



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 11:05 PM UTC

PDB ID : 1NXI / pdb_00001nxi
BMRB ID : 5589
Title : Solution structure of Vibrio cholerae protein VC0424
Authors : Ramelot, T.A.; Ni, S.; Goldsmith-Fischman, S.; Cort, J.R.; Honig, B.;
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Deposited on : 2003-02-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

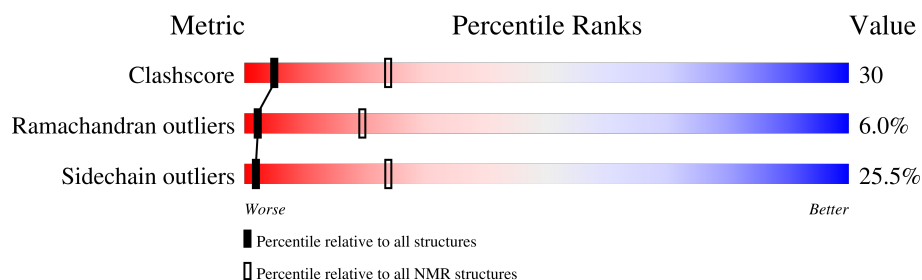
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	132	21% 54% 5% 20%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:11-A:73, A:80-A:121 (105)	0.61	2

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2073 atoms, of which 993 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called conserved hypothetical protein VC0424.

Mol	Chain	Residues	Atoms						Trace
1	A	132	Total	C	H	N	O	S	0
			2073	680	993	169	227	4	

There are 8 discrepancies between the modelled and reference sequences:

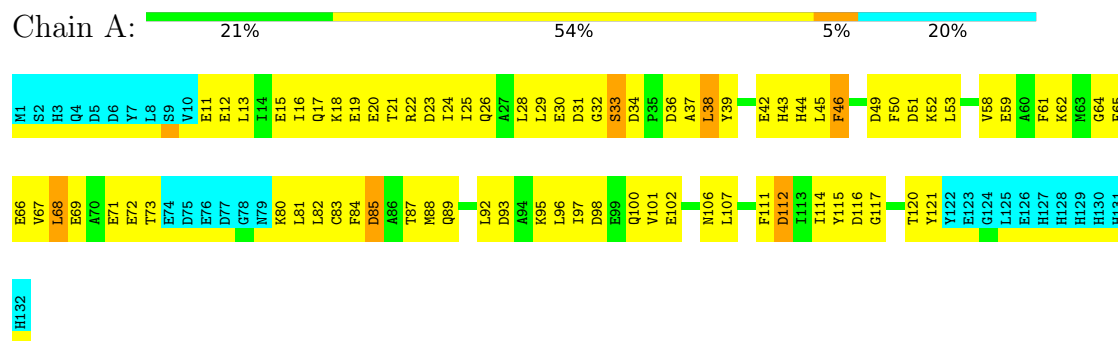
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	LEU	-	expression tag	UNP Q9KUU1
A	126	GLU	-	expression tag	UNP Q9KUU1
A	127	HIS	-	expression tag	UNP Q9KUU1
A	128	HIS	-	expression tag	UNP Q9KUU1
A	129	HIS	-	expression tag	UNP Q9KUU1
A	130	HIS	-	expression tag	UNP Q9KUU1
A	131	HIS	-	expression tag	UNP Q9KUU1
A	132	HIS	-	expression tag	UNP Q9KUU1

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: conserved hypothetical protein VC0424

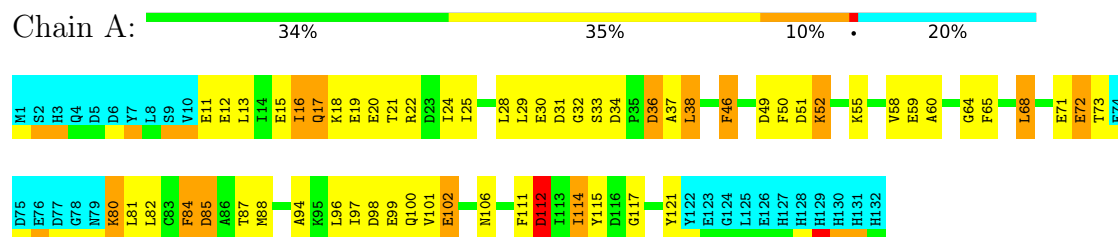


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

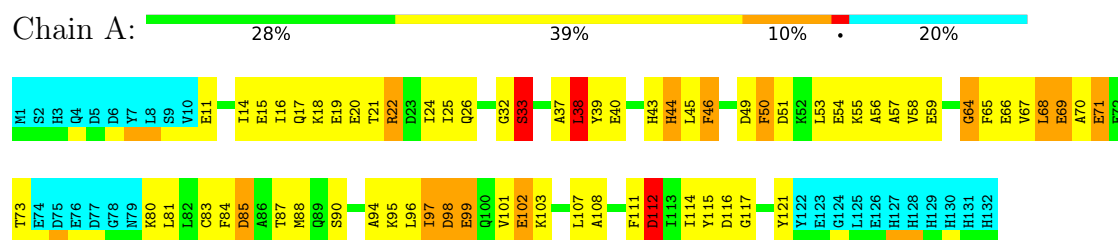
4.2.1 Score per residue for model 1

- Molecule 1: conserved hypothetical protein VC0424



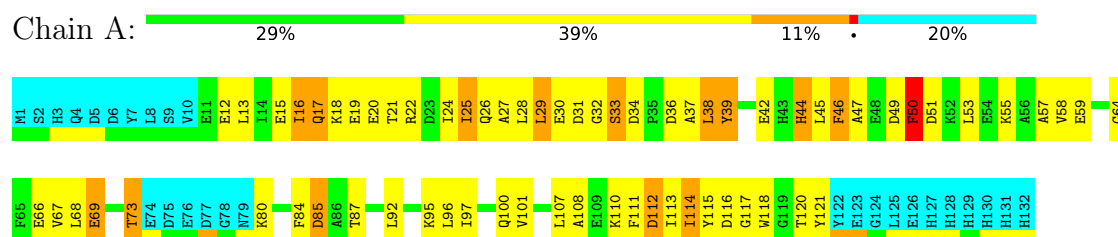
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: conserved hypothetical protein VC0424



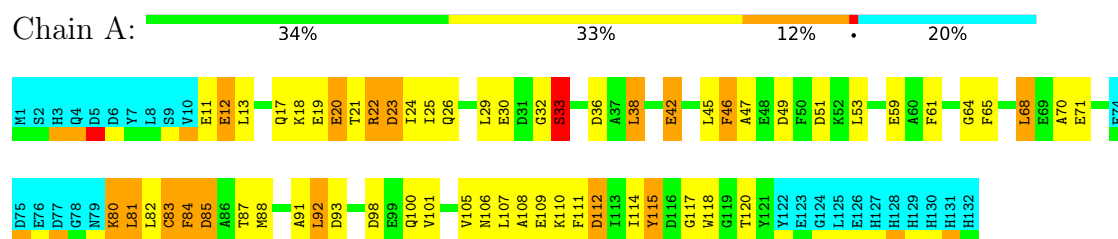
4.2.3 Score per residue for model 3

- Molecule 1: conserved hypothetical protein VC0424



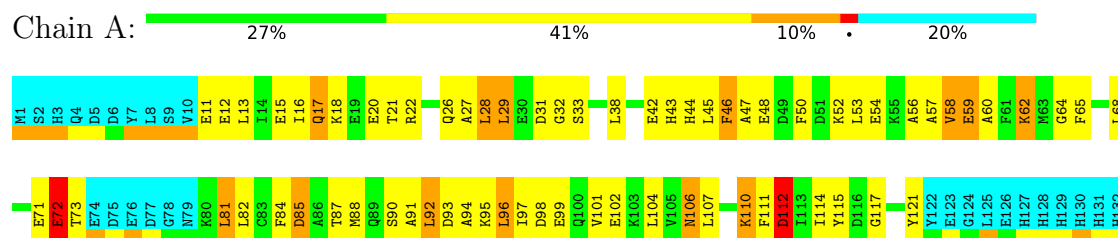
4.2.4 Score per residue for model 4

- Molecule 1: conserved hypothetical protein VC0424



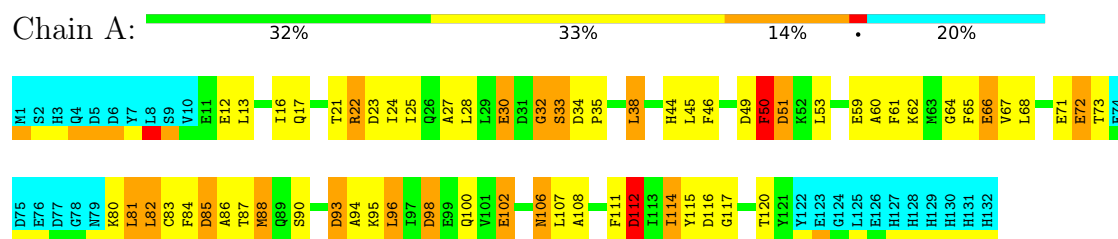
4.2.5 Score per residue for model 5

- Molecule 1: conserved hypothetical protein VC0424



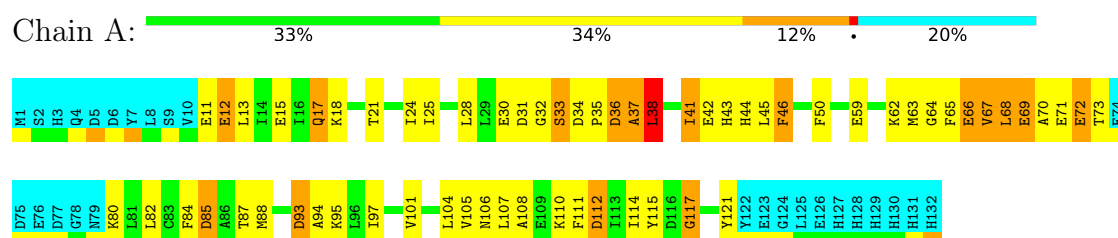
4.2.6 Score per residue for model 6

- Molecule 1: conserved hypothetical protein VC0424



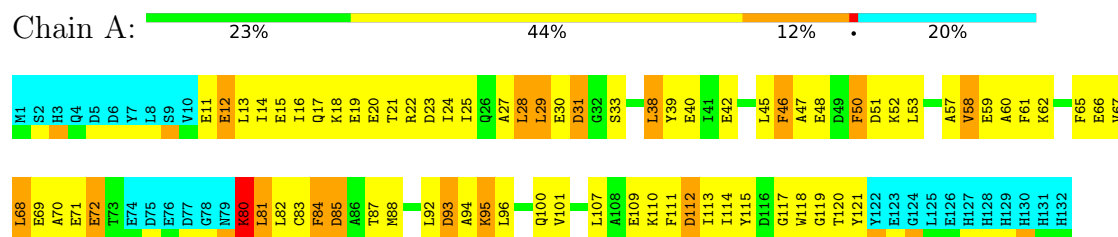
4.2.7 Score per residue for model 7

- Molecule 1: conserved hypothetical protein VC0424



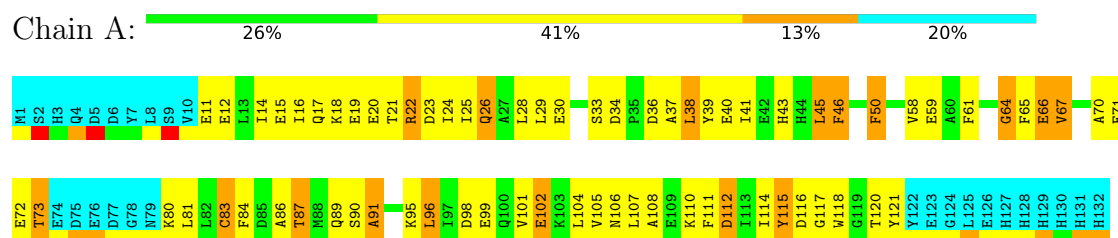
4.2.8 Score per residue for model 8

- Molecule 1: conserved hypothetical protein VC0424



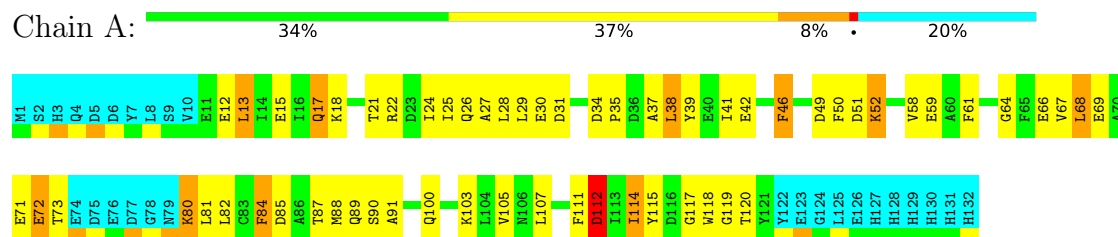
4.2.9 Score per residue for model 9

- Molecule 1: conserved hypothetical protein VC0424



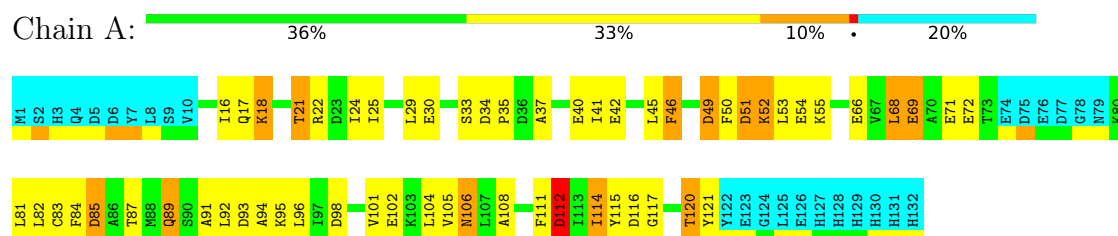
4.2.10 Score per residue for model 10

- Molecule 1: conserved hypothetical protein VC0424



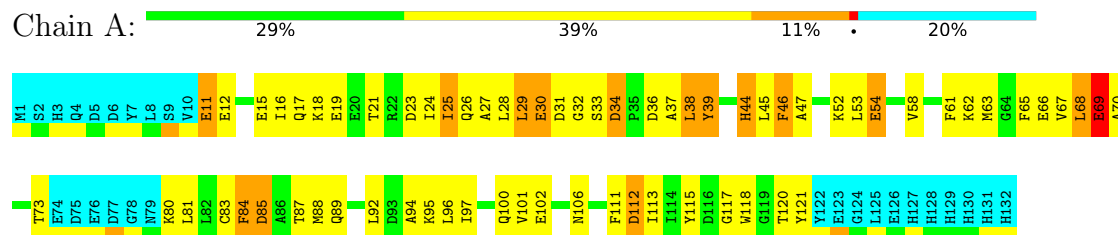
4.2.11 Score per residue for model 11

- Molecule 1: conserved hypothetical protein VC0424



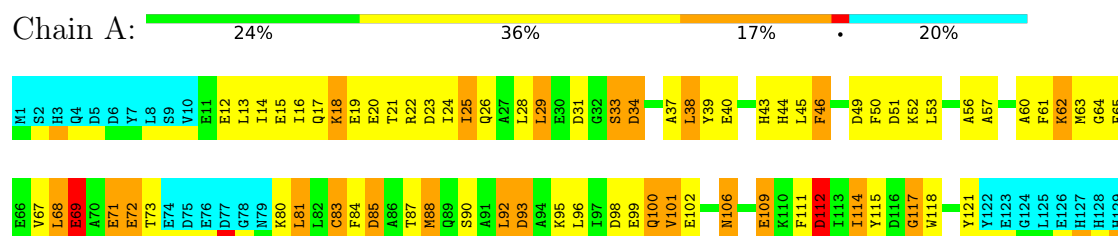
4.2.12 Score per residue for model 12

- Molecule 1: conserved hypothetical protein VC0424



4.2.13 Score per residue for model 13

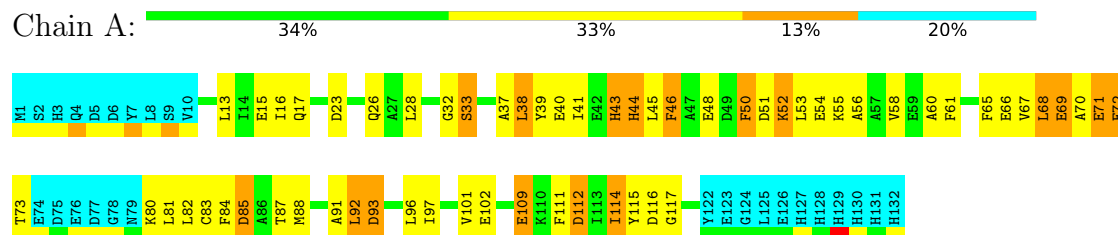
- Molecule 1: conserved hypothetical protein VC0424





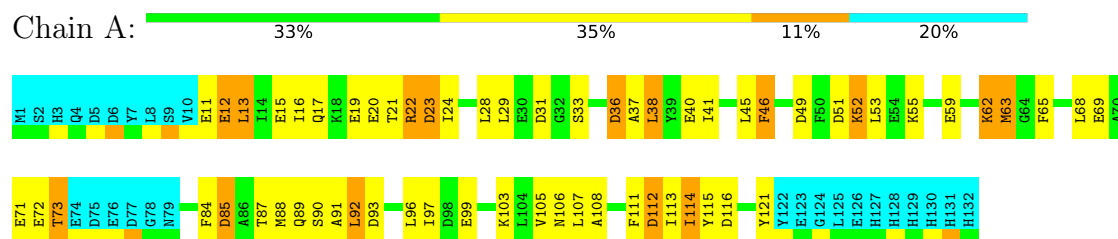
4.2.14 Score per residue for model 14

- Molecule 1: conserved hypothetical protein VC0424



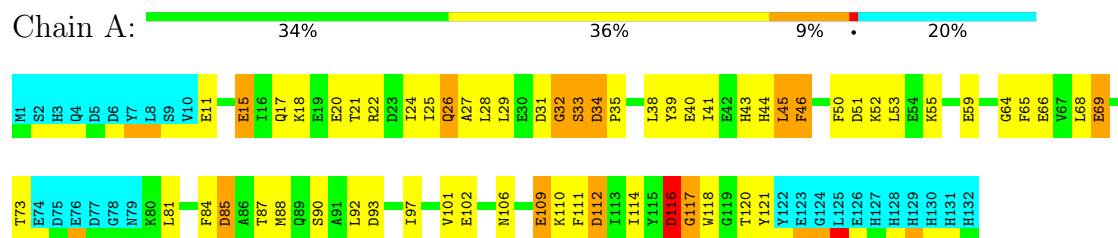
4.2.15 Score per residue for model 15

- Molecule 1: conserved hypothetical protein VC0424



4.2.16 Score per residue for model 16

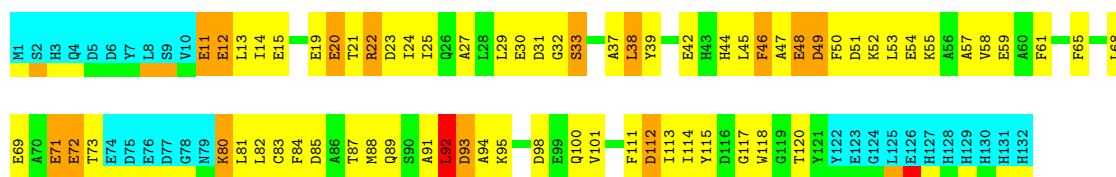
- Molecule 1: conserved hypothetical protein VC0424



4.2.17 Score per residue for model 17

- Molecule 1: conserved hypothetical protein VC0424

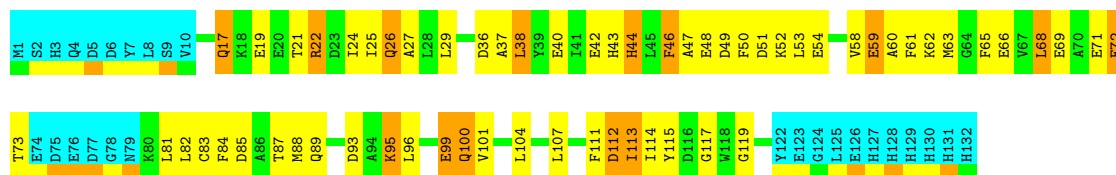




4.2.18 Score per residue for model 18

- Molecule 1: conserved hypothetical protein VC0424

Chain A: 33% 36% 11% 20%



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 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
X-PLOR	structure solution	NIH-2.0.4
X-PLOR	refinement	NIH-2.0.4

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	1545
Number of shifts mapped to atoms	1545
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.43±0.01	0±0/863 (0.0± 0.0%)	1.17±0.01	0±0/1165 (0.0± 0.0%)
All	All	1.43	1/17260 (0.0%)	1.17	0/23300 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	73	THR	N-CA	5.04	1.49	1.46	15	1

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	849	814	814	49±8
All	All	16980	16280	16280	985

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD12	1:A:45:LEU:N	0.81	1.90	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ILE:N	1:A:41:ILE:HD12	0.81	1.91	7	5
1:A:46:PHE:CD1	1:A:46:PHE:N	0.79	2.51	11	20
1:A:53:LEU:C	1:A:53:LEU:HD23	0.76	2.05	16	14
1:A:82:LEU:HD12	1:A:82:LEU:N	0.76	1.96	14	8
1:A:65:PHE:CZ	1:A:88:MET:SD	0.76	2.79	18	6
1:A:50:PHE:CD1	1:A:50:PHE:N	0.75	2.51	8	5
1:A:40:GLU:C	1:A:41:ILE:HD12	0.73	2.08	14	4
1:A:81:LEU:HD12	1:A:81:LEU:H	0.73	1.44	8	2
1:A:100:GLN:N	1:A:100:GLN:NE2	0.72	2.38	18	1
1:A:100:GLN:N	1:A:100:GLN:HE21	0.70	1.84	18	1
1:A:50:PHE:CD1	1:A:51:ASP:N	0.70	2.60	20	2
1:A:54:GLU:O	1:A:58:VAL:HG23	0.69	1.87	14	6
1:A:115:TYR:CD2	1:A:115:TYR:O	0.69	2.46	19	10
1:A:65:PHE:CD1	1:A:88:MET:SD	0.69	2.86	2	1
1:A:118:TRP:CG	1:A:118:TRP:O	0.69	2.46	12	3
1:A:84:PHE:CD1	1:A:84:PHE:N	0.69	2.61	12	18
1:A:64:GLY:O	1:A:65:PHE:CG	0.69	2.46	9	1
1:A:114:ILE:HD12	1:A:115:TYR:N	0.69	2.03	10	4
1:A:89:GLN:N	1:A:89:GLN:NE2	0.69	2.40	11	3
1:A:28:LEU:O	1:A:32:GLY:N	0.68	2.27	16	3
1:A:102:GLU:O	1:A:106:ASN:ND2	0.68	2.27	6	1
1:A:81:LEU:HD12	1:A:81:LEU:C	0.68	2.13	12	2
1:A:68:LEU:N	1:A:85:ASP:O	0.68	2.27	4	15
1:A:49:ASP:OD1	1:A:49:ASP:N	0.67	2.27	11	1
1:A:118:TRP:CE3	1:A:119:GLY:N	0.67	2.62	8	2
1:A:64:GLY:O	1:A:65:PHE:CD2	0.67	2.47	9	1
1:A:44:HIS:NE2	1:A:85:ASP:OD2	0.67	2.27	12	3
1:A:85:ASP:OD1	1:A:86:ALA:N	0.67	2.27	6	1
1:A:49:ASP:O	1:A:51:ASP:N	0.67	2.28	6	4
1:A:22:ARG:CG	1:A:22:ARG:HH11	0.67	2.03	2	5
1:A:31:ASP:N	1:A:31:ASP:OD1	0.66	2.28	8	1
1:A:89:GLN:N	1:A:89:GLN:CD	0.66	2.53	19	2
1:A:109:GLU:N	1:A:109:GLU:OE1	0.66	2.29	16	2
1:A:48:GLU:H	1:A:48:GLU:CD	0.66	1.99	17	1
1:A:100:GLN:N	1:A:100:GLN:OE1	0.66	2.29	13	2
1:A:66:GLU:N	1:A:66:GLU:OE1	0.66	2.28	6	1
1:A:44:HIS:NE2	1:A:85:ASP:CG	0.66	2.53	12	1
1:A:64:GLY:O	1:A:88:MET:SD	0.66	2.54	2	1
1:A:85:ASP:N	1:A:85:ASP:OD1	0.66	2.27	12	3
1:A:106:ASN:N	1:A:106:ASN:HD22	0.66	1.88	13	2
1:A:50:PHE:CE2	1:A:51:ASP:OD1	0.65	2.49	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:O	1:A:32:GLY:N	0.65	2.29	1	2
1:A:61:PHE:C	1:A:61:PHE:CD1	0.65	2.73	8	4
1:A:65:PHE:CE1	1:A:88:MET:CE	0.65	2.79	2	3
1:A:44:HIS:C	1:A:45:LEU:HD12	0.65	2.16	14	3
1:A:47:ALA:HB2	1:A:113:ILE:HG22	0.64	1.67	20	6
1:A:36:ASP:N	1:A:36:ASP:OD1	0.64	2.27	7	2
1:A:115:TYR:C	1:A:115:TYR:CD1	0.64	2.74	9	4
1:A:83:CYS:O	1:A:83:CYS:SG	0.64	2.55	6	5
1:A:89:GLN:OE1	1:A:89:GLN:N	0.64	2.31	12	1
1:A:26:GLN:O	1:A:26:GLN:NE2	0.64	2.31	4	2
1:A:85:ASP:CG	1:A:86:ALA:N	0.64	2.55	6	1
1:A:116:ASP:N	1:A:116:ASP:OD1	0.64	2.27	6	2
1:A:41:ILE:HD12	1:A:41:ILE:N	0.64	2.07	14	1
1:A:65:PHE:CE2	1:A:88:MET:SD	0.62	2.93	5	4
1:A:22:ARG:CG	1:A:22:ARG:NH1	0.62	2.61	4	4
1:A:73:THR:HG22	1:A:83:CYS:SG	0.62	2.35	20	1
1:A:41:ILE:N	1:A:41:ILE:CD1	0.62	2.61	7	5
1:A:65:PHE:CZ	1:A:88:MET:CE	0.62	2.83	14	1
1:A:59:GLU:OE1	1:A:59:GLU:N	0.62	2.33	3	1
1:A:18:LYS:NZ	1:A:98:ASP:OD2	0.61	2.33	5	3
1:A:72:GLU:N	1:A:72:GLU:OE1	0.61	2.33	1	2
1:A:106:ASN:ND2	1:A:106:ASN:N	0.61	2.47	6	2
1:A:91:ALA:O	1:A:92:LEU:C	0.61	2.44	15	6
1:A:28:LEU:O	1:A:31:ASP:N	0.61	2.33	16	3
1:A:64:GLY:C	1:A:65:PHE:CD2	0.61	2.78	9	1
1:A:51:ASP:CG	1:A:55:LYS:NZ	0.61	2.59	17	1
1:A:65:PHE:CE1	1:A:88:MET:SD	0.61	2.94	2	2
1:A:12:GLU:CG	1:A:13:LEU:N	0.61	2.64	3	4
1:A:115:TYR:O	1:A:115:TYR:CG	0.60	2.54	17	6
1:A:40:GLU:N	1:A:40:GLU:OE1	0.60	2.33	9	1
1:A:71:GLU:O	1:A:72:GLU:C	0.60	2.45	11	11
1:A:71:GLU:O	1:A:73:THR:N	0.60	2.35	18	4
1:A:49:ASP:C	1:A:51:ASP:N	0.59	2.59	6	5
1:A:95:LYS:O	1:A:98:ASP:N	0.59	2.36	9	2
1:A:111:PHE:O	1:A:112:ASP:CB	0.59	2.50	20	20
1:A:49:ASP:O	1:A:50:PHE:C	0.59	2.46	10	10
1:A:14:ILE:O	1:A:15:GLU:C	0.59	2.46	8	5
1:A:28:LEU:O	1:A:29:LEU:C	0.59	2.45	16	6
1:A:72:GLU:O	1:A:72:GLU:CD	0.59	2.45	9	1
1:A:45:LEU:O	1:A:84:PHE:CE1	0.59	2.56	11	3
1:A:111:PHE:O	1:A:112:ASP:CG	0.59	2.46	20	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:GLU:OE2	1:A:106:ASN:ND2	0.59	2.35	9	1
1:A:29:LEU:O	1:A:30:GLU:C	0.59	2.46	1	5
1:A:101:VAL:O	1:A:102:GLU:C	0.59	2.46	5	8
1:A:53:LEU:HD23	1:A:53:LEU:O	0.58	1.98	16	8
1:A:72:GLU:H	1:A:72:GLU:CD	0.58	1.99	8	2
1:A:45:LEU:N	1:A:45:LEU:CD1	0.58	2.60	9	3
1:A:114:ILE:HD12	1:A:114:ILE:C	0.58	2.23	10	3
1:A:59:GLU:O	1:A:60:ALA:C	0.58	2.46	19	4
1:A:101:VAL:O	1:A:105:VAL:HG23	0.58	1.99	11	2
1:A:96:LEU:O	1:A:97:ILE:C	0.58	2.46	19	6
1:A:94:ALA:O	1:A:95:LYS:C	0.58	2.45	7	8
1:A:11:GLU:CD	1:A:12:GLU:OE2	0.58	2.46	12	1
1:A:81:LEU:HD12	1:A:81:LEU:O	0.58	1.98	12	1
1:A:43:HIS:CD2	1:A:43:HIS:N	0.58	2.70	14	3
1:A:44:HIS:CE1	1:A:85:ASP:OD2	0.58	2.56	12	2
1:A:61:PHE:O	1:A:62:LYS:C	0.58	2.47	12	2
1:A:12:GLU:CD	1:A:12:GLU:C	0.58	2.71	15	1
1:A:21:THR:O	1:A:22:ARG:C	0.58	2.46	10	14
1:A:32:GLY:O	1:A:33:SER:C	0.58	2.45	2	4
1:A:48:GLU:CD	1:A:48:GLU:N	0.58	2.61	17	1
1:A:61:PHE:CD1	1:A:61:PHE:O	0.58	2.56	17	1
1:A:118:TRP:O	1:A:118:TRP:CD2	0.58	2.56	3	2
1:A:72:GLU:N	1:A:72:GLU:OE2	0.58	2.35	8	1
1:A:16:ILE:O	1:A:17:GLN:C	0.58	2.45	11	8
1:A:50:PHE:CG	1:A:51:ASP:N	0.58	2.72	20	1
1:A:82:LEU:CD1	1:A:82:LEU:N	0.57	2.67	7	1
1:A:37:ALA:O	1:A:38:LEU:O	0.57	2.22	17	11
1:A:101:VAL:HG13	1:A:115:TYR:CZ	0.57	2.34	18	6
1:A:24:ILE:O	1:A:26:GLN:N	0.57	2.37	13	4
1:A:19:GLU:O	1:A:20:GLU:C	0.57	2.46	2	9
1:A:30:GLU:OE1	1:A:30:GLU:C	0.57	2.47	17	1
1:A:33:SER:OG	1:A:34:ASP:N	0.57	2.34	20	1
1:A:81:LEU:HD12	1:A:81:LEU:N	0.57	2.13	8	3
1:A:52:LYS:NZ	1:A:112:ASP:O	0.57	2.36	5	1
1:A:68:LEU:O	1:A:69:GLU:O	0.57	2.23	2	6
1:A:92:LEU:O	1:A:93:ASP:CG	0.57	2.48	11	2
1:A:83:CYS:SG	1:A:83:CYS:O	0.57	2.62	17	1
1:A:26:GLN:O	1:A:29:LEU:N	0.56	2.38	18	1
1:A:115:TYR:CD1	1:A:115:TYR:O	0.56	2.58	6	2
1:A:69:GLU:CD	1:A:70:ALA:N	0.56	2.63	8	1
1:A:111:PHE:O	1:A:112:ASP:OD1	0.56	2.24	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ALA:O	1:A:57:ALA:C	0.56	2.46	2	3
1:A:93:ASP:O	1:A:94:ALA:C	0.56	2.48	5	6
1:A:30:GLU:OE2	1:A:30:GLU:O	0.56	2.22	9	1
1:A:32:GLY:O	1:A:33:SER:O	0.56	2.22	14	7
1:A:23:ASP:OD1	1:A:23:ASP:C	0.56	2.49	4	1
1:A:30:GLU:O	1:A:31:ASP:OD1	0.56	2.22	7	1
1:A:24:ILE:O	1:A:25:ILE:C	0.56	2.48	3	17
1:A:114:ILE:C	1:A:114:ILE:HD12	0.56	2.25	14	3
1:A:91:ALA:O	1:A:92:LEU:O	0.56	2.22	15	2
1:A:72:GLU:N	1:A:72:GLU:CD	0.56	2.64	17	1
1:A:12:GLU:O	1:A:13:LEU:C	0.56	2.48	10	3
1:A:47:ALA:C	1:A:48:GLU:OE2	0.56	2.48	5	1
1:A:20:GLU:O	1:A:23:ASP:N	0.56	2.39	9	2
1:A:27:ALA:O	1:A:28:LEU:C	0.56	2.49	12	4
1:A:82:LEU:HD23	1:A:82:LEU:N	0.56	2.15	6	1
1:A:20:GLU:O	1:A:21:THR:C	0.55	2.47	9	8
1:A:51:ASP:O	1:A:52:LYS:C	0.55	2.47	11	6
1:A:53:LEU:C	1:A:53:LEU:CD2	0.55	2.76	16	8
1:A:65:PHE:CE1	1:A:88:MET:HE2	0.55	2.36	2	2
1:A:96:LEU:O	1:A:98:ASP:N	0.55	2.39	2	2
1:A:32:GLY:O	1:A:34:ASP:N	0.55	2.39	6	2
1:A:17:GLN:O	1:A:18:LYS:C	0.55	2.46	2	4
1:A:44:HIS:ND1	1:A:117:GLY:O	0.55	2.39	16	3
1:A:22:ARG:O	1:A:26:GLN:CG	0.55	2.54	9	2
1:A:65:PHE:CZ	1:A:88:MET:HE2	0.55	2.36	7	1
1:A:14:ILE:CG2	1:A:18:LYS:HZ3	0.55	2.15	8	1
1:A:32:GLY:O	1:A:34:ASP:OD1	0.55	2.23	12	2
1:A:59:GLU:OE1	1:A:59:GLU:O	0.55	2.23	18	1
1:A:18:LYS:O	1:A:19:GLU:C	0.55	2.50	9	2
1:A:57:ALA:O	1:A:58:VAL:C	0.55	2.50	5	3
1:A:60:ALA:O	1:A:61:PHE:C	0.55	2.50	18	3
1:A:88:MET:C	1:A:89:GLN:NE2	0.55	2.65	20	1
1:A:101:VAL:HG13	1:A:115:TYR:CE2	0.54	2.37	20	5
1:A:30:GLU:CD	1:A:30:GLU:O	0.54	2.50	12	1
1:A:106:ASN:N	1:A:106:ASN:ND2	0.54	2.53	13	1
1:A:68:LEU:O	1:A:69:GLU:C	0.54	2.50	7	14
1:A:45:LEU:C	1:A:46:PHE:CD1	0.54	2.86	8	7
1:A:42:GLU:CD	1:A:42:GLU:C	0.54	2.76	4	1
1:A:49:ASP:C	1:A:51:ASP:H	0.54	2.10	6	3
1:A:97:ILE:O	1:A:101:VAL:HG23	0.54	2.03	3	4
1:A:34:ASP:N	1:A:35:PRO:CD	0.54	2.70	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:GLU:O	1:A:120:THR:OG1	0.54	2.22	9	1
1:A:68:LEU:HD23	1:A:69:GLU:N	0.54	2.17	11	2
1:A:21:THR:O	1:A:24:ILE:N	0.54	2.40	10	5
1:A:107:LEU:O	1:A:108:ALA:C	0.54	2.50	3	8
1:A:73:THR:HG22	1:A:81:LEU:O	0.54	2.02	6	1
1:A:107:LEU:O	1:A:110:LYS:N	0.53	2.41	4	4
1:A:48:GLU:N	1:A:48:GLU:CD	0.53	2.66	5	1
1:A:19:GLU:N	1:A:22:ARG:HH21	0.53	2.01	8	1
1:A:44:HIS:NE2	1:A:85:ASP:OD1	0.53	2.42	14	2
1:A:105:VAL:HG12	1:A:106:ASN:N	0.53	2.17	4	3
1:A:51:ASP:O	1:A:54:GLU:N	0.53	2.40	11	1
1:A:81:LEU:C	1:A:81:LEU:CD1	0.53	2.81	12	1
1:A:65:PHE:CE1	1:A:88:MET:HE3	0.53	2.38	13	2
1:A:17:GLN:O	1:A:21:THR:OG1	0.53	2.22	1	4
1:A:72:GLU:CD	1:A:72:GLU:N	0.53	2.66	8	2
1:A:101:VAL:O	1:A:104:LEU:N	0.53	2.42	5	2
1:A:45:LEU:HD12	1:A:45:LEU:H	0.52	1.64	9	2
1:A:121:TYR:N	1:A:121:TYR:CD1	0.52	2.77	9	1
1:A:106:ASN:N	1:A:106:ASN:OD1	0.52	2.41	5	1
1:A:82:LEU:N	1:A:82:LEU:CD1	0.52	2.69	14	2
1:A:116:ASP:C	1:A:116:ASP:OD1	0.52	2.52	14	2
1:A:71:GLU:CD	1:A:71:GLU:N	0.52	2.68	2	2
1:A:94:ALA:O	1:A:97:ILE:N	0.52	2.42	7	1
1:A:96:LEU:O	1:A:99:GLU:N	0.52	2.42	5	3
1:A:65:PHE:CG	1:A:88:MET:SD	0.52	3.02	2	1
1:A:12:GLU:OE1	1:A:12:GLU:CA	0.52	2.56	17	1
1:A:81:LEU:N	1:A:81:LEU:CD1	0.52	2.73	8	2
1:A:15:GLU:O	1:A:16:ILE:C	0.52	2.53	3	4
1:A:69:GLU:CD	1:A:70:ALA:H	0.52	2.11	8	1
1:A:96:LEU:C	1:A:98:ASP:N	0.52	2.67	2	2
1:A:11:GLU:O	1:A:12:GLU:C	0.52	2.51	15	3
1:A:106:ASN:ND2	1:A:106:ASN:H	0.52	2.03	11	1
1:A:116:ASP:O	1:A:116:ASP:CG	0.51	2.50	16	2
1:A:95:LYS:O	1:A:96:LEU:C	0.51	2.53	6	2
1:A:11:GLU:O	1:A:15:GLU:OE2	0.51	2.28	19	1
1:A:71:GLU:OE1	1:A:72:GLU:C	0.51	2.54	13	1
1:A:21:THR:O	1:A:23:ASP:N	0.51	2.44	15	1
1:A:26:GLN:O	1:A:27:ALA:C	0.51	2.50	18	5
1:A:65:PHE:O	1:A:67:VAL:N	0.51	2.44	9	2
1:A:30:GLU:O	1:A:30:GLU:OE1	0.51	2.28	12	1
1:A:84:PHE:C	1:A:85:ASP:OD1	0.51	2.54	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLU:OE1	1:A:15:GLU:C	0.51	2.54	3	2
1:A:91:ALA:O	1:A:93:ASP:N	0.51	2.44	14	2
1:A:11:GLU:O	1:A:15:GLU:OE1	0.51	2.29	7	1
1:A:27:ALA:O	1:A:31:ASP:OD1	0.51	2.28	8	1
1:A:69:GLU:OE2	1:A:70:ALA:O	0.51	2.28	8	1
1:A:88:MET:SD	1:A:100:GLN:NE2	0.51	2.84	1	3
1:A:24:ILE:C	1:A:26:GLN:N	0.51	2.69	13	4
1:A:85:ASP:OD1	1:A:85:ASP:C	0.50	2.54	6	1
1:A:43:HIS:ND1	1:A:104:LEU:CD1	0.50	2.75	5	1
1:A:82:LEU:N	1:A:82:LEU:HD12	0.50	2.20	7	1
1:A:43:HIS:CD2	1:A:104:LEU:CD1	0.50	2.94	7	2
1:A:51:ASP:C	1:A:51:ASP:OD1	0.50	2.54	1	1
1:A:81:LEU:C	1:A:82:LEU:HD12	0.50	2.31	8	2
1:A:47:ALA:HB3	1:A:53:LEU:HD12	0.50	1.81	4	1
1:A:53:LEU:O	1:A:53:LEU:HD23	0.50	2.07	12	1
1:A:94:ALA:O	1:A:98:ASP:CG	0.50	2.54	1	1
1:A:15:GLU:O	1:A:18:LYS:CB	0.50	2.59	3	1
1:A:102:GLU:O	1:A:106:ASN:CG	0.49	2.56	11	2
1:A:92:LEU:O	1:A:93:ASP:OD1	0.49	2.29	13	1
1:A:41:ILE:HD13	1:A:41:ILE:N	0.49	2.23	15	1
1:A:72:GLU:O	1:A:72:GLU:OE1	0.49	2.29	9	1
1:A:12:GLU:CD	1:A:12:GLU:H	0.49	2.15	17	1
1:A:62:LYS:O	1:A:63:MET:C	0.49	2.55	7	4
1:A:45:LEU:O	1:A:84:PHE:CD1	0.49	2.66	11	1
1:A:33:SER:C	1:A:34:ASP:CG	0.49	2.80	12	1
1:A:11:GLU:OE1	1:A:12:GLU:N	0.49	2.46	12	2
1:A:33:SER:O	1:A:34:ASP:C	0.49	2.54	13	2
1:A:44:HIS:CD2	1:A:83:CYS:SG	0.49	3.05	18	1
1:A:50:PHE:CD1	1:A:50:PHE:C	0.49	2.88	3	1
1:A:51:ASP:O	1:A:53:LEU:N	0.49	2.46	11	2
1:A:22:ARG:NH1	1:A:22:ARG:CG	0.49	2.75	17	1
1:A:116:ASP:OD1	1:A:116:ASP:O	0.48	2.31	14	2
1:A:39:TYR:CE2	1:A:92:LEU:HD13	0.48	2.43	16	1
1:A:100:GLN:O	1:A:101:VAL:C	0.48	2.56	4	1
1:A:37:ALA:O	1:A:38:LEU:CB	0.48	2.60	18	2
1:A:89:GLN:N	1:A:89:GLN:HE21	0.48	2.05	20	2
1:A:115:TYR:CD1	1:A:116:ASP:N	0.48	2.82	15	1
1:A:16:ILE:O	1:A:18:LYS:N	0.48	2.46	1	2
1:A:67:VAL:HG22	1:A:68:LEU:N	0.48	2.23	2	1
1:A:33:SER:C	1:A:34:ASP:OD1	0.48	2.57	3	1
1:A:110:LYS:HB3	1:A:110:LYS:HZ3	0.48	1.69	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:MET:C	1:A:89:GLN:HE21	0.48	2.16	20	1
1:A:44:HIS:CD2	1:A:85:ASP:OD2	0.48	2.66	3	1
1:A:61:PHE:O	1:A:63:MET:N	0.48	2.47	12	1
1:A:17:GLN:OE1	1:A:21:THR:OG1	0.48	2.31	12	1
1:A:109:GLU:OE1	1:A:109:GLU:CA	0.48	2.62	14	1
1:A:22:ARG:NH1	1:A:22:ARG:HG3	0.48	2.23	2	4
1:A:27:ALA:O	1:A:30:GLU:N	0.48	2.47	8	2
1:A:11:GLU:OE1	1:A:11:GLU:C	0.47	2.56	12	1
1:A:90:SER:OG	1:A:91:ALA:N	0.47	2.47	10	1
1:A:46:PHE:CD2	1:A:114:ILE:HG23	0.47	2.44	14	2
1:A:35:PRO:C	1:A:37:ALA:N	0.47	2.72	10	2
1:A:52:LYS:NZ	1:A:112:ASP:OD2	0.47	2.47	10	1
1:A:105:VAL:O	1:A:106:ASN:C	0.47	2.56	7	3
1:A:118:TRP:CE3	1:A:119:GLY:CA	0.47	2.98	8	1
1:A:89:GLN:N	1:A:89:GLN:OE1	0.47	2.48	15	1
1:A:100:GLN:HE21	1:A:100:GLN:CA	0.47	2.22	18	1
1:A:50:PHE:CE2	1:A:82:LEU:HD11	0.47	2.44	19	1
1:A:15:GLU:O	1:A:18:LYS:N	0.47	2.47	3	1
1:A:13:LEU:O	1:A:14:ILE:C	0.47	2.57	20	2
1:A:102:GLU:OE1	1:A:102:GLU:C	0.47	2.58	2	1
1:A:24:ILE:O	1:A:27:ALA:N	0.47	2.48	3	3
1:A:32:GLY:O	1:A:34:ASP:CG	0.47	2.58	12	1
1:A:73:THR:CG2	1:A:83:CYS:SG	0.47	3.03	20	1
1:A:104:LEU:O	1:A:108:ALA:HB2	0.47	2.10	11	1
1:A:53:LEU:HD23	1:A:53:LEU:C	0.46	2.35	12	1
1:A:118:TRP:CD2	1:A:118:TRP:C	0.46	2.93	17	2
1:A:64:GLY:C	1:A:65:PHE:CG	0.46	2.93	9	1
1:A:17:GLN:HG2	1:A:101:VAL:HG11	0.46	1.88	11	1
1:A:120:THR:OG1	1:A:121:TYR:N	0.46	2.49	11	1
1:A:70:ALA:CB	1:A:83:CYS:C	0.46	2.89	14	6
1:A:39:TYR:CD2	1:A:92:LEU:HD13	0.46	2.46	3	1
1:A:54:GLU:O	1:A:55:LYS:C	0.46	2.59	2	1
1:A:26:GLN:CD	1:A:26:GLN:C	0.46	2.82	14	2
1:A:88:MET:HE1	1:A:100:GLN:NE2	0.46	2.25	10	1
1:A:102:GLU:O	1:A:106:ASN:OD1	0.46	2.34	1	1
1:A:44:HIS:CE1	1:A:85:ASP:OD1	0.46	2.69	20	1
1:A:29:LEU:O	1:A:31:ASP:N	0.46	2.49	1	1
1:A:66:GLU:O	1:A:67:VAL:C	0.46	2.59	19	4
1:A:65:PHE:HB3	1:A:86:ALA:HB1	0.46	1.86	9	1
1:A:36:ASP:OD1	1:A:36:ASP:C	0.46	2.58	18	1
1:A:39:TYR:CZ	1:A:92:LEU:HD13	0.45	2.46	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ALA:CB	1:A:83:CYS:O	0.45	2.64	4	2
1:A:44:HIS:CD2	1:A:85:ASP:OD1	0.45	2.69	5	1
1:A:52:LYS:O	1:A:55:LYS:N	0.45	2.48	15	1
1:A:22:ARG:NH1	1:A:22:ARG:HG2	0.45	2.25	17	1
1:A:72:GLU:CD	1:A:72:GLU:H	0.45	2.16	17	1
1:A:111:PHE:O	1:A:112:ASP:OD2	0.45	2.35	19	1
1:A:58:VAL:HG12	1:A:59:GLU:N	0.45	2.26	8	1
1:A:115:TYR:O	1:A:115:TYR:CD2	0.45	2.70	12	1
1:A:43:HIS:C	1:A:44:HIS:CD2	0.45	2.94	16	2
1:A:115:TYR:CD1	1:A:115:TYR:C	0.45	2.95	6	1
1:A:27:ALA:O	1:A:29:LEU:N	0.45	2.50	8	1
1:A:12:GLU:HG2	1:A:13:LEU:N	0.45	2.27	4	1
1:A:65:PHE:C	1:A:66:GLU:OE1	0.45	2.59	6	1
1:A:68:LEU:HD23	1:A:69:GLU:H	0.45	1.69	13	1
1:A:118:TRP:O	1:A:118:TRP:CG	0.45	2.66	16	1
1:A:13:LEU:HD23	1:A:13:LEU:N	0.45	2.27	19	3
1:A:66:GLU:OE1	1:A:67:VAL:O	0.45	2.35	2	1
1:A:17:GLN:NE2	1:A:101:VAL:HG21	0.45	2.27	5	1
1:A:52:LYS:O	1:A:53:LEU:C	0.45	2.58	15	1
1:A:25:ILE:CD1	1:A:25:ILE:N	0.45	2.79	18	1
1:A:67:VAL:O	1:A:68:LEU:HD22	0.45	2.12	14	1
1:A:41:ILE:HG22	1:A:42:GLU:N	0.44	2.27	10	1
1:A:103:LYS:C	1:A:105:VAL:N	0.44	2.74	20	1
1:A:38:LEU:O	1:A:39:TYR:CD1	0.44	2.70	9	1
1:A:34:ASP:N	1:A:35:PRO:HD3	0.44	2.27	7	2
1:A:104:LEU:O	1:A:105:VAL:C	0.44	2.59	9	1
1:A:114:ILE:C	1:A:114:ILE:CD1	0.44	2.87	14	1
1:A:65:PHE:CD1	1:A:65:PHE:N	0.44	2.86	19	2
1:A:40:GLU:O	1:A:120:THR:CB	0.44	2.65	9	1
1:A:61:PHE:CD1	1:A:61:PHE:C	0.44	2.93	10	2
1:A:34:ASP:OD1	1:A:34:ASP:N	0.44	2.50	19	1
1:A:59:GLU:OE2	1:A:107:LEU:CD1	0.44	2.65	8	1
1:A:12:GLU:CD	1:A:12:GLU:N	0.44	2.71	17	1
1:A:101:VAL:O	1:A:103:LYS:N	0.44	2.51	19	1
1:A:53:LEU:HD21	1:A:84:PHE:CD1	0.44	2.48	3	2
1:A:30:GLU:CD	1:A:30:GLU:C	0.44	2.85	4	2
1:A:44:HIS:HE2	1:A:85:ASP:CG	0.44	2.21	12	1
1:A:109:GLU:CD	1:A:109:GLU:O	0.44	2.61	13	1
1:A:50:PHE:C	1:A:50:PHE:CD1	0.44	2.95	7	1
1:A:25:ILE:N	1:A:25:ILE:HD13	0.44	2.28	8	2
1:A:88:MET:HE1	1:A:100:GLN:HE22	0.44	1.73	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:N	1:A:38:LEU:CD2	0.43	2.81	3	1
1:A:34:ASP:HB3	1:A:37:ALA:HB2	0.43	1.88	13	1
1:A:70:ALA:HB1	1:A:83:CYS:C	0.43	2.39	14	2
1:A:17:GLN:OE1	1:A:118:TRP:CD1	0.43	2.71	4	1
1:A:99:GLU:O	1:A:103:LYS:NZ	0.43	2.44	15	1
1:A:44:HIS:CD2	1:A:44:HIS:N	0.43	2.87	2	1
1:A:45:LEU:HB2	1:A:84:PHE:CZ	0.43	2.48	6	6
1:A:42:GLU:OE2	1:A:121:TYR:CE2	0.43	2.72	7	1
1:A:35:PRO:C	1:A:37:ALA:H	0.43	2.20	10	1
1:A:11:GLU:O	1:A:13:LEU:N	0.43	2.52	15	1
1:A:25:ILE:N	1:A:25:ILE:HD12	0.43	2.28	18	1
1:A:90:SER:O	1:A:91:ALA:O	0.43	2.35	9	1
1:A:51:ASP:C	1:A:53:LEU:N	0.43	2.74	11	3
1:A:101:VAL:HG12	1:A:102:GLU:N	0.43	2.28	13	1
1:A:42:GLU:CG	1:A:119:GLY:O	0.43	2.67	18	1
1:A:95:LYS:O	1:A:99:GLU:OE2	0.43	2.37	18	1
1:A:100:GLN:NE2	1:A:100:GLN:CA	0.43	2.82	18	1
1:A:81:LEU:C	1:A:82:LEU:HD23	0.43	2.38	6	1
1:A:90:SER:OG	1:A:96:LEU:CD2	0.43	2.67	6	1
1:A:20:GLU:O	1:A:23:ASP:OD2	0.43	2.37	4	1
1:A:36:ASP:OD1	1:A:36:ASP:N	0.43	2.52	15	2
1:A:58:VAL:O	1:A:59:GLU:C	0.43	2.61	10	2
1:A:51:ASP:OD1	1:A:51:ASP:N	0.43	2.45	11	1
1:A:57:ALA:HB1	1:A:67:VAL:HG21	0.42	1.91	8	1
1:A:54:GLU:O	1:A:58:VAL:CG2	0.42	2.67	18	2
1:A:59:GLU:O	1:A:62:LYS:N	0.42	2.52	5	1
1:A:42:GLU:C	1:A:43:HIS:CD2	0.42	2.97	19	1
1:A:59:GLU:OE1	1:A:59:GLU:C	0.42	2.61	2	1
1:A:47:ALA:HB1	1:A:52:LYS:HE3	0.42	1.91	5	1
1:A:21:THR:C	1:A:23:ASP:N	0.42	2.75	15	1
1:A:61:PHE:CD2	1:A:62:LYS:N	0.42	2.88	12	1
1:A:109:GLU:N	1:A:109:GLU:CD	0.42	2.78	14	1
1:A:17:GLN:CD	1:A:17:GLN:O	0.42	2.62	12	1
1:A:54:GLU:OE1	1:A:54:GLU:C	0.42	2.62	12	1
1:A:32:GLY:C	1:A:33:SER:O	0.42	2.60	14	2
1:A:101:VAL:HG13	1:A:115:TYR:OH	0.42	2.15	4	1
1:A:105:VAL:HG22	1:A:115:TYR:CD2	0.42	2.48	10	1
1:A:44:HIS:C	1:A:45:LEU:CD1	0.42	2.89	14	1
1:A:40:GLU:C	1:A:41:ILE:HD13	0.42	2.40	15	1
1:A:60:ALA:O	1:A:63:MET:N	0.42	2.53	18	1
1:A:48:GLU:H	1:A:52:LYS:NZ	0.42	2.13	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ALA:HA	1:A:97:ILE:HD12	0.42	1.92	7	1
1:A:61:PHE:C	1:A:63:MET:N	0.42	2.77	12	1
1:A:82:LEU:N	1:A:82:LEU:CD2	0.42	2.76	6	1
1:A:30:GLU:OE1	1:A:31:ASP:N	0.42	2.53	17	1
1:A:18:LYS:CE	1:A:98:ASP:OD2	0.42	2.68	19	1
1:A:55:LYS:O	1:A:56:ALA:C	0.41	2.63	14	1
1:A:101:VAL:HG13	1:A:115:TYR:CE1	0.41	2.50	14	1
1:A:108:ALA:HB1	1:A:113:ILE:HG13	0.41	1.92	15	1
1:A:16:ILE:C	1:A:18:LYS:N	0.41	2.77	9	2
1:A:16:ILE:N	1:A:16:ILE:CD1	0.41	2.82	12	1
1:A:68:LEU:C	1:A:69:GLU:O	0.41	2.63	2	3
1:A:46:PHE:CZ	1:A:114:ILE:HG23	0.41	2.50	6	1
1:A:61:PHE:CD2	1:A:61:PHE:C	0.41	2.98	4	1
1:A:25:ILE:HG22	1:A:26:GLN:N	0.41	2.30	12	1
1:A:66:GLU:N	1:A:87:THR:O	0.41	2.53	9	1
1:A:28:LEU:O	1:A:31:ASP:C	0.41	2.63	16	1
1:A:46:PHE:CE2	1:A:114:ILE:HG23	0.41	2.51	20	1
1:A:22:ARG:HH11	1:A:22:ARG:HG2	0.41	1.76	2	1
1:A:70:ALA:HB1	1:A:83:CYS:N	0.41	2.31	2	1
1:A:42:GLU:OE2	1:A:121:TYR:CD2	0.41	2.74	7	1
1:A:43:HIS:ND1	1:A:118:TRP:HB2	0.41	2.30	9	1
1:A:57:ALA:O	1:A:60:ALA:HB3	0.41	2.14	8	1
1:A:65:PHE:CZ	1:A:88:MET:HE3	0.41	2.49	13	1
1:A:37:ALA:C	1:A:38:LEU:O	0.41	2.63	19	1
1:A:13:LEU:N	1:A:13:LEU:HD23	0.41	2.31	14	2
1:A:25:ILE:O	1:A:26:GLN:C	0.41	2.62	12	1
1:A:71:GLU:OE1	1:A:72:GLU:O	0.41	2.38	13	1
1:A:62:LYS:NZ	1:A:62:LYS:HB3	0.40	2.31	13	1
1:A:17:GLN:O	1:A:21:THR:CB	0.40	2.69	18	1
1:A:13:LEU:O	1:A:17:GLN:OE1	0.40	2.39	13	1
1:A:11:GLU:C	1:A:13:LEU:N	0.40	2.76	15	1
1:A:69:GLU:HG2	1:A:70:ALA:N	0.40	2.31	7	1
1:A:65:PHE:CZ	1:A:100:GLN:NE2	0.40	2.89	12	1
1:A:27:ALA:C	1:A:29:LEU:N	0.40	2.78	8	1
1:A:40:GLU:N	1:A:40:GLU:CD	0.40	2.79	9	1
1:A:70:ALA:HB1	1:A:83:CYS:H	0.40	1.76	9	1
1:A:45:LEU:HB2	1:A:84:PHE:CE2	0.40	2.52	11	1
1:A:39:TYR:CE1	1:A:92:LEU:HD13	0.40	2.51	12	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/132 (80%)	81±3 (77±3%)	18±4 (17±3%)	6±2 (6±2%)	2	19
All	All	2100/2640 (80%)	1616 (77%)	359 (17%)	125 (6%)	2	19

All 21 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	112	ASP	20
1	A	117	GLY	19
1	A	38	LEU	17
1	A	33	SER	14
1	A	64	GLY	13
1	A	69	GLU	9
1	A	92	LEU	5
1	A	80	LYS	4
1	A	72	GLU	4
1	A	50	PHE	3
1	A	16	ILE	2
1	A	97	ILE	2
1	A	25	ILE	2
1	A	32	GLY	2
1	A	66	GLU	2
1	A	116	ASP	2
1	A	37	ALA	1
1	A	91	ALA	1
1	A	22	ARG	1
1	A	51	ASP	1
1	A	67	VAL	1

6.3.2 Protein sidechains

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/115 (78%)	67±5 (74±5%)	23±5 (26±5%)	2	24
All	All	1800/2300 (78%)	1341 (74%)	459 (26%)	2	24

All 78 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	87	THR	20
1	A	46	PHE	19
1	A	114	ILE	19
1	A	68	LEU	15
1	A	81	LEU	15
1	A	85	ASP	14
1	A	52	LYS	12
1	A	38	LEU	10
1	A	93	ASP	10
1	A	34	ASP	9
1	A	96	LEU	9
1	A	120	THR	9
1	A	66	GLU	9
1	A	17	GLN	8
1	A	72	GLU	8
1	A	39	TYR	8
1	A	44	HIS	8
1	A	15	GLU	7
1	A	50	PHE	7
1	A	80	LYS	7
1	A	84	PHE	7
1	A	112	ASP	7
1	A	22	ARG	7
1	A	71	GLU	7
1	A	90	SER	7
1	A	29	LEU	7
1	A	23	ASP	7
1	A	59	GLU	7
1	A	89	GLN	7
1	A	36	ASP	6
1	A	49	ASP	6
1	A	121	TYR	6
1	A	42	GLU	6
1	A	95	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	12	GLU	6
1	A	106	ASN	6
1	A	28	LEU	5
1	A	102	GLU	5
1	A	33	SER	5
1	A	98	ASP	5
1	A	31	ASP	5
1	A	109	GLU	5
1	A	107	LEU	5
1	A	51	ASP	5
1	A	67	VAL	5
1	A	55	LYS	4
1	A	73	THR	4
1	A	40	GLU	4
1	A	99	GLU	4
1	A	100	GLN	4
1	A	83	CYS	4
1	A	62	LYS	4
1	A	88	MET	4
1	A	18	LYS	4
1	A	11	GLU	4
1	A	58	VAL	3
1	A	20	GLU	3
1	A	82	LEU	3
1	A	110	LYS	3
1	A	30	GLU	3
1	A	92	LEU	3
1	A	26	GLN	3
1	A	48	GLU	3
1	A	103	LYS	2
1	A	115	TYR	2
1	A	54	GLU	2
1	A	45	LEU	2
1	A	13	LEU	2
1	A	69	GLU	2
1	A	43	HIS	2
1	A	41	ILE	1
1	A	21	THR	1
1	A	25	ILE	1
1	A	101	VAL	1
1	A	63	MET	1
1	A	116	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	19	GLU	1
1	A	113	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 87% 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	1545
Number of shifts mapped to atoms	1545
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	124	-0.46 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	118	-0.12 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	121	-0.09 ± 0.10	None needed (< 0.5 ppm)
^{15}N	124	0.03 ± 0.13	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 93%, i.e. 1339 atoms were assigned a chemical shift out of a possible 1434. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	523/527 (99%)	212/213 (100%)	207/210 (99%)	104/104 (100%)
Sidechain	726/794 (91%)	496/513 (97%)	226/265 (85%)	4/16 (25%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	90/113 (80%)	45/56 (80%)	44/54 (81%)	1/3 (33%)
Overall	1339/1434 (93%)	753/782 (96%)	477/529 (90%)	109/123 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1544 atoms were assigned a chemical shift out of a possible 1778. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	621/664 (94%)	252/269 (94%)	245/264 (93%)	124/131 (95%)
Sidechain	817/934 (87%)	557/601 (93%)	255/315 (81%)	5/18 (28%)
Aromatic	106/180 (59%)	53/92 (58%)	52/78 (67%)	1/10 (10%)
Overall	1544/1778 (87%)	862/962 (90%)	552/657 (84%)	130/159 (82%)

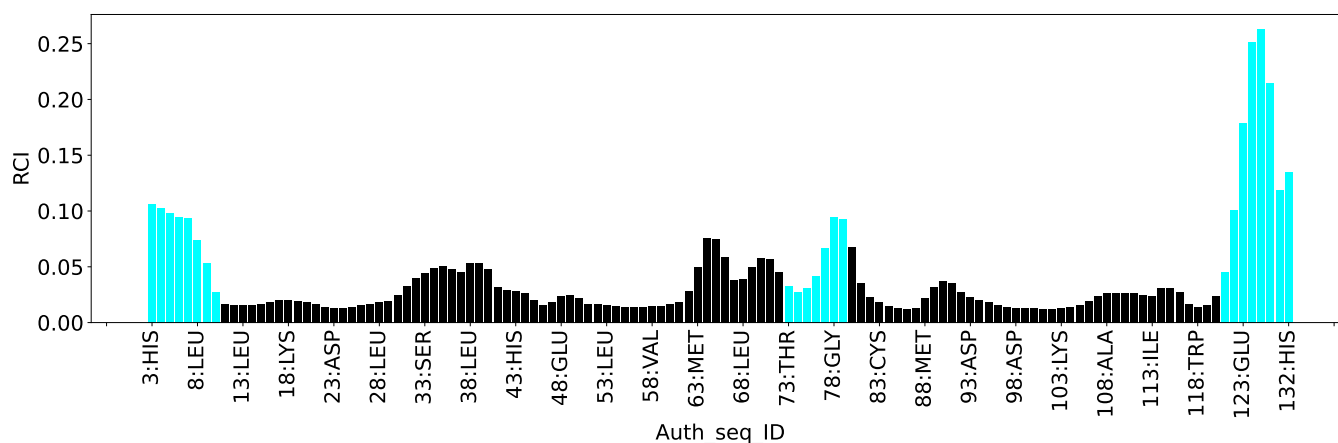
7.1.4 Statistically unusual chemical shifts [i](#)

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

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	1151
Intra-residue ($ i-j =0$)	5
Sequential ($ i-j =1$)	255
Medium range ($ i-j >1$ and $ i-j <5$)	329
Long range ($ i-j \geq 5$)	446
Inter-chain	0
Hydrogen bond restraints	116
Disulfide bond restraints	0
Total dihedral-angle restraints	117
Number of unmapped restraints	0
Number of restraints per residue	9.6
Number of long range restraints per residue ¹	3.6

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.1	0.14
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

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

9 Distance violation analysis ⓘ

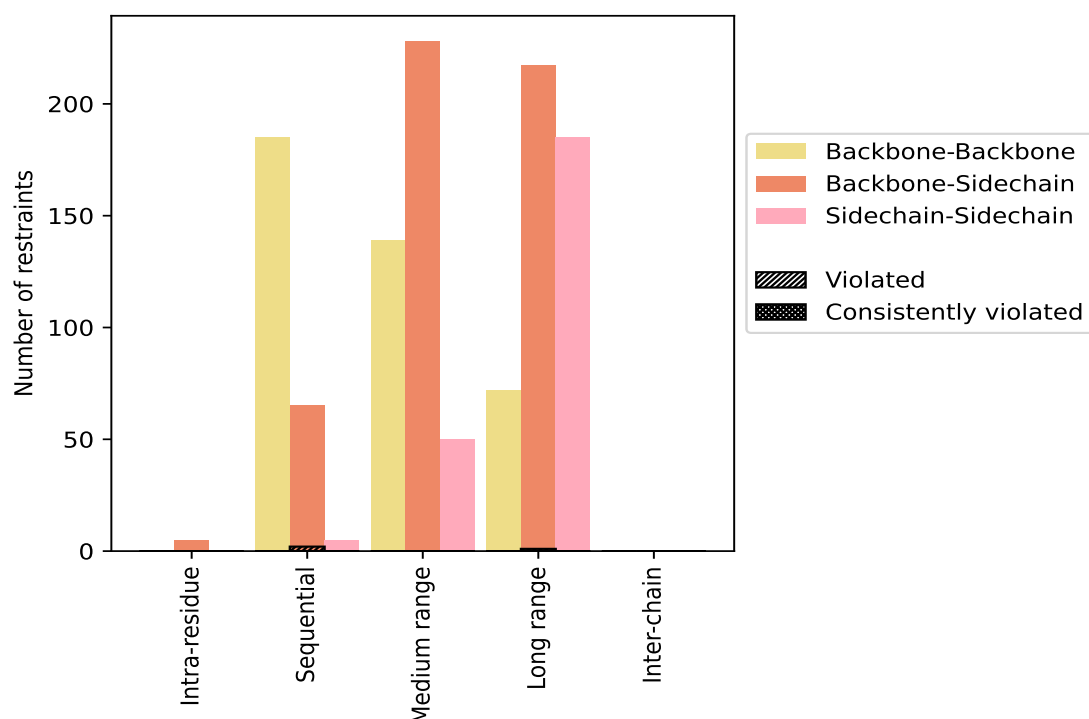
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	5	0.4	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	5	0.4	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 ($i-j =1$)	255	22.2	2	0.8	0.2	0	0.0	0.0
Backbone-Backbone	185	16.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	65	5.6	2	3.1	0.2	0	0.0	0.0
Sidechain-Sidechain	5	0.4	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	329	28.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	139	12.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	140	12.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	50	4.3	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	446	38.7	1	0.2	0.1	0	0.0	0.0
Backbone-Backbone	72	6.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	189	16.4	1	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	185	16.1	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	116	10.1	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	1151	100.0	3	0.3	0.3	0	0.0	0.0
Backbone-Backbone	396	34.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	515	44.7	3	0.6	0.3	0	0.0	0.0
Sidechain-Sidechain	240	20.9	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 disulfid 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	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	1	0	0	0	1	0.11	0.11	0.0	0.11
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	1	0	1	0.11	0.11	0.0	0.11
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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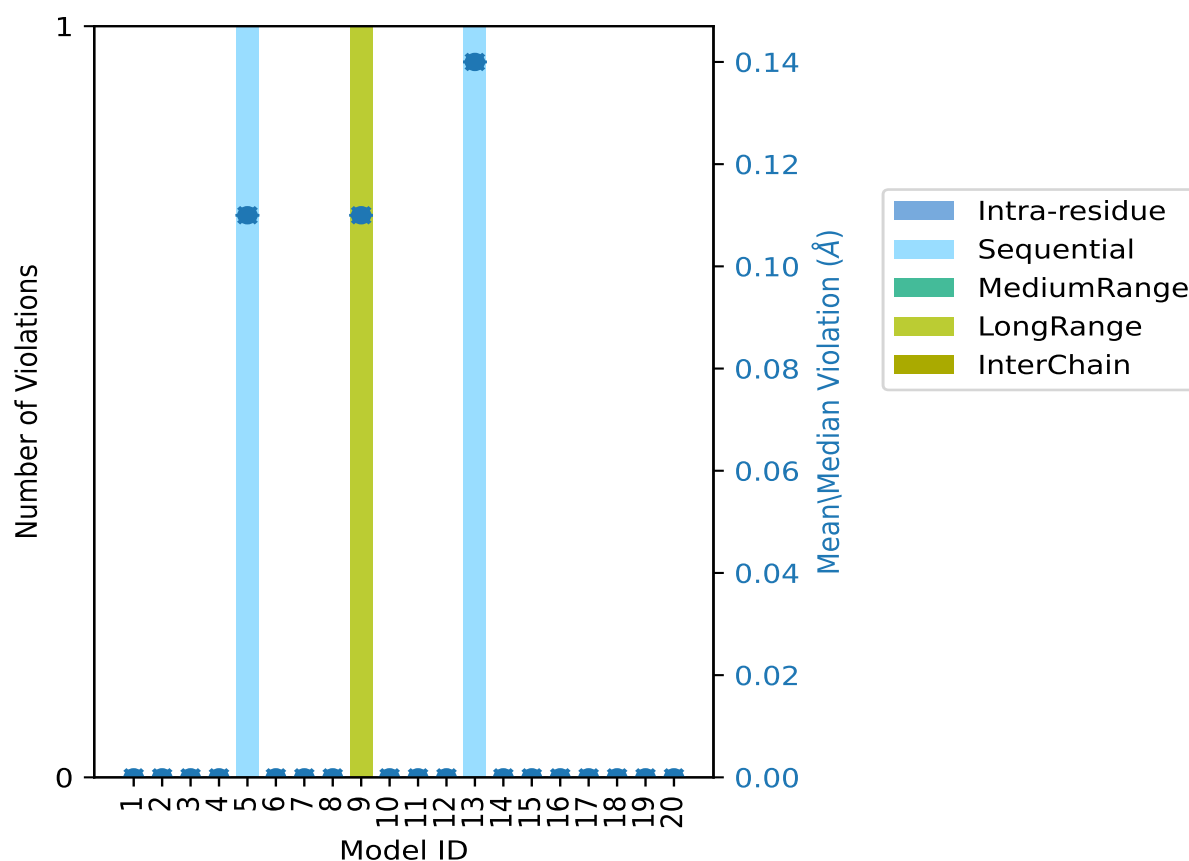
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	1	0	0	0	1	0.14	0.14	0.0	0.14
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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 ⓘ



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

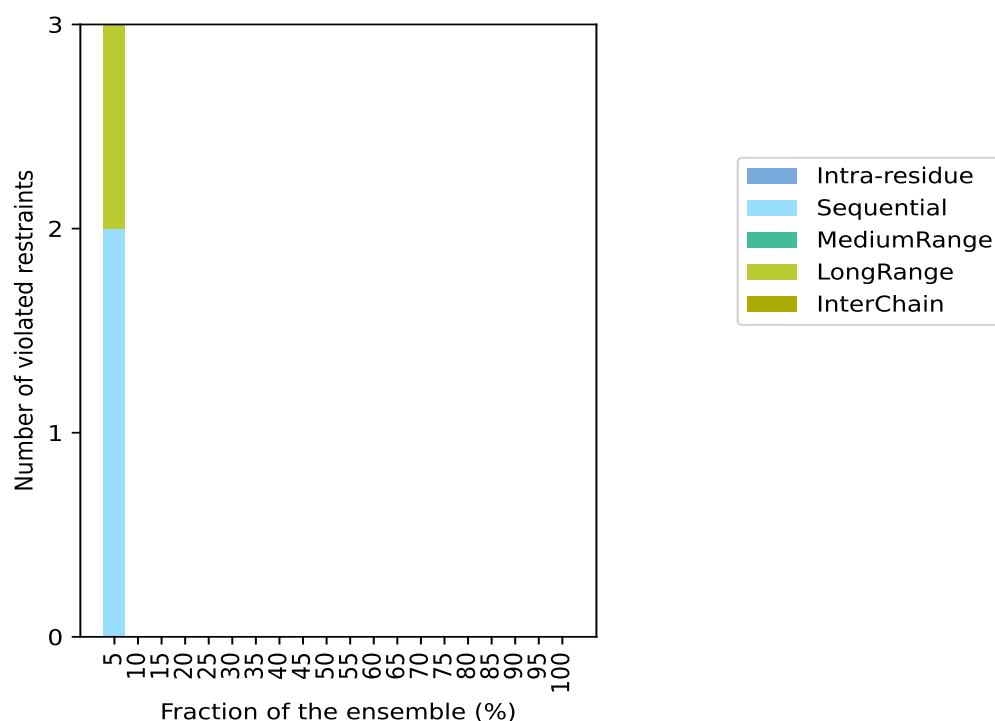
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1032(IR:5, SQ:253, MR:329, LR:445, IC:0) restraints are not 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	2	0	1	0	3	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	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](#)



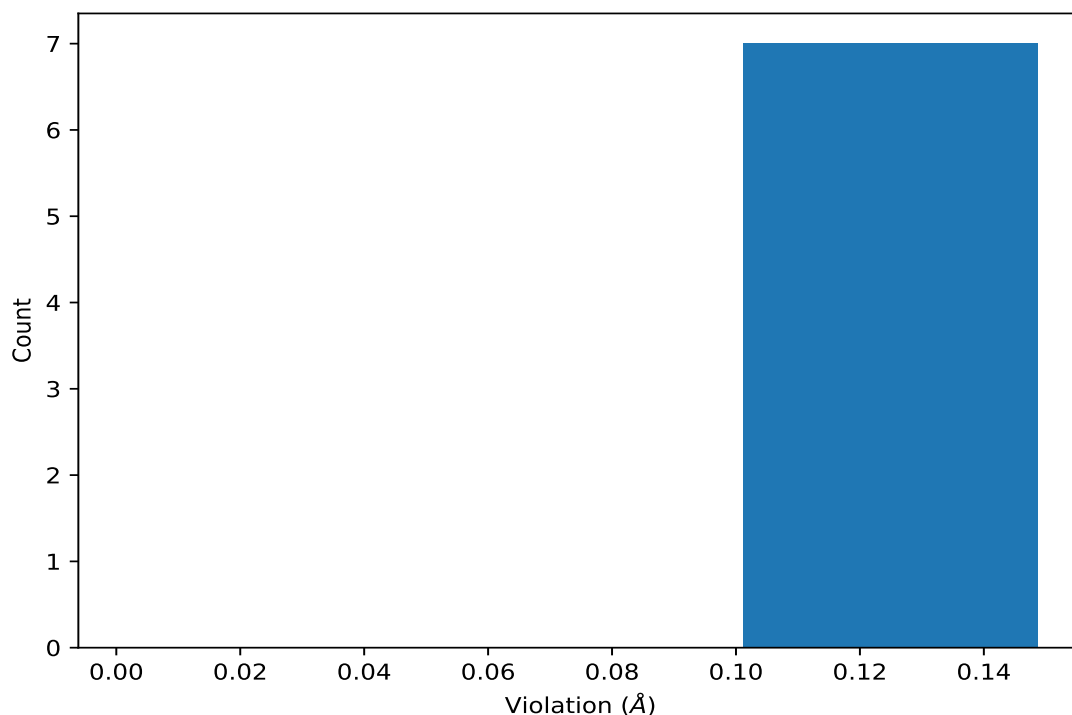
9.4 Most violated distance restraints in the ensemble [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:75:A:ASP:HB2	1:76:A:GLU:H	13	0.14
(2,330)	1:75:A:ASP:HB3	1:76:A:GLU:H	13	0.14
(2,602)	1:70:A:ALA:HB1	1:83:A:CYS:H	9	0.11
(2,602)	1:70:A:ALA:HB2	1:83:A:CYS:H	9	0.11
(2,602)	1:70:A:ALA:HB3	1:83:A:CYS:H	9	0.11
(2,331)	1:79:A:ASN:HB2	1:80:A:LYS:H	5	0.11
(2,331)	1:79:A:ASN:HB3	1:80:A:LYS:H	5	0.11

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

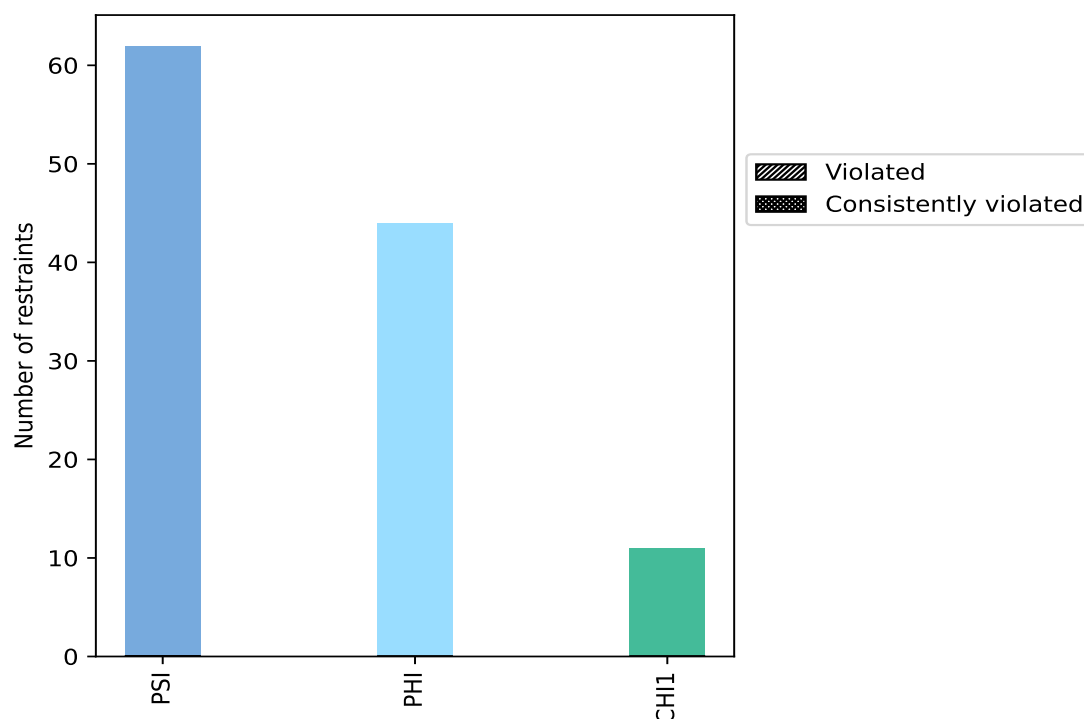
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	62	53.0	0	0.0	0.0	0	0.0	0.0
PHI	44	37.6	0	0.0	0.0	0	0.0	0.0
CHI1	11	9.4	0	0.0	0.0	0	0.0	0.0
Total	117	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