



Full wwPDB NMR Structure Validation Report ⓘ

Jul 9, 2026 – 12:51 AM JST

PDB ID : 9VHS / pdb_00009vhs
BMRB ID : 36766
Title : Keratin 14 120 - 144 peptide fragment
Authors : Li, Z.Y.; Zhang, W.B.; Li, H.W.; Wang, C.X.
Deposited on : 2025-06-17

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) : 2.50

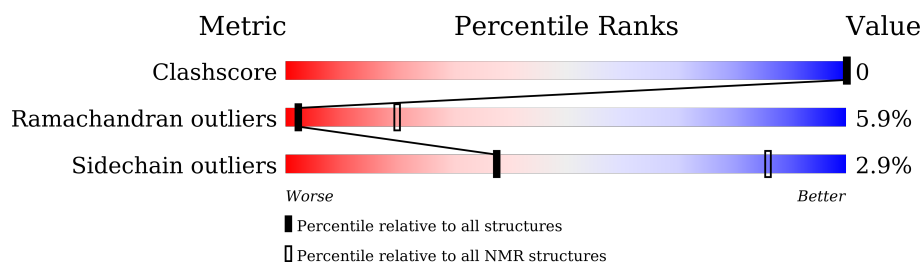
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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	25	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:8-A:25 (18)	0.54	3

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 396 atoms, of which 195 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Keratin, type I cytoskeletal 14.

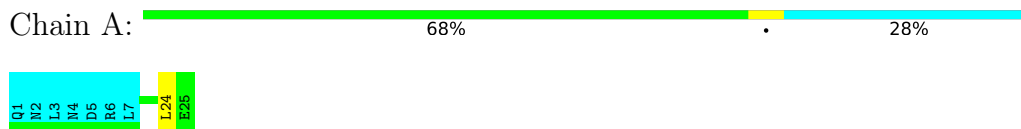
Mol	Chain	Residues	Atoms					Trace
1	A	25	Total	C	H	N	O	0
			396	121	195	36	44	

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: Keratin, type I cytoskeletal 14

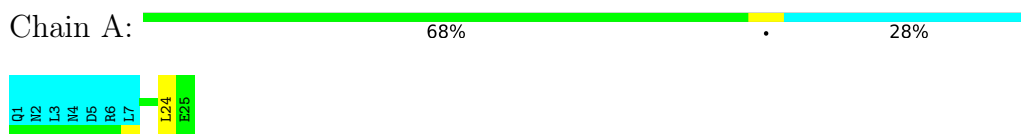


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Keratin, type I cytoskeletal 14



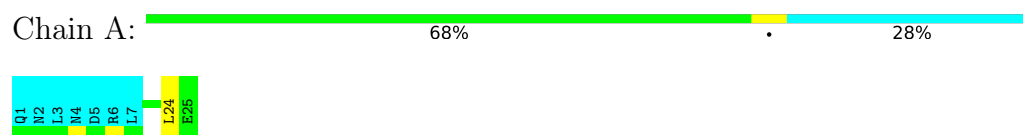
4.2.2 Score per residue for model 2

- Molecule 1: Keratin, type I cytoskeletal 14



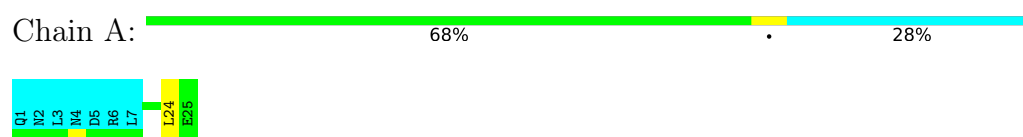
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Keratin, type I cytoskeletal 14



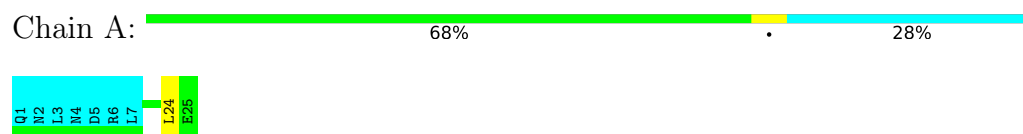
4.2.4 Score per residue for model 4

- Molecule 1: Keratin, type I cytoskeletal 14



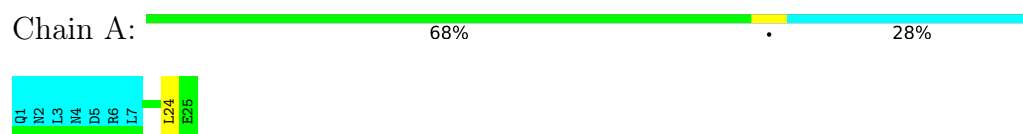
4.2.5 Score per residue for model 5

- Molecule 1: Keratin, type I cytoskeletal 14



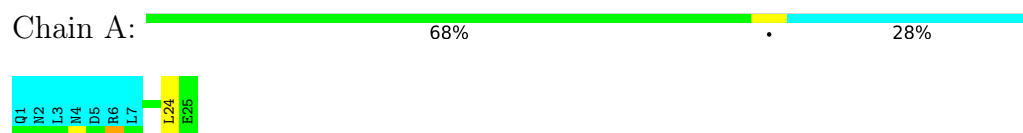
4.2.6 Score per residue for model 6

- Molecule 1: Keratin, type I cytoskeletal 14



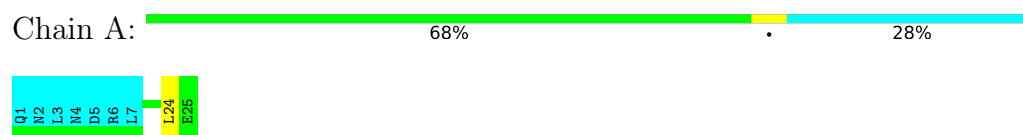
4.2.7 Score per residue for model 7

- Molecule 1: Keratin, type I cytoskeletal 14



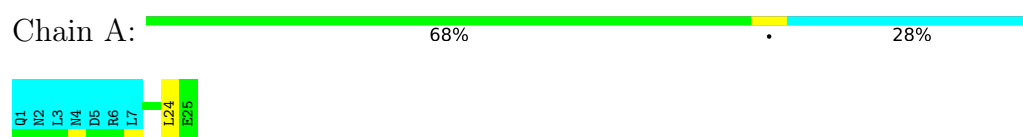
4.2.8 Score per residue for model 8

- Molecule 1: Keratin, type I cytoskeletal 14



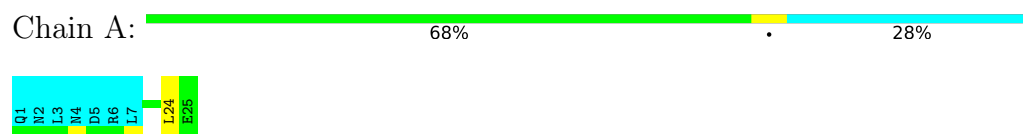
4.2.9 Score per residue for model 9

- Molecule 1: Keratin, type I cytoskeletal 14



4.2.10 Score per residue for model 10

- Molecule 1: Keratin, type I cytoskeletal 14



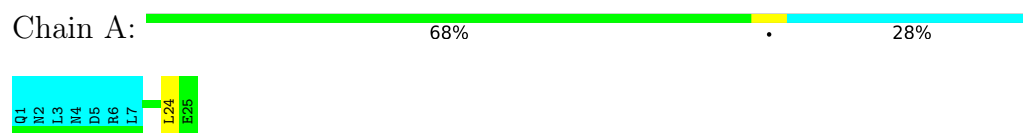
4.2.11 Score per residue for model 11

- Molecule 1: Keratin, type I cytoskeletal 14



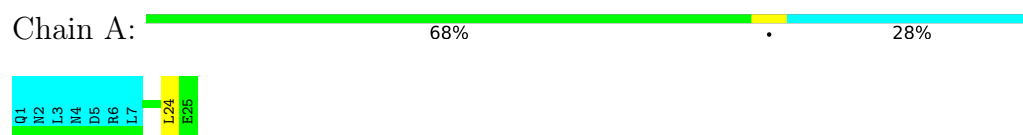
4.2.12 Score per residue for model 12

- Molecule 1: Keratin, type I cytoskeletal 14



4.2.13 Score per residue for model 13

- Molecule 1: Keratin, type I cytoskeletal 14



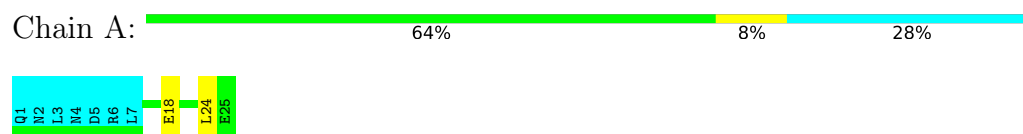
4.2.14 Score per residue for model 14

- Molecule 1: Keratin, type I cytoskeletal 14



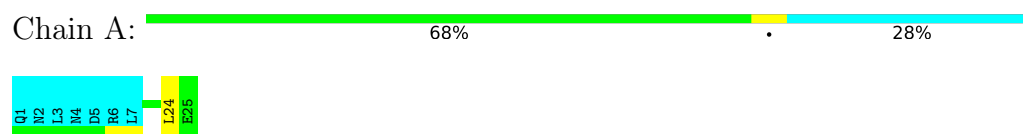
4.2.15 Score per residue for model 15

- Molecule 1: Keratin, type I cytoskeletal 14



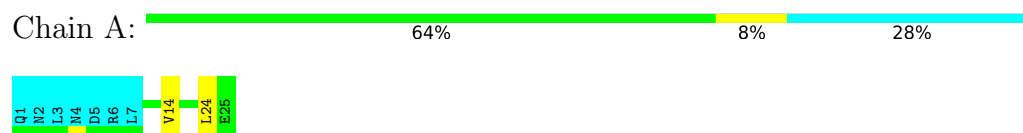
4.2.16 Score per residue for model 16

- Molecule 1: Keratin, type I cytoskeletal 14



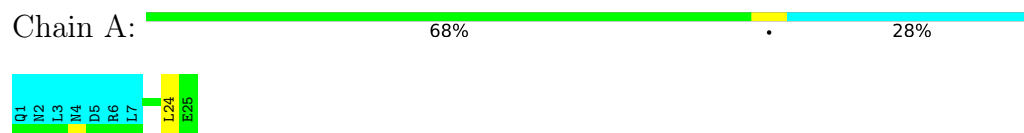
4.2.17 Score per residue for model 17

- Molecule 1: Keratin, type I cytoskeletal 14



4.2.18 Score per residue for model 18

- Molecule 1: Keratin, type I cytoskeletal 14



4.2.19 Score per residue for model 19

- Molecule 1: Keratin, type I cytoskeletal 14



4.2.20 Score per residue for model 20

- Molecule 1: Keratin, type I cytoskeletal 14



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	
Amber	refinement	

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	253
Number of shifts mapped to atoms	253
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

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	0.89±0.02	0±0/141 (0.0± 0.0%)	1.39±0.06	0±0/188 (0.1± 0.2%)
All	All	0.89	0/2820 (0.0%)	1.39	3/3760 (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	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	ARG	NE-CZ-NH2	5.84	124.46	119.20	2	2
1	A	15	ARG	N-CA-C	5.43	118.70	111.75	20	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	15	ARG	Sidechain	1

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
All	All	2820	2680	2680	-

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 -.

There are no clashes.

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	17/25 (68%)	14±1 (80±6%)	2±1 (14±6%)	1±0 (6±0%)	2	20
All	All	340/500 (68%)	273 (80%)	47 (14%)	20 (6%)	2	20

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	24	LEU	20

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	14/21 (67%)	14±1 (97±5%)	0±1 (3±5%)	38	86
All	All	280/420 (67%)	272 (97%)	8 (3%)	38	86

All 5 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	21	ASN	3
1	A	18	GLU	2
1	A	25	GLU	1
1	A	14	VAL	1
1	A	13	LYS	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 42% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	253
Number of shifts mapped to atoms	253
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

- Can not parse the chemical shift value. All 120 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	GLN	HB2	2.039	.	.
1	A	1	GLN	HB3	1.943	.	.
1	A	1	GLN	HG2	2.340	.	.
1	A	1	GLN	HG3	2.340	.	.
1	A	2	ASN	HB2	2.781	.	.
1	A	2	ASN	HB3	2.870	.	.
1	A	2	ASN	HD21	7.644	.	.
1	A	2	ASN	HD22	6.923	.	.
1	A	3	LEU	HB2	1.653	.	.
1	A	3	LEU	HB3	1.656	.	.
1	A	3	LEU	HD11	0.853	.	.
1	A	3	LEU	HD12	0.853	.	.
1	A	3	LEU	HD13	0.853	.	.
1	A	3	LEU	HD21	0.912	.	.
1	A	3	LEU	HD22	0.912	.	.
1	A	3	LEU	HD23	0.912	.	.
1	A	3	LEU	CD1	23.643	.	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	LEU	CD2	23.178	.	.
1	A	4	ASN	HB2	2.758	.	.
1	A	4	ASN	HB3	2.835	.	.
1	A	4	ASN	HD21	7.619	.	.
1	A	4	ASN	HD22	6.908	.	.
1	A	5	ASP	HB2	2.678	.	.
1	A	5	ASP	HB3	2.678	.	.
1	A	6	ARG	HB2	1.817	.	.
1	A	6	ARG	HB3	1.878	.	.
1	A	6	ARG	HD2	3.179	.	.
1	A	6	ARG	HD3	3.179	.	.
1	A	6	ARG	HG2	1.658	.	.
1	A	6	ARG	HG3	1.616	.	.
1	A	7	LEU	HB2	1.676	.	.
1	A	7	LEU	HB3	1.632	.	.
1	A	7	LEU	HD11	0.934	.	.
1	A	7	LEU	HD12	0.934	.	.
1	A	7	LEU	HD13	0.934	.	.
1	A	7	LEU	HD21	0.872	.	.
1	A	7	LEU	HD22	0.872	.	.
1	A	7	LEU	HD23	0.872	.	.
1	A	7	LEU	CD1	24.813	.	.
1	A	7	LEU	CD2	24.813	.	.
1	A	9	SER	HB2	3.908	.	.
1	A	9	SER	HB3	3.849	.	.
1	A	10	TYR	HB2	3.098	.	.
1	A	10	TYR	HB3	3.098	.	.
1	A	10	TYR	HD1	7.119	.	.
1	A	10	TYR	HD2	7.108	.	.
1	A	10	TYR	HE1	6.819	.	.
1	A	10	TYR	HE2	6.805	.	.
1	A	11	LEU	HB2	1.536	.	.
1	A	11	LEU	HB3	1.511	.	.
1	A	11	LEU	HD11	0.896	.	.
1	A	11	LEU	HD12	0.896	.	.
1	A	11	LEU	HD13	0.896	.	.
1	A	11	LEU	HD21	0.861	.	.
1	A	11	LEU	HD22	0.861	.	.
1	A	11	LEU	HD23	0.861	.	.
1	A	11	LEU	CD1	23.468	.	.
1	A	11	LEU	CD2	23.468	.	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	ASP	HB2	2.691	.	.
1	A	12	ASP	HB3	2.691	.	.
1	A	13	LYS	HB2	1.860	.	.
1	A	13	LYS	HB3	1.823	.	.
1	A	13	LYS	HD2	1.677	.	.
1	A	13	LYS	HD3	1.672	.	.
1	A	13	LYS	HE2	2.987	.	.
1	A	13	LYS	HE3	2.976	.	.
1	A	13	LYS	HG2	1.488	.	.
1	A	13	LYS	HG3	1.407	.	.
1	A	14	VAL	HG11	0.894	.	.
1	A	14	VAL	HG12	0.894	.	.
1	A	14	VAL	HG13	0.894	.	.
1	A	14	VAL	HG21	0.894	.	.
1	A	14	VAL	HG22	0.894	.	.
1	A	14	VAL	HG23	0.894	.	.
1	A	14	VAL	CG1	21.250	.	.
1	A	14	VAL	CG2	21.250	.	.
1	A	15	ARG	HB2	1.845	.	.
1	A	15	ARG	HB3	1.803	.	.
1	A	15	ARG	HD2	3.181	.	.
1	A	15	ARG	HD3	3.197	.	.
1	A	15	ARG	HG2	1.673	.	.
1	A	15	ARG	HG3	1.619	.	.
1	A	17	LEU	HB2	1.687	.	.
1	A	17	LEU	HB3	1.728	.	.
1	A	17	LEU	HD11	0.875	.	.
1	A	17	LEU	HD12	0.875	.	.
1	A	17	LEU	HD13	0.875	.	.
1	A	17	LEU	HD21	0.925	.	.
1	A	17	LEU	HD22	0.925	.	.
1	A	17	LEU	HD23	0.925	.	.
1	A	17	LEU	CD1	25.127	.	.
1	A	17	LEU	CD2	25.127	.	.
1	A	18	GLU	HB2	1.955	.	.
1	A	18	GLU	HB3	2.071	.	.
1	A	18	GLU	HG2	2.244	.	.
1	A	18	GLU	HG3	2.292	.	.
1	A	19	GLU	HB2	2.063	.	.
1	A	19	GLU	HB3	1.974	.	.
1	A	19	GLU	HG2	2.324	.	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	GLU	HG3	2.258	.	.
1	A	21	ASN	HB2	2.766	.	.
1	A	21	ASN	HB3	2.860	.	.
1	A	21	ASN	HD21	7.626	.	.
1	A	21	ASN	HD22	6.918	.	.
1	A	23	ASP	HB2	2.734	.	.
1	A	23	ASP	HB3	2.620	.	.
1	A	24	LEU	HB2	1.621	.	.
1	A	24	LEU	HB3	1.654	.	.
1	A	24	LEU	HD11	0.867	.	.
1	A	24	LEU	HD12	0.867	.	.
1	A	24	LEU	HD13	0.867	.	.
1	A	24	LEU	HD21	0.935	.	.
1	A	24	LEU	HD22	0.935	.	.
1	A	24	LEU	HD23	0.935	.	.
1	A	24	LEU	CD1	25.176	.	.
1	A	24	LEU	CD2	25.176	.	.
1	A	25	GLU	HB2	2.016	.	.
1	A	25	GLU	HB3	2.016	.	.
1	A	25	GLU	HG2	2.332	.	.
1	A	25	GLU	HG3	2.332	.	.

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
$^{13}\text{C}_\alpha$	24	—	None (insufficient data)
$^{13}\text{C}_\beta$	25	0.18 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

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 42%, i.e. 100 atoms were assigned a chemical shift out of a possible 237. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	54/90 (60%)	36/36 (100%)	18/36 (50%)	0/18 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Sidechain	46/138 (33%)	17/89 (19%)	29/44 (66%)	0/5 (0%)
Aromatic	0/9 (0%)	0/4 (0%)	0/5 (0%)	0/0 (—%)
Overall	100/237 (42%)	53/129 (41%)	47/85 (55%)	0/23 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 133 atoms were assigned a chemical shift out of a possible 344. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	73/125 (58%)	49/50 (98%)	24/50 (48%)	0/25 (0%)
Sidechain	60/210 (29%)	19/134 (14%)	41/65 (63%)	0/11 (0%)
Aromatic	0/9 (0%)	0/4 (0%)	0/5 (0%)	0/0 (—%)
Overall	133/344 (39%)	68/188 (36%)	65/120 (54%)	0/36 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

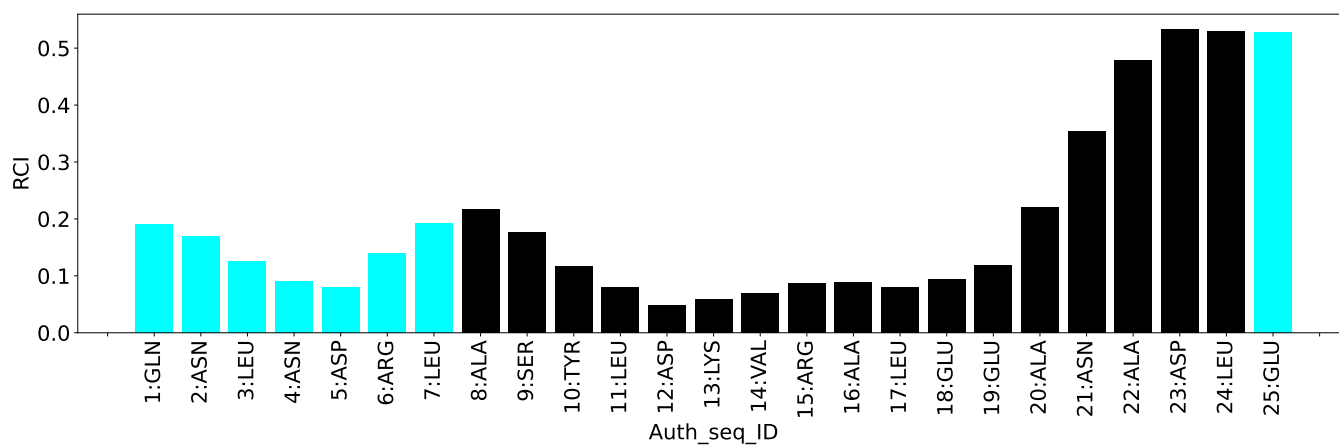
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	7	LEU	CG	18.78	21.37 – 32.19	-7.4

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	255
Intra-residue ($ i-j =0$)	127
Sequential ($ i-j =1$)	59
Medium range ($ i-j >1$ and $ i-j <5$)	51
Long range ($ i-j \geq 5$)	18
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	10.2
Number of long range restraints per residue ¹	0.7

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)	0.7	0.19
0.2-0.5 (Medium)	1.1	0.48
>0.5 (Large)	3.6	3.37

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 ⓘ

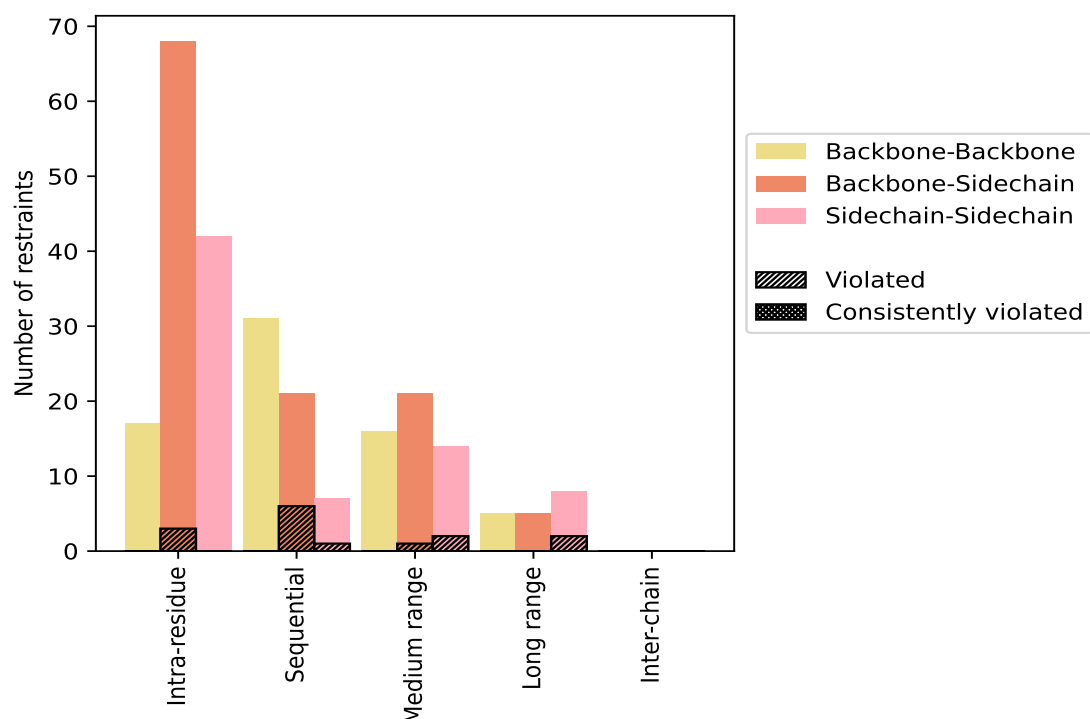
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	127	49.8	3	2.4	1.2	0	0.0	0.0
Backbone-Backbone	17	6.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	68	26.7	3	4.4	1.2	0	0.0	0.0
Sidechain-Sidechain	42	16.5	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	59	23.1	7	11.9	2.7	0	0.0	0.0
Backbone-Backbone	31	12.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	21	8.2	6	28.6	2.4	0	0.0	0.0
Sidechain-Sidechain	7	2.7	1	14.3	0.4	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	51	20.0	3	5.9	1.2	0	0.0	0.0
Backbone-Backbone	16	6.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	21	8.2	1	4.8	0.4	0	0.0	0.0
Sidechain-Sidechain	14	5.5	2	14.3	0.8	0	0.0	0.0
Long range ($i-j \geq 5$)	18	7.1	2	11.1	0.8	0	0.0	0.0
Backbone-Backbone	5	2.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	5	2.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	3.1	2	25.0	0.8	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	255	100.0	15	5.9	5.9	0	0.0	0.0
Backbone-Backbone	69	27.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	115	45.1	10	8.7	3.9	0	0.0	0.0
Sidechain-Sidechain	71	27.8	5	7.0	2.0	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	2	1	1	0	0	4	0.94	2.42	0.88	0.6
2	0	4	1	2	0	7	1.68	2.88	0.96	1.87
3	0	4	1	2	0	7	1.79	2.79	0.95	2.16
4	2	1	1	0	0	4	0.96	2.53	0.92	0.59
5	3	1	1	0	0	5	0.85	2.77	0.98	0.57
6	2	1	2	0	0	5	0.59	1.9	0.67	0.22
7	0	4	1	2	0	7	1.88	3.07	1.06	2.22
8	2	3	1	0	0	6	0.63	2.38	0.8	0.33
9	0	4	1	2	0	7	1.88	3.25	1.06	2.17
10	2	0	1	0	0	3	0.74	1.8	0.75	0.21

Continued on next page...

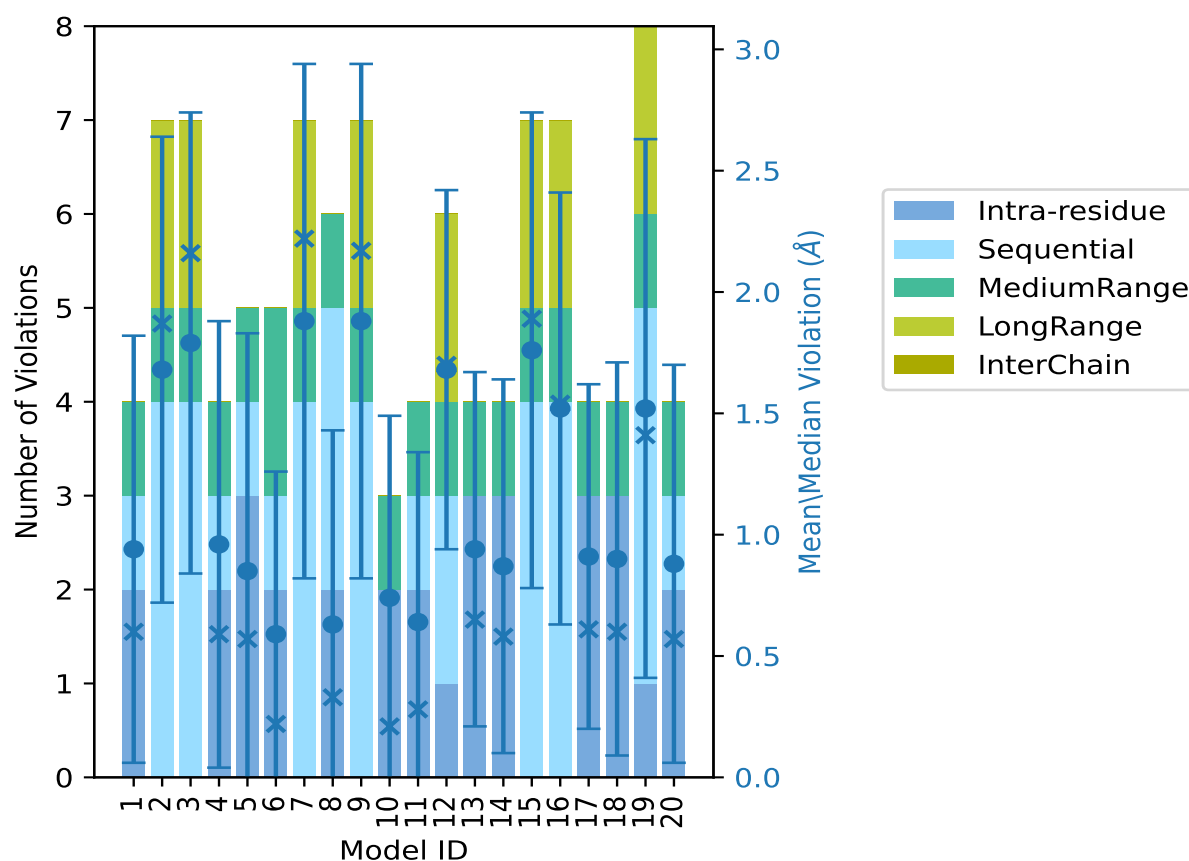
Continued from previous page...

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	2	1	1	0	0	4	0.64	1.85	0.7	0.28
12	1	2	1	2	0	6	1.68	2.8	0.74	1.7
13	3	0	1	0	0	4	0.94	2.18	0.73	0.65
14	3	0	1	0	0	4	0.87	2.17	0.77	0.58
15	0	4	1	2	0	7	1.76	2.92	0.98	1.89
16	0	4	1	2	0	7	1.52	2.7	0.89	1.54
17	3	0	1	0	0	4	0.91	2.12	0.71	0.61
18	3	0	1	0	0	4	0.9	2.27	0.81	0.6
19	1	4	1	2	0	8	1.52	3.37	1.11	1.41
20	2	1	1	0	0	4	0.88	2.26	0.82	0.57

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

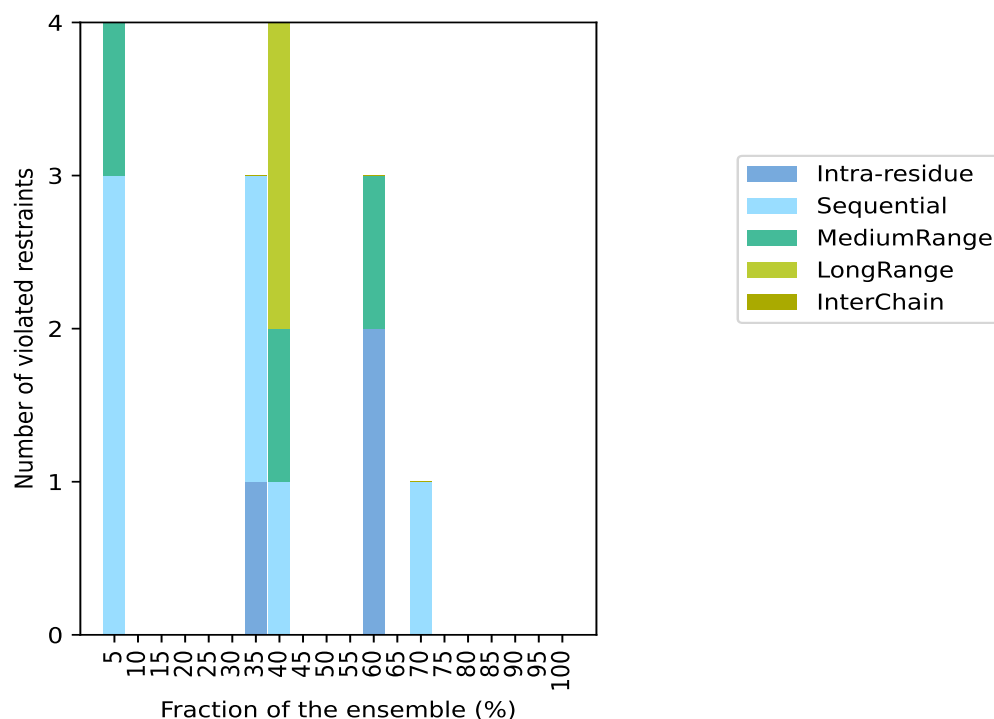
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 240(IR:124, SQ:52, MR:48, LR:16, IC:0) restraints are not 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	3	1	0	0	4	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
1	2	0	0	0	3	7	35.0
0	1	1	2	0	4	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
2	0	1	0	0	3	12	60.0
0	0	0	0	0	0	13	65.0
0	1	0	0	0	1	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

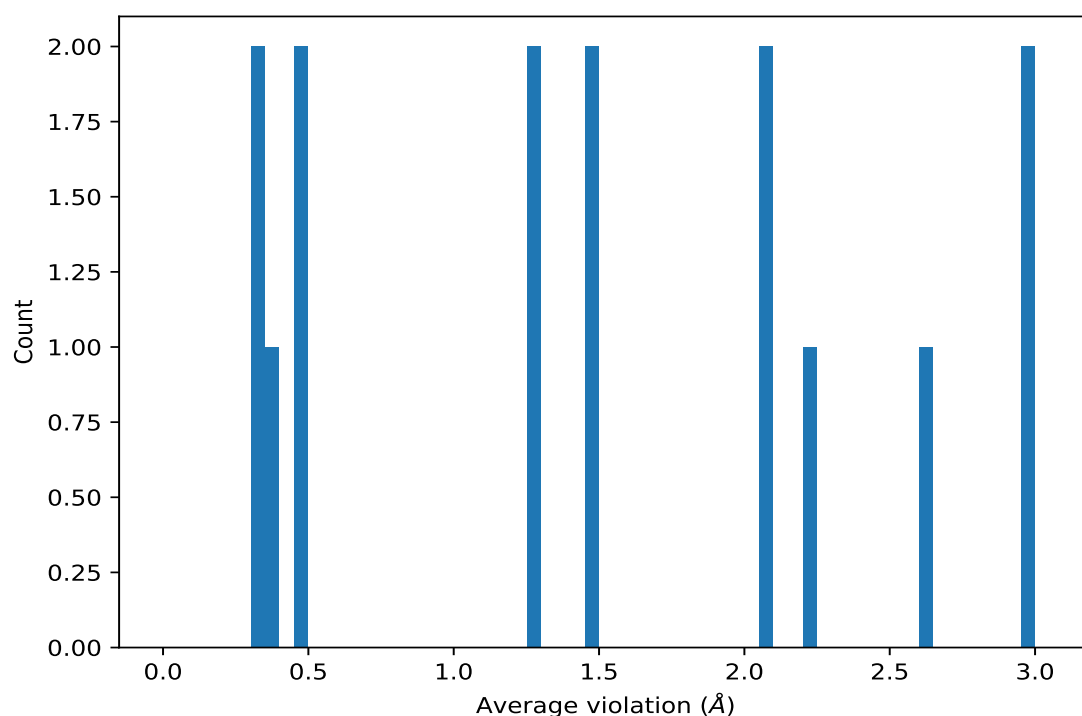
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

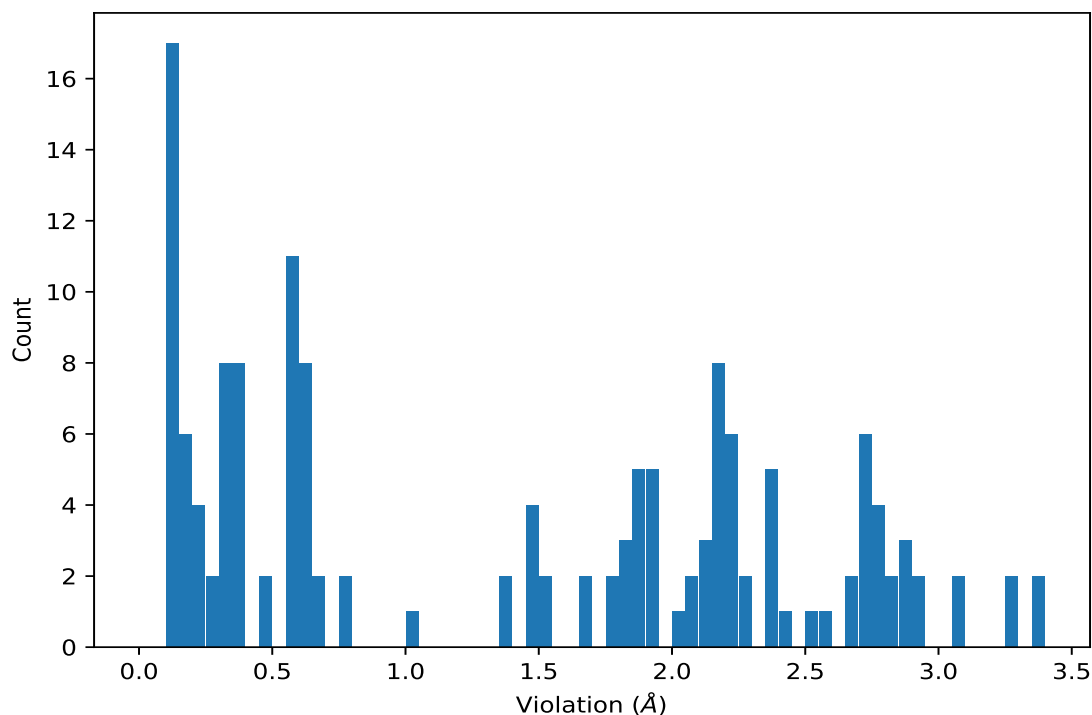
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	14	1.28	0.94	1.58
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	14	1.28	0.94	1.58
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	12	2.22	0.27	2.22
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	12	0.49	0.17	0.57
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	12	0.49	0.17	0.57
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	8	2.97	0.22	2.9
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	8	2.97	0.22	2.9
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	8	2.63	0.24	2.71
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	8	2.05	0.33	2.13
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	8	2.05	0.33	2.13
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	8	1.49	0.49	1.65
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	8	1.49	0.49	1.65
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	7	0.37	0.3	0.28
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	7	0.33	0.02	0.33
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	7	0.33	0.02	0.33

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)
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	19	3.37
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	19	3.37
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	9	3.25
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	9	3.25
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	7	3.07
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	7	3.07
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	15	2.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	15	2.92
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	2	2.88
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	2	2.88
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	9	2.85
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	12	2.8
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	12	2.8
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	3	2.79
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	3	2.79
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	5	2.77
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	15	2.75
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	3	2.73
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	2	2.72
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	16	2.7
(2,89)	1:10:A:TYR:HD1	1:14:A:VAL:HB	16	2.7
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	7	2.7
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	19	2.7
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	7	2.65
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	7	2.65
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	16	2.57
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	4	2.53
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	1	2.42
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	9	2.38
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	9	2.38
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	8	2.38
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	15	2.36
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	15	2.36
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	18	2.27
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	20	2.26
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	7	2.22
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	7	2.22
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	12	2.22
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	12	2.22
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	3	2.21
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	3	2.21
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	13	2.18
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	14	2.17
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	9	2.17
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	9	2.17
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	2	2.16
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	2	2.16
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	3	2.16
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	3	2.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	17	2.12
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	19	2.11
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	19	2.11
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	19	2.06
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	19	2.06
(2,25)	1:10:A:TYR:HD1	1:11:A:LEU:HA	12	2.02
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	3	1.93
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	3	1.93
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	7	1.92
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	7	1.92
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	6	1.9
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	15	1.89
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	15	1.89
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	2	1.87
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	2	1.87
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	11	1.85
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	9	1.82
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	9	1.82
(2,24)	1:10:A:TYR:HD1	1:7:A:LEU:HA	10	1.8
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	16	1.79
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	16	1.79
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	15	1.67
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	15	1.67
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG2	16	1.54
(1,6)	1:10:A:TYR:HD1	1:18:A:GLU:HG3	16	1.54
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	2	1.48
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	2	1.48
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	16	1.47
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	16	1.47
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	12	1.37
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	12	1.37
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	12	1.02
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	19	0.76
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	19	0.76
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	13	0.65
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	13	0.65
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB2	12	0.62
(1,4)	1:10:A:TYR:HD1	1:21:A:ASN:HB3	12	0.62
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	17	0.61
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	17	0.61
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	1	0.6
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	18	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	1	0.6
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	18	0.6
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	4	0.59
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	4	0.59
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	14	0.58
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	14	0.58
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	5	0.57
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	20	0.57
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	5	0.57
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	20	0.57
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	8	0.55
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	8	0.55
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	19	0.55
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	6	0.48
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	6	0.48
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	11	0.38
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	11	0.38
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	3	0.35
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	9	0.35
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	15	0.35
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	3	0.35
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	9	0.35
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	15	0.35
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	2	0.33
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	2	0.33
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	19	0.32
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	19	0.32
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	7	0.3
(2,64)	1:10:A:TYR:HD1	1:11:A:LEU:H	16	0.3
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	7	0.3
(2,60)	1:11:A:LEU:H	1:10:A:TYR:HD1	16	0.3
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	17	0.29
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	13	0.28
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	6	0.22
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	6	0.22
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	10	0.21
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	10	0.21
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	5	0.19
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	5	0.19
(2,65)	1:10:A:TYR:HD1	1:10:A:TYR:H	11	0.17
(2,59)	1:10:A:TYR:H	1:10:A:TYR:HD1	11	0.17
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	5	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	14	0.15
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	4	0.14
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	4	0.14
(2,156)	1:2:A:ASN:HB2	1:4:A:ASN:HB2	6	0.13
(2,156)	1:2:A:ASN:HB2	1:4:A:ASN:HB3	6	0.13
(2,156)	1:2:A:ASN:HB3	1:4:A:ASN:HB2	6	0.13
(2,156)	1:2:A:ASN:HB3	1:4:A:ASN:HB3	6	0.13
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	20	0.13
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	20	0.13
(2,23)	1:10:A:TYR:HD1	1:10:A:TYR:HA	18	0.13
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB2	1	0.12
(2,88)	1:10:A:TYR:HD1	1:11:A:LEU:HB3	1	0.12
(2,206)	1:2:A:ASN:HB2	1:3:A:LEU:H	8	0.11
(2,206)	1:2:A:ASN:HB3	1:3:A:LEU:H	8	0.11
(2,204)	1:2:A:ASN:HB2	1:3:A:LEU:H	8	0.11
(2,204)	1:2:A:ASN:HB3	1:3:A:LEU:H	8	0.11
(2,32)	1:3:A:LEU:H	1:2:A:ASN:HB2	8	0.11
(2,32)	1:3:A:LEU:H	1:2:A:ASN:HB3	8	0.11

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found