



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 AM UTC

PDB ID : 2V6Z / pdb_00002v6z
BMRB ID : 7419
Title : Solution Structure of Amino-Terminal Domain of Human DNA Polymerase Epsilon Subunit B
Authors : Nuutinen, T.; Fredriksson, K.; Tossavainen, H.; Pospiech, H.; Pirila, P.; Permi, P.; Annala, A.; Syvaoja, J.E.
Deposited on : 2007-07-24

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

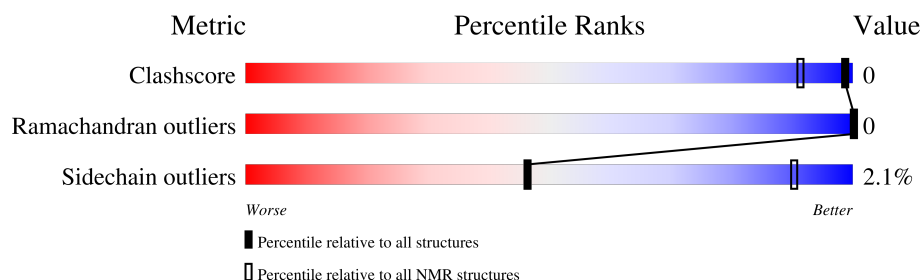
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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	M	99	

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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	M:34-M:99 (66)	0.42	12

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1101 atoms, of which 513 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA POLYMERASE EPSILON SUBUNIT 2.

Mol	Chain	Residues	Atoms						Trace
1	M	75	Total	C	H	N	O	S	0
			1101	367	513	103	116	2	

There are 25 discrepancies between the modelled and reference sequences:

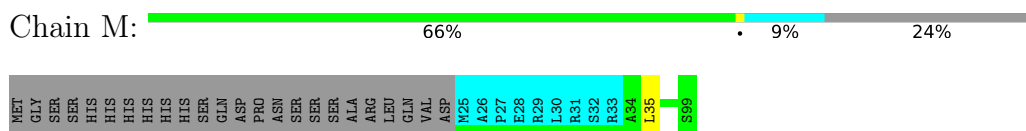
Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MET	-	expression tag	UNP P56282
M	2	GLY	-	expression tag	UNP P56282
M	3	SER	-	expression tag	UNP P56282
M	4	SER	-	expression tag	UNP P56282
M	5	HIS	-	expression tag	UNP P56282
M	6	HIS	-	expression tag	UNP P56282
M	7	HIS	-	expression tag	UNP P56282
M	8	HIS	-	expression tag	UNP P56282
M	9	HIS	-	expression tag	UNP P56282
M	10	HIS	-	expression tag	UNP P56282
M	11	SER	-	expression tag	UNP P56282
M	12	GLN	-	expression tag	UNP P56282
M	13	ASP	-	expression tag	UNP P56282
M	14	PRO	-	expression tag	UNP P56282
M	15	ASN	-	expression tag	UNP P56282
M	16	SER	-	expression tag	UNP P56282
M	17	SER	-	expression tag	UNP P56282
M	18	SER	-	expression tag	UNP P56282
M	19	ALA	-	expression tag	UNP P56282
M	20	ARG	-	expression tag	UNP P56282
M	21	LEU	-	expression tag	UNP P56282
M	22	GLN	-	expression tag	UNP P56282
M	23	VAL	-	expression tag	UNP P56282
M	24	ASP	-	expression tag	UNP P56282
M	98	SER	CYS	engineered mutation	UNP P56282

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2

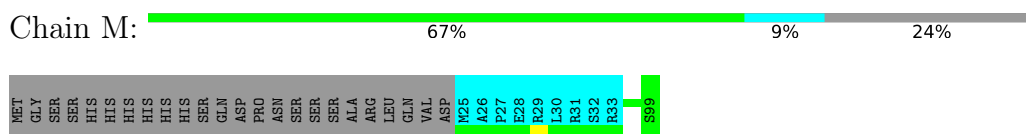


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

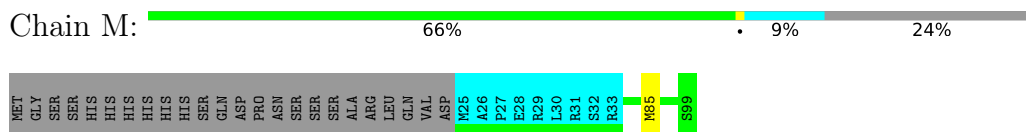
4.2.1 Score per residue for model 1

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



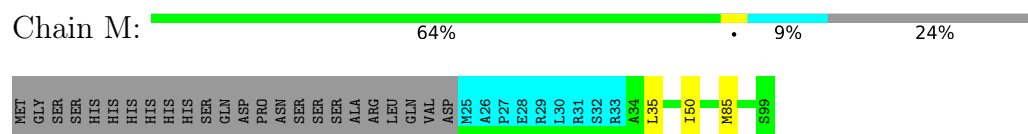
4.2.2 Score per residue for model 2

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



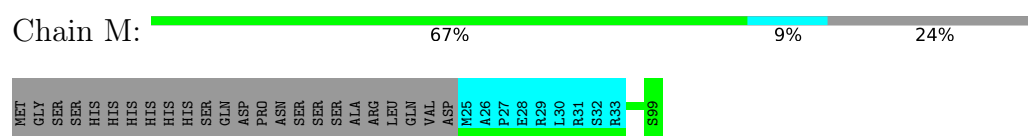
4.2.3 Score per residue for model 3

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



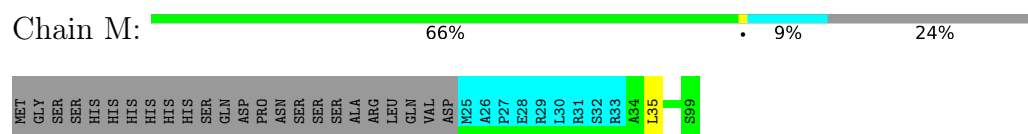
4.2.4 Score per residue for model 4

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



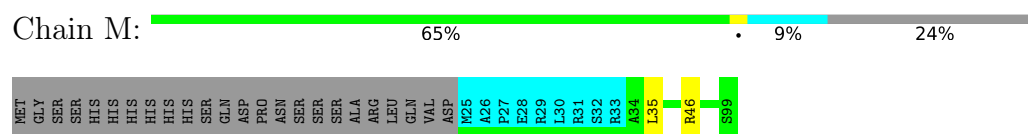
4.2.5 Score per residue for model 5

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



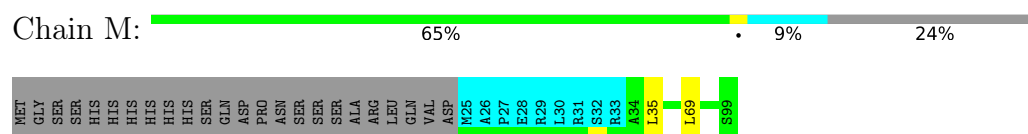
4.2.6 Score per residue for model 6

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



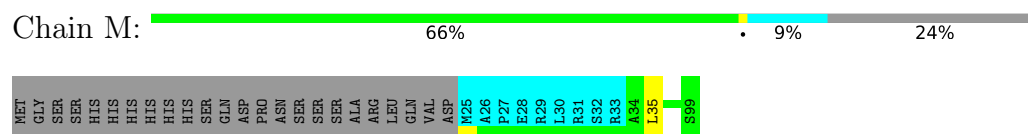
4.2.7 Score per residue for model 7

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



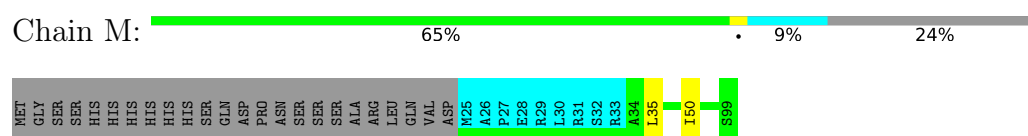
4.2.8 Score per residue for model 8

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



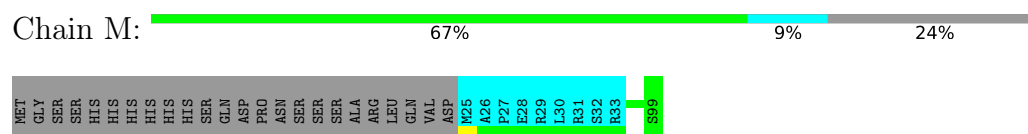
4.2.9 Score per residue for model 9

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



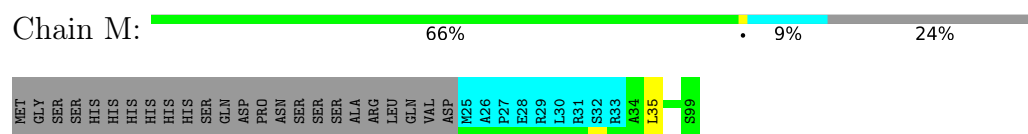
4.2.10 Score per residue for model 10

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



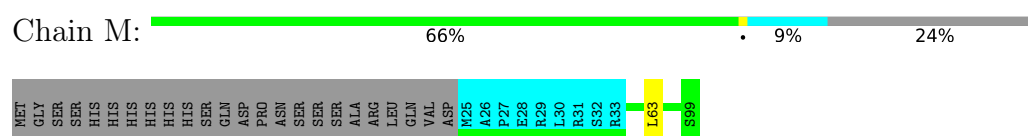
4.2.11 Score per residue for model 11

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



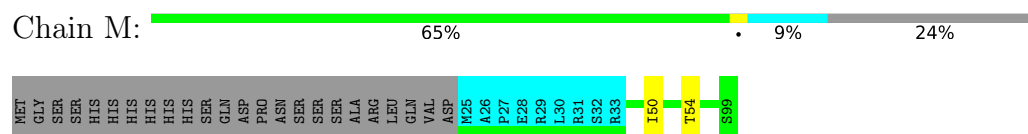
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



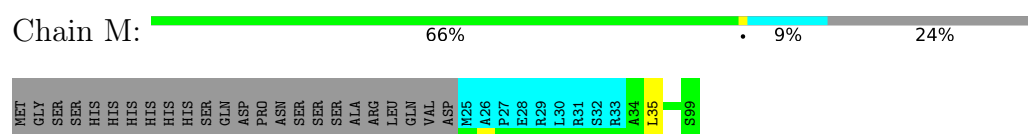
4.2.13 Score per residue for model 13

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



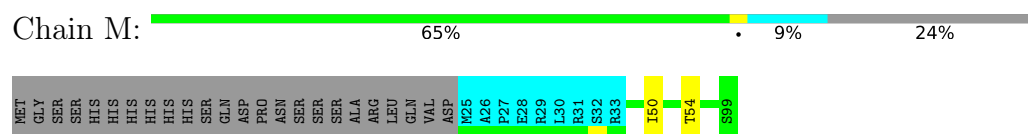
4.2.14 Score per residue for model 14

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



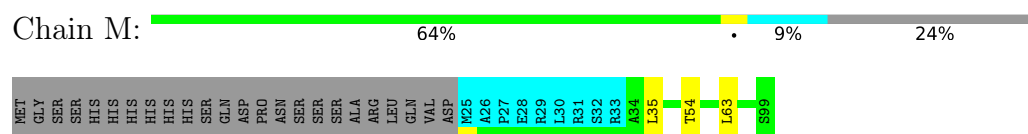
4.2.15 Score per residue for model 15

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



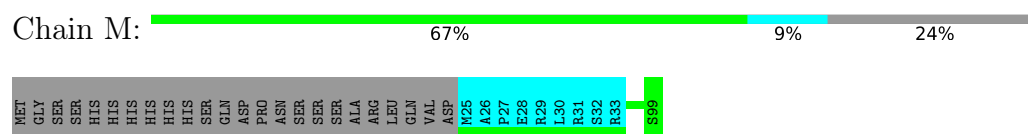
4.2.16 Score per residue for model 16

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



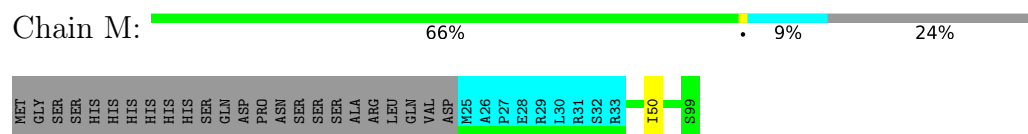
4.2.17 Score per residue for model 17

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



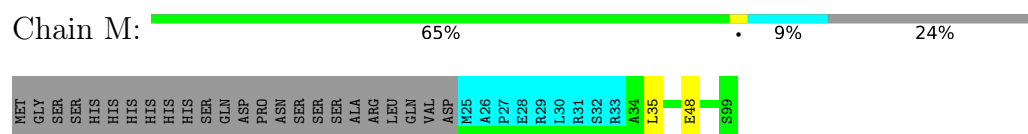
4.2.18 Score per residue for model 18

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



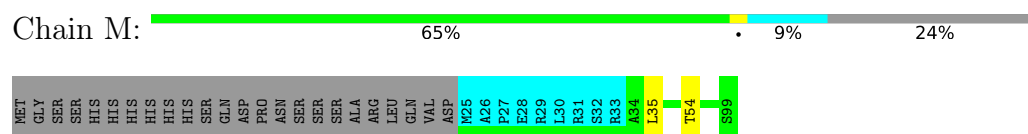
4.2.19 Score per residue for model 19

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



4.2.20 Score per residue for model 20

- Molecule 1: DNA POLYMERASE EPSILON SUBUNIT 2



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *LOWEST NOE RESTRAINT VIOLATION ENERGIES*.

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

Software name	Classification	Version
Amber	refinement	8
CYANA	structure solution	
Amber	structure solution	8
PROCHECK / PROCHECK-NMR	structure solution	NMR

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	1122
Number of shifts mapped to atoms	872
Number of unparsed shifts	0
Number of shifts with mapping errors	250
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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	M	0.82±0.01	0±0/514 (0.0± 0.0%)	1.35±0.03	0±0/688 (0.0± 0.0%)
All	All	0.82	0/10280 (0.0%)	1.35	1/13760 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	M	46	ARG	N-CA-C	5.28	119.20	112.34	6	1

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	M	512	449	538	0±0
All	All	10240	8980	10760	2

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:M:63:LEU:H	1:M:63:LEU:HD23	0.42	1.75	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:M:63:LEU:HD23	1:M:63:LEU:H	0.41	1.76	16	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	M	65/99 (66%)	64±2 (98±3%)	1±1 (1±2%)	0±0 (0±0%)	100	100
All	All	1292/1980 (65%)	1273 (99%)	19 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	M	57/87 (66%)	56±1 (97±2%)	1±1 (2±2%)	46	90
All	All	1135/1740 (65%)	1111 (98%)	24 (2%)	46	90

All 6 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	M	35	LEU	11
1	M	50	ILE	5
1	M	54	THR	4
1	M	85	MET	2
1	M	69	LEU	1
1	M	48	GLU	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 94% for the well-defined parts and 92% 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	1122
Number of shifts mapped to atoms	872
Number of unparsed shifts	0
Number of shifts with mapping errors	250
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. All 250 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	M	11	SER	HA	4.41	0.02	1
1	M	11	SER	HB2	3.87	0.02	1
1	M	11	SER	HB3	3.87	0.02	1
1	M	11	SER	C	174.34	0.20	1
1	M	11	SER	CA	58.57	0.20	1
1	M	11	SER	CB	63.86	0.20	1
1	M	12	GLN	H	8.48	0.02	1
1	M	12	GLN	HA	4.38	0.02	1
1	M	12	GLN	HB2	2.12	0.02	2
1	M	12	GLN	HB3	2.02	0.02	2
1	M	12	GLN	HG2	2.36	0.02	1
1	M	12	GLN	HG3	2.36	0.02	1
1	M	12	GLN	C	175.35	0.20	1
1	M	12	GLN	CA	55.68	0.20	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	M	12	GLN	CB	29.56	0.20	1
1	M	12	GLN	CG	33.79	0.20	1
1	M	12	GLN	N	121.99	0.20	1
1	M	13	ASP	H	8.36	0.02	1
1	M	13	ASP	HA	4.85	0.02	1
1	M	13	ASP	HB2	2.79	0.02	2
1	M	13	ASP	HB3	2.6	0.02	2
1	M	13	ASP	CA	52.19	0.20	1
1	M	13	ASP	CB	41.31	0.20	1
1	M	13	ASP	N	123.31	0.20	1
1	M	14	PRO	HA	4.43	0.02	1
1	M	14	PRO	HB2	2.31	0.02	2
1	M	14	PRO	HB3	1.97	0.02	2
1	M	14	PRO	HD2	3.86	0.02	1
1	M	14	PRO	HD3	3.86	0.02	1
1	M	14	PRO	HG2	2.01	0.02	1
1	M	14	PRO	HG3	2.01	0.02	1
1	M	14	PRO	C	177.17	0.20	1
1	M	14	PRO	CA	63.86	0.20	1
1	M	14	PRO	CB	32.09	0.20	1
1	M	14	PRO	CD	50.91	0.20	1
1	M	14	PRO	CG	27.05	0.20	1
1	M	15	ASN	H	8.55	0.02	1
1	M	15	ASN	HA	4.75	0.02	1
1	M	15	ASN	HB2	2.89	0.02	2
1	M	15	ASN	HB3	2.8	0.02	2
1	M	15	ASN	C	175.58	0.20	1
1	M	15	ASN	CA	53.57	0.20	1
1	M	15	ASN	CB	38.83	0.20	1
1	M	15	ASN	N	117.35	0.20	1
1	M	16	SER	H	8.01	0.02	1
1	M	16	SER	HA	4.46	0.02	1
1	M	16	SER	HB2	3.95	0.02	1
1	M	16	SER	HB3	3.95	0.02	1
1	M	16	SER	C	174.96	0.20	1
1	M	16	SER	CA	58.77	0.20	1
1	M	16	SER	CB	63.85	0.20	1
1	M	16	SER	N	115.74	0.20	1
1	M	17	SER	H	8.39	0.02	1
1	M	17	SER	HA	4.5	0.02	1
1	M	17	SER	HB2	3.97	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	M	17	SER	HB3	3.93	0.02	2
1	M	17	SER	C	175.02	0.20	1
1	M	17	SER	CA	58.88	0.20	1
1	M	17	SER	CB	63.7	0.20	1
1	M	17	SER	N	117.89	0.20	1
1	M	18	SER	H	8.28	0.02	1
1	M	18	SER	HA	4.44	0.02	1
1	M	18	SER	HB2	3.91	0.02	1
1	M	18	SER	HB3	3.91	0.02	1
1	M	18	SER	C	174.53	0.20	1
1	M	18	SER	CA	58.81	0.20	1
1	M	18	SER	CB	63.67	0.20	1
1	M	18	SER	N	117.62	0.20	1
1	M	19	ALA	H	8.16	0.02	1
1	M	19	ALA	HA	4.32	0.02	1
1	M	19	ALA	HB1	1.4	0.02	1
1	M	19	ALA	HB2	1.4	0.02	1
1	M	19	ALA	HB3	1.4	0.02	1
1	M	19	ALA	C	177.8	0.20	1
1	M	19	ALA	CA	52.93	0.20	1
1	M	19	ALA	CB	19.16	0.20	1
1	M	19	ALA	N	125.71	0.20	1
1	M	20	ARG	H	8.14	0.02	1
1	M	20	ARG	HA	4.32	0.02	1
1	M	20	ARG	HB2	1.87	0.02	2
1	M	20	ARG	HB3	1.79	0.02	2
1	M	20	ARG	HD2	3.22	0.02	1
1	M	20	ARG	HD3	3.22	0.02	1
1	M	20	ARG	HG2	1.65	0.02	1
1	M	20	ARG	HG3	1.65	0.02	1
1	M	20	ARG	C	176.26	0.20	1
1	M	20	ARG	CA	56.23	0.20	1
1	M	20	ARG	CB	30.71	0.20	1
1	M	20	ARG	CD	43.36	0.20	1
1	M	20	ARG	CG	27.11	0.20	1
1	M	20	ARG	N	119.69	0.20	1
1	M	21	LEU	H	8.18	0.02	1
1	M	21	LEU	HA	4.35	0.02	1
1	M	21	LEU	HB2	1.67	0.02	2
1	M	21	LEU	HB3	1.59	0.02	2
1	M	21	LEU	HD11	0.94	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	M	21	LEU	HD12	0.94	0.02	2
1	M	21	LEU	HD13	0.94	0.02	2
1	M	21	LEU	HD21	0.87	0.02	2
1	M	21	LEU	HD22	0.87	0.02	2
1	M	21	LEU	HD23	0.87	0.02	2
1	M	21	LEU	HG	1.63	0.02	1
1	M	21	LEU	C	177.17	0.20	1
1	M	21	LEU	CA	55.3	0.20	1
1	M	21	LEU	CB	42.44	0.20	1
1	M	21	LEU	CD1	24.95	0.20	2
1	M	21	LEU	CD2	23.57	0.20	2
1	M	21	LEU	CG	26.98	0.20	1
1	M	21	LEU	N	123.03	0.20	1
1	M	22	GLN	H	8.32	0.02	1
1	M	22	GLN	HA	4.38	0.02	1
1	M	22	GLN	HB2	2.11	0.02	2
1	M	22	GLN	HB3	1.96	0.02	2
1	M	22	GLN	HG2	2.36	0.02	1
1	M	22	GLN	HG3	2.36	0.02	1
1	M	22	GLN	C	175.75	0.20	1
1	M	22	GLN	CA	55.79	0.20	1
1	M	22	GLN	CB	29.44	0.20	1
1	M	22	GLN	CG	33.79	0.20	1
1	M	22	GLN	N	121.68	0.20	1
1	M	23	VAL	H	8.11	0.02	1
1	M	23	VAL	HA	4.17	0.02	1
1	M	23	VAL	HB	2.12	0.02	1
1	M	23	VAL	HG11	0.94	0.02	1
1	M	23	VAL	HG12	0.94	0.02	1
1	M	23	VAL	HG13	0.94	0.02	1
1	M	23	VAL	HG21	0.94	0.02	1
1	M	23	VAL	HG22	0.94	0.02	1
1	M	23	VAL	HG23	0.94	0.02	1
1	M	23	VAL	C	175.69	0.20	1
1	M	23	VAL	CA	62.14	0.20	1
1	M	23	VAL	CB	33.06	0.20	1
1	M	23	VAL	CG1	20.3	0.20	2
1	M	23	VAL	CG2	21.27	0.20	2
1	M	23	VAL	N	121.24	0.20	1
1	M	24	ASP	H	8.39	0.02	1
1	M	24	ASP	HA	4.64	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	M	24	ASP	HB2	2.75	0.02	2
1	M	24	ASP	HB3	2.61	0.02	2
1	M	24	ASP	C	176.32	0.20	1
1	M	24	ASP	CA	54.61	0.20	1
1	M	24	ASP	CB	41.34	0.20	1
1	M	24	ASP	N	124.01	0.20	1
1	M	25	MET	HB2	2.08	0.02	2
1	M	25	MET	HG2	2.59	0.02	1
1	M	27	PRO	HB2	2.35	0.02	2
1	M	27	PRO	HD2	3.91	0.02	2
1	M	27	PRO	HG2	2.18	0.02	2
1	M	28	GLU	HB2	2.07	0.02	1
1	M	28	GLU	HG2	2.35	0.02	1
1	M	29	ARG	HB2	1.98	0.02	1
1	M	29	ARG	HD2	3.29	0.02	1
1	M	29	ARG	HG2	1.76	0.02	2
1	M	30	LEU	HB2	1.74	0.02	2
1	M	31	ARG	HB2	1.91	0.02	2
1	M	31	ARG	HD2	3.22	0.02	1
1	M	31	ARG	HG2	1.5	0.02	2
1	M	32	SER	HB2	4.04	0.02	1
1	M	33	ARG	HB2	2.01	0.02	2
1	M	33	ARG	HD2	3.25	0.02	2
1	M	33	ARG	HG2	1.73	0.02	1
1	M	35	LEU	HB2	1.97	0.02	2
1	M	36	SER	HB2	4.06	0.02	2
1	M	38	PHE	HB2	3.1	0.02	2
1	M	39	LYS	HB2	2.08	0.02	1
1	M	39	LYS	HD2	1.74	0.02	2
1	M	39	LYS	HE2	2.98	0.02	1
1	M	39	LYS	HG2	1.53	0.02	1
1	M	40	LEU	HB2	1.87	0.02	2
1	M	41	ARG	HB2	2.24	0.02	2
1	M	41	ARG	HD2	3.18	0.02	2
1	M	41	ARG	HG2	1.67	0.02	2
1	M	43	LEU	HB2	2.04	0.02	2
1	M	44	LEU	HB2	1.73	0.02	2
1	M	45	LEU	HB2	1.41	0.02	2
1	M	46	ARG	HB2	2.25	0.02	2
1	M	46	ARG	HD2	3.37	0.02	2
1	M	46	ARG	HG2	1.77	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	M	48	GLU	HB2	2.14	0.02	1
1	M	48	GLU	HG2	2.45	0.02	1
1	M	50	ILE	HG12	1.39	0.02	2
1	M	51	LYS	HB2	1.92	0.02	2
1	M	51	LYS	HD2	1.7	0.02	1
1	M	51	LYS	HE2	2.98	0.02	1
1	M	51	LYS	HG2	1.49	0.02	2
1	M	52	TYR	HB2	3.13	0.02	2
1	M	53	LEU	HB2	1.69	0.02	2
1	M	55	GLU	HB2	2.05	0.02	2
1	M	55	GLU	HG2	2.38	0.02	2
1	M	57	LEU	HB2	1.74	0.02	2
1	M	58	GLN	HB2	2.24	0.02	2
1	M	58	GLN	HG2	2.48	0.02	1
1	M	59	SER	HB2	3.96	0.02	1
1	M	60	ILE	HG12	1.49	0.02	2
1	M	61	SER	HB2	4.22	0.02	2
1	M	62	GLU	HB2	2.16	0.02	2
1	M	62	GLU	HG2	2.36	0.02	1
1	M	63	LEU	HB2	1.72	0.02	2
1	M	64	GLU	HB2	2.21	0.02	2
1	M	64	GLU	HG2	2.33	0.02	2
1	M	65	LEU	HB2	1.82	0.02	2
1	M	66	GLU	HB2	2.08	0.02	2
1	M	66	GLU	HG2	2.37	0.02	2
1	M	67	ASP	HB2	2.73	0.02	2
1	M	68	LYS	HB2	1.99	0.02	2
1	M	68	LYS	HD2	1.77	0.02	2
1	M	68	LYS	HE2	2.86	0.02	2
1	M	68	LYS	HG2	1.5	0.02	1
1	M	69	LEU	HB2	1.97	0.02	2
1	M	70	GLU	HB2	2.14	0.02	1
1	M	70	GLU	HG2	2.26	0.02	1
1	M	71	LYS	HB2	2.07	0.02	2
1	M	71	LYS	HD2	1.74	0.02	2
1	M	71	LYS	HE2	3.04	0.02	1
1	M	71	LYS	HG2	1.74	0.02	2
1	M	72	ILE	HG12	2.04	0.02	2
1	M	73	ILE	HG12	1.17	0.02	2
1	M	74	ASN	HB2	2.96	0.02	2
1	M	77	GLU	HB2	2.15	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	M	77	GLU	HG2	2.54	0.02	2
1	M	78	LYS	HB2	1.98	0.02	2
1	M	78	LYS	HD2	1.71	0.02	1
1	M	78	LYS	HE2	2.99	0.02	1
1	M	78	LYS	HG2	1.65	0.02	2
1	M	79	GLN	HB2	2.2	0.02	2
1	M	79	GLN	HG2	2.57	0.02	1
1	M	80	PRO	HB2	2.09	0.02	1
1	M	80	PRO	HD2	3.75	0.02	2
1	M	80	PRO	HG2	2.16	0.02	2
1	M	81	LEU	HB2	1.77	0.02	2
1	M	82	SER	HB2	4.03	0.02	2
1	M	83	SER	HB2	4.1	0.02	2
1	M	84	ASN	HB2	3.46	0.02	2
1	M	85	MET	HB2	1.96	0.02	2
1	M	85	MET	HG2	2.46	0.02	2
1	M	86	ILE	HG12	1.92	0.02	2
1	M	87	GLU	HB2	2.44	0.02	2
1	M	87	GLU	HG2	2.48	0.02	1
1	M	88	ARG	HB2	1.87	0.02	2
1	M	88	ARG	HD2	3.11	0.02	2
1	M	88	ARG	HG2	1.33	0.02	1
1	M	89	SER	HB2	3.907	0.02	2
1	M	92	GLU	HB2	1.76	0.02	2
1	M	92	GLU	HG2	1.89	0.02	2
1	M	96	GLN	HB2	2.23	0.02	1
1	M	96	GLN	HG2	2.57	0.02	2
1	M	97	GLU	HB2	2.14	0.02	1
1	M	97	GLU	HG2	2.4	0.02	2
1	M	98	SER	HB2	3.94	0.02	2
1	M	99	SER	HB2	3.93	0.02	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	89	-0.22 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	87	0.19 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	83	-0.27 ± 0.19	None needed (< 0.5 ppm)
^{15}N	85	0.20 ± 0.29	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 94%, i.e. 862 atoms were assigned a chemical shift out of a possible 917. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	326/330 (99%)	133/133 (100%)	128/132 (97%)	65/65 (100%)
Sidechain	518/568 (91%)	356/371 (96%)	157/178 (88%)	5/19 (26%)
Aromatic	18/19 (95%)	9/9 (100%)	9/10 (90%)	0/0 (—%)
Overall	862/917 (94%)	498/513 (97%)	294/320 (92%)	70/84 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 979 atoms were assigned a chemical shift out of a possible 1060. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	368/373 (99%)	150/150 (100%)	145/150 (97%)	73/73 (100%)
Sidechain	593/668 (89%)	408/435 (94%)	180/205 (88%)	5/28 (18%)
Aromatic	18/19 (95%)	9/9 (100%)	9/10 (90%)	0/0 (—%)
Overall	979/1060 (92%)	567/594 (95%)	334/365 (92%)	78/101 (77%)

7.1.4 Statistically unusual chemical shifts [i](#)

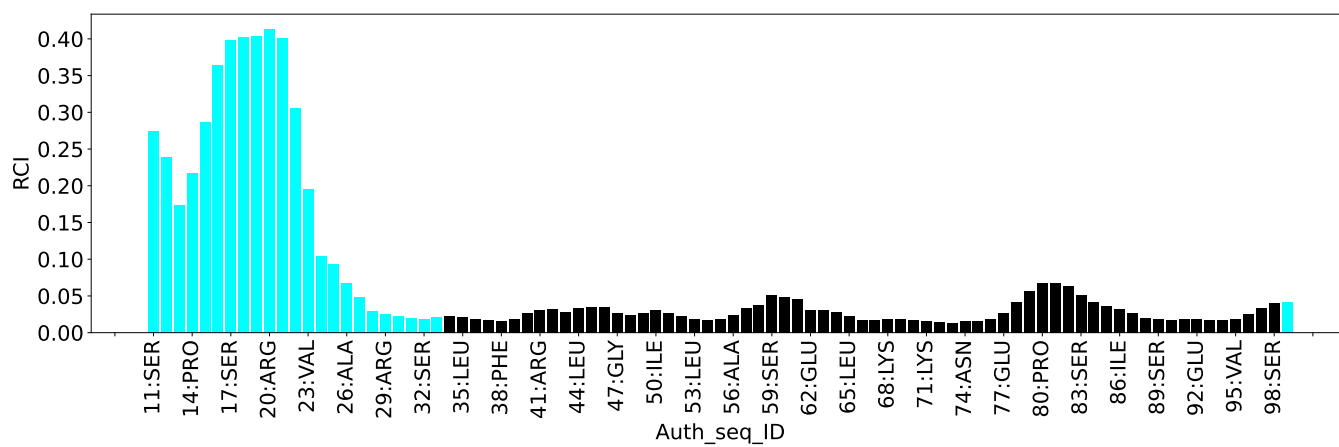
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	M	88	ARG	NE	109.68	76.53 – 92.65	15.6
1	M	73	ILE	HG13	-0.90	-0.82 – 3.23	-5.2

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 M:



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	1395
Intra-residue ($ i-j =0$)	387
Sequential ($ i-j =1$)	363
Medium range ($ i-j >1$ and $ i-j <5$)	330
Long range ($ i-j \geq 5$)	315
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	51
Number of restraints per residue	14.1
Number of long range restraints per residue ¹	3.2

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)	1.5	0.17
0.2-0.5 (Medium)	0.1	0.23
>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 ⓘ

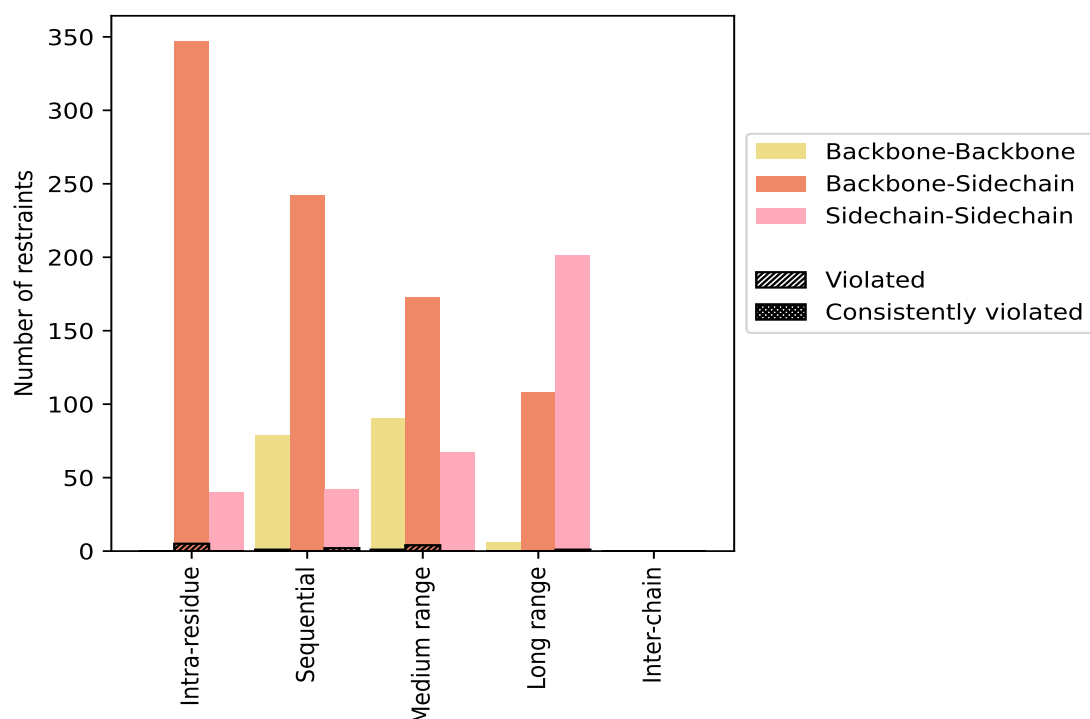
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	387	27.7	5	1.3	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	347	24.9	5	1.4	0.4	0	0.0	0.0
Sidechain-Sidechain	40	2.9	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	363	26.0	3	0.8	0.2	0	0.0	0.0
Backbone-Backbone	79	5.7	1	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	242	17.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	42	3.0	2	4.8	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	330	23.7	5	1.5	0.4	0	0.0	0.0
Backbone-Backbone	90	6.5	1	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	173	12.4	4	2.3	0.3	0	0.0	0.0
Sidechain-Sidechain	67	4.8	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	315	22.6	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	6	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	108	7.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	201	14.4	1	0.5	0.1	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	0	0.0	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	1395	100.0	14	1.0	1.0	0	0.0	0.0
Backbone-Backbone	175	12.5	2	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	870	62.4	9	1.0	0.6	0	0.0	0.0
Sidechain-Sidechain	350	25.1	3	0.9	0.2	0	0.0	0.0

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

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



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

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

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	1	0	0	2	0.12	0.13	0.02	0.12
2	2	0	1	0	0	3	0.12	0.14	0.02	0.11
3	2	1	1	0	0	4	0.12	0.14	0.02	0.12
4	0	1	1	0	0	2	0.14	0.14	0.01	0.14
5	2	0	1	0	0	3	0.11	0.12	0.0	0.11
6	2	1	1	0	0	4	0.14	0.23	0.05	0.12
7	0	1	0	0	0	1	0.11	0.11	0.0	0.11
8	0	1	0	0	0	1	0.13	0.13	0.0	0.13
9	0	0	1	0	0	1	0.1	0.1	0.0	0.1
10	0	0	2	0	0	2	0.11	0.11	0.0	0.11

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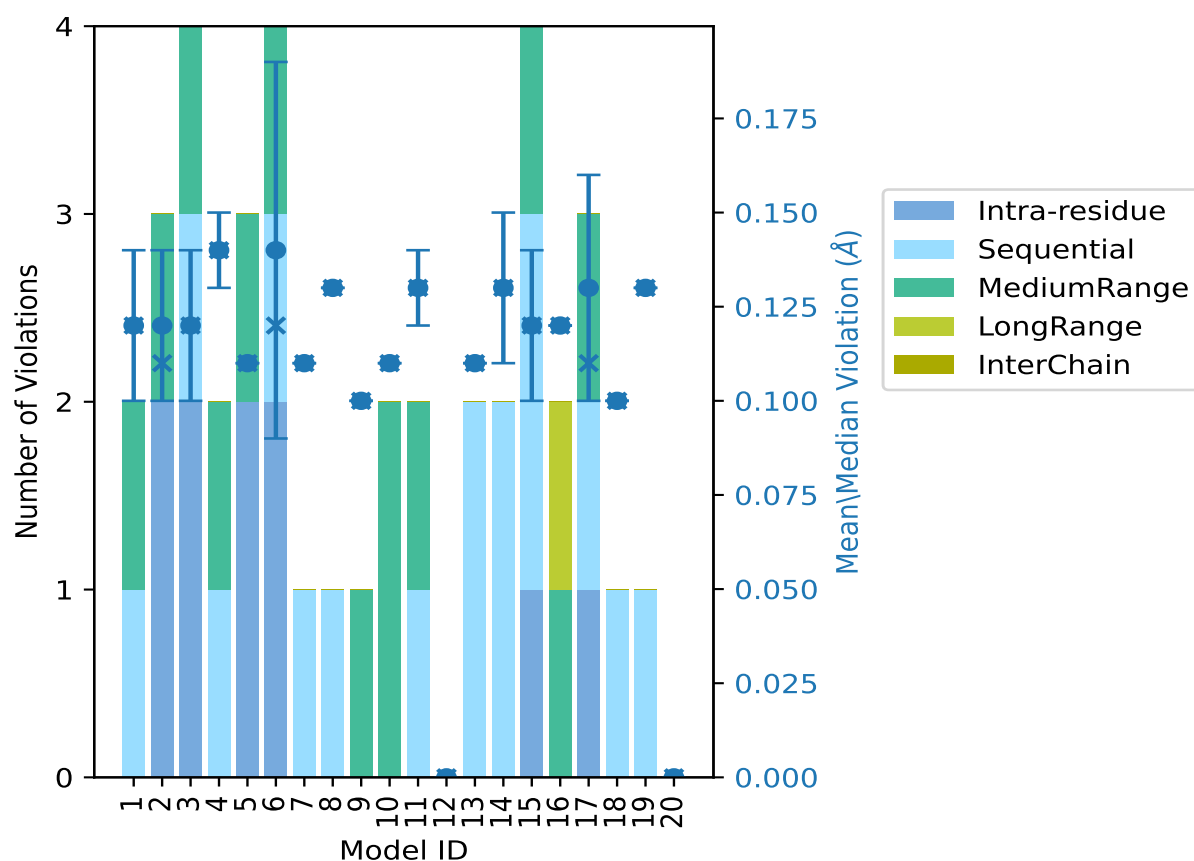
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	1	0	0	2	0.13	0.14	0.01	0.13
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	2	0	0	0	2	0.11	0.11	0.0	0.11
14	0	2	0	0	0	2	0.13	0.15	0.02	0.13
15	1	2	1	0	0	4	0.12	0.16	0.02	0.12
16	0	0	1	1	0	2	0.12	0.12	0.0	0.12
17	1	1	1	0	0	3	0.13	0.17	0.03	0.11
18	0	1	0	0	0	1	0.1	0.1	0.0	0.1
19	0	1	0	0	0	1	0.13	0.13	0.0	0.13
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

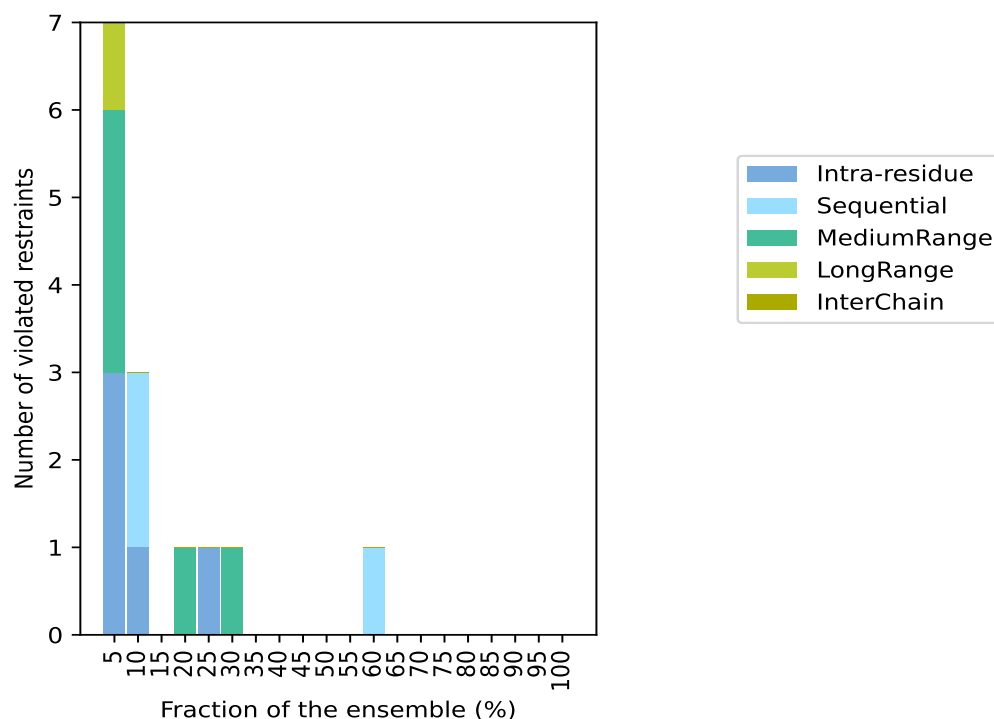
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1381(IR:382, SQ:360, MR:325, LR:314, IC:0) restraints are 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	%
3	0	3	1	0	7	1	5.0
1	2	0	0	0	3	2	10.0
0	0	0	0	0	0	3	15.0
0	0	1	0	0	1	4	20.0
1	0	0	0	0	1	5	25.0
0	0	1	0	0	1	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	1	0	0	0	1	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

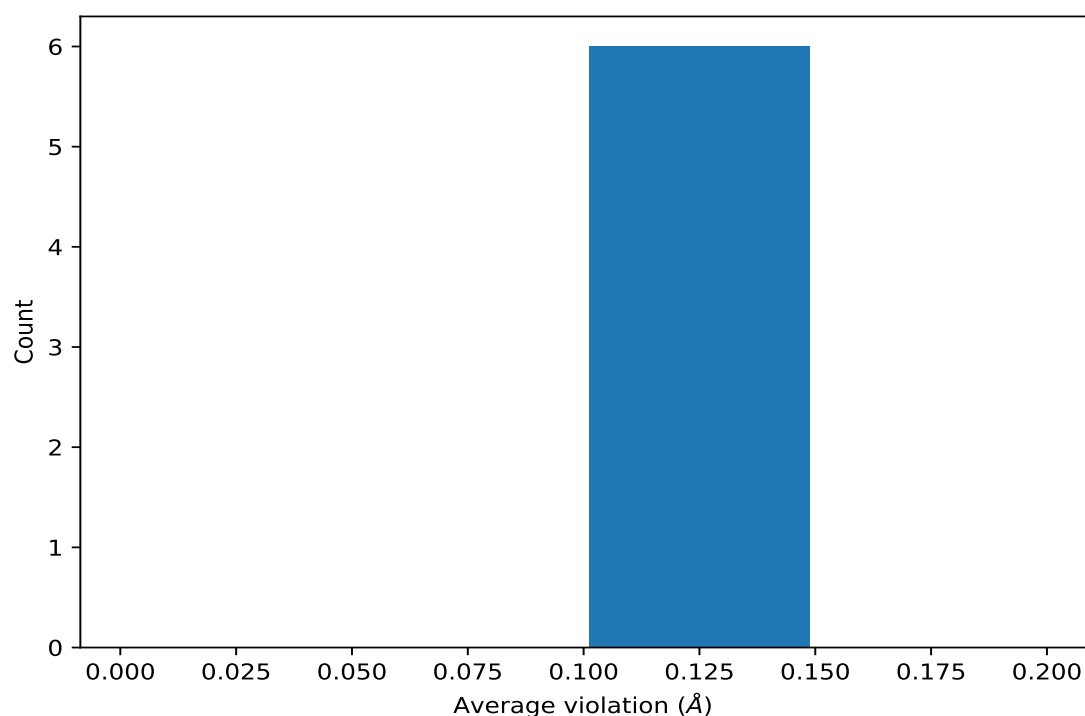
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

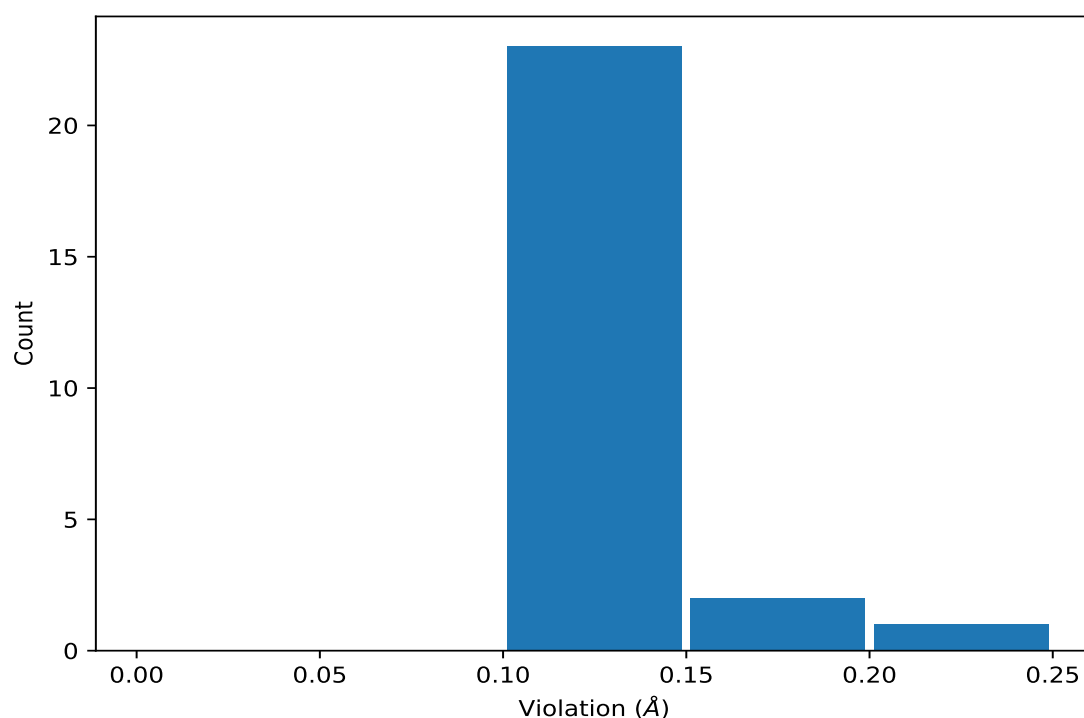
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,934)	1:47:M:GLY:HA3	1:50:M:ILE:HB	6	0.11	0.01	0.11
(1,182)	1:30:M:LEU:H	1:30:M:LEU:HG	5	0.14	0.02	0.14
(1,919)	1:36:M:SER:HA	1:39:M:LYS:HE3	4	0.12	0.01	0.12
(1,191)	1:25:M:MET:H	1:26:M:ALA:H	2	0.12	0.01	0.12
(1,1361)	1:88:M:ARG:HB3	1:89:M:SER:HB3	2	0.11	0.0	0.11
(1,1392)	1:97:M:GLU:H	1:97:M:GLU:HG3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

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)
(1,1182)	1:46:M:ARG:H	1:46:M:ARG:HG3	6	0.23
(1,182)	1:30:M:LEU:H	1:30:M:LEU:HG	17	0.17
(1,182)	1:30:M:LEU:H	1:30:M:LEU:HG	15	0.16
(1,182)	1:30:M:LEU:H	1:30:M:LEU:HG	2	0.14
(1,934)	1:47:M:GLY:HA3	1:50:M:ILE:HB	1	0.13
(1,919)	1:36:M:SER:HA	1:39:M:LYS:HE3	4	0.13
(1,563)	1:51:M:LYS:H	1:51:M:LYS:HE3	3	0.13
(1,191)	1:25:M:MET:H	1:26:M:ALA:H	15	0.13
(1,934)	1:47:M:GLY:HA3	1:50:M:ILE:HB	11	0.12
(1,919)	1:36:M:SER:HA	1:39:M:LYS:HE3	6	0.12
(1,919)	1:36:M:SER:HA	1:39:M:LYS:HE3	16	0.12
(1,182)	1:30:M:LEU:H	1:30:M:LEU:HG	5	0.12
(1,182)	1:30:M:LEU:H	1:30:M:LEU:HG	6	0.12
(1,1392)	1:97:M:GLU:H	1:97:M:GLU:HG3	2	0.11
(1,1392)	1:97:M:GLU:H	1:97:M:GLU:HG3	3	0.11
(1,1361)	1:88:M:ARG:HB3	1:89:M:SER:HB3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:88:M:ARG:HB3	1:89:M:SER:HB3	13	0.11
(1,934)	1:47:M:GLY:HA3	1:50:M:ILE:HB	5	0.11
(1,934)	1:47:M:GLY:HA3	1:50:M:ILE:HB	10	0.11
(1,191)	1:25:M:MET:H	1:26:M:ALA:H	14	0.11
(1,48)	1:81:M:LEU:HA	1:83:M:SER:H	10	0.11
(1,934)	1:47:M:GLY:HA3	1:50:M:ILE:HB	2	0.1
(1,934)	1:47:M:GLY:HA3	1:50:M:ILE:HB	17	0.1
(1,932)	1:63:M:LEU:HG	1:65:M:LEU:H	15	0.1
(1,919)	1:36:M:SER:HA	1:39:M:LYS:HE3	9	0.1
(1,281)	1:95:M:VAL:HA	1:99:M:SER:HB3	3	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found