



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:45 AM UTC

PDB ID : 2MMG / pdb_00002mmg
BMRB ID : 19854
Title : Structural Characterization of the Mengovirus Leader Protein Bound to Ran GTPase by Nuclear Magnetic Resonance
Authors : Bacot-Davis, V.R.; Palmenberg, A.C.; Cornilescu, C.C.; Markley, J.L.
Deposited on : 2014-03-15

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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

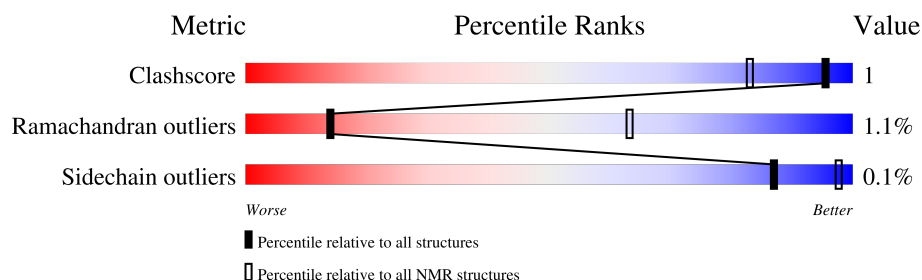
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	216	

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 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:9-A:175 (167)	0.22	6
2	A:182-A:190 (9)	0.97	9
3	A:199-A:207 (9)	0.15	2

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	7, 8, 9
2	2, 6, 10
3	1, 4
Single-model clusters	3; 5

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3449 atoms, of which 1725 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTP-binding nuclear protein Ran.

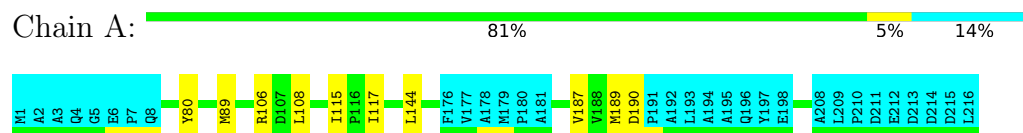
Mol	Chain	Residues	Atoms						Trace
1	A	216	Total	C	H	N	O	S	0
			3449	1109	1725	295	313	7	

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: GTP-binding nuclear protein Ran

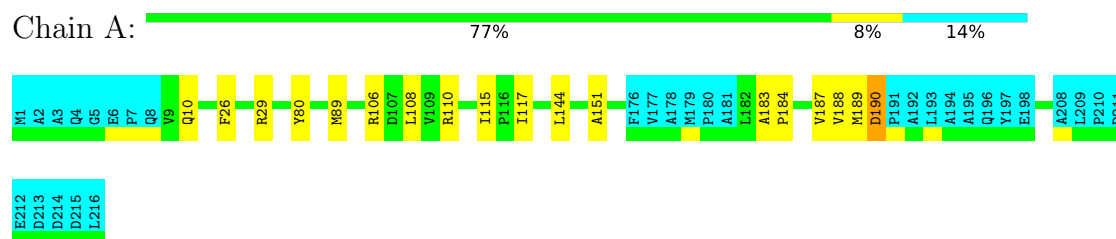


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

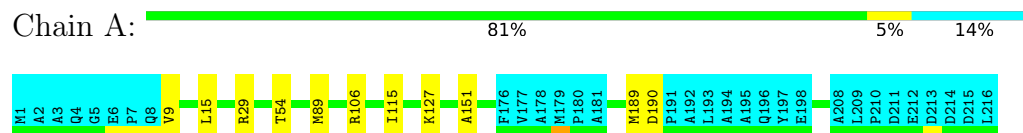
4.2.1 Score per residue for model 1

- Molecule 1: GTP-binding nuclear protein Ran



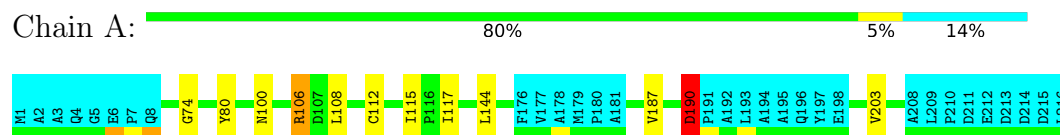
4.2.2 Score per residue for model 2

- Molecule 1: GTP-binding nuclear protein Ran



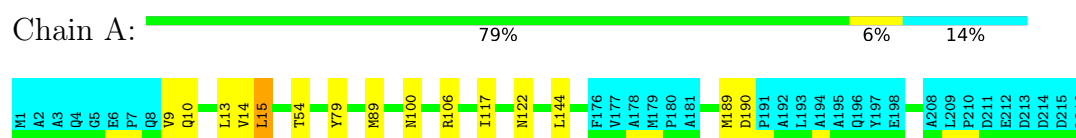
4.2.3 Score per residue for model 3

- Molecule 1: GTP-binding nuclear protein Ran



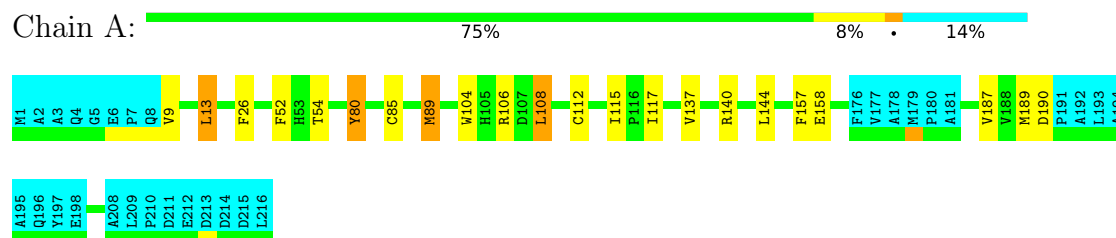
4.2.4 Score per residue for model 4

- Molecule 1: GTP-binding nuclear protein Ran



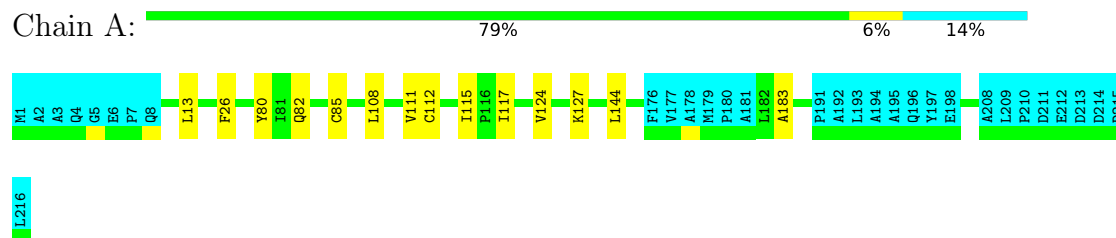
4.2.5 Score per residue for model 5

- Molecule 1: GTP-binding nuclear protein Ran



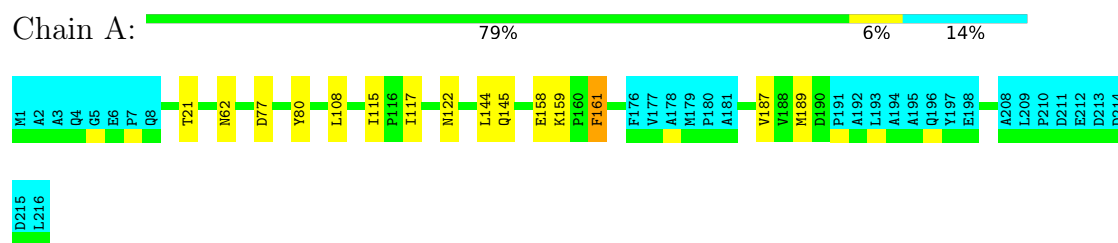
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: GTP-binding nuclear protein Ran



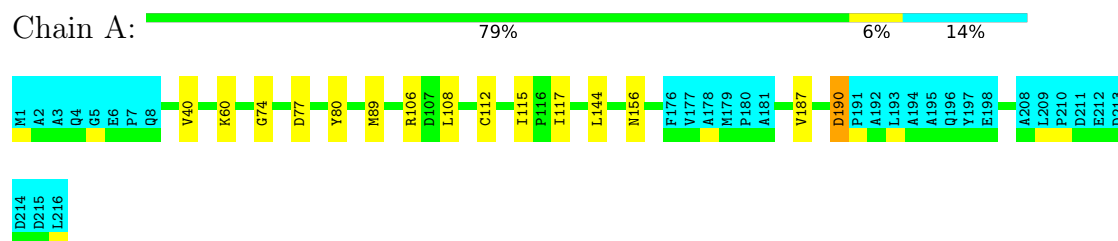
4.2.7 Score per residue for model 7

- Molecule 1: GTP-binding nuclear protein Ran



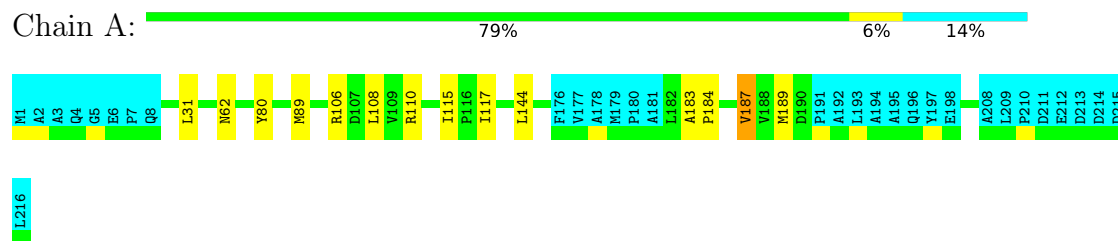
4.2.8 Score per residue for model 8

- Molecule 1: GTP-binding nuclear protein Ran



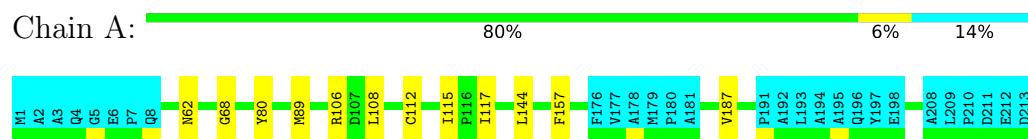
4.2.9 Score per residue for model 9

- Molecule 1: GTP-binding nuclear protein Ran



4.2.10 Score per residue for model 10

- Molecule 1: GTP-binding nuclear protein Ran



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 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	
TALOS	geometry optimization	
SPARTA+	geometry optimization	
CYANA	refinement	

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	2631
Number of shifts mapped to atoms	2625
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

6 Model quality

6.1 Standard geometry

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	1.13±0.02	0±0/1532 (0.0± 0.0%)	1.55±0.03	10±2/2076 (0.5± 0.1%)
All	All	1.13	0/15320 (0.0%)	1.55	95/20760 (0.5%)

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	0.9±0.9
All	All	0	9

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	115	ILE	N-CA-C	-8.22	102.45	109.19	10	8
1	A	80	TYR	N-CA-C	8.13	120.22	111.36	5	1
1	A	112	CYS	N-CA-C	7.45	119.48	111.36	5	5
1	A	9	VAL	N-CA-C	7.14	118.57	108.36	4	3
1	A	115	ILE	N-CA-CB	6.89	119.01	111.64	9	8
1	A	13	LEU	CB-CA-C	-6.78	97.99	109.72	5	1
1	A	190	ASP	N-CA-C	6.78	124.79	109.81	3	2
1	A	157	PHE	N-CA-CB	6.50	119.67	110.12	5	1
1	A	159	LYS	N-CA-C	6.40	121.46	112.75	7	1
1	A	110	ARG	CB-CA-C	-6.19	100.51	110.79	9	2
1	A	60	LYS	N-CA-CB	6.18	121.07	110.68	8	1
1	A	184	PRO	N-CA-C	5.99	116.22	110.47	9	1
1	A	62	ASN	N-CA-C	-5.97	98.80	108.41	7	2
1	A	189	MET	CA-C-N	5.87	128.74	123.10	7	2
1	A	189	MET	C-N-CA	5.87	128.74	123.10	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	62	ASN	N-CA-CB	5.86	119.53	110.21	9	1
1	A	183	ALA	N-CA-C	-5.86	101.09	109.24	9	1
1	A	40	VAL	N-CA-C	-5.80	99.99	108.11	8	1
1	A	183	ALA	CA-C-N	5.78	123.82	119.66	1	3
1	A	183	ALA	C-N-CA	5.78	123.82	119.66	1	3
1	A	190	ASP	N-CA-CB	5.76	120.62	110.37	1	1
1	A	77	ASP	N-CA-C	5.68	117.48	111.28	7	1
1	A	184	PRO	N-CA-CB	5.52	106.09	103.22	1	1
1	A	145	GLN	N-CA-CB	5.48	119.56	110.52	7	1
1	A	13	LEU	CA-C-N	-5.42	116.47	123.19	5	1
1	A	13	LEU	C-N-CA	-5.42	116.47	123.19	5	1
1	A	158	GLU	CB-CA-C	-5.41	99.33	109.72	5	1
1	A	80	TYR	CA-CB-CG	-5.36	104.26	113.90	5	1
1	A	127	LYS	N-CA-C	5.32	116.76	111.07	2	2
1	A	68	GLY	CA-C-N	5.31	127.83	120.29	10	1
1	A	68	GLY	C-N-CA	5.31	127.83	120.29	10	1
1	A	54	THR	CA-C-N	5.30	127.39	120.28	5	3
1	A	54	THR	C-N-CA	5.30	127.39	120.28	5	3
1	A	106	ARG	N-CA-C	-5.29	99.54	110.80	3	3
1	A	74	GLY	CA-C-N	5.29	127.36	120.28	8	2
1	A	74	GLY	C-N-CA	5.29	127.36	120.28	8	2
1	A	111	VAL	N-CA-C	5.28	115.49	110.53	6	1
1	A	100	ASN	CA-C-N	5.27	123.56	120.24	3	2
1	A	100	ASN	C-N-CA	5.27	123.56	120.24	3	2
1	A	79	TYR	CB-CA-C	-5.26	102.06	110.79	4	1
1	A	52	PHE	N-CA-CB	5.21	119.89	110.83	5	1
1	A	161	PHE	N-CA-CB	5.21	117.86	110.16	7	1
1	A	188	VAL	CA-C-N	5.16	131.40	121.54	1	1
1	A	188	VAL	C-N-CA	5.16	131.40	121.54	1	1
1	A	108	LEU	CB-CA-C	-5.14	102.80	110.88	5	1
1	A	15	LEU	N-CA-CB	5.13	118.78	110.42	4	2
1	A	203	VAL	N-CA-CB	5.12	117.50	110.54	3	1
1	A	157	PHE	CA-CB-CG	5.05	118.85	113.80	10	1
1	A	124	VAL	CA-C-N	5.04	127.03	120.28	6	1
1	A	124	VAL	C-N-CA	5.04	127.03	120.28	6	1
1	A	26	PHE	CA-CB-CG	5.04	118.84	113.80	6	1
1	A	31	LEU	N-CA-C	5.04	116.46	111.07	9	1
1	A	156	ASN	CA-C-N	5.02	126.97	120.44	8	1
1	A	156	ASN	C-N-CA	5.02	126.97	120.44	8	1

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	89	MET	Mainchain	5
1	A	189	MET	Mainchain	3
1	A	80	TYR	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	1495	1516	1516	3±1
All	All	14950	15160	15160	30

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HD22	1:A:85:CYS:SG	0.74	2.23	5	1
1:A:29:ARG:HH21	1:A:151:ALA:HA	0.55	1.61	1	2
1:A:117:ILE:HB	1:A:144:LEU:HD22	0.51	1.82	5	9
1:A:26:PHE:CD2	1:A:89:MET:HE1	0.49	2.42	5	1
1:A:80:TYR:CE1	1:A:108:LEU:HG	0.48	2.43	3	7
1:A:104:TRP:O	1:A:108:LEU:HD13	0.47	2.09	5	1
1:A:13:LEU:HD23	1:A:14:VAL:N	0.47	2.24	4	1
1:A:13:LEU:HD22	1:A:15:LEU:CD1	0.44	2.43	4	1
1:A:89:MET:HB3	1:A:122:ASN:HD21	0.42	1.74	4	1
1:A:26:PHE:CG	1:A:89:MET:HE1	0.42	2.50	1	1
1:A:13:LEU:CD2	1:A:85:CYS:HB2	0.41	2.45	6	1
1:A:137:VAL:HG12	1:A:140:ARG:HH21	0.41	1.76	5	1
1:A:13:LEU:HD22	1:A:15:LEU:HD12	0.41	1.92	4	1
1:A:21:THR:HG22	1:A:122:ASN:HD21	0.41	1.74	7	1
1:A:158:GLU:HA	1:A:161:PHE:CE2	0.40	2.51	7	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	185/216 (86%)	181±1 (98±1%)	2±1 (1±0%)	2±1 (1±1%)	14	63
All	All	1850/2160 (86%)	1809 (98%)	21 (1%)	20 (1%)	14	63

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	187	VAL	7
1	A	106	ARG	6
1	A	190	ASP	6
1	A	189	MET	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	163/185 (88%)	163±0 (100±0%)	0±0 (0±0%)	87	98
All	All	1630/1850 (88%)	1628 (100%)	2 (0%)	87	98

All 2 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	82	GLN	1
1	A	77	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 85% 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	2631
Number of shifts mapped to atoms	2625
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	92

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

- No matching atom found in the structure. All 6 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	HIS	HE2	11.376	0.020	1
1	A	48	HIS	HE2	11.298	0.020	1
1	A	53	HIS	HE2	11.083	0.020	1
1	A	105	HIS	HE2	11.112	0.020	1
1	A	139	HIS	HE2	12.494	0.020	1
1	A	199	HIS	HE2	12.445	0.020	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	212	-1.32 ± 0.31	Should be checked
$^{13}\text{C}_\beta$	196	-0.40 ± 0.18	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}'$	211	-0.48 ± 0.18	None needed (< 0.5 ppm)
^{15}N	215	0.64 ± 0.38	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 2236 atoms were assigned a chemical shift out of a possible 2630. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	740/922 (80%)	202/375 (54%)	362/370 (98%)	176/177 (99%)
Sidechain	1249/1461 (85%)	880/948 (93%)	308/452 (68%)	61/61 (100%)
Aromatic	247/247 (100%)	120/120 (100%)	112/112 (100%)	15/15 (100%)
Overall	2236/2630 (85%)	1202/1443 (83%)	782/934 (84%)	252/253 (100%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 2542 atoms were assigned a chemical shift out of a possible 3007. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	856/1070 (80%)	230/434 (53%)	423/432 (98%)	203/204 (100%)
Sidechain	1420/1671 (85%)	1008/1086 (93%)	348/521 (67%)	64/64 (100%)
Aromatic	266/266 (100%)	129/129 (100%)	122/122 (100%)	15/15 (100%)
Overall	2542/3007 (85%)	1367/1649 (83%)	893/1075 (83%)	282/283 (100%)

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	114	ASN	ND2	1114.29	101.55 – 123.95	447.1
1	A	104	TRP	CE3	174.81	111.58 – 129.41	30.5
1	A	32	THR	HG1	6.41	0.08 – 2.19	25.0
1	A	66	THR	HG1	6.01	0.08 – 2.19	23.1
1	A	207	THR	HG1	5.99	0.08 – 2.19	23.0
1	A	206	THR	HG1	5.96	0.08 – 2.19	22.8
1	A	24	THR	HG1	5.91	0.08 – 2.19	22.6
1	A	54	THR	HG1	5.59	0.08 – 2.19	21.1

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	93	THR	HG1	5.56	0.08 – 2.19	21.0
1	A	97	THR	HG1	5.48	0.08 – 2.19	20.6
1	A	25	THR	HG1	5.39	0.08 – 2.19	20.1
1	A	127	LYS	HB3	6.92	0.46 – 3.04	20.0
1	A	42	THR	HG1	5.31	0.08 – 2.19	19.8
1	A	127	LYS	HD2	5.61	0.58 – 2.64	19.4
1	A	127	LYS	HD3	5.66	0.54 – 2.65	19.3
1	A	84	GLN	HB3	6.96	0.71 – 3.33	18.9
1	A	21	THR	HG1	5.08	0.08 – 2.19	18.7
1	A	127	LYS	HG2	5.43	0.13 – 2.61	16.4
1	A	127	LYS	HG3	5.58	0.04 – 2.67	16.1
1	A	140	ARG	NE	108.39	76.53 – 92.65	14.8
1	A	127	LYS	HE3	5.80	1.92 – 3.89	14.7
1	A	127	LYS	HE2	5.73	1.95 – 3.88	14.6
1	A	127	LYS	HB2	5.20	0.58 – 2.97	14.3
1	A	104	TRP	CD2	155.17	118.40 – 137.65	14.1
1	A	134	LYS	CB	54.58	24.03 – 41.47	12.5
1	A	82	GLN	NE2	132.38	103.38 – 120.35	12.1
1	A	183	ALA	HB1	4.16	0.14 – 2.58	11.5
1	A	183	ALA	HB2	4.16	0.14 – 2.58	11.5
1	A	183	ALA	HB3	4.16	0.14 – 2.58	11.5
1	A	36	GLU	CB	48.14	21.56 – 38.37	10.8
1	A	85	CYS	HB3	7.56	0.69 – 5.10	10.6
1	A	139	HIS	HB3	6.88	1.18 – 4.91	10.3
1	A	85	CYS	HB2	7.31	0.81 – 5.11	10.1
1	A	28	LYS	NZ	59.20	19.79 – 46.09	10.0
1	A	84	GLN	NE2	128.39	103.38 – 120.35	9.7
1	A	205	GLN	NE2	128.39	103.38 – 120.35	9.7
1	A	139	HIS	HB2	6.46	1.36 – 4.85	9.6
1	A	175	GLU	CA	76.25	47.03 – 67.62	9.2
1	A	45	VAL	CB	17.10	23.86 – 41.50	-8.8
1	A	68	GLY	C	189.53	164.92 – 182.89	8.7
1	A	151	ALA	C	160.74	167.61 – 188.05	-8.4
1	A	60	LYS	CA	74.29	46.18 – 67.77	8.0
1	A	84	GLN	HB2	4.01	0.80 – 3.29	7.9
1	A	123	LYS	NZ	53.49	19.79 – 46.09	7.8
1	A	23	LYS	NZ	53.30	19.79 – 46.09	7.7
1	A	99	LYS	NZ	53.30	19.79 – 46.09	7.7
1	A	127	LYS	NZ	53.29	19.79 – 46.09	7.7
1	A	37	LYS	NZ	53.20	19.79 – 46.09	7.7
1	A	32	THR	CG2	29.98	16.06 – 27.03	7.7
1	A	82	GLN	CD	170.41	173.59 – 185.85	-7.6

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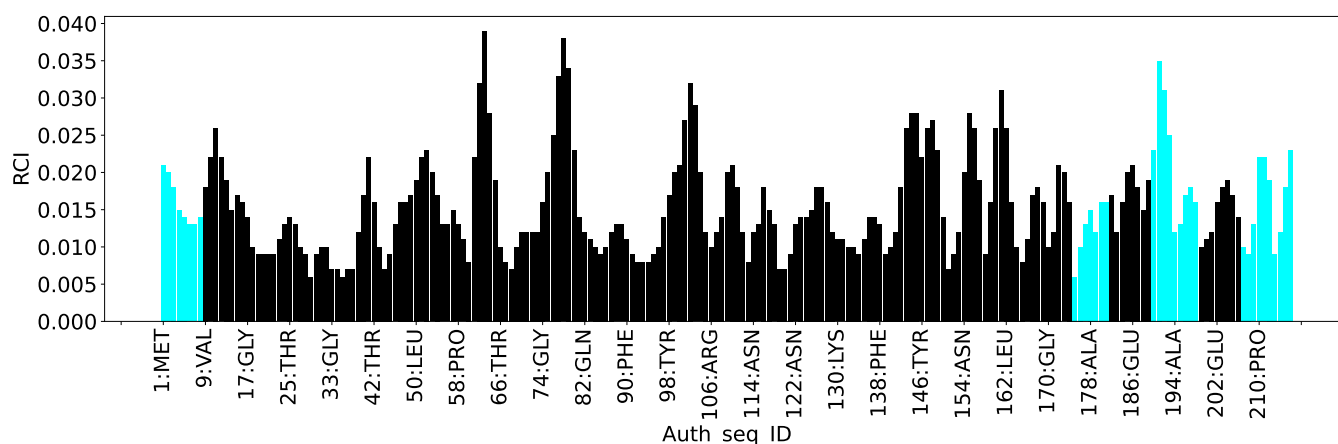
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	186	GLU	CD	198.61	171.45 – 193.13	7.5
1	A	38	LYS	NZ	52.40	19.79 – 46.09	7.4
1	A	143	ASN	ND2	129.29	101.55 – 123.95	7.4
1	A	158	GLU	CA	72.15	47.03 – 67.62	7.2
1	A	44	GLY	CA	54.58	38.93 – 51.79	7.2
1	A	99	LYS	CE	47.85	37.57 – 46.21	6.9
1	A	29	ARG	CA	72.15	45.44 – 68.13	6.8
1	A	33	GLY	C	161.91	164.92 – 182.89	-6.7
1	A	23	LYS	CE	47.55	37.57 – 46.21	6.6
1	A	60	LYS	NZ	49.99	19.79 – 46.09	6.5
1	A	62	ASN	ND2	98.29	101.55 – 123.95	-6.5
1	A	12	LYS	NZ	49.89	19.79 – 46.09	6.5
1	A	170	GLY	C	162.50	164.92 – 182.89	-6.3
1	A	132	LYS	NZ	49.59	19.79 – 46.09	6.3
1	A	94	SER	C	163.97	166.15 – 183.14	-6.3
1	A	134	LYS	NZ	49.30	19.79 – 46.09	6.2
1	A	141	LYS	NZ	49.24	19.79 – 46.09	6.2
1	A	89	MET	CE	27.93	8.39 – 25.85	6.2
1	A	142	LYS	NZ	49.22	19.79 – 46.09	6.2
1	A	152	LYS	NZ	49.22	19.79 – 46.09	6.2
1	A	71	LYS	NZ	49.00	19.79 – 46.09	6.1
1	A	119	LEU	CA	42.87	45.17 – 66.21	-6.1
1	A	22	GLY	C	184.81	164.92 – 182.89	6.1
1	A	99	LYS	HE2	4.08	1.95 – 3.88	6.1
1	A	124	VAL	CG1	29.68	14.71 – 28.29	6.0
1	A	84	GLN	HG3	3.94	0.91 – 3.68	5.9
1	A	165	ALA	C	165.72	167.61 – 188.05	-5.9
1	A	127	LYS	CE	46.97	37.57 – 46.21	5.9
1	A	110	ARG	NE	94.02	76.53 – 92.65	5.8
1	A	104	TRP	CD1	137.30	117.34 – 135.80	5.8
1	A	113	GLU	CA	69.22	47.03 – 67.62	5.8
1	A	124	VAL	CB	42.57	23.86 – 41.50	5.6
1	A	154	ASN	ND2	125.21	101.55 – 123.95	5.6
1	A	213	ASP	CB	49.61	32.98 – 48.76	5.5
1	A	99	LYS	CD	34.95	23.50 – 34.42	5.5
1	A	99	LYS	HE3	3.98	1.92 – 3.89	5.5
1	A	29	ARG	NE	93.29	76.53 – 92.65	5.4
1	A	76	ARG	NE	93.29	76.53 – 92.65	5.4
1	A	194	ALA	C	166.90	167.61 – 188.05	-5.3
1	A	167	LYS	NZ	46.77	19.79 – 46.09	5.3
1	A	84	GLN	HG2	3.66	1.01 – 3.62	5.2
1	A	140	ARG	CB	39.64	21.74 – 39.52	5.1

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 [i](#)

8.1 Conformationally restricting restraints [i](#)

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	0
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	144
Number of unmapped restraints	0
Number of restraints per residue	0
Number of long range restraints per residue ¹	0

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 [i](#)

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 [i](#)

Distance violations less than 0.1 Å are not included in the calculation. There are no distance restraints

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)	8.9	9.98

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Bins (°)	Average number of violations per model	Max (°)
10.0-20.0 (Medium)	2.7	18.9
>20.0 (Large)	21.9	156.72

9 Distance violation analysis ⓘ

No distance restraints data found

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

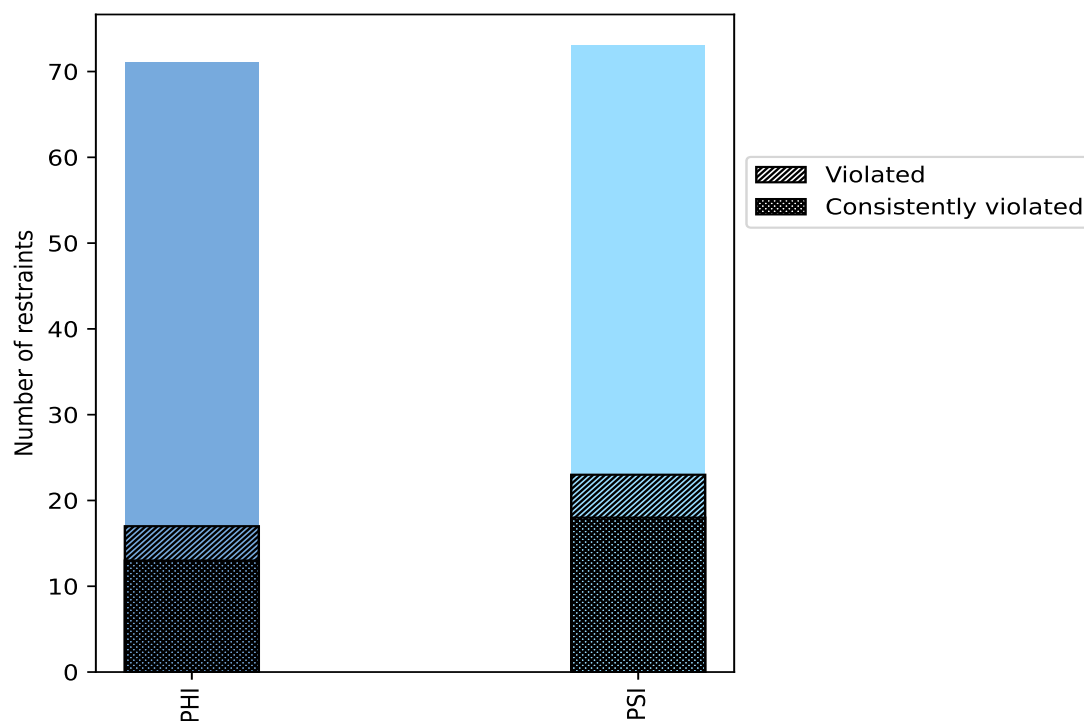
10.1 Summary of dihedral-angle violations [i](#)

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	71	49.3	17	23.9	11.8	13	18.3	9.0
PSI	73	50.7	23	31.5	16.0	18	24.7	12.5
Total	144	100.0	40	27.8	27.8	31	21.5	21.5

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

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



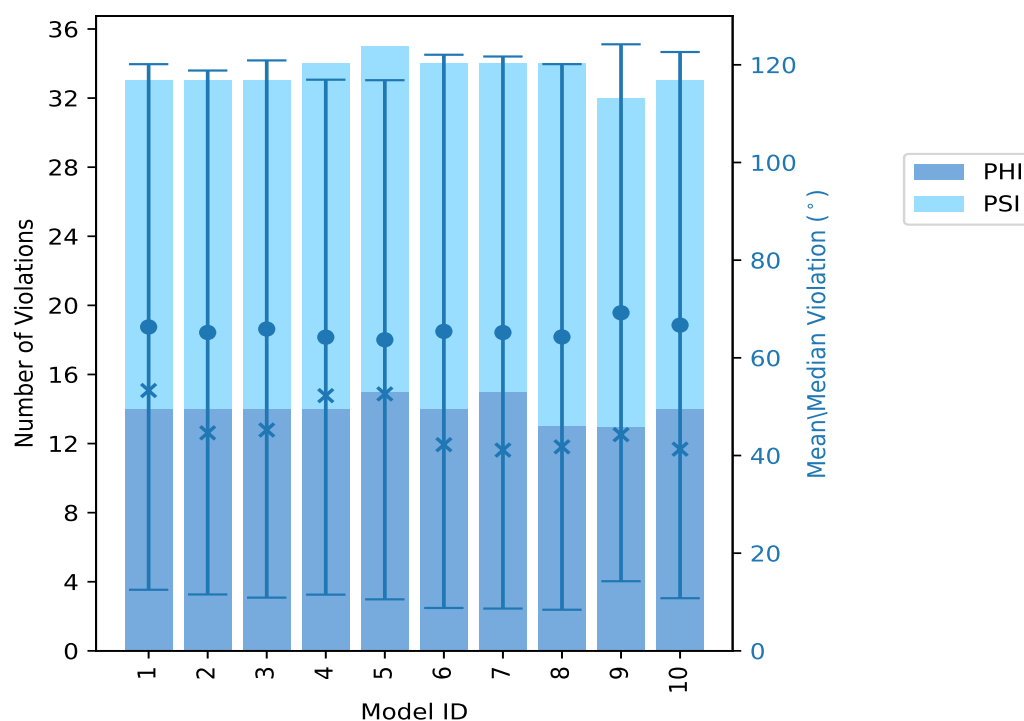
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	14	19	33	66.32	147.08	53.81	53.31
2	14	19	33	65.19	147.69	53.64	44.64
3	14	19	33	65.9	146.17	55.0	45.22
4	14	20	34	64.23	149.12	52.72	52.26
5	15	20	35	63.7	153.3	53.15	52.61
6	14	20	34	65.42	148.35	56.64	42.22
7	15	19	34	65.18	153.02	56.52	41.11
8	13	21	34	64.28	145.75	55.86	41.78
9	13	19	32	69.23	156.72	54.97	44.27
10	14	19	33	66.7	147.83	55.92	41.3

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

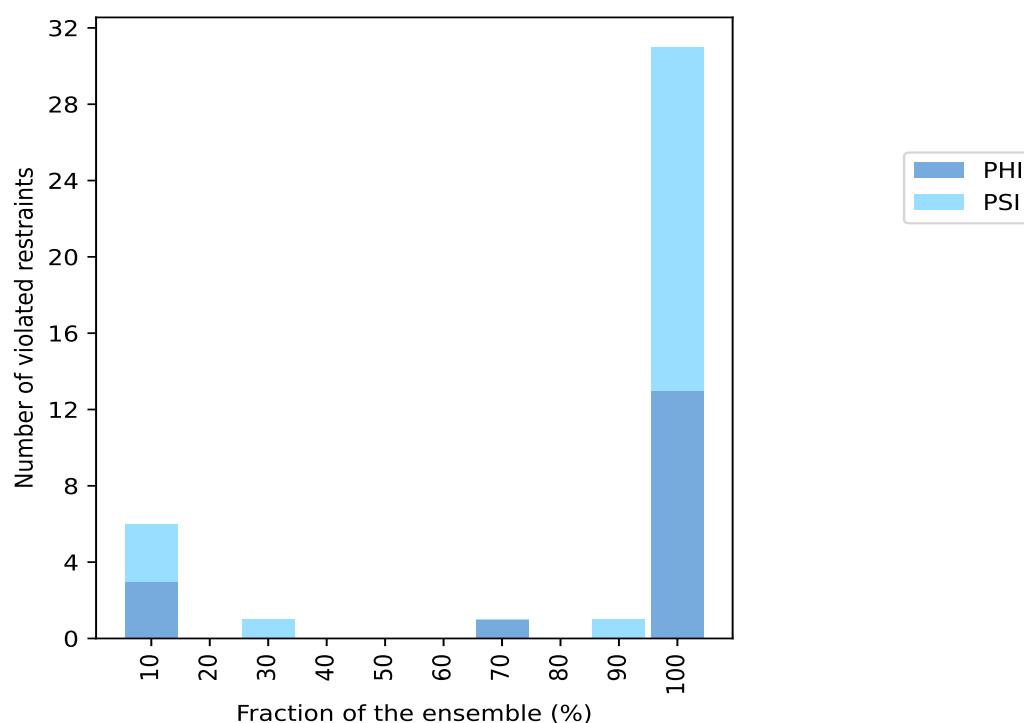
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
3	3	6	1	10.0
0	0	0	2	20.0
0	1	1	3	30.0
0	0	0	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
1	0	1	7	70.0
0	0	0	8	80.0
0	1	1	9	90.0
13	18	31	10	100.0

¹ Number of models with violations

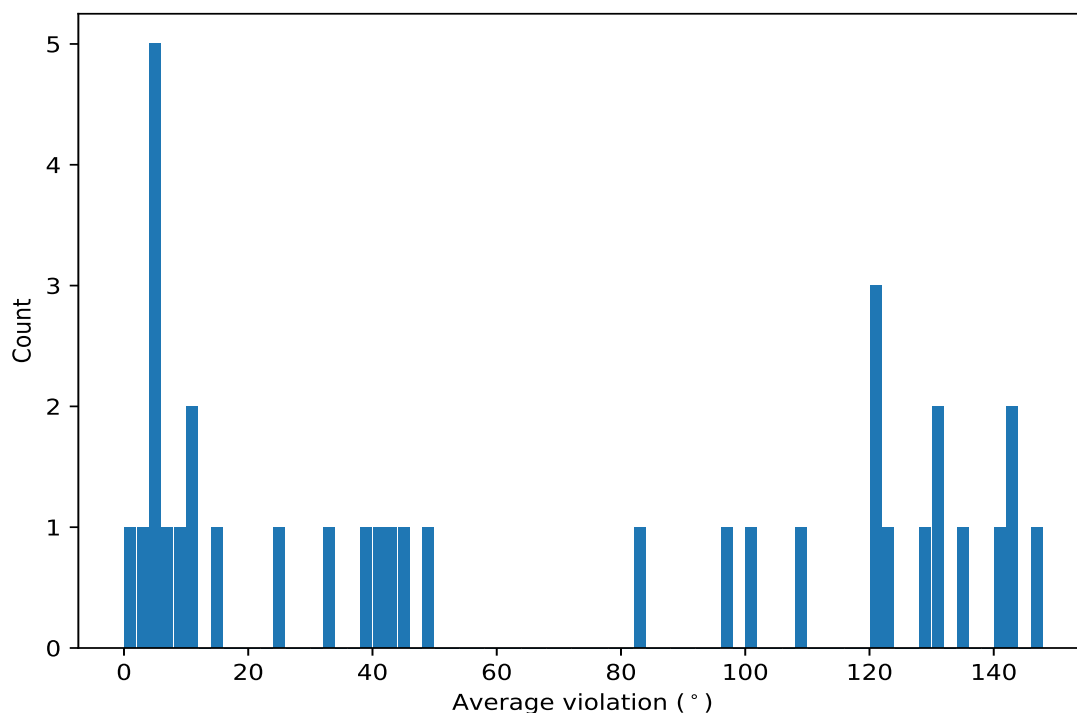
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	10	146.24	1.32	146.0
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	10	143.63	5.78	143.27
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	10	142.03	6.7	142.24
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	10	140.5	5.5	139.54
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	10	135.74	5.94	136.38
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	10	130.36	3.88	131.2
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	10	130.36	3.88	131.2
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	10	128.13	5.12	130.45
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	10	123.85	1.8	124.16
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	10	121.65	1.98	121.15
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	10	121.17	3.76	122.28
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	10	120.7	1.32	120.32
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	10	108.05	35.53	119.24

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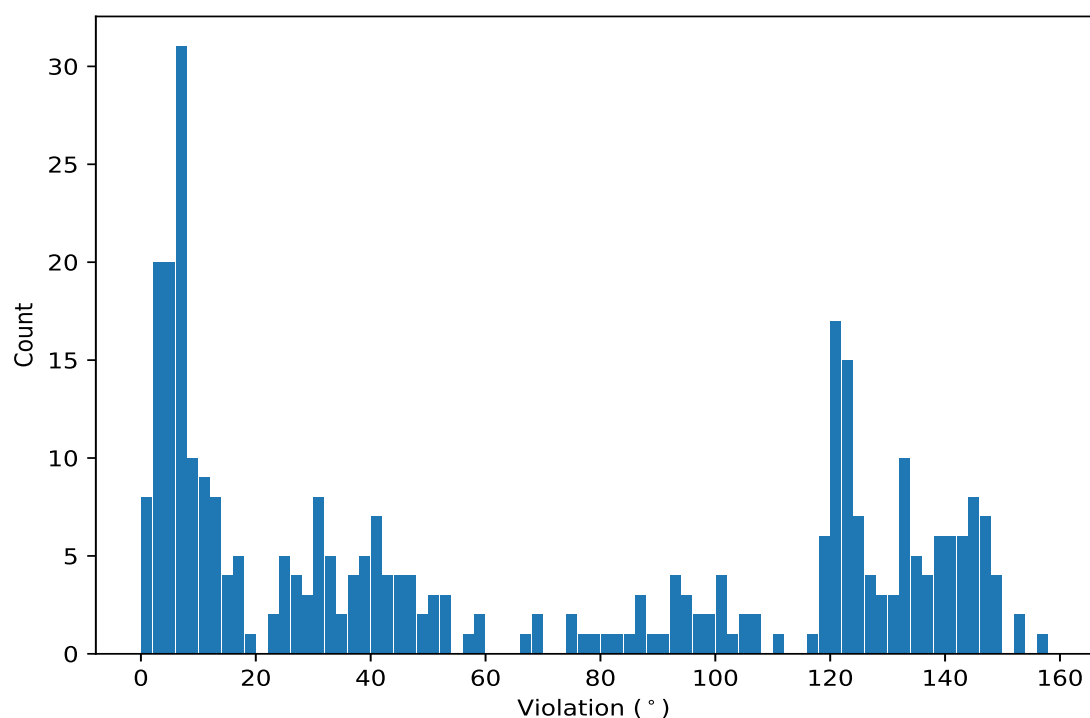
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	10	100.01	4.31	99.92
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	10	97.23	4.99	95.73
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	10	82.14	5.21	82.76
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	10	48.54	2.96	49.24
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	10	44.05	2.28	44.06
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	10	42.15	13.47	36.38
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	10	41.52	16.99	31.04
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	10	39.83	1.07	39.82
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	10	32.05	1.86	32.86
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	10	25.36	1.72	25.31
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	10	15.22	3.05	15.93
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	10	11.85	1.21	11.72
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	10	10.02	2.24	10.54
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	10	8.08	1.04	8.07
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	10	5.8	0.62	5.89
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	10	5.75	1.06	5.97
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	10	5.6	1.46	6.34
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	10	5.29	1.52	5.56
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	10	3.04	0.55	3.12
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	9	4.32	2.29	3.6
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	7	6.31	4.37	7.07
(1,113)	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	1:176:A:PHE:N	3	1.77	0.26	1.76

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	9	156.72
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	5	153.3
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	7	153.02
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	4	149.12
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	9	148.44
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	6	148.35
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	6	148.18
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	10	147.83
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	2	147.69
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	7	147.46
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	1	147.08
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	1	146.78
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	3	146.17
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	2	146.01
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	1	145.99
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	8	145.75
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	10	145.45
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	2	145.32
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	7	145.03
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	4	144.89
(1,2)	1:2:A:ALA:N	1:2:A:ALA:CA	1:2:A:ALA:C	1:3:A:ALA:N	5	144.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	1	144.07
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	8	143.81
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	3	142.74
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	3	142.73
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	6	142.64
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	8	142.32
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	7	142.15
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	10	141.87
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	10	141.49
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	6	140.64
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	9	140.48
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	3	140.44
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	9	140.2
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	6	139.27
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	7	139.19
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	10	139.16
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	5	139.08
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	3	138.63
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	5	138.6
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	4	137.89
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	9	136.69
(1,22)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:TYR:N	2	136.64
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	2	136.08
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	8	135.67
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	6	135.37
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	7	135.1
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	4	134.82
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	7	134.17
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	6	133.89
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	8	133.73
(1,73)	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	1:113:A:GLU:N	10	133.47
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	8	133.18
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	8	133.0
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	8	132.88
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	1	132.63
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	1	132.56
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	6	132.48
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	3	132.13
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	10	131.98
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	2	131.81
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	10	130.6
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	1	129.71
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	9	128.93
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	4	128.23
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	9	127.94
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	3	126.82
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	5	126.25
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	5	126.15
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	4	125.92
(1,137)	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	1:210:A:PRO:N	4	125.32
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	5	125.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,133)	1:207:A:THR:N	1:207:A:THR:CA	1:207:A:THR:C	1:208:A:ALA:N	5	124.7
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	7	124.66
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	1	124.53
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	3	124.04
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	6	123.8
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	3	123.54
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	9	123.48
(1,121)	1:194:A:ALA:N	1:194:A:ALA:CA	1:194:A:ALA:C	1:195:A:ALA:N	5	123.47
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	10	123.2
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	8	123.05
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	6	123.01
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	7	122.98
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	1	122.76
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	10	122.51
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	2	122.49
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	2	122.25
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	10	122.12
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	9	122.06
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	5	122.05
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	9	121.96
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	9	121.95
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	4	121.82
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	2	121.81
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	4	121.79
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	9	121.75
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	8	121.69
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	8	121.44
(1,44)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	2	121.39
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	4	121.32
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	6	121.1
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	6	120.98
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	3	120.74
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1	120.66
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	10	120.41
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	2	120.22
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	1	120.04
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	8	119.93
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	4	119.57
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	3	119.16
(1,135)	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1:209:A:LEU:N	7	119.11
(1,26)	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1:44:A:GLY:N	7	118.88
(1,122)	1:194:A:ALA:C	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	7	118.62
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	3	116.51
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:GLY:N	5	110.07
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	7	106.35
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	9	106.19
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	6	105.21
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	7	104.0
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	8	102.77
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	10	101.81
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	9	101.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	6	101.22
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	10	100.54
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	3	98.61
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	5	98.52
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	2	97.55
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	8	96.18
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	4	95.28
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	5	95.01
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	4	94.58
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	5	93.69
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	2	92.79
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	1	92.66
(1,24)	1:39:A:TYR:N	1:39:A:TYR:CA	1:39:A:TYR:C	1:40:A:VAL:N	1	92.55
(1,47)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ASP:N	3	90.15
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	2	88.6
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	5	87.6
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1	87.22
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	4	86.95
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	3	84.27
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	4	83.85
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	8	81.26
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	7	78.89
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	6	77.13
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	10	75.48
(1,64)	1:105:A:HIS:C	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	9	74.01
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	5	69.07
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	2	68.74
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	1	67.68
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	5	59.59
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	4	58.62
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	1	57.97
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1	53.31
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	4	52.7
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	5	52.61
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	4	51.82
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	2	50.6
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	3	50.56
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	1	49.89
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	8	48.6
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	9	47.65
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	5	46.91
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	6	46.9
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	4	46.27
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	10	45.39
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	3	45.22
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	7	44.77
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	2	44.64
(1,94)	1:149:A:ILE:C	1:150:A:SER:N	1:150:A:SER:CA	1:150:A:SER:C	6	43.5
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	8	43.47
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	1	43.36
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	7	42.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	5	41.43
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	10	41.3
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	6	40.95
(1,138)	1:210:A:PRO:N	1:210:A:PRO:CA	1:210:A:PRO:C	1:211:A:ASP:N	2	40.89
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	9	40.89
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	3	40.54
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	8	40.09
(1,112)	1:174:A:LEU:C	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	9	39.74
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	7	39.54
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	1	39.09
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	2	38.92
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	4	38.86
(1,9)	1:16:A:VAL:C	1:17:A:GLY:N	1:17:A:GLY:CA	1:17:A:GLY:C	10	37.95
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	6	37.83
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	9	36.62
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	2	36.13
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	3	35.69
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	2	34.74
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	4	33.01
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	7	32.98
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	9	32.96
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	3	32.89
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	1	32.84
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	5	31.92
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	3	31.65
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	10	31.3
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	10	30.44
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	9	30.37
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	10	30.36
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	6	30.33
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	8	30.23
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	7	29.9
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	7	29.68
(1,142)	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	1:214:A:ASP:N	8	29.05
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	9	27.88
(1,80)	1:136:A:ILE:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	6	27.65
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	5	27.63
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	8	27.0
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	4	25.52
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	2	25.31
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	6	25.31
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	7	25.01
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	1	24.54
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	10	23.13
(1,38)	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1:55:A:ASN:N	3	22.27
(1,141)	1:212:A:GLU:C	1:213:A:ASP:N	1:213:A:ASP:CA	1:213:A:ASP:C	8	18.9
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	9	17.66
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	7	17.02
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	6	16.76
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	8	16.74
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	1	16.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	10	15.85
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	2	15.76
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	5	15.01
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	4	15.0
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	2	13.78
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	6	13.39
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	9	13.37
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	8	13.04
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	10	12.84
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	1	12.64
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1	12.64
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	8	12.04
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	10	11.89
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	2	11.55
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	7	11.47
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	3	11.29
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	9	10.93
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	4	10.82
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	5	10.28
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	5	10.26
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	4	10.22
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	10	9.98
(1,25)	1:42:A:THR:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	5	9.67
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	9	9.13
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	2	8.94
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	10	8.72
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	7	8.67
(1,119)	1:193:A:LEU:N	1:193:A:LEU:CA	1:193:A:LEU:C	1:194:A:ALA:N	5	8.64
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	6	8.47
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	1	8.42
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	6	8.29
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	7	7.88
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	8	7.86
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	3	7.79
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	5	7.7
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	4	7.32
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	9	7.19
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	5	7.12
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	3	7.11
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	3	7.07
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	8	6.96
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	4	6.89
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	4	6.87
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	10	6.81
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	2	6.73
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	9	6.69
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	7	6.59
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	10	6.59
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	4	6.51
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	5	6.5
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	9	6.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:ARG:N	3	6.4
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	1	6.4
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	6	6.4
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	7	6.37
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	6	6.35
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	4	6.28
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	8	6.25
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	1	6.19
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	3	6.17
(1,8)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:GLY:N	2	6.08
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	9	6.04
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	9	5.95
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1	5.83
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	2	5.75
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	3	5.72
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	7	5.39
(1,97)	1:153:A:SER:N	1:153:A:SER:CA	1:153:A:SER:C	1:154:A:ASN:N	3	5.36
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	3	5.36
(1,123)	1:195:A:ALA:N	1:195:A:ALA:CA	1:195:A:ALA:C	1:196:A:GLN:N	4	5.23
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	4	5.2
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	3	5.19
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	2	5.14
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	8	5.07
(1,136)	1:208:A:ALA:C	1:209:A:LEU:N	1:209:A:LEU:CA	1:209:A:LEU:C	7	4.82
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	6	4.82
(1,17)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	5	4.78
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	6	4.41
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	1	4.4
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	10	4.33
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1	4.04
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	8	4.02
(1,72)	1:111:A:VAL:C	1:112:A:CYS:N	1:112:A:CYS:CA	1:112:A:CYS:C	5	3.93
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	5	3.76
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	7	3.74
(1,129)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:GLN:N	6	3.63
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	7	3.6
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	7	3.41
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	4	3.29
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	9	3.22
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	8	3.2
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	6	3.13
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	2	3.12
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	7	3.04
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	5	2.98
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	8	2.79
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	10	2.66
(1,11)	1:18:A:ASP:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	10	2.62
(1,134)	1:207:A:THR:C	1:208:A:ALA:N	1:208:A:ALA:CA	1:208:A:ALA:C	1	2.34
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	5	2.14
(1,113)	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	1:176:A:PHE:N	8	2.1
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	4	2.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:53:A:HIS:C	1:54:A:THR:N	1:54:A:THR:CA	1:54:A:THR:C	2	1.98
(1,65)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:ASP:N	1	1.8
(1,39)	1:54:A:THR:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	3	1.79
(1,113)	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	1:176:A:PHE:N	2	1.76
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	6	1.54
(1,113)	1:175:A:GLU:N	1:175:A:GLU:CA	1:175:A:GLU:C	1:176:A:PHE:N	6	1.46
(1,103)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:TRP:N	8	1.46
(1,114)	1:176:A:PHE:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	10	1.13