



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:21 PM UTC

PDB ID : 6YEG / pdb_00006yeg
EMDB ID : EMD-10792
BMRB ID : 27468
Title : Hybrid structure of the SPP1 tail tube by solid-state NMR and cryo EM - Final EM Refinement
Authors : Zinke, M.; Sachowsky, K.A.A.; Zinn-Justin, S.; Ravelli, R.; Schroder, G.F.; Habeck, M.; Lange, A.
Deposited on : 2020-03-24

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **NOT EXECUTED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **NOT EXECUTED**
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

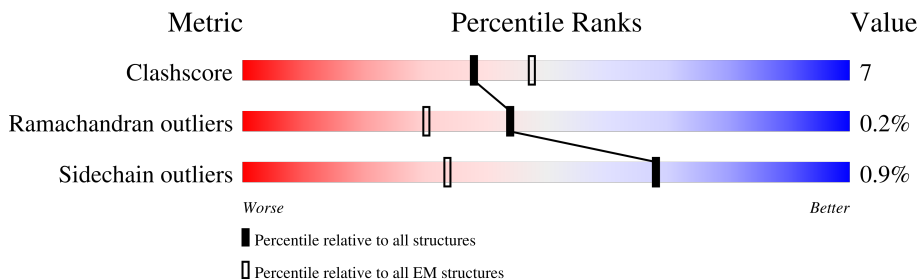
The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY, SOLID-STATE NMR

The reported resolution of this entry is 4.00 Å.

The overall completeness of chemical shifts assignment is 4%.

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	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	180	75% 20% . .
1	B	180	78% 17% . .
1	C	180	75% 20% . .
1	D	180	79% 16% . .
1	E	180	78% 17% . .
1	F	180	81% 15% .
1	G	180	71% 24% . .
1	H	180	77% 18% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	180	 76%19% . .
1	J	180	 75%20% . .
1	K	180	 76%19% . .
1	L	180	 72%23% . .

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tail tube protein gp17.1*.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	B	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	C	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	D	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	E	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	F	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	G	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	H	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	I	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	J	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	K	172	Total	C	N	O	S	0	
			1313	821	216	275	1		
1	L	172	Total	C	N	O	S	0	
			1313	821	216	275	1		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP O48449
A	178	HIS	-	expression tag	UNP O48449
A	179	HIS	-	expression tag	UNP O48449
A	180	HIS	-	expression tag	UNP O48449
A	181	HIS	-	expression tag	UNP O48449
A	182	HIS	-	expression tag	UNP O48449

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	-	expression tag	UNP O48449
B	4	MET	-	initiating methionine	UNP O48449
B	178	HIS	-	expression tag	UNP O48449
B	179	HIS	-	expression tag	UNP O48449
B	180	HIS	-	expression tag	UNP O48449
B	181	HIS	-	expression tag	UNP O48449
B	182	HIS	-	expression tag	UNP O48449
B	183	HIS	-	expression tag	UNP O48449
C	4	MET	-	initiating methionine	UNP O48449
C	178	HIS	-	expression tag	UNP O48449
C	179	HIS	-	expression tag	UNP O48449
C	180	HIS	-	expression tag	UNP O48449
C	181	HIS	-	expression tag	UNP O48449
C	182	HIS	-	expression tag	UNP O48449
C	183	HIS	-	expression tag	UNP O48449
D	4	MET	-	initiating methionine	UNP O48449
D	178	HIS	-	expression tag	UNP O48449
D	179	HIS	-	expression tag	UNP O48449
D	180	HIS	-	expression tag	UNP O48449
D	181	HIS	-	expression tag	UNP O48449
D	182	HIS	-	expression tag	UNP O48449
D	183	HIS	-	expression tag	UNP O48449
E	4	MET	-	initiating methionine	UNP O48449
E	178	HIS	-	expression tag	UNP O48449
E	179	HIS	-	expression tag	UNP O48449
E	180	HIS	-	expression tag	UNP O48449
E	181	HIS	-	expression tag	UNP O48449
E	182	HIS	-	expression tag	UNP O48449
E	183	HIS	-	expression tag	UNP O48449
F	4	MET	-	initiating methionine	UNP O48449
F	178	HIS	-	expression tag	UNP O48449
F	179	HIS	-	expression tag	UNP O48449
F	180	HIS	-	expression tag	UNP O48449
F	181	HIS	-	expression tag	UNP O48449
F	182	HIS	-	expression tag	UNP O48449
F	183	HIS	-	expression tag	UNP O48449
G	4	MET	-	initiating methionine	UNP O48449
G	178	HIS	-	expression tag	UNP O48449
G	179	HIS	-	expression tag	UNP O48449
G	180	HIS	-	expression tag	UNP O48449
G	181	HIS	-	expression tag	UNP O48449
G	182	HIS	-	expression tag	UNP O48449

Continued on next page...

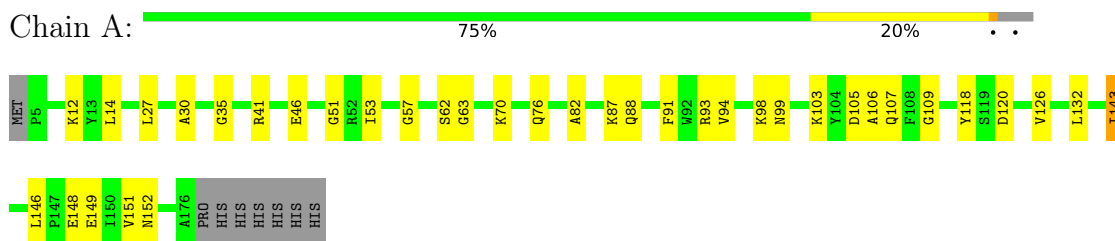
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	183	HIS	-	expression tag	UNP O48449
H	4	MET	-	initiating methionine	UNP O48449
H	178	HIS	-	expression tag	UNP O48449
H	179	HIS	-	expression tag	UNP O48449
H	180	HIS	-	expression tag	UNP O48449
H	181	HIS	-	expression tag	UNP O48449
H	182	HIS	-	expression tag	UNP O48449
H	183	HIS	-	expression tag	UNP O48449
I	4	MET	-	initiating methionine	UNP O48449
I	178	HIS	-	expression tag	UNP O48449
I	179	HIS	-	expression tag	UNP O48449
I	180	HIS	-	expression tag	UNP O48449
I	181	HIS	-	expression tag	UNP O48449
I	182	HIS	-	expression tag	UNP O48449
I	183	HIS	-	expression tag	UNP O48449
J	4	MET	-	initiating methionine	UNP O48449
J	178	HIS	-	expression tag	UNP O48449
J	179	HIS	-	expression tag	UNP O48449
J	180	HIS	-	expression tag	UNP O48449
J	181	HIS	-	expression tag	UNP O48449
J	182	HIS	-	expression tag	UNP O48449
J	183	HIS	-	expression tag	UNP O48449
K	4	MET	-	initiating methionine	UNP O48449
K	178	HIS	-	expression tag	UNP O48449
K	179	HIS	-	expression tag	UNP O48449
K	180	HIS	-	expression tag	UNP O48449
K	181	HIS	-	expression tag	UNP O48449
K	182	HIS	-	expression tag	UNP O48449
K	183	HIS	-	expression tag	UNP O48449
L	4	MET	-	initiating methionine	UNP O48449
L	178	HIS	-	expression tag	UNP O48449
L	179	HIS	-	expression tag	UNP O48449
L	180	HIS	-	expression tag	UNP O48449
L	181	HIS	-	expression tag	UNP O48449
L	182	HIS	-	expression tag	UNP O48449
L	183	HIS	-	expression tag	UNP O48449

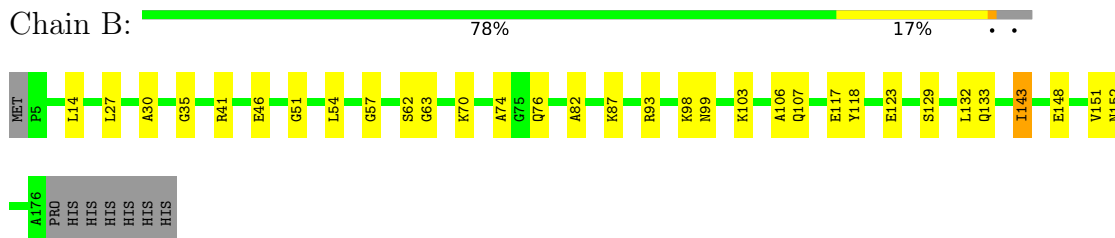
4 Residue-property plots [i](#)

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.

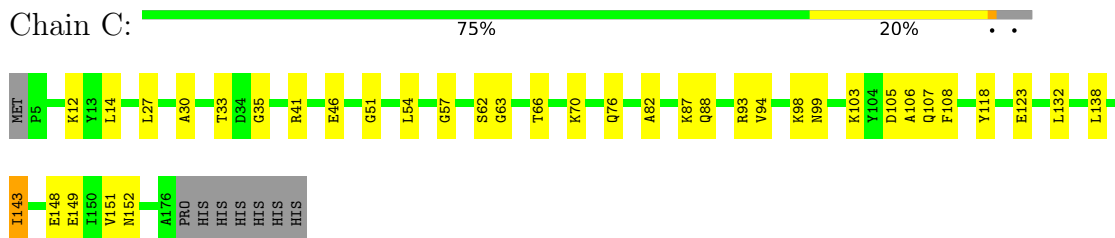
• Molecule 1: Tail tube protein gp17.1*



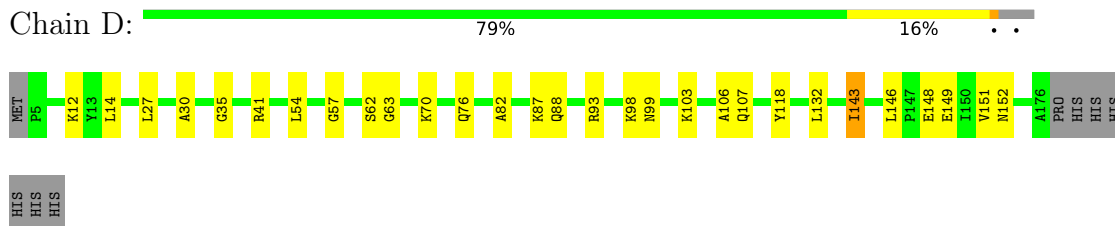
• Molecule 1: Tail tube protein gp17.1*



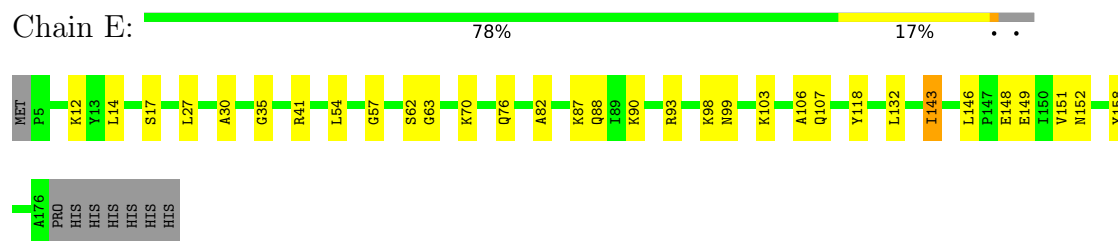
• Molecule 1: Tail tube protein gp17.1*



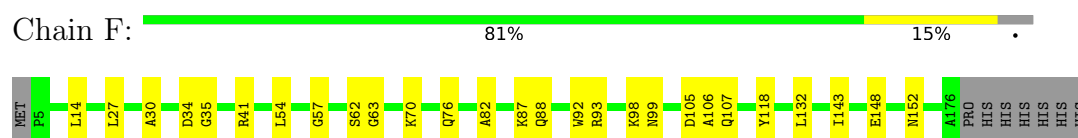
• Molecule 1: Tail tube protein gp17.1*



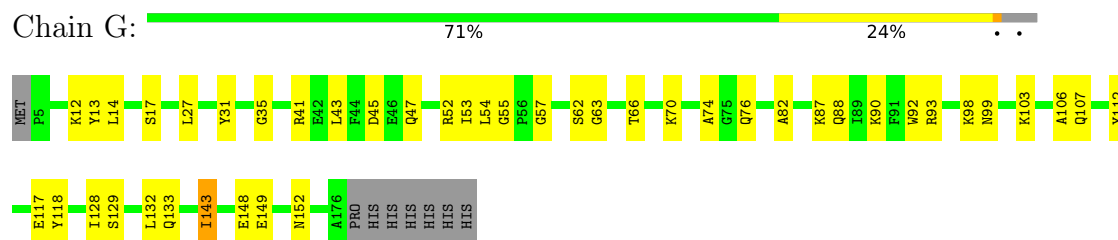
- Molecule 1: Tail tube protein gp17.1*



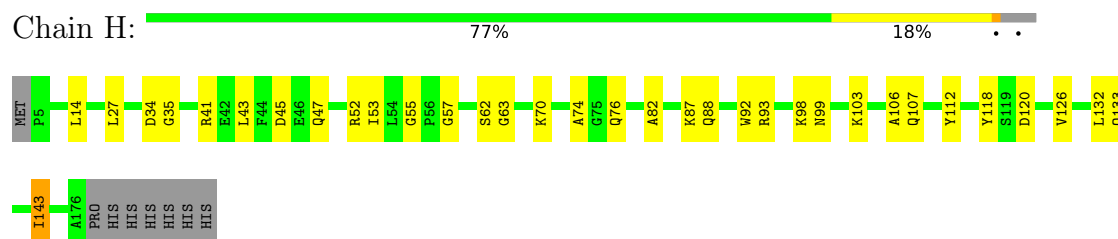
- Molecule 1: Tail tube protein gp17.1*



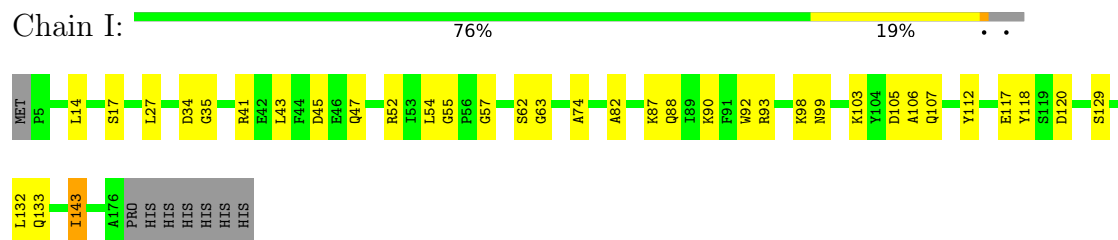
- Molecule 1: Tail tube protein gp17.1*



- Molecule 1: Tail tube protein gp17.1*

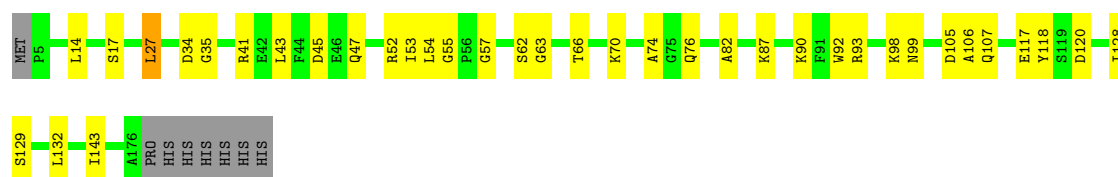


- Molecule 1: Tail tube protein gp17.1*



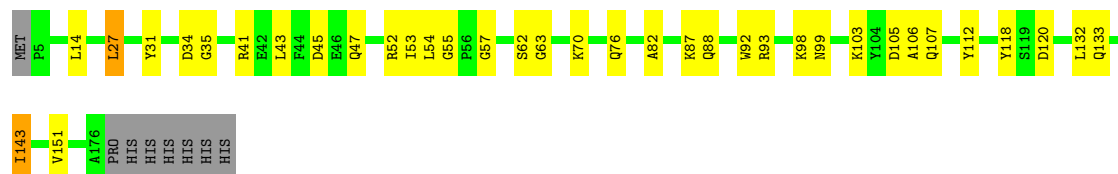
- Molecule 1: Tail tube protein gp17.1*





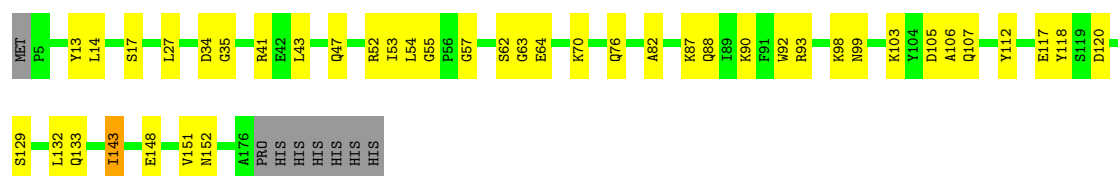
- Molecule 1: Tail tube protein gp17.1*

Chain K: 76% 19% ..



- Molecule 1: Tail tube protein gp17.1*

Chain L: 72% 23% ..



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *all calculated structures submitted*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Inferential Structure Determination (ISD)	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	963
Number of shifts mapped to atoms	655
Number of unparsed shifts	0
Number of shifts with mapping errors	308
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	0.28	0/1338 (0.0%)	0.65	1/1809 (0.1%)
1	B	0.29	0/1338 (0.0%)	0.65	1/1809 (0.1%)
1	C	0.28	0/1338 (0.0%)	0.65	1/1809 (0.1%)
1	D	0.28	0/1338 (0.0%)	0.64	1/1809 (0.1%)
1	E	0.27	0/1338 (0.0%)	0.64	1/1809 (0.1%)
1	F	0.27	0/1338 (0.0%)	0.64	0/1809 (0.0%)
1	G	0.27	0/1338 (0.0%)	0.65	0/1809 (0.0%)
1	H	0.28	0/1338 (0.0%)	0.65	0/1809 (0.0%)
1	I	0.28	0/1338 (0.0%)	0.66	0/1809 (0.0%)
1	J	0.27	0/1338 (0.0%)	0.66	2/1809 (0.1%)
1	K	0.27	0/1338 (0.0%)	0.64	3/1809 (0.2%)
1	L	0.27	0/1338 (0.0%)	0.62	1/1809 (0.1%)
All	All	0.27	0/16056 (0.0%)	0.65	11/21708 (0.1%)

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	E	0	1
All	All	0	1

There are no bond-length outliers.

5 of 11 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	27	LEU	CA-C-N	-5.78	108.79	122.31
1	J	27	LEU	C-N-CA	-5.78	108.79	122.31
1	E	151	VAL	N-CA-C	-5.67	106.78	113.42
1	K	27	LEU	CA-C-N	-5.54	109.35	122.31
1	K	27	LEU	C-N-CA	-5.54	109.35	122.31

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	E	158	TYR	Peptide

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	1313	0	1243	23
1	B	1313	0	1243	19
1	C	1313	0	1243	23
1	D	1313	0	1243	18
1	E	1313	0	1243	19
1	F	1313	0	1243	19
1	G	1313	0	1243	26
1	H	1313	0	1243	21
1	I	1313	0	1243	22
1	J	1313	0	1243	22
1	K	1313	0	1243	23
1	L	1313	0	1243	27
All	All	15756	0	14916	226

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 7.

5 of 226 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:L:14:LEU:O	1:L:92:TRP:HB2	0.77	1.80
1:I:14:LEU:O	1:I:92:TRP:HB2	0.74	1.81
1:G:14:LEU:O	1:G:92:TRP:HB2	0.72	1.85
1:A:93:ARG:O	1:A:106:ALA:HA	0.71	1.85
1:K:14:LEU:O	1:K:92:TRP:HB2	0.71	1.86

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	170/180 (94%)	143 (84%)	27 (16%)	0 (0%)	100	100
1	B	170/180 (94%)	142 (84%)	27 (16%)	1 (1%)	23	72
1	C	170/180 (94%)	144 (85%)	26 (15%)	0 (0%)	100	100
1	D	170/180 (94%)	141 (83%)	29 (17%)	0 (0%)	100	100
1	E	170/180 (94%)	143 (84%)	27 (16%)	0 (0%)	100	100
1	F	170/180 (94%)	142 (84%)	28 (16%)	0 (0%)	100	100
1	G	170/180 (94%)	143 (84%)	26 (15%)	1 (1%)	23	72
1	H	170/180 (94%)	144 (85%)	25 (15%)	1 (1%)	23	72
1	I	170/180 (94%)	145 (85%)	24 (14%)	1 (1%)	23	72
1	J	170/180 (94%)	143 (84%)	26 (15%)	1 (1%)	23	72
1	K	170/180 (94%)	147 (86%)	23 (14%)	0 (0%)	100	100
1	L	170/180 (94%)	144 (85%)	26 (15%)	0 (0%)	100	100
All	All	2040/2160 (94%)	1721 (84%)	314 (15%)	5 (0%)	44	80

All 5 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	74	ALA
1	G	74	ALA
1	H	74	ALA
1	I	74	ALA
1	J	74	ALA

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	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	B	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	C	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	D	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	E	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	F	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	G	137/145 (94%)	135 (99%)	2 (1%)	55	93
1	H	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	I	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	J	137/145 (94%)	136 (99%)	1 (1%)	73	96
1	K	137/145 (94%)	135 (99%)	2 (1%)	55	93
1	L	137/145 (94%)	136 (99%)	1 (1%)	73	96
All	All	1644/1740 (94%)	1630 (99%)	14 (1%)	68	95

5 of 14 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	143	ILE
1	B	143	ILE
1	C	143	ILE
1	D	143	ILE
1	E	143	ILE

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

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 4% for the well-defined parts and 4% 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	963
Number of shifts mapped to atoms	655
Number of unparsed shifts	0
Number of shifts with mapping errors	308
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 308) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	ILE	H	8.408	0.016	1
1	A	6	ILE	HD11	0.905	0.006	1
1	A	6	ILE	HD12	0.905	0.006	1
1	A	6	ILE	HD13	0.905	0.006	1
1	A	6	ILE	HG21	0.969	0.000	1
1	A	6	ILE	HG22	0.969	0.000	1
1	A	6	ILE	HG23	0.969	0.000	1
1	A	7	MET	H	9.277	0.020	1
1	A	7	MET	HE1	2.105	0.000	1
1	A	7	MET	HE2	2.105	0.000	1
1	A	7	MET	HE3	2.105	0.000	1
1	A	8	GLY	H	9.068	0.012	1
1	A	9	GLN	H	9.15	0.018	1
1	A	10	ASP	H	7.58	0.025	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	VAL	H	7.711	0.016	1
1	A	12	LYS	H	8.967	0.016	1
1	A	13	TYR	H	8.305	0.033	1
1	A	14	LEU	H	9.392	0.008	1
1	A	14	LEU	HD11	0.466	0.000	1
1	A	14	LEU	HD12	0.466	0.000	1
1	A	14	LEU	HD13	0.466	0.000	1
1	A	15	PHE	H	9.197	0.008	1
1	A	16	GLN	H	9.328	0.011	1
1	A	17	SER	H	9.922	0.023	1
1	A	18	ILE	H	9.49	0.031	1
1	A	18	ILE	HD11	1.01	0.007	1
1	A	18	ILE	HD12	1.01	0.007	1
1	A	18	ILE	HD13	1.01	0.007	1
1	A	18	ILE	HG21	1.048	0.000	1
1	A	18	ILE	HG22	1.048	0.000	1
1	A	18	ILE	HG23	1.048	0.000	1
1	A	19	ASP	H	8.241	0.012	1
1	A	20	ALA	H	7.233	0.011	1
1	A	20	ALA	HB1	1.628	0.012	1
1	A	20	ALA	HB2	1.628	0.012	1
1	A	20	ALA	HB3	1.628	0.012	1
1	A	21	ALA	H	8.815	0.027	1
1	A	21	ALA	HB1	1.537	0.007	1
1	A	21	ALA	HB2	1.537	0.007	1
1	A	21	ALA	HB3	1.537	0.007	1
1	A	22	THR	H	9.05	0.034	1
1	A	22	THR	HG21	1.241	0.000	1
1	A	22	THR	HG22	1.241	0.000	1
1	A	22	THR	HG23	1.241	0.000	1
1	A	23	GLY	H	9.895	0.010	1
1	A	24	SER	H	7.459	0.013	1
1	A	25	ALA	H	8.568	0.014	1
1	A	25	ALA	HB1	1.441	0.006	1
1	A	25	ALA	HB2	1.441	0.006	1
1	A	25	ALA	HB3	1.441	0.006	1
1	A	27	LEU	H	9.156	0.010	1
1	A	27	LEU	HD11	0.9	0.000	1
1	A	27	LEU	HD12	0.9	0.000	1
1	A	27	LEU	HD13	0.9	0.000	1
1	A	28	PHE	H	9.356	0.015	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	ALA	H	7.917	0.018	1
1	A	30	ALA	HB1	0.729	0.022	1
1	A	30	ALA	HB2	0.729	0.022	1
1	A	30	ALA	HB3	0.729	0.022	1
1	A	31	TYR	H	8.541	0.013	1
1	A	32	GLN	H	9.85	0.023	1
1	A	33	THR	H	9.119	0.011	1
1	A	35	GLY	H	8.437	0.025	1
1	A	36	SER	H	9.423	0.011	1
1	A	37	VAL	H	8.192	0.010	1
1	A	38	SER	H	9.2	0.012	1
1	A	39	GLY	H	8.535	0.013	1
1	A	40	GLU	H	8.552	0.012	1
1	A	43	LEU	HD11	0.832	0.000	5
1	A	43	LEU	HD12	0.832	0.000	5
1	A	43	LEU	HD13	0.832	0.000	5
1	A	45	ASP	H	8.239	0.025	1
1	A	46	GLU	H	8.297	0.042	1
1	A	47	GLN	H	8.728	0.011	1
1	A	48	THR	H	7.585	0.025	1
1	A	49	LYS	H	9.71	0.019	1
1	A	50	ASN	H	8.645	0.009	1
1	A	51	GLY	H	7.801	0.015	1
1	A	52	ARG	H	8.742	0.014	1
1	A	53	ILE	H	9.506	0.013	1
1	A	53	ILE	HD11	0.517	0.019	1
1	A	53	ILE	HD12	0.517	0.019	1
1	A	53	ILE	HD13	0.517	0.019	1
1	A	53	ILE	HG21	0.93	0.000	1
1	A	53	ILE	HG22	0.93	0.000	1
1	A	53	ILE	HG23	0.93	0.000	1
1	A	54	LEU	H	8.151	0.021	1
1	A	54	LEU	HD11	0.832	0.000	5
1	A	54	LEU	HD12	0.832	0.000	5
1	A	54	LEU	HD13	0.832	0.000	5
1	A	60	ALA	H	8.851	0.011	1
1	A	60	ALA	HB1	1.561	0.009	1
1	A	60	ALA	HB2	1.561	0.009	1
1	A	60	ALA	HB3	1.561	0.009	1
1	A	61	ASP	H	9.882	0.026	1
1	A	62	SER	H	9.468	0.016	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	63	GLY	H	8.771	0.011	1
1	A	64	GLU	H	9.385	0.022	1
1	A	65	VAL	H	8.108	0.021	1
1	A	66	THR	H	8.067	0.013	1
1	A	66	THR	HG21	1.096	0.000	1
1	A	66	THR	HG22	1.096	0.000	1
1	A	66	THR	HG23	1.096	0.000	1
1	A	67	TYR	H	8.63	0.011	1
1	A	68	TYR	H	8.448	0.009	1
1	A	69	GLY	H	8.73	0.013	1
1	A	70	LYS	H	9.094	0.010	1
1	A	71	ARG	H	8.864	0.009	1
1	A	72	GLY	H	9.111	0.020	1
1	A	73	ASP	H	7.392	0.014	1
1	A	74	ALA	H	9.263	0.012	1
1	A	74	ALA	HB1	1.625	0.007	1
1	A	74	ALA	HB2	1.625	0.007	1
1	A	74	ALA	HB3	1.625	0.007	1
1	A	75	GLY	H	8.855	0.017	1
1	A	76	GLN	H	8.634	0.033	1
1	A	77	LYS	H	8.397	0.021	1
1	A	78	ALA	H	8.019	0.013	1
1	A	78	ALA	HB1	1.561	0.006	1
1	A	78	ALA	HB2	1.561	0.006	1
1	A	78	ALA	HB3	1.561	0.006	1
1	A	79	ILE	H	7.363	0.022	1
1	A	79	ILE	HD11	-0.083	0.009	1
1	A	79	ILE	HD12	-0.083	0.009	1
1	A	79	ILE	HD13	-0.083	0.009	1
1	A	79	ILE	HG21	0.955	0.000	1
1	A	79	ILE	HG22	0.955	0.000	1
1	A	79	ILE	HG23	0.955	0.000	1
1	A	80	GLU	H	7.776	0.010	1
1	A	81	ASP	H	8.554	0.011	1
1	A	82	ALA	H	7.901	0.012	1
1	A	82	ALA	HB1	1.721	0.008	1
1	A	82	ALA	HB2	1.721	0.008	1
1	A	82	ALA	HB3	1.721	0.008	1
1	A	83	TYR	H	9.024	0.016	1
1	A	84	GLN	H	9.369	0.012	1
1	A	85	ASN	H	7.711	0.034	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	GLY	H	7.755	0.020	1
1	A	87	LYS	H	8.366	0.044	1
1	A	88	GLN	H	8.355	0.008	1
1	A	89	ILE	H	9.223	0.014	1
1	A	89	ILE	HD11	0.967	0.011	1
1	A	89	ILE	HD12	0.967	0.011	1
1	A	89	ILE	HD13	0.967	0.011	1
1	A	89	ILE	HG21	0.869	0.000	1
1	A	89	ILE	HG22	0.869	0.000	1
1	A	89	ILE	HG23	0.869	0.000	1
1	A	90	LYS	H	7.962	0.014	1
1	A	91	PHE	H	8.241	0.013	1
1	A	92	TRP	H	8.679	0.010	1
1	A	92	TRP	HE1	9.8	0.000	1
1	A	93	ARG	H	8.264	0.025	1
1	A	94	VAL	H	8.631	0.030	1
1	A	94	VAL	HG11	0.663	0.000	1
1	A	94	VAL	HG12	0.663	0.000	1
1	A	94	VAL	HG13	0.663	0.000	1
1	A	95	ASP	H	8.491	0.010	1
1	A	96	THR	H	8.378	0.009	1
1	A	96	THR	HG21	0.946	0.000	1
1	A	96	THR	HG22	0.946	0.000	1
1	A	96	THR	HG23	0.946	0.000	1
1	A	97	VAL	H	8.044	0.012	1
1	A	97	VAL	HG11	0.924	0.000	1
1	A	97	VAL	HG12	0.924	0.000	1
1	A	97	VAL	HG13	0.924	0.000	1
1	A	98	LYS	H	8.389	0.018	1
1	A	99	ASN	H	9.138	0.007	1
1	A	100	GLU	H	8.854	0.015	1
1	A	101	ASN	H	8.238	0.015	1
1	A	102	ASP	H	8.392	0.023	1
1	A	103	LYS	H	7.448	0.018	1
1	A	104	TYR	H	8.185	0.013	1
1	A	105	ASP	H	9.966	0.014	1
1	A	106	ALA	H	8.849	0.012	1
1	A	106	ALA	HB1	1.606	0.004	1
1	A	106	ALA	HB2	1.606	0.004	1
1	A	106	ALA	HB3	1.606	0.004	1
1	A	107	GLN	H	8.5	0.013	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	PHE	H	9.465	0.009	1
1	A	109	GLY	H	7.222	0.011	1
1	A	110	PHE	H	7.323	0.015	1
1	A	111	ALA	H	9.344	0.008	1
1	A	111	ALA	HB1	1.086	0.020	1
1	A	111	ALA	HB2	1.086	0.020	1
1	A	111	ALA	HB3	1.086	0.020	1
1	A	112	TYR	H	8.343	0.012	1
1	A	113	ILE	H	10.249	0.027	1
1	A	113	ILE	HG21	1.128	0.000	1
1	A	113	ILE	HG22	1.128	0.000	1
1	A	113	ILE	HG23	1.128	0.000	1
1	A	114	GLU	H	8.786	0.019	1
1	A	115	SER	H	7.644	0.018	1
1	A	116	ARG	H	8.402	0.008	1
1	A	117	GLU	H	9.247	0.013	1
1	A	118	TYR	H	9.402	0.009	1
1	A	119	SER	H	9.082	0.013	1
1	A	120	ASP	H	9.273	0.013	1
1	A	121	GLY	H	8.371	0.011	1
1	A	122	VAL	H	7.931	0.023	1
1	A	123	GLU	H	8.882	0.013	1
1	A	124	GLY	H	7.879	0.015	1
1	A	125	ALA	H	8.826	0.020	1
1	A	126	VAL	H	9.236	0.016	1
1	A	126	VAL	HG11	1.101	0.000	1
1	A	126	VAL	HG12	1.101	0.000	1
1	A	126	VAL	HG13	1.101	0.000	1
1	A	127	GLU	H	8.694	0.019	1
1	A	128	ILE	H	9.683	0.013	1
1	A	128	ILE	HD11	1.127	0.008	1
1	A	128	ILE	HD12	1.127	0.008	1
1	A	128	ILE	HD13	1.127	0.008	1
1	A	128	ILE	HG21	0.343	0.000	1
1	A	128	ILE	HG22	0.343	0.000	1
1	A	128	ILE	HG23	0.343	0.000	1
1	A	129	SER	H	8.448	0.010	1
1	A	130	ILE	H	8.948	0.013	1
1	A	130	ILE	HD11	0.801	0.009	1
1	A	130	ILE	HD12	0.801	0.009	1
1	A	130	ILE	HD13	0.801	0.009	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ILE	HG21	0.817	0.000	1
1	A	130	ILE	HG22	0.817	0.000	1
1	A	130	ILE	HG23	0.817	0.000	1
1	A	131	SER	H	7.926	0.036	1
1	A	132	LEU	H	9.521	0.015	1
1	A	132	LEU	HD11	0.053	0.000	1
1	A	132	LEU	HD12	0.053	0.000	1
1	A	132	LEU	HD13	0.053	0.000	1
1	A	133	GLN	H	9.022	0.016	1
1	A	134	VAL	H	7.771	0.029	1
1	A	135	ILE	H	9.008	0.021	1
1	A	135	ILE	HD11	0.581	0.014	1
1	A	135	ILE	HD12	0.581	0.014	1
1	A	135	ILE	HD13	0.581	0.014	1
1	A	135	ILE	HG21	1.341	0.000	1
1	A	135	ILE	HG22	1.341	0.000	1
1	A	135	ILE	HG23	1.341	0.000	1
1	A	136	GLY	H	9.229	0.019	1
1	A	137	GLU	H	7.658	0.008	1
1	A	138	LEU	H	9.829	0.021	1
1	A	139	LYS	H	9.583	0.017	1
1	A	140	ASN	H	9.226	0.017	1
1	A	141	GLY	H	8.418	0.010	1
1	A	142	GLU	H	7.723	0.021	1
1	A	143	ILE	H	9.809	0.012	1
1	A	143	ILE	HD11	0.356	0.007	1
1	A	143	ILE	HD12	0.356	0.007	1
1	A	143	ILE	HD13	0.356	0.007	1
1	A	143	ILE	HG21	0.889	0.000	1
1	A	143	ILE	HG22	0.889	0.000	1
1	A	143	ILE	HG23	0.889	0.000	1
1	A	144	ASP	H	8.751	0.009	1
1	A	145	THR	H	7.73	0.009	1
1	A	145	THR	HG21	1.149	0.000	1
1	A	145	THR	HG22	1.149	0.000	1
1	A	145	THR	HG23	1.149	0.000	1
1	A	146	LEU	H	8.002	0.010	1
1	A	146	LEU	HD11	-0.299	0.000	1
1	A	146	LEU	HD12	-0.299	0.000	1
1	A	146	LEU	HD13	-0.299	0.000	1
1	A	148	GLU	H	9.014	0.009	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	149	GLU	H	9.316	0.013	1
1	A	150	ILE	H	7.54	0.011	1
1	A	150	ILE	HD11	0.776	0.017	1
1	A	150	ILE	HD12	0.776	0.017	1
1	A	150	ILE	HD13	0.776	0.017	1
1	A	150	ILE	HG21	0.31	0.000	1
1	A	150	ILE	HG22	0.31	0.000	1
1	A	150	ILE	HG23	0.31	0.000	1
1	A	151	VAL	H	6.919	0.010	1
1	A	151	VAL	HG11	0.788	0.000	5
1	A	151	VAL	HG12	0.788	0.000	5
1	A	151	VAL	HG13	0.788	0.000	5
1	A	152	ASN	H	9.561	0.026	1
1	A	153	VAL	H	8.519	0.019	1
1	A	153	VAL	HG11	0.788	0.000	5
1	A	153	VAL	HG12	0.788	0.000	5
1	A	153	VAL	HG13	0.788	0.000	5
1	A	154	SER	H	9.055	0.013	1
1	A	158	TYR	H	6.934	0.008	1
1	A	159	ASP	H	9.08	0.017	1
1	A	160	PHE	H	9.031	0.010	1
1	A	161	GLN	H	8.777	0.000	1
1	A	162	GLN	H	8.223	0.006	1
1	A	164	GLY	H	10.269	0.031	1
1	A	165	GLN	H	7.775	0.015	1
1	A	166	THR	H	7.64	0.003	1
1	A	167	THR	H	8.836	0.011	1
1	A	167	THR	HG21	1.192	0.000	1
1	A	167	THR	HG22	1.192	0.000	1
1	A	167	THR	HG23	1.192	0.000	1
1	A	168	GLY	H	8.879	0.011	1
1	A	169	GLU	H	8.327	0.011	1
1	A	170	ALA	H	9.109	0.024	1
1	A	170	ALA	HB1	0.408	0.002	1
1	A	170	ALA	HB2	0.408	0.002	1
1	A	170	ALA	HB3	0.408	0.002	1
1	A	172	GLY	H	8.619	0.006	1
1	A	173	THR	H	9.63	0.010	1
1	A	173	THR	HG21	1.252	0.000	1
1	A	173	THR	HG22	1.252	0.000	1
1	A	173	THR	HG23	1.252	0.000	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	174	VAL	H	8.351	0.013	1
1	A	174	VAL	HG11	1.081	0.000	1
1	A	174	VAL	HG12	1.081	0.000	1
1	A	174	VAL	HG13	1.081	0.000	1
1	A	176	ALA	HB1	1.408	0.000	1
1	A	176	ALA	HB2	1.408	0.000	1
1	A	176	ALA	HB3	1.408	0.000	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	161	-0.09 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	126	0.58 ± 0.15	Should be checked
$^{13}\text{C}'$	161	0.04 ± 0.26	None needed (< 0.5 ppm)
^{15}N	151	-0.00 ± 0.44	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 4%, i.e. 963 atoms were assigned a chemical shift out of a possible 26317. 0 out of 228 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	624/10392 (6%)	151/4296 (4%)	322/4128 (8%)	151/1968 (8%)
Sidechain	337/13980 (2%)	156/8988 (2%)	181/4476 (4%)	0/516 (0%)
Aromatic	2/1945 (0%)	1/924 (0%)	0/1020 (0%)	1/1 (100%)
Overall	963/26317 (4%)	308/14208 (2%)	503/9624 (5%)	152/2485 (6%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

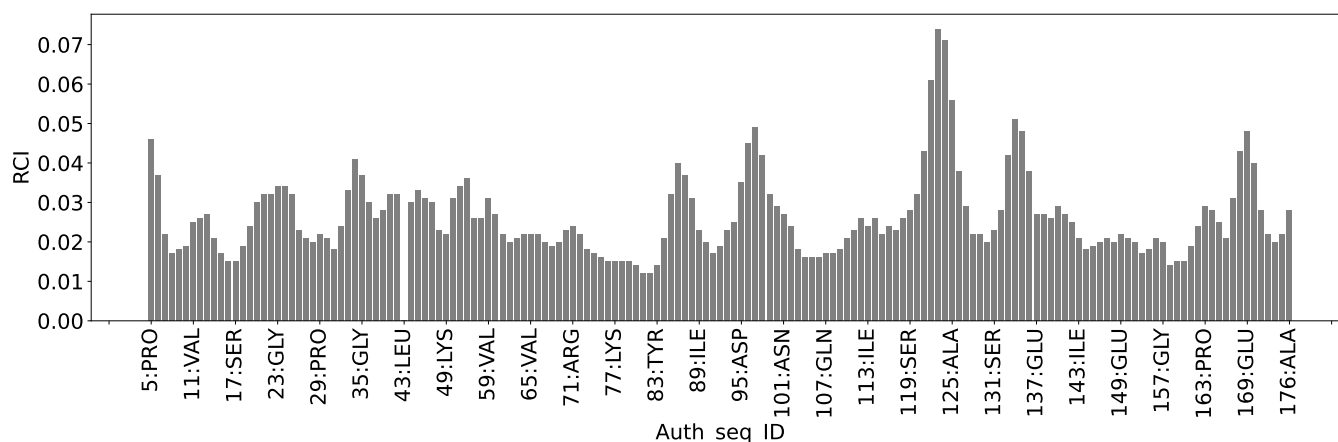
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis [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	1384
Intra-residue ($ i-j =0$)	24
Sequential ($ i-j =1$)	188
Medium range ($ i-j >1$ and $ i-j <5$)	144
Long range ($ i-j \geq 5$)	920
Inter-chain	0
Hydrogen bond restraints	108
Disulfide bond restraints	0
Total dihedral-angle restraints	2880
Number of unmapped restraints	0
Number of restraints per residue	2.0
Number of long range restraints per residue ¹	0.5

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.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	31.0	0.2
0.2-0.5 (Medium)	35.0	0.5
>0.5 (Large)	773.0	70.24

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)	530.0	10.0
10.0-20.0 (Medium)	352.0	19.96
>20.0 (Large)	1137.0	174.36

9 Distance violation analysis ⓘ

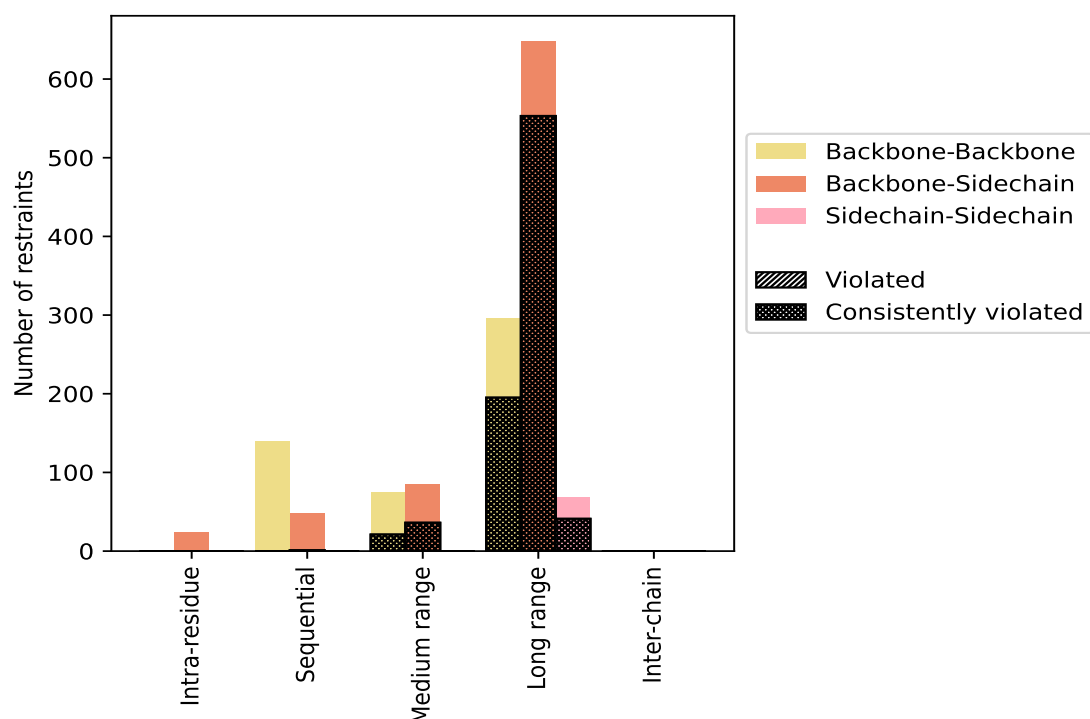
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	24	1.7	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	24	1.7	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
Sequential (i-j =1)	188	13.6	1	0.5	0.1	1	0.5	0.1
Backbone-Backbone	140	10.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	48	3.5	1	2.1	0.1	1	2.1	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	144	10.4	45	31.2	3.3	45	31.2	3.3
Backbone-Backbone	75	5.4	21	28.0	1.5	21	28.0	1.5
Backbone-Sidechain	69	5.0	24	34.8	1.7	24	34.8	1.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	920	66.5	706	76.7	51.0	706	76.7	51.0
Backbone-Backbone	296	21.4	195	65.9	14.1	195	65.9	14.1
Backbone-Sidechain	556	40.2	470	84.5	34.0	470	84.5	34.0
Sidechain-Sidechain	68	4.9	41	60.3	3.0	41	60.3	3.0
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	108	7.8	95	88.0	6.9	95	88.0	6.9
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1384	100.0	847	61.2	61.2	847	61.2	61.2
Backbone-Backbone	511	36.9	216	42.3	15.6	216	42.3	15.6
Backbone-Sidechain	805	58.2	590	73.3	42.6	590	73.3	42.6
Sidechain-Sidechain	68	4.9	41	60.3	3.0	41	60.3	3.0

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

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



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

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

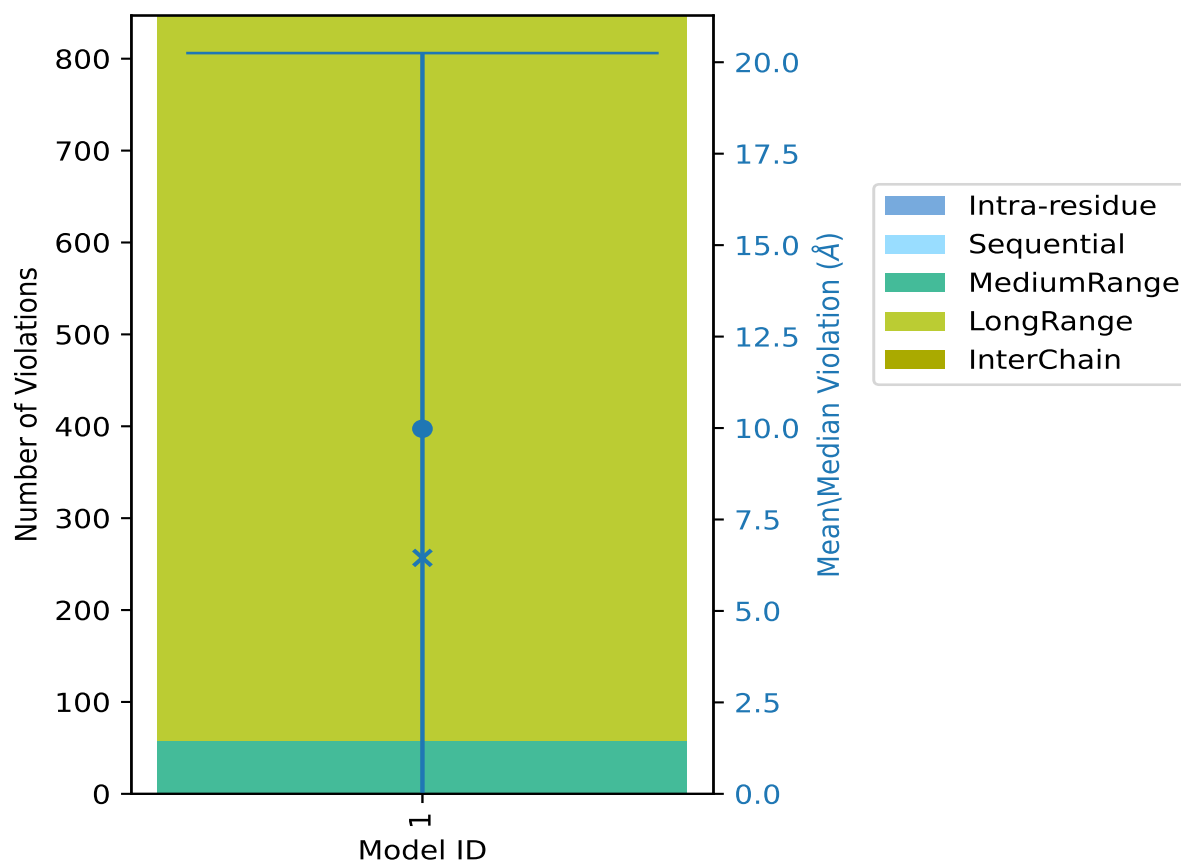
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	1	57	789	0	847	9.98	70.24	10.27	6.45

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

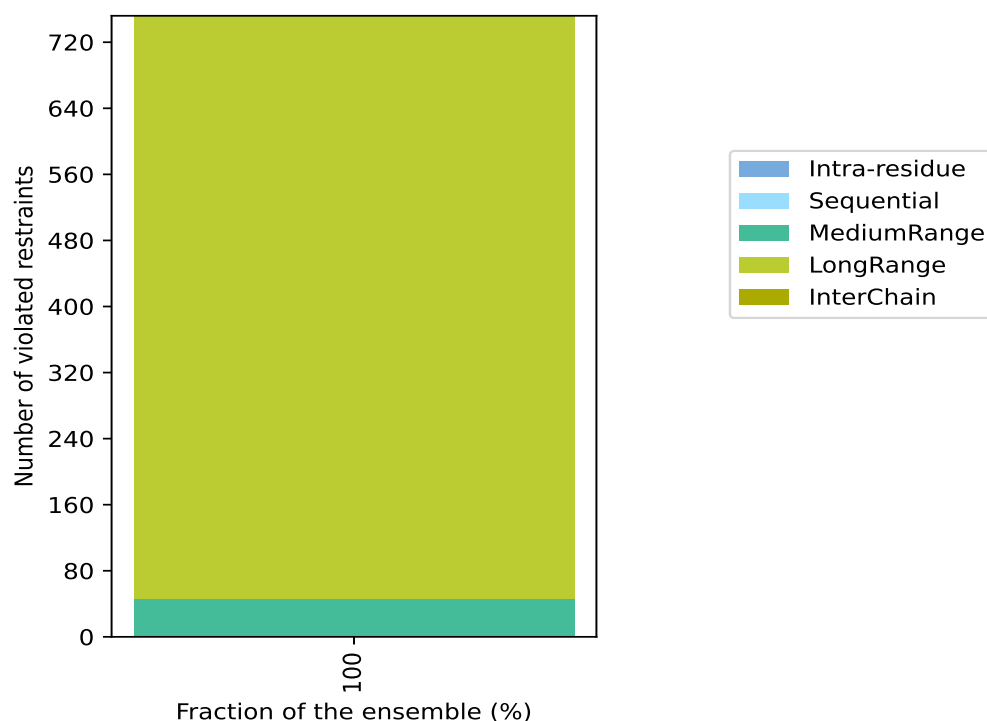
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 524(IR:24, SQ:187, MR:99, LR:214, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	45	706	0	752	1	100.0

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

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

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



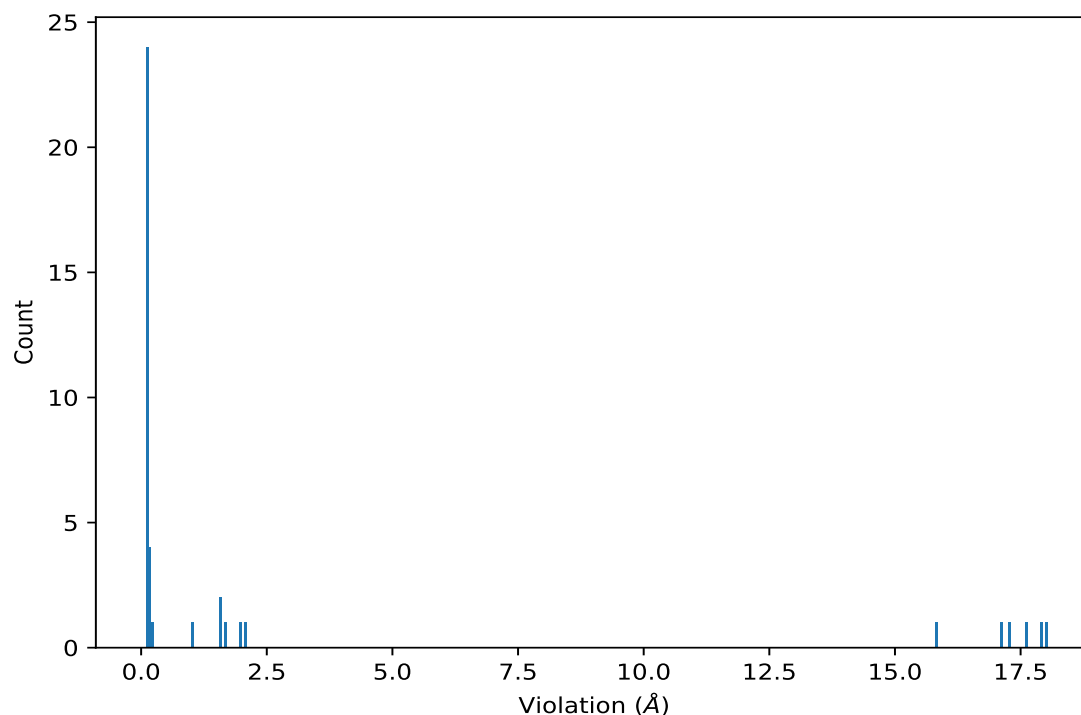
9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



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

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,11)	1:38:A:SER:N	1:116:A:ARG:O	1	18.01
(5,5)	1:116:A:ARG:N	1:38:A:SER:O	1	17.91
(5,3)	1:118:A:TYR:N	1:36:A:SER:O	1	17.64
(5,9)	1:36:A:SER:N	1:118:A:TYR:O	1	17.29
(5,7)	1:34:A:ASP:N	1:120:A:ASP:O	1	17.13
(5,1)	1:120:A:ASP:N	1:34:A:ASP:O	1	15.83
(4,1)	1:77:A:LYS:N	1:73:A:ASP:O	1	2.09
(4,93)	1:106:A:ALA:N	1:140:A:ASN:O	1	1.96
(4,87)	1:140:A:ASN:N	1:106:A:ALA:O	1	1.66
(4,31)	1:115:A:SER:N	1:131:A:SER:O	1	1.57

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

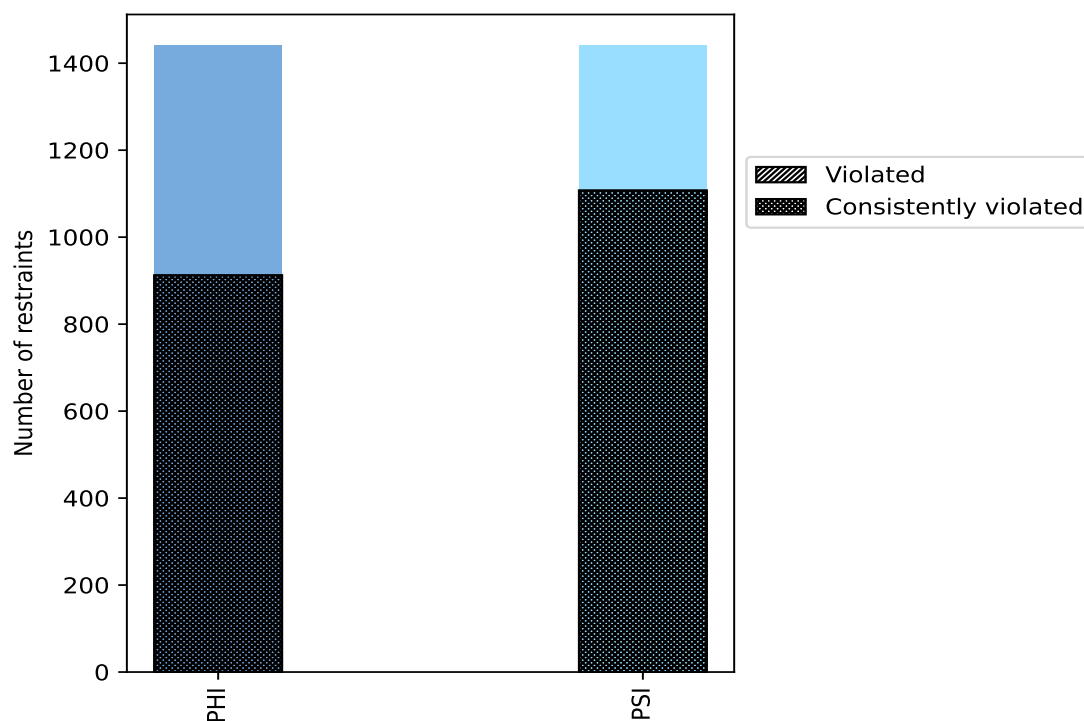
10.1 Summary of dihedral-angle violations [i](#)

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	1440	50.0	912	63.3	31.7	912	63.3	31.7
PSI	1440	50.0	1107	76.9	38.4	1107	76.9	38.4
Total	2880	100.0	2019	70.1	70.1	2019	70.1	70.1

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](#)



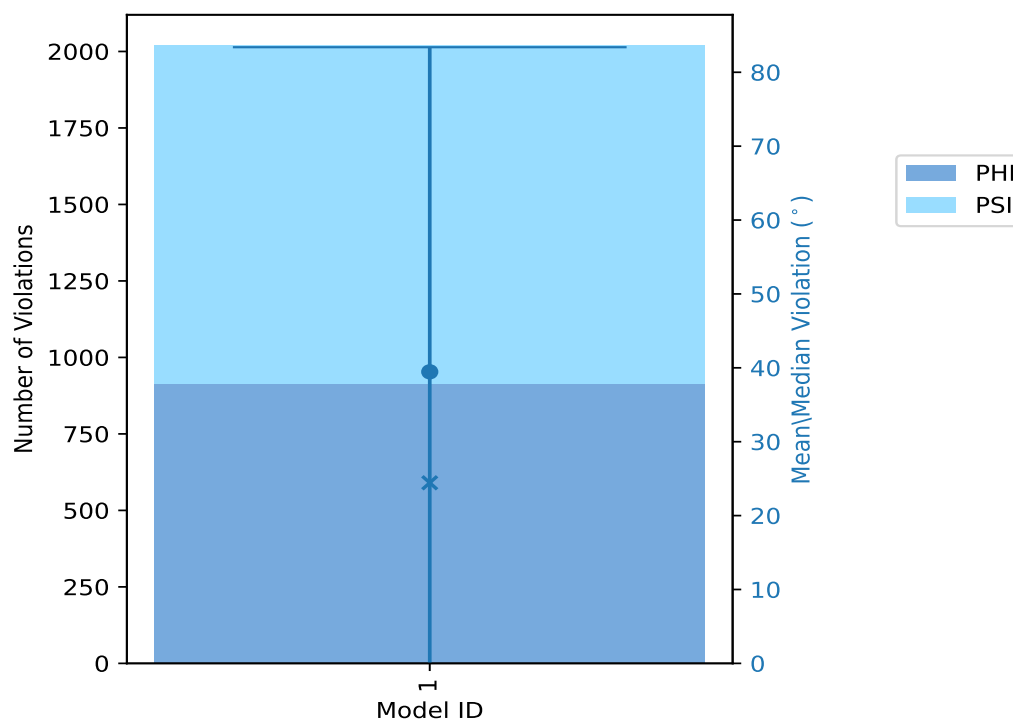
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	912	1107	2019	39.46	174.36	43.93	24.44

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

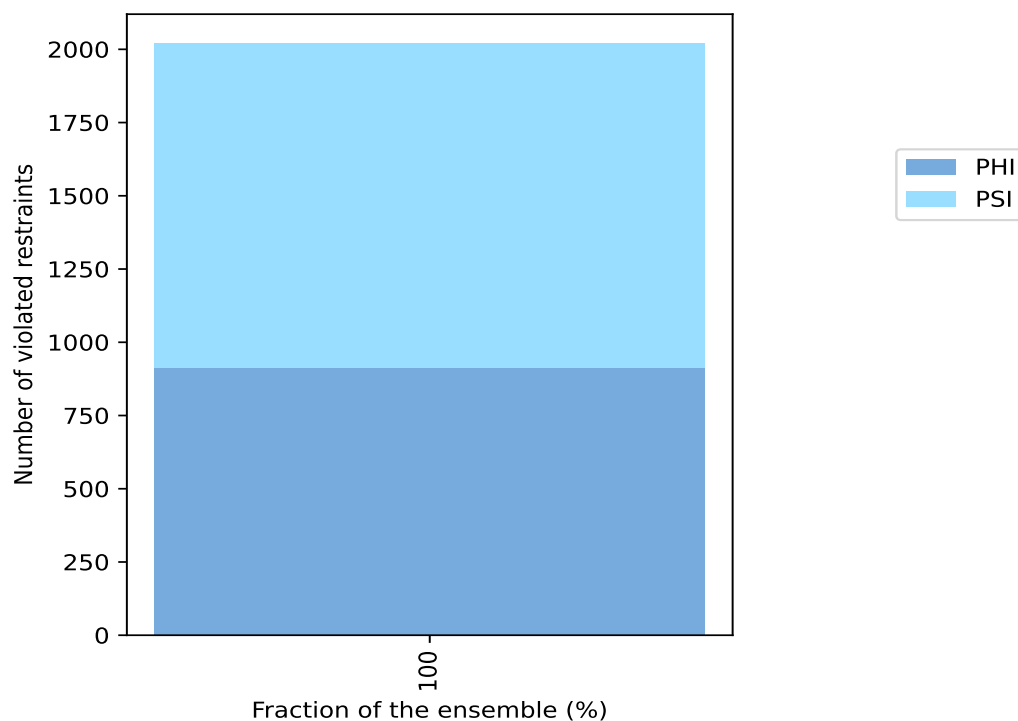
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
912	1107	2019	1	100.0

¹ Number of models with violations

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



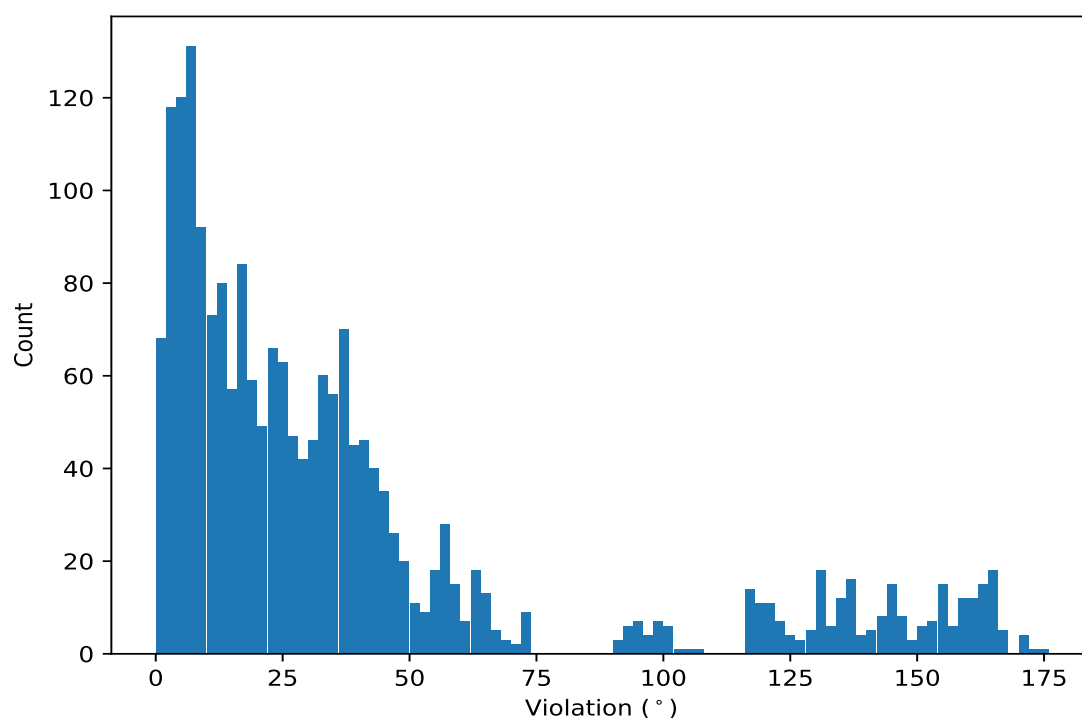
10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

No violations found

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation 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 (°)
(1,1538)	1:101:I:ASN:C	1:102:I:ASP:N	1:102:I:ASP:CA	1:102:I:ASP:C	1	174.36
(1,2702)	1:163:J:PRO:N	1:163:J:PRO:CA	1:163:J:PRO:C	1:164:J:GLY:N	1	172.43
(1,2704)	1:163:I:PRO:N	1:163:I:PRO:CA	1:163:I:PRO:C	1:164:I:GLY:N	1	171.93
(1,2701)	1:163:G:PRO:N	1:163:G:PRO:CA	1:163:G:PRO:C	1:164:G:GLY:N	1	171.63
(1,2707)	1:163:L:PRO:N	1:163:L:PRO:CA	1:163:L:PRO:C	1:164:L:GLY:N	1	171.56
(1,2706)	1:163:K:PRO:N	1:163:K:PRO:CA	1:163:K:PRO:C	1:164:K:GLY:N	1	171.51
(1,1541)	1:101:K:ASN:C	1:102:K:ASP:N	1:102:K:ASP:CA	1:102:K:ASP:C	1	167.95
(1,2708)	1:163:H:PRO:N	1:163:H:PRO:CA	1:163:H:PRO:C	1:164:H:GLY:N	1	167.94
(1,1544)	1:101:G:ASN:C	1:102:G:ASP:N	1:102:G:ASP:CA	1:102:G:ASP:C	1	167.5
(1,2373)	1:143:J:ILE:N	1:143:J:ILE:CA	1:143:J:ILE:C	1:144:J:ASP:N	1	167.21