Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 10:13 AM EDT

PDB ID	:	2RT6
BMRB ID	:	11525
Title	:	Backbone 1H, 13C, and 15N Chemical Shift Assignments for PriC N-terminal domain
Authors	:	Aramaki, T.; Abe, Y.; Katayama, T.; Ueda, T.
Deposited on	:	2013-04-24

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 (i) 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 (1)) were used in the production of this report:

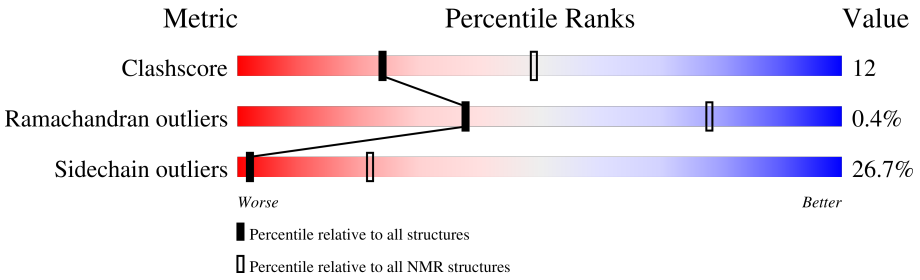
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	98	50% 30% • 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 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:12-A:90 (79)	0.70	17

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	4, 6, 11, 12, 14, 15, 17, 18, 19, 20
2	3, 5, 7, 10
3	1, 2, 9, 13
Single-model clusters	8; 16

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1551 atoms, of which 777 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Primosomal replication protein N".

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	98	1551	485	777	144	142	3	0

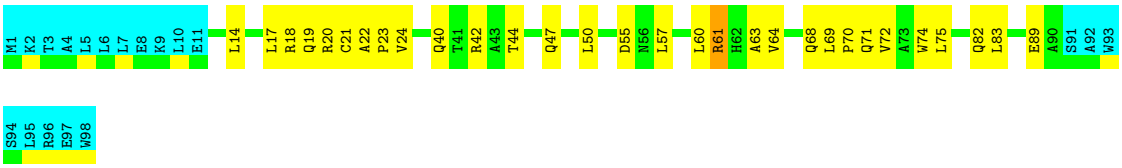
4 Residue-property plots (i)

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: Primosomal replication protein N"

Chain A: 50% 30% • 19%



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

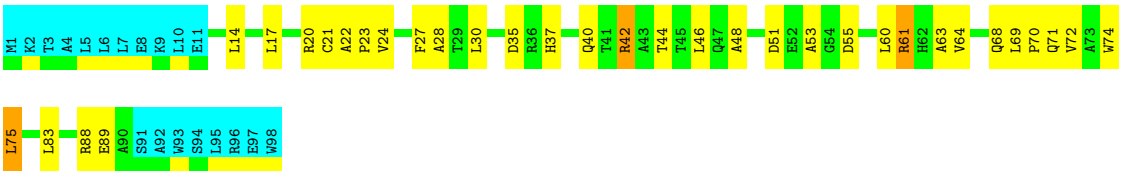
• Molecule 1: Primosomal replication protein N"

Chain A: 46% 34% • 19%

4.2.2 Score per residue for model 2

• Molecule 1: Primosomal replication protein N"

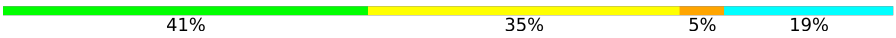
Chain A: 46% 32% • 19%



4.2.3 Score per residue for model 3

- Molecule 1: Primosomal replication protein N"

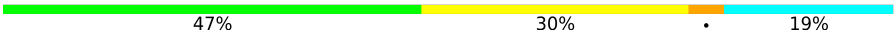
Chain A:

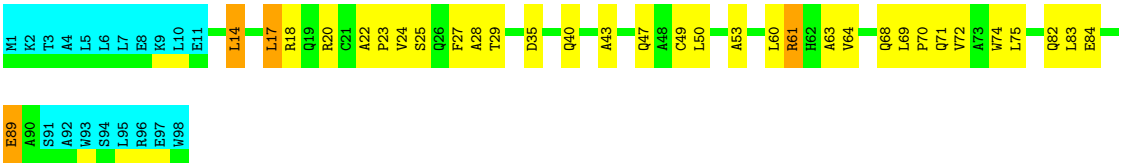


4.2.4 Score per residue for model 4

- Molecule 1: Primosomal replication protein N"

Chain A:

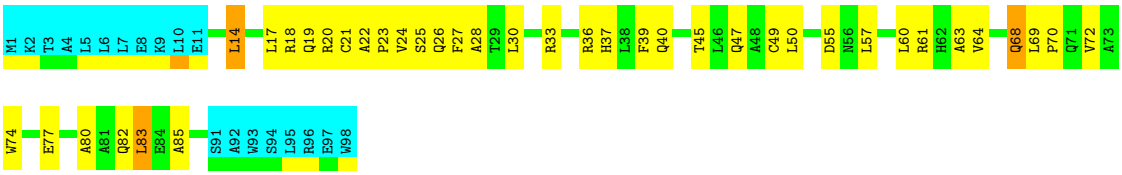




4.2.5 Score per residue for model 5

- Molecule 1: Primosomal replication protein N"

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Primosomal replication protein N"

Chain A: 49% 30% • 19%

M1 K2 T3 A4 L5 L6 L7 E8 K9 L10 E11 G12 Q13 L14 R18 C21 A22 P23 T29 L30 F39 R42 A43 T44 L50 D51 D55 N56 L57 A58 R61 V64 E65 L69 P70 Q71 W74 L75 L79 Q82 L83 E84 A85 R88 E89 A90

S91 A92 W93 S94 L95 R96 E97 W98

4.2.7 Score per residue for model 7

- Molecule 1: Primosomal replication protein N"

Chain A: 51% 26% • 19%

M1 K2 T3 A4 L5 L6 L7 E8 K9 L10 E11 L14 L17 R18 Q19 R20 C21 A22 P23 V24 R36 F39 Q40 T41 R42 C49 L50 L57 L60 R61 H62 A63 V64 Q68 L69 P70 Q71 V72 A73 W74 Q82 L83 E84 A85 E89 A90 S91 A92 W93 S94

L95 R96 E97 W98

4.2.8 Score per residue for model 8

- Molecule 1: Primosomal replication protein N"

Chain A: 49% 29% • 19%

M1 K2 T3 A4 L5 L6 L7 E8 K9 L10 E11 G12 Q13 L14 R20 C21 A22 P23 V24 L30 R33 L38 F39 Q40 T41 R42 A43 T44 D55 L60 R61 H62 A63 V64 Q68 L69 P70 Q71 V72 A73 W74 L75 A81 Q82 L83 E84 A85 R88 E89 A90 S91

A92 W93 S94 L95 R96 E97 W98

4.2.9 Score per residue for model 9

- Molecule 1: Primosomal replication protein N"

Chain A: 44% 35% • 19%

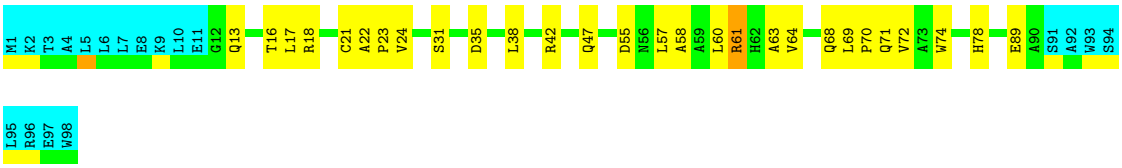
M1 K2 T3 A4 L5 L6 L7 E8 K9 L10 E11 G12 Q13 L14 L17 R18 Q19 R20 C21 A22 P23 V24 A28 D35 R36 H37 Q40 T41 R42 A43 T44 T45 L46 Q47 A48 C49 L50 L60 R61 H62 A63 V64 E65 Q66 Q67 Q68 L69 P70 Q71 V72 A73 W74 L83 E84

R88 S91 A92 W93 S94 L95 R96 E97 W98

4.2.10 Score per residue for model 10

- Molecule 1: Primosomal replication protein N"

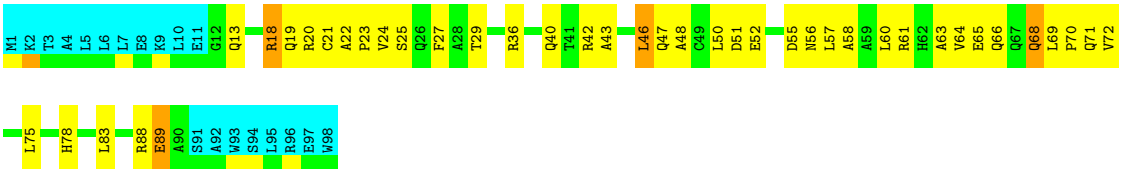
Chain A: 52% 28% • 19%



4.2.11 Score per residue for model 11

- Molecule 1: Primosomal replication protein N"

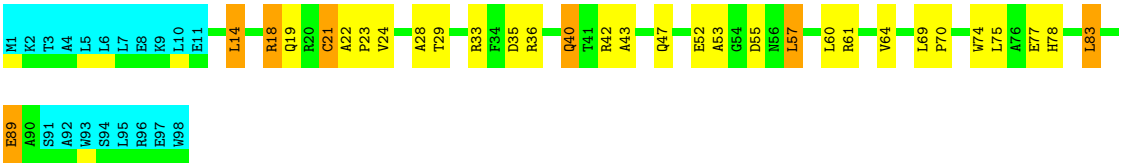
Chain A: 39% 38% • 19%



4.2.12 Score per residue for model 12

- Molecule 1: Primosomal replication protein N"

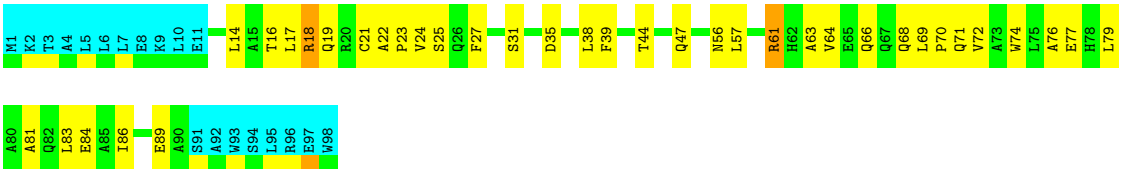
Chain A: 49% 24% 7% 19%



4.2.13 Score per residue for model 13

- Molecule 1: Primosomal replication protein N"

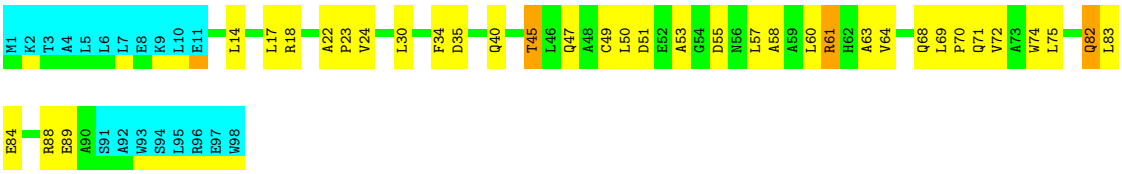
Chain A: 43% 36% • 19%



4.2.14 Score per residue for model 14

- Molecule 1: Primosomal replication protein N"

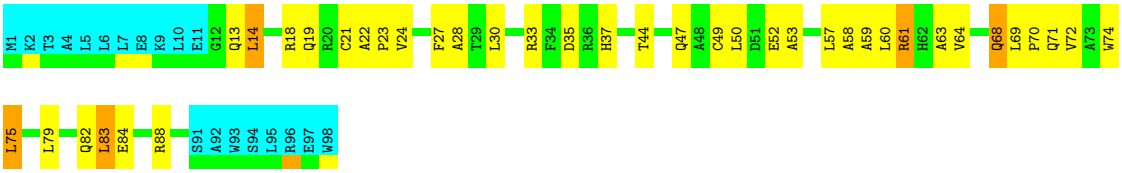
Chain A: 45% 33% • 19%



4.2.15 Score per residue for model 15

- Molecule 1: Primosomal replication protein N"

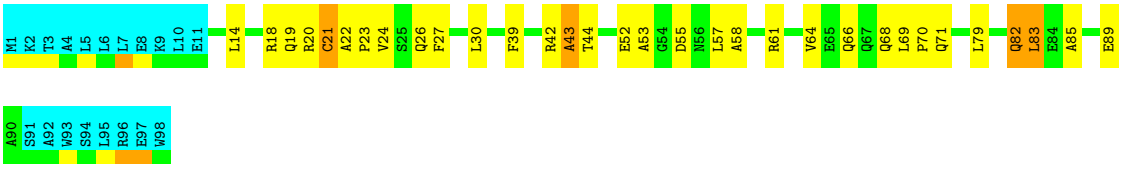
Chain A: 41% 35% 5% 19%



4.2.16 Score per residue for model 16

- Molecule 1: Primosomal replication protein N"

Chain A: 48% 29% • 19%



4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Primosomal replication protein N"

Chain A: 48% 30% • 19%

4.2.18 Score per residue for model 18

- Molecule 1: Primosomal replication protein N"

Chain A: 52% 27% • 19%

M1 K2 T3 A4 L5 L6 L7 E8 K9 L10 E11 L14 R18 Q19 R20 C21 A22 P23 V24 A28 R42 Q47 A48 C49 L50 D55 L60 R61 V64 E65 Q66 Q67 Q68 L69 P70 Q71 V72 L75 H78 L83 E89 A90 S91 A92 W93 S94 L95 R96

E97 W98

4.2.19 Score per residue for model 19

- Molecule 1: Primosomal replication protein N"

Chain A: 44% 33% • 19%

M1 K2 T3 A4 L5 L6 L7 E8 K9 L10 E11 L14 L17 R18 Q19 R20 C21 A22 P23 V24 S25 A28 S31 R36 H37 Q40 T41 R42 A43 T44 Q47 A48 C49 L50 D55 N56 L57 A58 A59 L60 R61 H62 A63 V64 L69 P70 Q71 V72 E77 H78

Q82 L83 R88 E89 A90 S91 A92 W93 S94 L95 R96 E97 W98

4.2.20 Score per residue for model 20

- Molecule 1: Primosomal replication protein N"

Chain A: 48% 32% • 19%

M1 K2 T3 A4 L5 L6 L7 E8 K9 L10 E11 Q12 Q13 L14 L17 R18 Q19 A22 P23 V24 A28 T29 L30 R33 A43 T44 T45 L46 C49 L50 D51 E52 D55 N56 L57 A58 A59 L60 R61 H62 A63 V64 E65 Q66 Q67 Q68 L69 P70 Q71 W74 L83

E89 A90 S91 A92 W93 S94 L95 R96 E97 W98

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 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	1.21
CNS	structure solution	1.21

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	1231
Number of shifts mapped to atoms	1231
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	612	610	607	15±3
All	All	12240	12200	12140	292

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD11	1:A:72:VAL:HG13	0.91	1.42	9	7
1:A:14:LEU:HD11	1:A:53:ALA:HB1	0.87	1.47	14	4
1:A:61:ARG:O	1:A:64:VAL:HG22	0.74	1.83	2	20
1:A:21:CYS:O	1:A:24:VAL:HG22	0.74	1.82	9	8
1:A:18:ARG:O	1:A:22:ALA:HB2	0.72	1.84	3	13
1:A:22:ALA:HB3	1:A:23:PRO:HD3	0.71	1.62	3	20
1:A:60:LEU:HD11	1:A:72:VAL:HG22	0.68	1.63	17	1
1:A:57:LEU:HD12	1:A:58:ALA:N	0.68	2.01	16	8
1:A:63:ALA:HB1	1:A:68:GLN:HB2	0.68	1.64	9	9
1:A:17:LEU:HD21	1:A:86:ILE:HG21	0.67	1.66	3	3
1:A:17:LEU:HD22	1:A:83:LEU:HD23	0.65	1.65	13	1
1:A:50:LEU:HD12	1:A:51:ASP:N	0.65	2.07	14	1
1:A:68:GLN:O	1:A:72:VAL:HG23	0.64	1.91	18	7
1:A:24:VAL:O	1:A:28:ALA:HB2	0.63	1.93	18	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD12	1:A:75:LEU:HB2	0.62	1.71	14	2
1:A:63:ALA:HB1	1:A:68:GLN:HB3	0.62	1.72	11	2
1:A:60:LEU:HD12	1:A:75:LEU:HB3	0.62	1.72	3	2
1:A:17:LEU:HD23	1:A:50:LEU:HD21	0.62	1.70	4	1
1:A:30:LEU:HD11	1:A:49:CYS:SG	0.61	2.36	20	2
1:A:63:ALA:HB1	1:A:68:GLN:CB	0.60	2.25	5	7
1:A:18:ARG:HA	1:A:50:LEU:HD11	0.60	1.73	3	2
1:A:69:LEU:O	1:A:72:VAL:HG23	0.59	1.97	8	1
1:A:14:LEU:HD13	1:A:14:LEU:O	0.59	1.97	18	2
1:A:60:LEU:HG	1:A:72:VAL:HG13	0.58	1.72	11	2
1:A:60:LEU:HD22	1:A:75:LEU:HB3	0.57	1.76	17	1
1:A:17:LEU:HD21	1:A:86:ILE:CG2	0.57	2.29	3	2
1:A:14:LEU:HD11	1:A:53:ALA:CB	0.57	2.27	14	1
1:A:38:LEU:HD22	1:A:81:ALA:HB1	0.57	1.74	17	3
1:A:14:LEU:CD1	1:A:57:LEU:HD11	0.57	2.30	5	1
1:A:14:LEU:HB2	1:A:83:LEU:HD11	0.57	1.76	7	3
1:A:30:LEU:HD12	1:A:44:THR:C	0.56	2.20	8	7
1:A:14:LEU:CB	1:A:83:LEU:HD21	0.56	2.30	14	1
1:A:38:LEU:HB2	1:A:81:ALA:HB1	0.56	1.77	13	1
1:A:60:LEU:HD12	1:A:75:LEU:CB	0.56	2.30	2	4
1:A:39:PHE:CZ	1:A:85:ALA:HB1	0.56	2.36	7	3
1:A:18:ARG:HA	1:A:50:LEU:HD13	0.56	1.77	15	1
1:A:44:THR:O	1:A:45:THR:HG23	0.56	2.01	17	2
1:A:22:ALA:HB3	1:A:23:PRO:CD	0.55	2.31	5	12
1:A:53:ALA:HB2	1:A:82:GLN:NE2	0.55	2.16	16	2
1:A:56:ASN:OD1	1:A:79:LEU:HD21	0.54	2.03	13	1
1:A:60:LEU:HD13	1:A:75:LEU:HD13	0.54	1.80	18	2
1:A:24:VAL:HG12	1:A:24:VAL:O	0.54	2.02	14	1
1:A:24:VAL:O	1:A:24:VAL:HG12	0.54	2.03	2	8
1:A:57:LEU:HA	1:A:79:LEU:HD11	0.53	1.80	15	3
1:A:39:PHE:CE2	1:A:85:ALA:HB1	0.53	2.38	8	1
1:A:18:ARG:HA	1:A:50:LEU:HD21	0.53	1.80	9	2
1:A:18:ARG:HG2	1:A:50:LEU:HD13	0.53	1.81	14	1
1:A:30:LEU:HD12	1:A:45:THR:N	0.53	2.18	14	2
1:A:63:ALA:HB1	1:A:68:GLN:CG	0.53	2.33	8	1
1:A:18:ARG:HH21	1:A:53:ALA:HB3	0.53	1.62	12	1
1:A:56:ASN:OD1	1:A:75:LEU:HD23	0.52	2.03	11	1
1:A:21:CYS:CB	1:A:50:LEU:HD11	0.52	2.35	5	1
1:A:14:LEU:HD22	1:A:57:LEU:HD12	0.52	1.82	12	1
1:A:60:LEU:HD11	1:A:72:VAL:CG1	0.52	2.29	9	1
1:A:69:LEU:N	1:A:70:PRO:CD	0.52	2.73	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:CYS:O	1:A:24:VAL:HG12	0.52	2.04	3	1
1:A:18:ARG:NH2	1:A:53:ALA:HB3	0.51	2.20	12	1
1:A:18:ARG:HG2	1:A:50:LEU:HD21	0.51	1.83	6	1
1:A:43:ALA:HA	1:A:48:ALA:HB1	0.51	1.83	11	1
1:A:59:ALA:O	1:A:63:ALA:HB2	0.51	2.06	20	3
1:A:43:ALA:HB1	1:A:49:CYS:SG	0.51	2.46	20	1
1:A:57:LEU:O	1:A:57:LEU:HD12	0.50	2.06	20	1
1:A:14:LEU:HD23	1:A:83:LEU:HG	0.50	1.83	19	1
1:A:69:LEU:N	1:A:70:PRO:HD2	0.50	2.22	15	8
1:A:63:ALA:HB1	1:A:68:GLN:CD	0.49	2.28	8	1
1:A:14:LEU:HB2	1:A:83:LEU:HD21	0.49	1.84	14	1
1:A:39:PHE:CZ	1:A:85:ALA:HB3	0.49	2.42	6	1
1:A:21:CYS:O	1:A:24:VAL:HG13	0.49	2.08	10	1
1:A:14:LEU:HD11	1:A:57:LEU:HD11	0.48	1.83	5	1
1:A:71:GLN:O	1:A:75:LEU:HD12	0.48	2.08	8	2
1:A:60:LEU:C	1:A:60:LEU:HD23	0.47	2.30	14	1
1:A:60:LEU:HD13	1:A:75:LEU:HB3	0.47	1.86	15	1
1:A:63:ALA:HB1	1:A:68:GLN:NE2	0.47	2.24	8	1
1:A:17:LEU:CD2	1:A:50:LEU:HD21	0.46	2.41	4	1
1:A:28:ALA:HA	1:A:46:LEU:HD12	0.46	1.87	20	2
1:A:60:LEU:HD13	1:A:75:LEU:HB2	0.46	1.87	4	1
1:A:42:ARG:O	1:A:48:ALA:HB1	0.45	2.11	2	3
1:A:14:LEU:HD12	1:A:83:LEU:HD11	0.45	1.88	12	1
1:A:14:LEU:HD22	1:A:57:LEU:HD13	0.45	1.87	7	1
1:A:39:PHE:CZ	1:A:85:ALA:CB	0.45	3.00	16	2
1:A:24:VAL:HG22	1:A:24:VAL:O	0.45	2.11	3	1
1:A:38:LEU:HD23	1:A:81:ALA:HB1	0.45	1.87	3	1
1:A:21:CYS:HB2	1:A:50:LEU:HD11	0.45	1.88	5	1
1:A:44:THR:HG23	1:A:45:THR:HG23	0.45	1.89	20	1
1:A:72:VAL:O	1:A:76:ALA:HB2	0.44	2.13	13	1
1:A:39:PHE:CE2	1:A:85:ALA:CB	0.43	3.01	6	1
1:A:17:LEU:HD23	1:A:50:LEU:CD2	0.43	2.41	4	1
1:A:17:LEU:HD12	1:A:20:ARG:HH12	0.43	1.73	17	1
1:A:14:LEU:CD1	1:A:83:LEU:HD12	0.43	2.44	6	1
1:A:22:ALA:N	1:A:23:PRO:CD	0.43	2.81	14	1
1:A:43:ALA:HB2	1:A:52:GLU:OE2	0.43	2.14	16	1
1:A:60:LEU:HD13	1:A:75:LEU:CB	0.43	2.44	4	1
1:A:17:LEU:HD21	1:A:86:ILE:CB	0.43	2.44	13	1
1:A:60:LEU:HD22	1:A:75:LEU:CB	0.43	2.43	17	1
1:A:39:PHE:N	1:A:39:PHE:CD1	0.42	2.86	5	1
1:A:30:LEU:HD12	1:A:44:THR:CA	0.42	2.45	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:CYS:SG	1:A:24:VAL:HG11	0.42	2.54	12	1
1:A:29:THR:H	1:A:46:LEU:HD12	0.42	1.75	11	1
1:A:21:CYS:HB3	1:A:50:LEU:HD11	0.42	1.91	15	2
1:A:13:GLN:HB3	1:A:83:LEU:HD11	0.42	1.91	15	1
1:A:60:LEU:CD1	1:A:72:VAL:HG13	0.41	2.45	10	1
1:A:22:ALA:CB	1:A:23:PRO:CD	0.41	2.98	5	5
1:A:14:LEU:CG	1:A:83:LEU:HD21	0.41	2.45	14	1
1:A:34:PHE:CD1	1:A:36:ARG:NH2	0.41	2.88	1	1
1:A:14:LEU:O	1:A:14:LEU:HD23	0.41	2.14	8	1
1:A:21:CYS:O	1:A:50:LEU:HD22	0.41	2.15	11	1
1:A:69:LEU:CB	1:A:70:PRO:CD	0.41	2.99	7	2
1:A:14:LEU:HD13	1:A:14:LEU:C	0.41	2.36	18	1
1:A:17:LEU:HD12	1:A:20:ARG:NH1	0.41	2.30	17	1
1:A:40:GLN:OE1	1:A:78:HIS:CE1	0.41	2.74	12	1
1:A:34:PHE:CD1	1:A:34:PHE:O	0.40	2.74	14	1
1:A:45:THR:OG1	1:A:48:ALA:HB2	0.40	2.17	9	1
1:A:60:LEU:CG	1:A:72:VAL:HG13	0.40	2.46	14	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	79/98 (81%)	77±1 (98±1%)	1±1 (2±1%)	0±0 (0±1%)	38	78
All	All	1580/1960 (81%)	1547 (98%)	26 (2%)	7 (0%)	38	78

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	43	ALA	7

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	60/77 (78%)	44±3 (73±5%)	16±3 (27±5%)	2 22
All	All	1200/1540 (78%)	880 (73%)	320 (27%)	2 22

All 47 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	74	TRP	16
1	A	83	LEU	16
1	A	71	GLN	15
1	A	47	GLN	13
1	A	19	GLN	12
1	A	40	GLN	12
1	A	55	ASP	12
1	A	61	ARG	12
1	A	42	ARG	11
1	A	20	ARG	11
1	A	17	LEU	10
1	A	88	ARG	10
1	A	18	ARG	9
1	A	35	ASP	9
1	A	14	LEU	9
1	A	27	PHE	8
1	A	66	GLN	8
1	A	82	GLN	8
1	A	13	GLN	7
1	A	75	LEU	7
1	A	89	GLU	7
1	A	36	ARG	7
1	A	65	GLU	6
1	A	21	CYS	6
1	A	37	HIS	6
1	A	33	ARG	6
1	A	49	CYS	6
1	A	78	HIS	5
1	A	51	ASP	5
1	A	25	SER	5
1	A	84	GLU	5
1	A	68	GLN	5
1	A	77	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	44	THR	4
1	A	57	LEU	4
1	A	31	SER	4
1	A	52	GLU	4
1	A	29	THR	3
1	A	26	GLN	2
1	A	45	THR	2
1	A	16	THR	2
1	A	38	LEU	1
1	A	46	LEU	1
1	A	39	PHE	1
1	A	67	GLN	1
1	A	69	LEU	1
1	A	60	LEU	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 monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% 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 (i)

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	1231
Number of shifts mapped to atoms	1231
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	96	-0.53 ± 0.09	Should be checked
$^{13}C_{\beta}$	94	0.17 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	96	-0.37 ± 0.13	None needed (< 0.5 ppm)
^{15}N	93	-0.31 ± 0.37	None needed (< 0.5 ppm)

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 91%, i.e. 989 atoms were assigned a chemical shift out of a possible 1087. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	393/393 (100%)	158/158 (100%)	158/158 (100%)	77/77 (100%)
Sidechain	550/628 (88%)	377/410 (92%)	157/186 (84%)	16/32 (50%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	46/66 (70%)	23/33 (70%)	22/26 (85%)	1/7 (14%)
Overall	989/1087 (91%)	558/601 (93%)	337/370 (91%)	94/116 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1231 atoms were assigned a chemical shift out of a possible 1372. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	476/488 (98%)	191/196 (97%)	192/196 (98%)	93/96 (97%)
Sidechain	689/794 (87%)	472/519 (91%)	201/238 (84%)	16/37 (43%)
Aromatic	66/90 (73%)	33/45 (73%)	30/36 (83%)	3/9 (33%)
Overall	1231/1372 (90%)	696/760 (92%)	423/470 (90%)	112/142 (79%)

7.1.4 Statistically unusual chemical shifts (i)

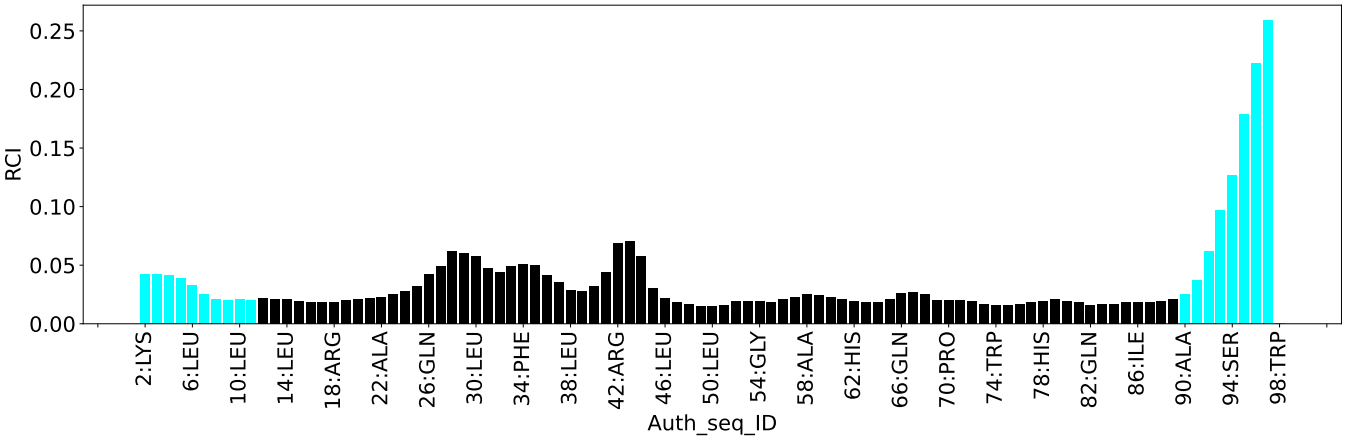
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	82	GLN	HG3	0.70	0.91 – 3.68	-5.8
1	A	40	GLN	H	11.23	5.39 – 11.05	5.3

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:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
2:LYS
6:LEU
10:LEU
14:LEU
18:ARG
22:ALA
26:GLN
30:LEU
34:PHE
38:LEU
42:ARG
46:LEU
50:LEU
54:GLY
58:ALA
62:HIS
66:GLN
70:PRO
74:TRP
78:HIS
82:GLN
86:ILE
90:ALA
94:SER
98:TRP
Auth_seq_ID

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	992
Intra-residue (|i-j|=0)	296
Sequential (|i-j|=1)	309
Medium range (|i-j|>1 and |i-j|<5)	172
Long range (|i-j|≥5)	123
Inter-chain	0
Hydrogen bond restraints	92
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	1.3

[1]Long 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 violations

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

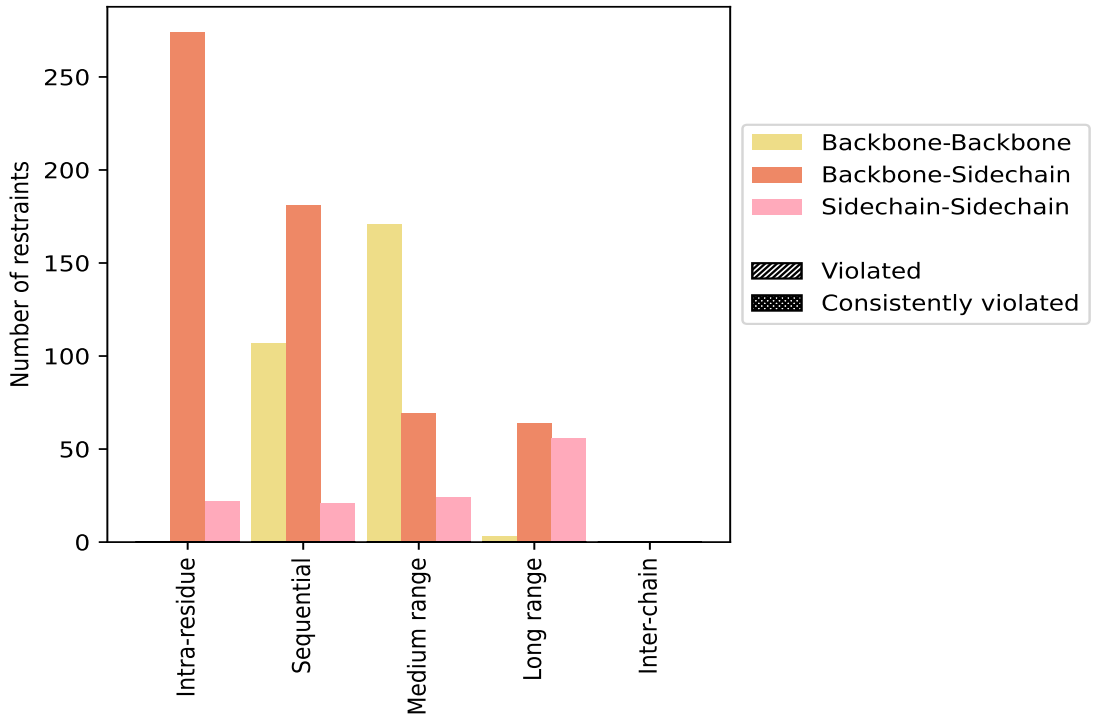
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	296	29.8	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	274	27.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	22	2.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	309	31.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	107	10.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	181	18.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	21	2.1	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	172	17.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	79	8.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	69	7.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	24	2.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	123	12.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	3	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	64	6.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	56	5.6	0	0.0	0.0	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	9.3	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	992	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	281	28.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	588	59.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	123	12.4	0	0.0	0.0	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)

No violations found

9.3 Distance violation statistics for the ensemble (i)

No violations found

9.4 Most violated distance restraints in the ensemble (i)

No violations found

9.5 All violated distance restraints (i)

No violations found

10 Dihedral-angle violation analysis (i)

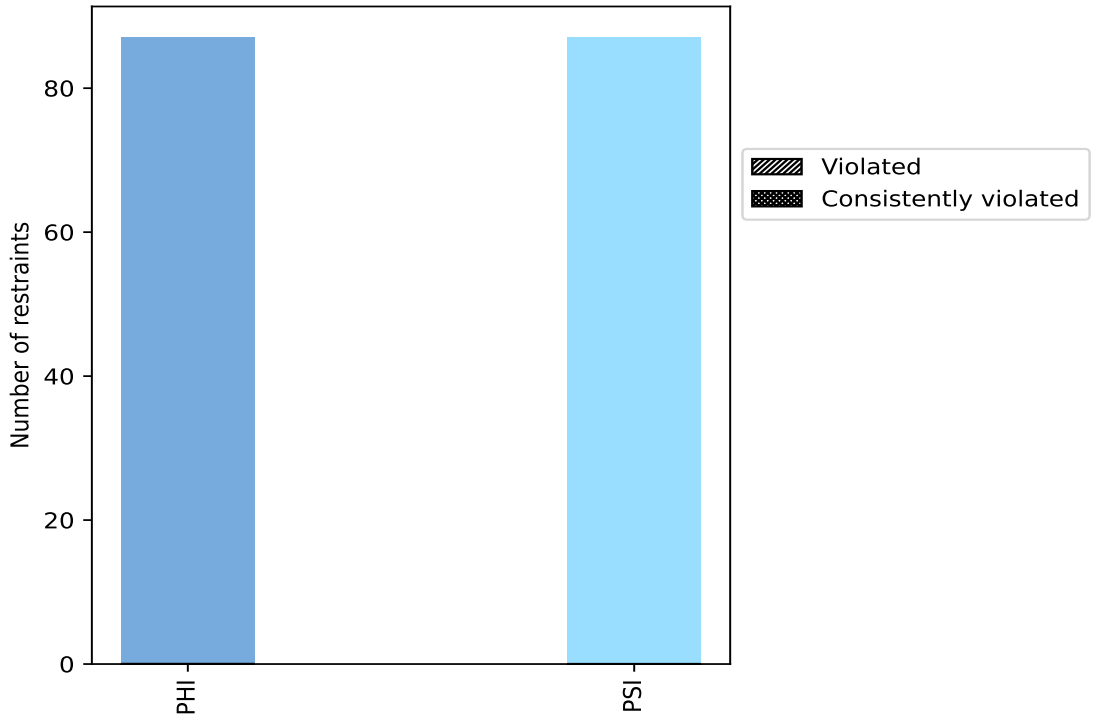
10.1 Summary of dihedral-angle violations (i)

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	87	50.0	0	0.0	0.0	0	0.0	0.0
PSI	87	50.0	0	0.0	0.0	0	0.0	0.0
Total	174	100.0	0	0.0	0.0	0	0.0	0.0

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

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



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

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

No violations found

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

No violations found

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

No violations found

10.5 All violated dihedral-angle restraints (i)

No violations found