Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 10:17 AM EDT

PDB ID	:	2RU8
BMRB ID	:	11549
Title	:	DnaT C-terminal domain
Authors	:	Abe, Y.; Tani, J.; Fujiyama, S.; Urabe, M.; Sato, K.; Aramaki, T.; Katayama, T.; Ueda, T.
Deposited on	:	2014-01-29

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

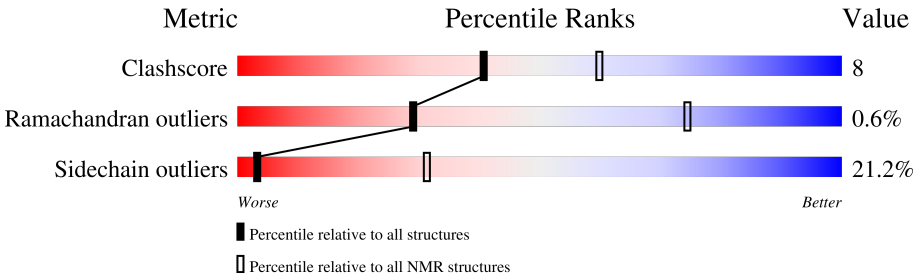
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 92%.

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	51% 13% • 29% 6%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:88-A:151 (64)	0.82	15

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. No single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 7, 9, 10, 11, 13, 15, 17, 18, 19, 20
2	4, 8, 12, 14
3	2, 5, 16

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1451 atoms, of which 715 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Primosomal protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	92	1451	473	715	130	131	2	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	expression tag	UNP P0A8J2
A	180	HIS	-	expression tag	UNP P0A8J2
A	181	HIS	-	expression tag	UNP P0A8J2
A	182	HIS	-	expression tag	UNP P0A8J2
A	183	HIS	-	expression tag	UNP P0A8J2
A	184	HIS	-	expression tag	UNP P0A8J2
A	185	HIS	-	expression tag	UNP P0A8J2

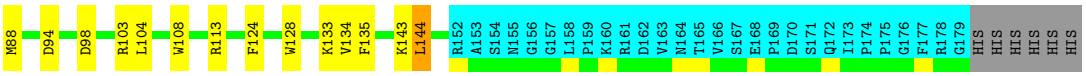
4 Residue-property plots

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 protein 1

Chain A:



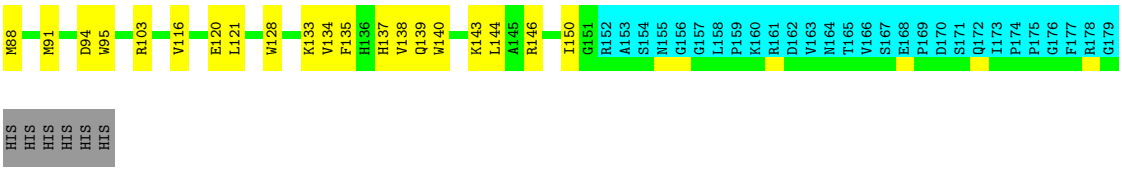
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Primosomal protein 1

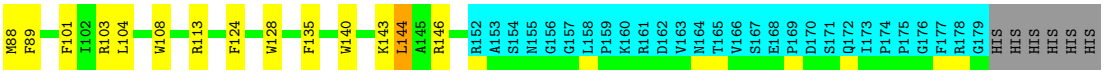
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Primosomal protein 1

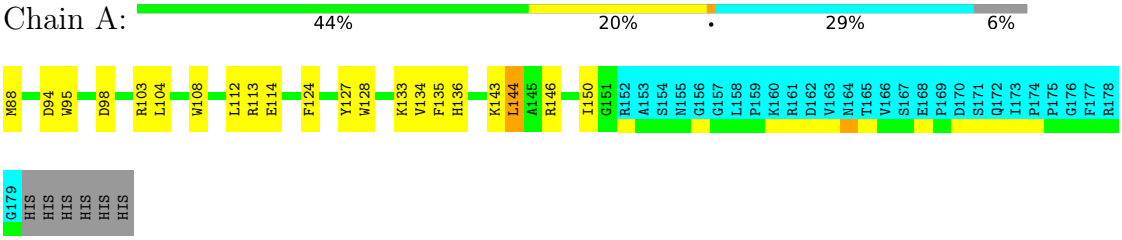
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Primosomal protein 1

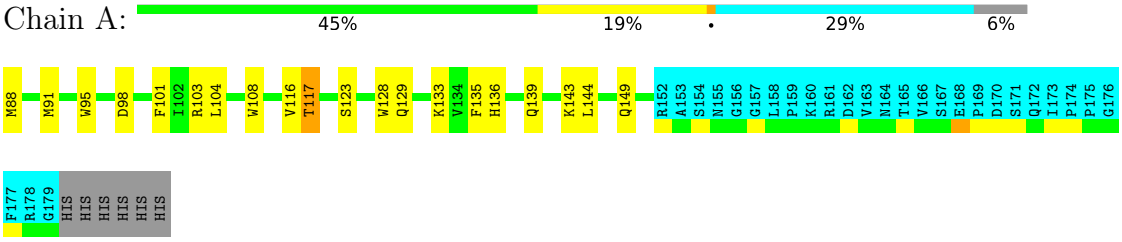
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Primosomal protein 1

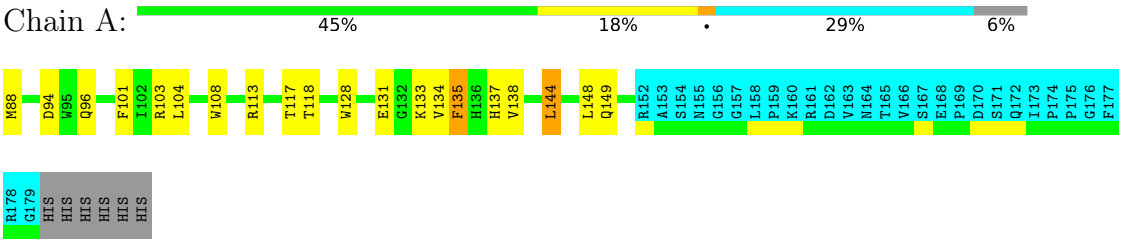
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Primosomal protein 1

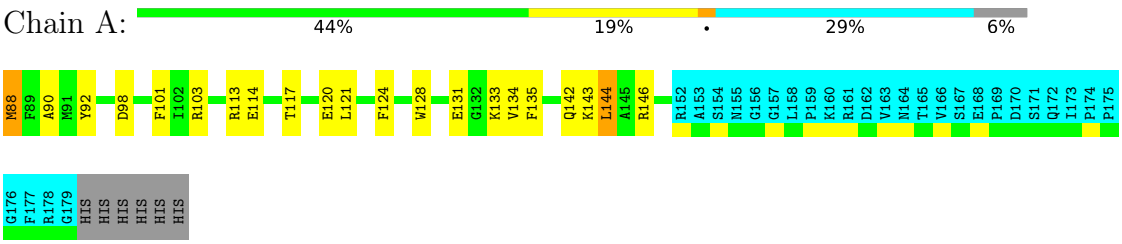
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Primosomal protein 1

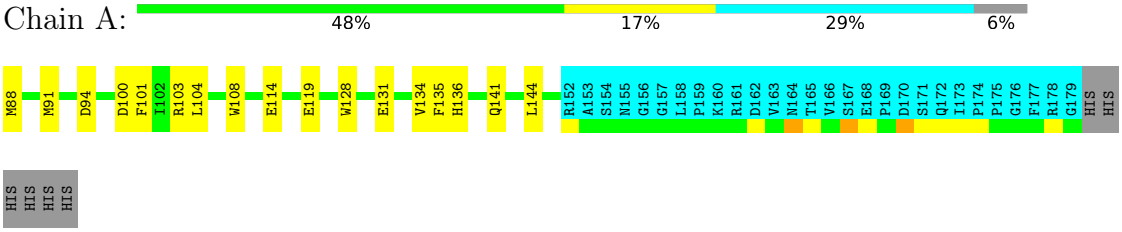
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Primosomal protein 1

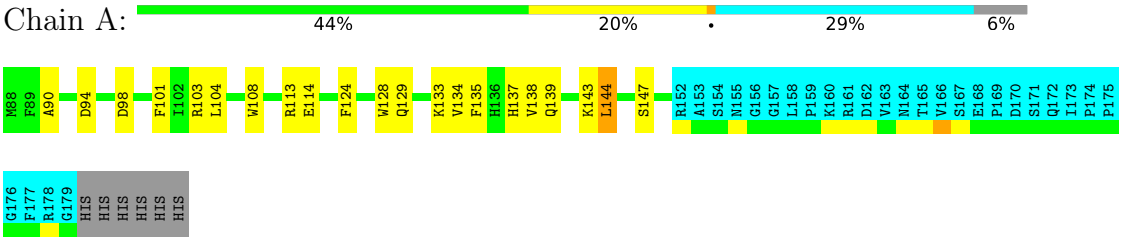
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Primosomal protein 1

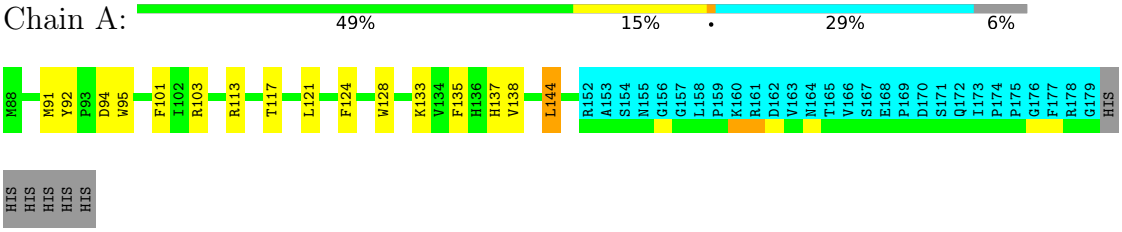
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Primosomal protein 1

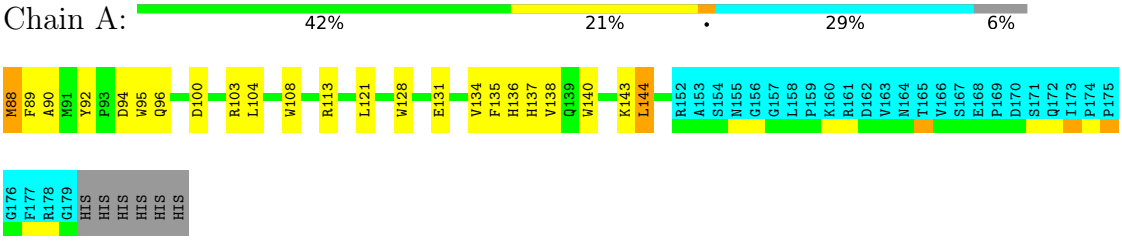
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Primosomal protein 1

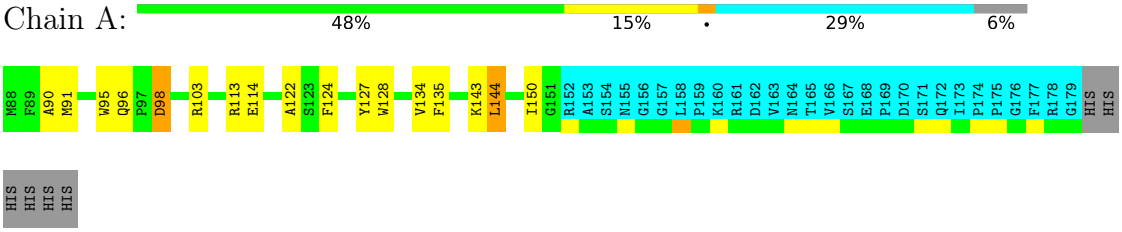
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Primosomal protein 1

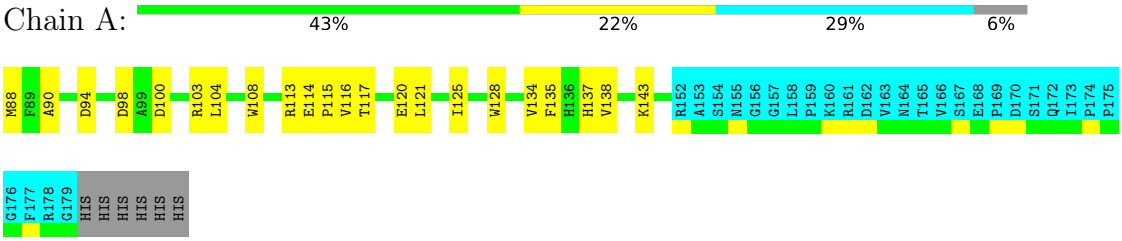
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Primosomal protein 1

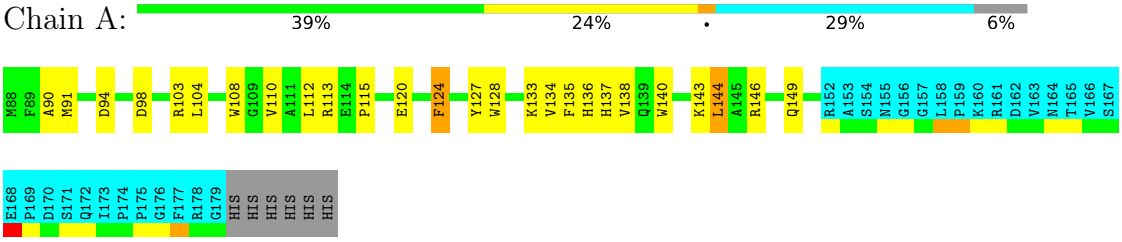
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Primosomal protein 1

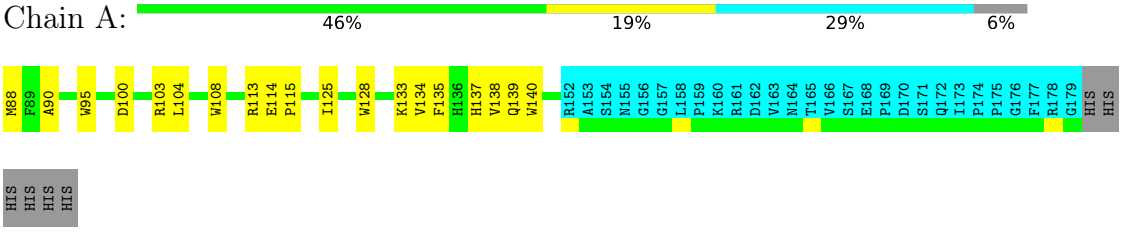
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Primosomal protein 1

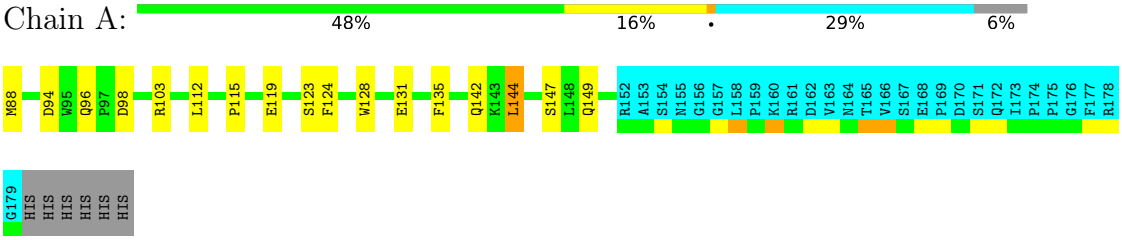
Chain A:



4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Primosomal protein 1

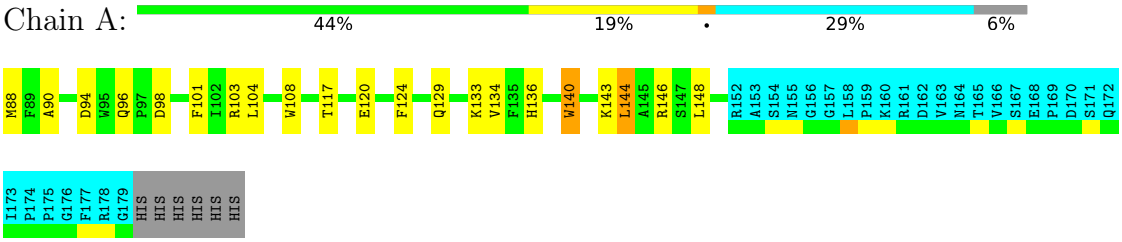
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Primosomal protein 1

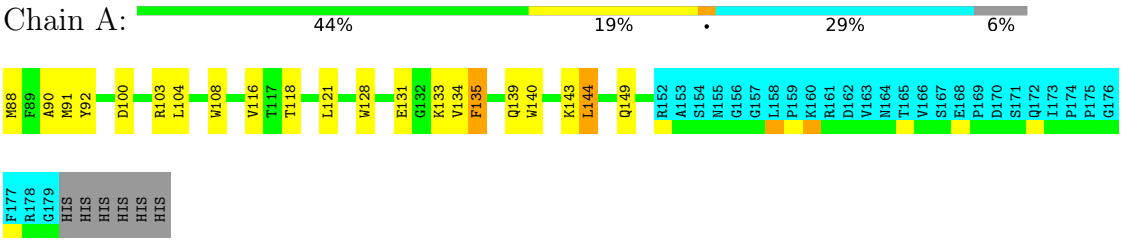
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Primosomal protein 1

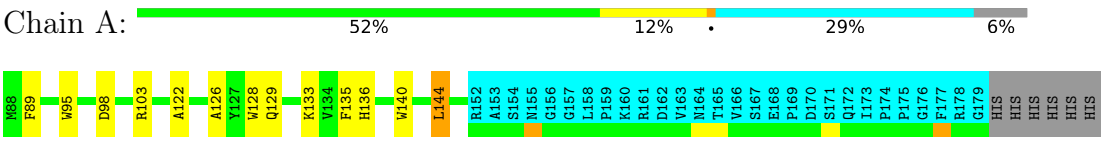
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Primosomal protein 1

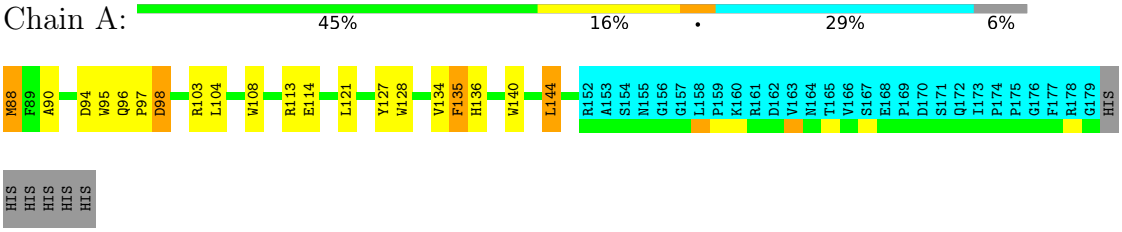
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Primosomal protein 1

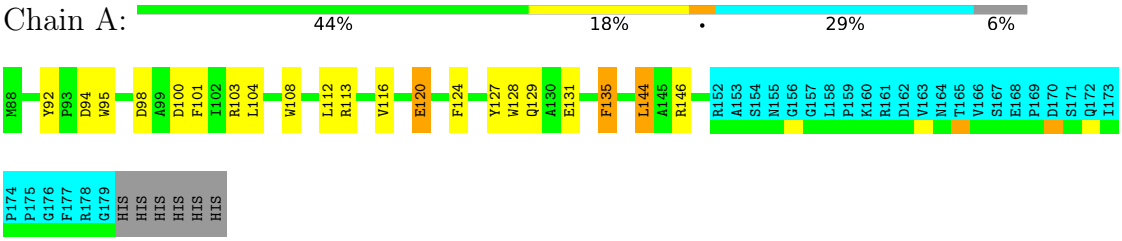
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Primosomal protein 1

Chain A:



5 Refinement protocol and experimental data overview

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
CNS	refinement	
CYANA	structure solution	2.1

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	1123
Number of shifts mapped to atoms	1123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	529	513	508	8±3
All	All	10580	10260	10160	156

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LEU:HD23	1:A:108:TRP:CZ2	0.82	2.09	12	6
1:A:124:PHE:CZ	1:A:144:LEU:HD12	0.80	2.11	20	8
1:A:116:VAL:HG11	1:A:121:LEU:HD13	0.80	1.52	1	2
1:A:116:VAL:HG23	1:A:120:GLU:OE1	0.72	1.84	12	2
1:A:97:PRO:CG	1:A:121:LEU:HD21	0.70	2.17	19	1
1:A:137:HIS:CD2	1:A:138:VAL:HG23	0.69	2.23	8	1
1:A:90:ALA:HB2	1:A:134:VAL:HG13	0.69	1.63	19	2
1:A:137:HIS:CE1	1:A:138:VAL:HG23	0.67	2.24	14	5
1:A:101:PHE:CZ	1:A:144:LEU:HD21	0.65	2.27	6	1
1:A:104:LEU:HD13	1:A:108:TRP:CZ2	0.65	2.26	16	5
1:A:140:TRP:CH2	1:A:144:LEU:HD13	0.63	2.29	17	4
1:A:140:TRP:CZ3	1:A:144:LEU:HD13	0.61	2.30	16	3
1:A:104:LEU:HD22	1:A:108:TRP:CZ2	0.59	2.33	20	3
1:A:124:PHE:CE2	1:A:144:LEU:HD12	0.59	2.33	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:LEU:HD22	1:A:148:LEU:HD11	0.57	1.74	5	1
1:A:110:VAL:HG12	1:A:112:LEU:HD12	0.56	1.76	13	1
1:A:101:PHE:CE1	1:A:112:LEU:HD11	0.56	2.36	20	1
1:A:104:LEU:HD23	1:A:108:TRP:CH2	0.56	2.36	17	4
1:A:88:MET:HB3	1:A:134:VAL:HG12	0.55	1.77	10	9
1:A:90:ALA:HB2	1:A:134:VAL:HG22	0.52	1.80	10	4
1:A:128:TRP:CZ3	1:A:135:PHE:CZ	0.52	2.97	19	1
1:A:90:ALA:CB	1:A:134:VAL:HG13	0.51	2.33	19	2
1:A:128:TRP:CZ3	1:A:135:PHE:CE2	0.51	2.99	8	17
1:A:116:VAL:CG1	1:A:121:LEU:HD13	0.51	2.31	1	1
1:A:128:TRP:CE3	1:A:135:PHE:CE2	0.50	3.00	6	6
1:A:104:LEU:HD22	1:A:108:TRP:CE2	0.50	2.41	14	2
1:A:137:HIS:CE1	1:A:138:VAL:CG2	0.48	2.97	14	4
1:A:90:ALA:N	1:A:134:VAL:HG13	0.48	2.24	10	8
1:A:137:HIS:NE2	1:A:138:VAL:HG23	0.48	2.24	10	2
1:A:110:VAL:HG12	1:A:112:LEU:CD1	0.48	2.39	13	1
1:A:104:LEU:CD2	1:A:108:TRP:CZ2	0.46	2.98	17	2
1:A:88:MET:HB2	1:A:134:VAL:HG12	0.45	1.88	7	1
1:A:122:ALA:O	1:A:126:ALA:HB2	0.45	2.11	18	1
1:A:140:TRP:CH2	1:A:144:LEU:CD1	0.45	2.99	19	2
1:A:144:LEU:O	1:A:148:LEU:HD23	0.45	2.11	16	1
1:A:104:LEU:HD22	1:A:108:TRP:NE1	0.45	2.26	14	2
1:A:97:PRO:HG3	1:A:121:LEU:HD11	0.45	1.89	19	1
1:A:92:TYR:CD1	1:A:92:TYR:N	0.44	2.85	9	1
1:A:108:TRP:CE2	1:A:141:GLN:HB3	0.43	2.49	7	1
1:A:136:HIS:CD2	1:A:136:HIS:N	0.43	2.87	7	2
1:A:121:LEU:O	1:A:125:ILE:HD12	0.43	2.14	12	1
1:A:116:VAL:HG12	1:A:117:THR:N	0.42	2.29	4	1
1:A:90:ALA:CB	1:A:134:VAL:HG22	0.42	2.43	19	1
1:A:104:LEU:HD13	1:A:108:TRP:CH2	0.42	2.49	20	1
1:A:137:HIS:CD2	1:A:138:VAL:CG2	0.42	2.99	8	1
1:A:95:TRP:O	1:A:95:TRP:CE3	0.42	2.73	11	9
1:A:101:PHE:CE1	1:A:112:LEU:CD1	0.42	3.02	20	1
1:A:128:TRP:O	1:A:128:TRP:CE3	0.41	2.73	19	1
1:A:146:ARG:CD	1:A:150:ILE:HD11	0.41	2.45	1	1
1:A:90:ALA:HB2	1:A:134:VAL:CG1	0.41	2.40	19	1
1:A:135:PHE:CD1	1:A:135:PHE:N	0.41	2.89	19	1
1:A:104:LEU:O	1:A:108:TRP:CG	0.41	2.74	3	7
1:A:88:MET:O	1:A:89:PHE:CD1	0.41	2.74	2	1
1:A:108:TRP:CE2	1:A:141:GLN:CB	0.41	3.03	7	1
1:A:97:PRO:HG2	1:A:121:LEU:HD21	0.41	1.91	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:TRP:CZ2	1:A:125:ILE:HG12	0.40	2.52	14	1
1:A:146:ARG:O	1:A:150:ILE:HD12	0.40	2.15	1	1
1:A:89:PHE:CD1	1:A:89:PHE:O	0.40	2.74	10	1
1:A:95:TRP:CE3	1:A:95:TRP:O	0.40	2.74	20	1
1:A:100:ASP:OD1	1:A:104:LEU:HD13	0.40	2.15	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	63/98 (64%)	59±1 (93±2%)	4±1 (7±2%)	0±0 (1±1%)	29	74
All	All	1260/1960 (64%)	1171 (93%)	82 (7%)	7 (1%)	29	74

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	115	PRO	4
1	A	98	ASP	3

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	52/81 (64%)	41±3 (79±5%)	11±3 (21±5%)	3	31
All	All	1040/1620 (64%)	819 (79%)	221 (21%)	3	31

All 35 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	103	ARG	20
1	A	144	LEU	18
1	A	94	ASP	13
1	A	113	ARG	13
1	A	133	LYS	12
1	A	143	LYS	12
1	A	98	ASP	11
1	A	114	GLU	8
1	A	91	MET	7
1	A	101	PHE	7
1	A	131	GLU	7
1	A	146	ARG	6
1	A	136	HIS	6
1	A	88	MET	6
1	A	117	THR	6
1	A	96	GLN	6
1	A	120	GLU	5
1	A	139	GLN	5
1	A	127	TYR	5
1	A	129	GLN	5
1	A	149	GLN	5
1	A	100	ASP	5
1	A	140	TRP	4
1	A	135	PHE	4
1	A	92	TYR	4
1	A	124	PHE	3
1	A	121	LEU	3
1	A	112	LEU	2
1	A	150	ILE	2
1	A	123	SER	2
1	A	118	THR	2
1	A	142	GLN	2
1	A	119	GLU	2
1	A	147	SER	2
1	A	89	PHE	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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 88% 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	1123
Number of shifts mapped to atoms	1123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	91	-0.17 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	84	-0.16 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	83	-0.31 ± 0.09	None needed (< 0.5 ppm)
^{15}N	84	0.02 ± 0.25	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 92%, i.e. 840 atoms were assigned a chemical shift out of a possible 913. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	311/317 (98%)	127/128 (99%)	124/128 (97%)	60/61 (98%)
Sidechain	425/474 (90%)	291/311 (94%)	129/146 (88%)	5/17 (29%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	104/122 (85%)	52/60 (87%)	48/54 (89%)	4/8 (50%)
Overall	840/913 (92%)	470/499 (94%)	301/328 (92%)	69/86 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1123 atoms were assigned a chemical shift out of a possible 1269. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	440/453 (97%)	182/184 (99%)	174/184 (95%)	84/85 (99%)
Sidechain	575/684 (84%)	397/445 (89%)	173/209 (83%)	5/30 (17%)
Aromatic	108/132 (82%)	54/65 (83%)	50/59 (85%)	4/8 (50%)
Overall	1123/1269 (88%)	633/694 (91%)	397/452 (88%)	93/123 (76%)

7.1.4 Statistically unusual chemical shifts (i)

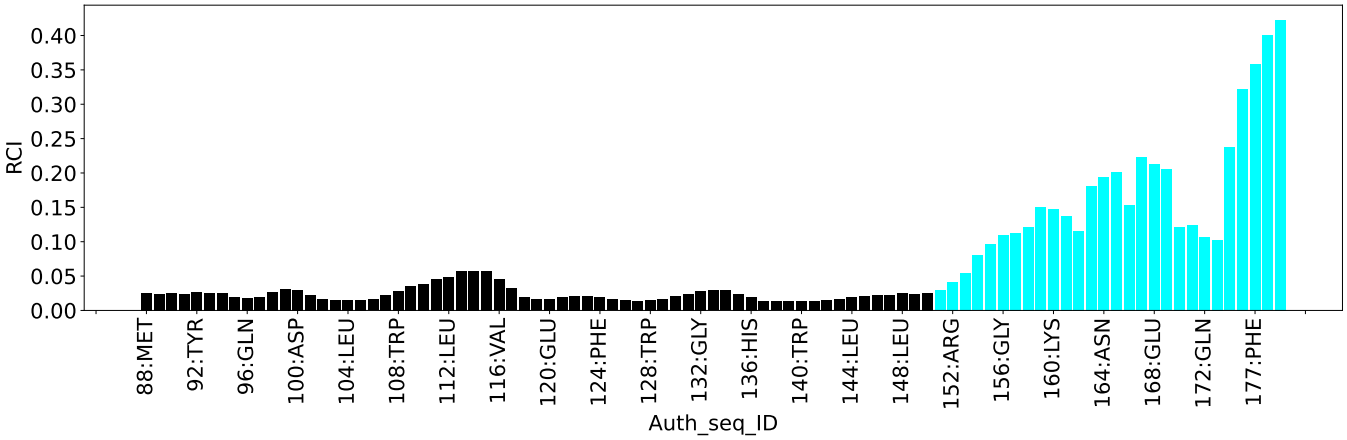
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	143	LYS	HE3	1.30	1.92 – 3.89	-8.1
1	A	143	LYS	HE2	1.37	1.95 – 3.88	-8.0
1	A	135	PHE	HB3	-0.10	1.03 – 4.85	-8.0
1	A	91	MET	HE1	-0.71	-0.03 – 3.80	-6.8
1	A	91	MET	HE2	-0.71	-0.03 – 3.80	-6.8
1	A	91	MET	HE3	-0.71	-0.03 – 3.80	-6.8
1	A	142	GLN	HG3	0.43	0.91 – 3.68	-6.7
1	A	143	LYS	HD3	0.29	0.54 – 2.65	-6.2
1	A	135	PHE	HD2	5.50	5.52 – 8.61	-5.0
1	A	135	PHE	HD1	5.50	5.51 – 8.60	-5.0

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
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
88:MET
92:TYR
96:GLN
100:ASP
104:LEU
108:TRP
112:LEU
116:VAL
120:GLU
124:PHE
128:TRP
132:GLY
136:HIS
140:TRP
144:LEU
148:LEU
152:ARG
156:GLY
160:LYS
164:ASN
168:GLU
172:GLN
177:PHE
Auth_seq_ID

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	804
Intra-residue (|i-j|=0)	251
Sequential (|i-j|=1)	243
Medium range (|i-j|>1 and |i-j|<5)	157
Long range (|i-j|≥5)	101
Inter-chain	0
Hydrogen bond restraints	52
Disulfide bond restraints	0
Total dihedral-angle restraints	110
Number of unmapped restraints	0
Number of restraints per residue	9.3
Number of long range restraints per residue[1]	1.1

[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

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.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis (i)

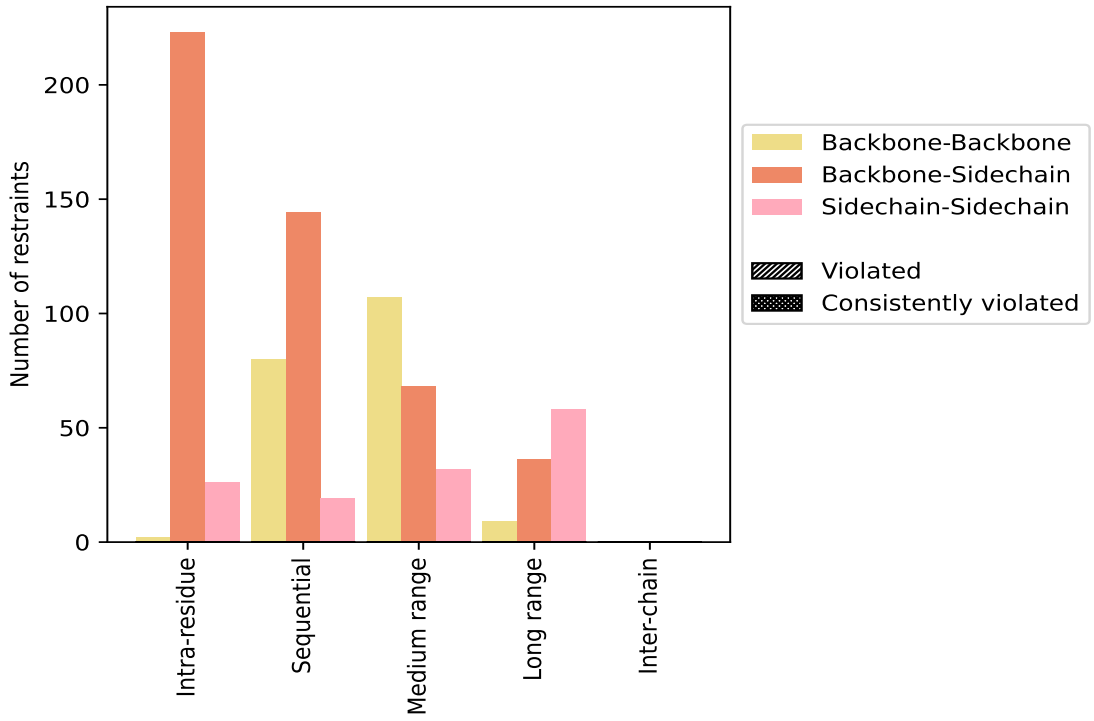
9.1 Summary of distance violations (i)

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)	251	31.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	223	27.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	26	3.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	243	30.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	80	10.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	144	17.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	19	2.4	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	157	19.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	57	7.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	68	8.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	32	4.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	101	12.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	7	0.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	36	4.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	58	7.2	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	52	6.5	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	804	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	198	24.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	471	58.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	135	16.8	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



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

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis

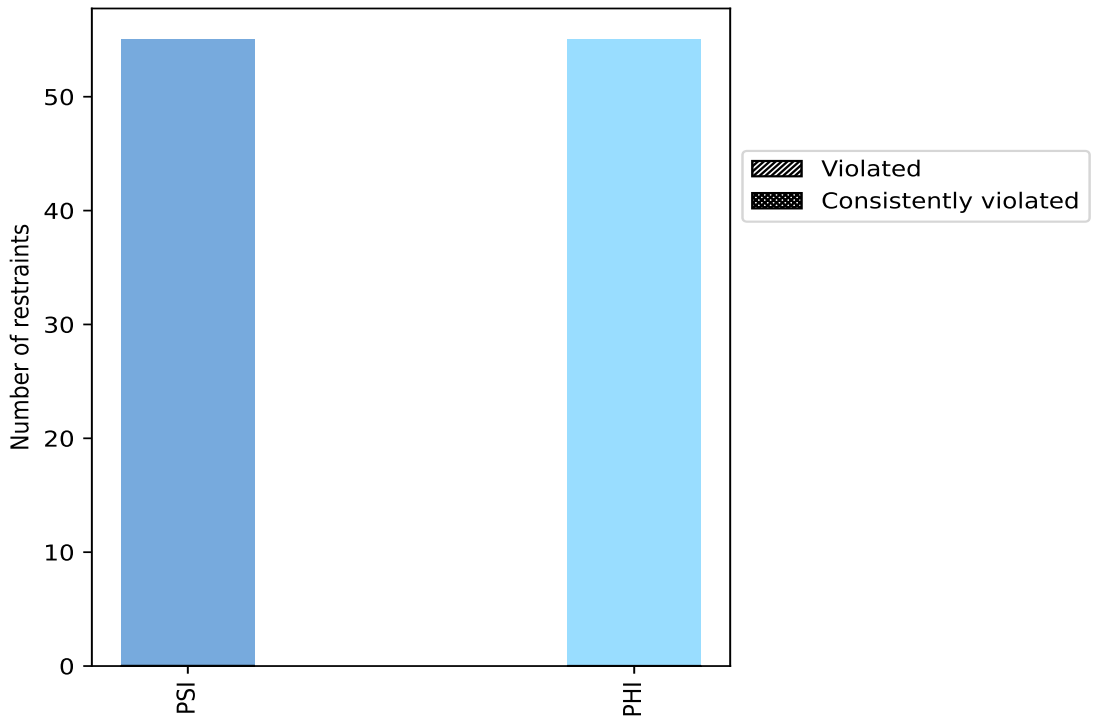
10.1 Summary of dihedral-angle violations

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]
PSI	55	50.0	0	0.0	0.0	0	0.0	0.0
PHI	55	50.0	0	0.0	0.0	0	0.0	0.0
Total	110	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



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