23	76.7
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	0	0	30	100.0

¹ Number of models with violations

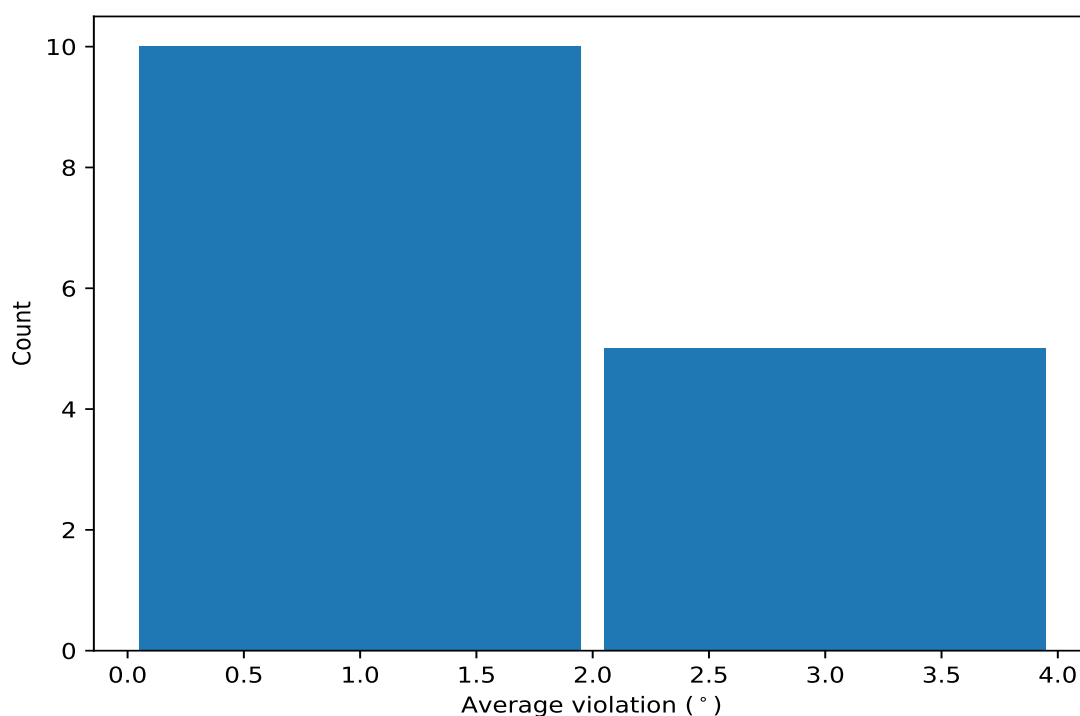
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

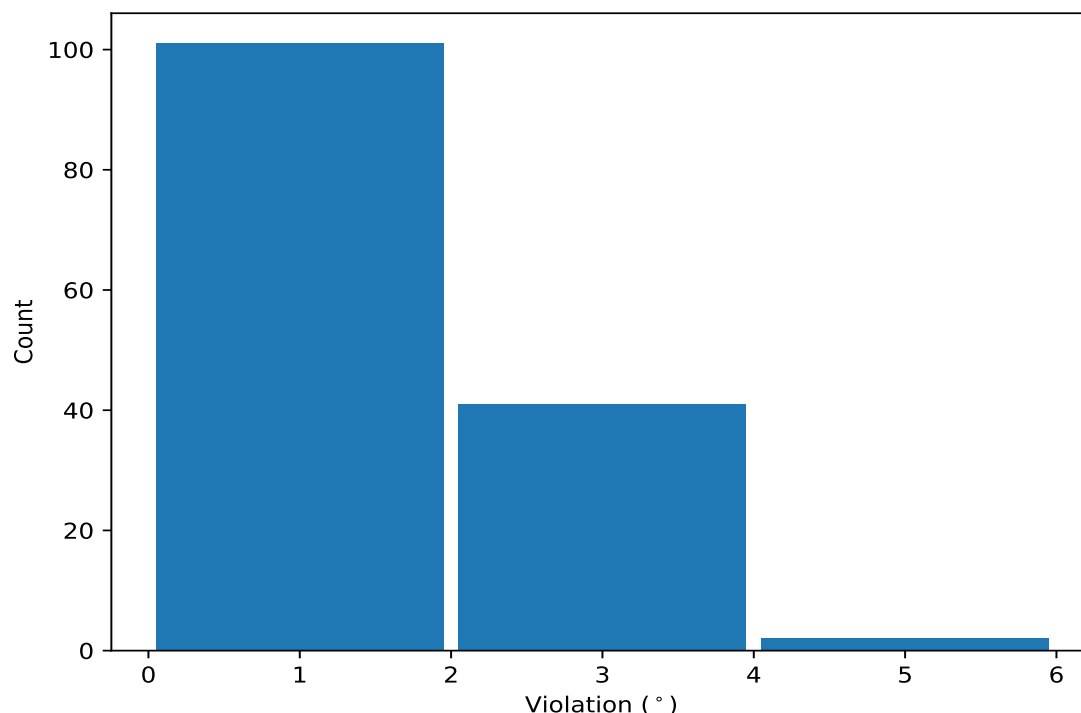
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	21	1.54	0.27	1.51
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	21	1.3	0.26	1.19
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	17	2.2	0.81	2.13
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	16	1.68	0.61	1.52
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	15	2.03	0.82	2.19
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	10	2.38	0.71	2.7
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	9	1.73	0.32	1.76
(1,14)	1:32:A:VAL:N	1:32:A:VAL:CA	1:32:A:VAL:C	1:33:A:PRO:N	4	1.9	0.99	1.52
(1,86)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASP:N	3	3.93	1.93	4.54
(1,157)	1:111:A:SER:C	1:112:A:SER:N	1:112:A:SER:CA	1:112:A:SER:C	3	1.7	0.55	1.58
(1,164)	1:115:A:HIS:N	1:115:A:HIS:CA	1:115:A:HIS:C	1:116:A:THR:N	3	1.56	0.21	1.67
(1,138)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ASP:N	3	1.12	0.13	1.07
(1,87)	1:76:A:ALA:C	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	2	3.75	0.2	3.75
(1,174)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ARG:N	2	1.54	0.14	1.54
(1,92)	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	1:80:A:LEU:N	2	1.32	0.28	1.32

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 (°)
(1,86)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASP:N	27	5.93
(1,86)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASP:N	22	4.54
(1,87)	1:76:A:ALA:C	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	22	3.95
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	30	3.82
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	17	3.72
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	30	3.68
(1,87)	1:76:A:ALA:C	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	27	3.55
(1,14)	1:32:A:VAL:N	1:32:A:VAL:CA	1:32:A:VAL:C	1:33:A:PRO:N	25	3.54
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	17	3.29
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	14	3.27
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	24	3.11
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	3	2.94
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	2	2.92
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	21	2.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	17	2.74
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	18	2.71
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	18	2.68
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	16	2.68
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	6	2.67
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	11	2.66
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	24	2.66
(1,91)	1:78:A:PRO:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	17	2.54
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	27	2.53
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	15	2.44
(1,157)	1:111:A:SER:C	1:112:A:SER:N	1:112:A:SER:CA	1:112:A:SER:C	15	2.43
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	27	2.4
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	24	2.39
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	6	2.38
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	24	2.37
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	14	2.36
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	11	2.27
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	3	2.26
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	7	2.26
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	10	2.2
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	26	2.19
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	1	2.19
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	11	2.19
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	25	2.17
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	10	2.13
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	14	2.12
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	16	2.08
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	27	2.08
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	4	2.03
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	30	1.91
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	10	1.91
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	21	1.89
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	18	1.88
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	2	1.87
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	16	1.86
(1,93)	1:79:A:GLU:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	18	1.85
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	5	1.84
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	13	1.84
(1,75)	1:69:A:HIS:C	1:70:A:ASP:N	1:70:A:ASP:CA	1:70:A:ASP:C	21	1.83
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	1	1.82
(1,14)	1:32:A:VAL:N	1:32:A:VAL:CA	1:32:A:VAL:C	1:33:A:PRO:N	4	1.82
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	29	1.79
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	9	1.78
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	21	1.78
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	11	1.76
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	6	1.76
(1,164)	1:115:A:HIS:N	1:115:A:HIS:CA	1:115:A:HIS:C	1:116:A:THR:N	18	1.74
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	2	1.73
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	8	1.73
(1,169)	1:118:A:GLN:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	6	1.71
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	27	1.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,174)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ARG:N	20	1.67
(1,164)	1:115:A:HIS:N	1:115:A:HIS:CA	1:115:A:HIS:C	1:116:A:THR:N	27	1.67
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	20	1.64
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	12	1.6
(1,92)	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	1:80:A:LEU:N	2	1.6
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	20	1.6
(1,157)	1:111:A:SER:C	1:112:A:SER:N	1:112:A:SER:CA	1:112:A:SER:C	12	1.58
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	20	1.57
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	25	1.53
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	18	1.51
(1,90)	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	1:79:A:GLU:N	27	1.47
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	10	1.45
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	28	1.45
(1,128)	1:97:A:GLY:N	1:97:A:GLY:CA	1:97:A:GLY:C	1:98:A:TRP:N	18	1.41
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	26	1.41
(1,174)	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	1:122:A:ARG:N	29	1.4
(1,154)	1:110:A:GLN:N	1:110:A:GLN:CA	1:110:A:GLN:C	1:111:A:SER:N	19	1.39
(1,45)	1:51:A:LEU:C	1:52:A:GLN:N	1:52:A:GLN:CA	1:52:A:GLN:C	16	1.39
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1	1.36
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	17	1.36
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	28	1.34
(1,86)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASP:N	2	1.33
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	19	1.32
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	14	1.32
(1,138)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ASP:N	5	1.3
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	7	1.3
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	15	1.3
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	14	1.29
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	30	1.29
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	29	1.28
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	22	1.28
(1,164)	1:115:A:HIS:N	1:115:A:HIS:CA	1:115:A:HIS:C	1:116:A:THR:N	13	1.27
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	10	1.27
(1,12)	1:27:A:PHE:N	1:27:A:PHE:CA	1:27:A:PHE:C	1:28:A:GLY:N	14	1.27
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	23	1.26
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	12	1.26
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	23	1.25
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	5	1.22
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	16	1.21
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	16	1.21
(1,14)	1:32:A:VAL:N	1:32:A:VAL:CA	1:32:A:VAL:C	1:33:A:PRO:N	6	1.21
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	4	1.19
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	13	1.19
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	24	1.19
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	22	1.19
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	7	1.18
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	25	1.18
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	10	1.18
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	28	1.17
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	12	1.16
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	25	1.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	28	1.16
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	28	1.16
(1,51)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1	1.14
(1,156)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:SER:N	28	1.13
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	26	1.13
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	17	1.12
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	4	1.12
(1,151)	1:108:A:PHE:C	1:109:A:GLU:N	1:109:A:GLU:CA	1:109:A:GLU:C	9	1.11
(1,85)	1:75:A:GLY:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	25	1.11
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	6	1.11
(1,157)	1:111:A:SER:C	1:112:A:SER:N	1:112:A:SER:CA	1:112:A:SER:C	30	1.1
(1,137)	1:101:A:TYR:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	26	1.1
(1,47)	1:53:A:GLY:C	1:54:A:ASN:N	1:54:A:ASN:CA	1:54:A:ASN:C	17	1.1
(1,89)	1:77:A:ASP:C	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	25	1.09
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	8	1.08
(1,138)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ASP:N	14	1.07
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	20	1.07
(1,126)	1:96:A:GLN:N	1:96:A:GLN:CA	1:96:A:GLN:C	1:97:A:GLY:N	3	1.06
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	23	1.05
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	17	1.05
(1,136)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:GLY:N	10	1.04
(1,92)	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	1:80:A:LEU:N	3	1.04
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	27	1.04
(1,14)	1:32:A:VAL:N	1:32:A:VAL:CA	1:32:A:VAL:C	1:33:A:PRO:N	10	1.04
(1,52)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:LEU:N	1	1.03
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	23	1.03
(1,44)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:GLN:N	19	1.01
(1,138)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ASP:N	2	1.0