



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:36 AM UTC

PDB ID : 2M3G / pdb_00002m3g
BMRB ID : 18595
Title : Structure of Anabaena Sensory Rhodopsin Determined by Solid State NMR Spectroscopy
Authors : Wang, S.; Munro, R.A.; Shi, L.; Kawamura, I.; Okitsu, T.; Wada, A.; Kim, S.; Jung, K.; Brown, L.S.; Ladizhansky, V.
Deposited on : 2013-01-17

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

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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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 13%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 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:6-A:22, A:34-A:149, A:158-A:186, A:198-A:221, B:6-B:22, B:35-B:149, B:159-B:185, B:197-B:221, C:6-C:21, C:35-C:123, C:127-C:148, C:159-C:186, C:197-C:221 (550)	1.12	6

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	1, 3, 6
2	4, 5, 9
3	7, 8
Single-model clusters	2; 10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11379 atoms, of which 5715 are hydrogens and 0 are deuteriums.

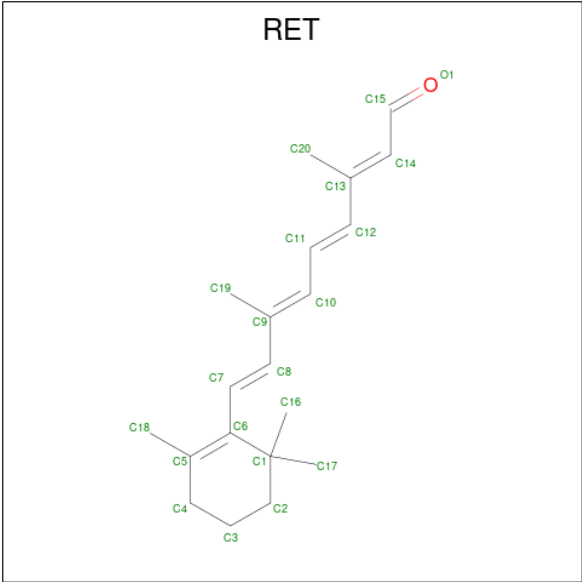
- Molecule 1 is a protein called Anabaena Sensory Rhodopsin.

Mol	Chain	Residues	Atoms						Trace
1	A	229	Total	C	H	N	O	S	0
			3745	1248	1877	298	311	11	
1	B	229	Total	C	H	N	O	S	0
			3745	1248	1877	298	311	11	
1	C	229	Total	C	H	N	O	S	0
			3745	1248	1877	298	311	11	

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	HIS	-	expression tag	UNP Q8YSC4
A	231	HIS	-	expression tag	UNP Q8YSC4
A	232	HIS	-	expression tag	UNP Q8YSC4
A	233	HIS	-	expression tag	UNP Q8YSC4
A	234	HIS	-	expression tag	UNP Q8YSC4
A	235	HIS	-	expression tag	UNP Q8YSC4
B	230	HIS	-	expression tag	UNP Q8YSC4
B	231	HIS	-	expression tag	UNP Q8YSC4
B	232	HIS	-	expression tag	UNP Q8YSC4
B	233	HIS	-	expression tag	UNP Q8YSC4
B	234	HIS	-	expression tag	UNP Q8YSC4
B	235	HIS	-	expression tag	UNP Q8YSC4
C	230	HIS	-	expression tag	UNP Q8YSC4
C	231	HIS	-	expression tag	UNP Q8YSC4
C	232	HIS	-	expression tag	UNP Q8YSC4
C	233	HIS	-	expression tag	UNP Q8YSC4
C	234	HIS	-	expression tag	UNP Q8YSC4
C	235	HIS	-	expression tag	UNP Q8YSC4

- Molecule 2 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O).



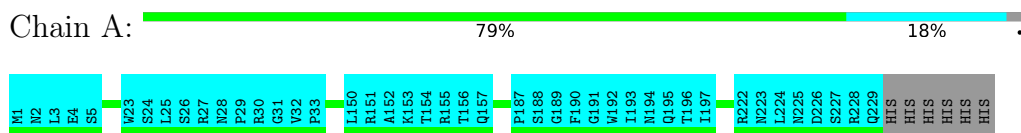
Mol	Chain	Residues	Atoms		
2	A	1	Total	C	H
			48	20	28
2	B	1	Total	C	H
			48	20	28
2	C	1	Total	C	H
			48	20	28

4 Residue-property plots

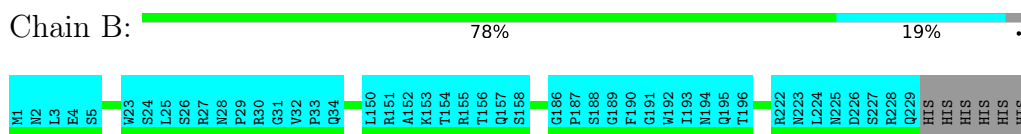
4.1 Average score per residue in the NMR ensemble

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.

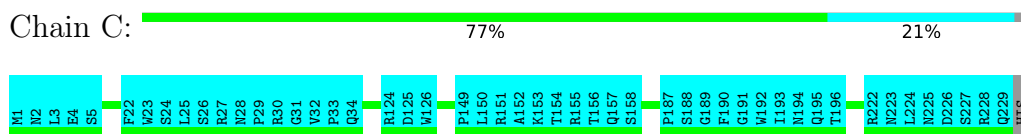
- Molecule 1: Anabaena Sensory Rhodopsin



- Molecule 1: Anabaena Sensory Rhodopsin



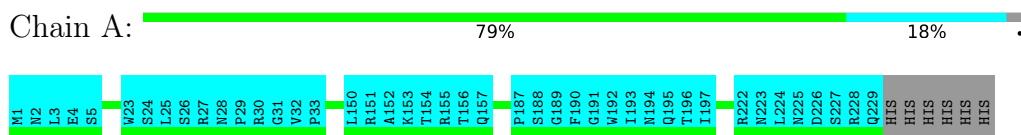
- Molecule 1: Anabaena Sensory Rhodopsin



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 6. Colouring as in section 4.1 above.

- Molecule 1: Anabaena Sensory Rhodopsin

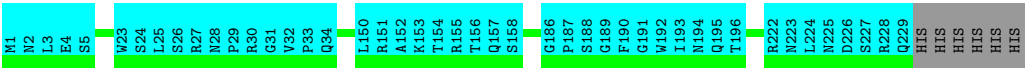


- Molecule 1: Anabaena Sensory Rhodopsin

Chain B:

78%

19%

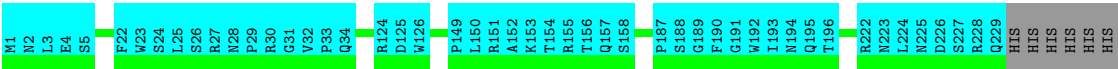


● Molecule 1: Anabaena Sensory Rhodopsin

Chain C:

77%

21%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 10 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
ARIA	structure solution	
CNS	structure solution	
CNS	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	2
Total number of shifts	1186
Number of shifts mapped to atoms	1186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

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6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 11% 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	1143
Number of shifts mapped to atoms	1143
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	205	-1.33 ± 0.20	Should be checked
$^{13}\text{C}_\beta$	176	0.53 ± 0.10	Should be checked
$^{13}\text{C}'$	203	-0.40 ± 0.24	None needed (< 0.5 ppm)
^{15}N	205	1.40 ± 0.35	Should be applied

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 12%, i.e. 976 atoms were assigned a chemical shift out of a possible 7924. 0 out of 117 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	536/2760 (19%)	0/1124 (0%)	360/1100 (33%)	176/536 (33%)
Sidechain	372/4037 (9%)	0/2718 (0%)	366/1261 (29%)	6/58 (10%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	68/1127 (6%)	0/547 (0%)	64/524 (12%)	4/56 (7%)
Overall	976/7924 (12%)	0/4389 (0%)	790/2885 (27%)	186/650 (29%)

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

7.1.4 Statistically unusual chemical shifts ⓘ

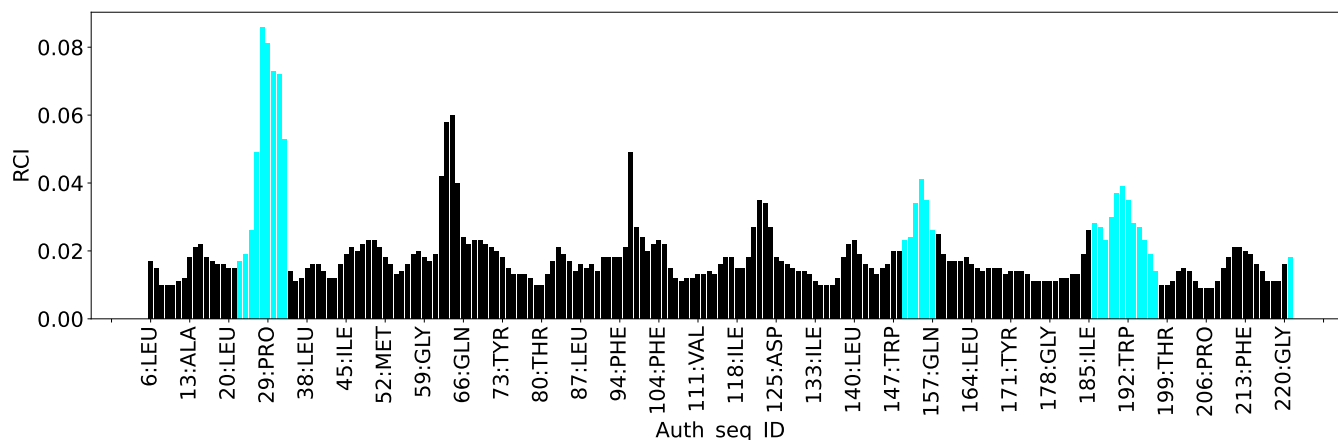
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	210	LYS	NZ	177.20	19.79 – 46.09	54.9
1	A	210	LYS	CE	55.67	37.57 – 46.21	15.9
1	A	109	GLN	NE2	98.30	103.38 – 120.35	-8.0
1	A	128	ARG	CD	37.40	38.57 – 47.75	-6.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_dup*

7.2.1 Bookkeeping [i](#)

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	43
Number of shifts mapped to atoms	43
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

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 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 0%, i.e. 34 atoms were assigned a chemical shift out of a possible 7924. 0 out of 117 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	18/2760 (1%)	0/1124 (0%)	12/1100 (1%)	6/536 (1%)
Sidechain	12/4037 (0%)	0/2718 (0%)	12/1261 (1%)	0/58 (0%)
Aromatic	4/1127 (0%)	0/547 (0%)	4/524 (1%)	0/56 (0%)
Overall	34/7924 (0%)	0/4389 (0%)	28/2885 (1%)	6/650 (1%)

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

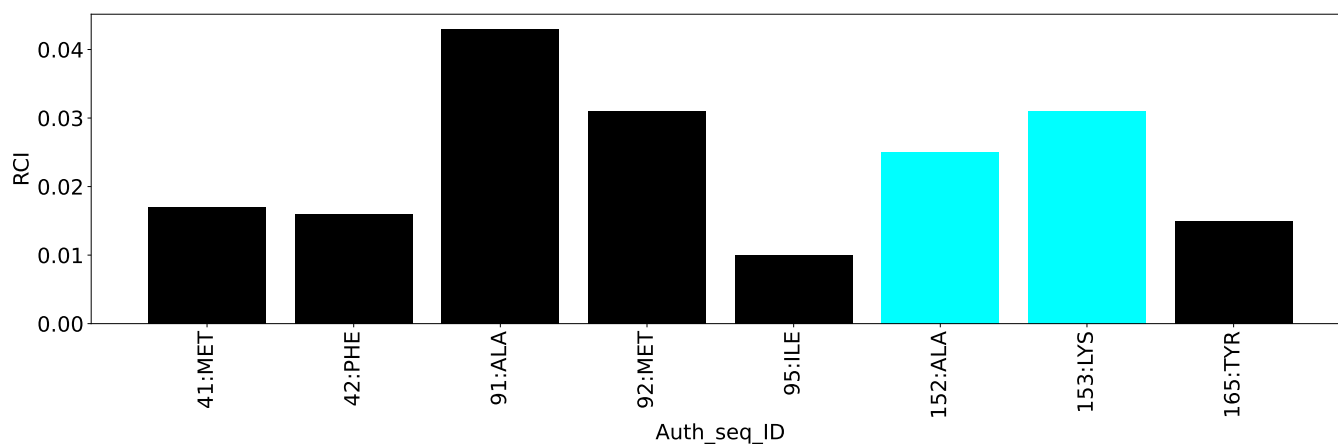
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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 B:



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	10266
Intra-residue ($ i-j =0$)	4599
Sequential ($ i-j =1$)	1980
Medium range ($ i-j >1$ and $ i-j <5$)	1599
Long range ($ i-j \geq 5$)	1098
Inter-chain	990
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.5
Number of long range restraints per residue ¹	1.6

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)	9.8	0.2
0.2-0.5 (Medium)	16.4	0.5
>0.5 (Large)	84.4	9.14

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

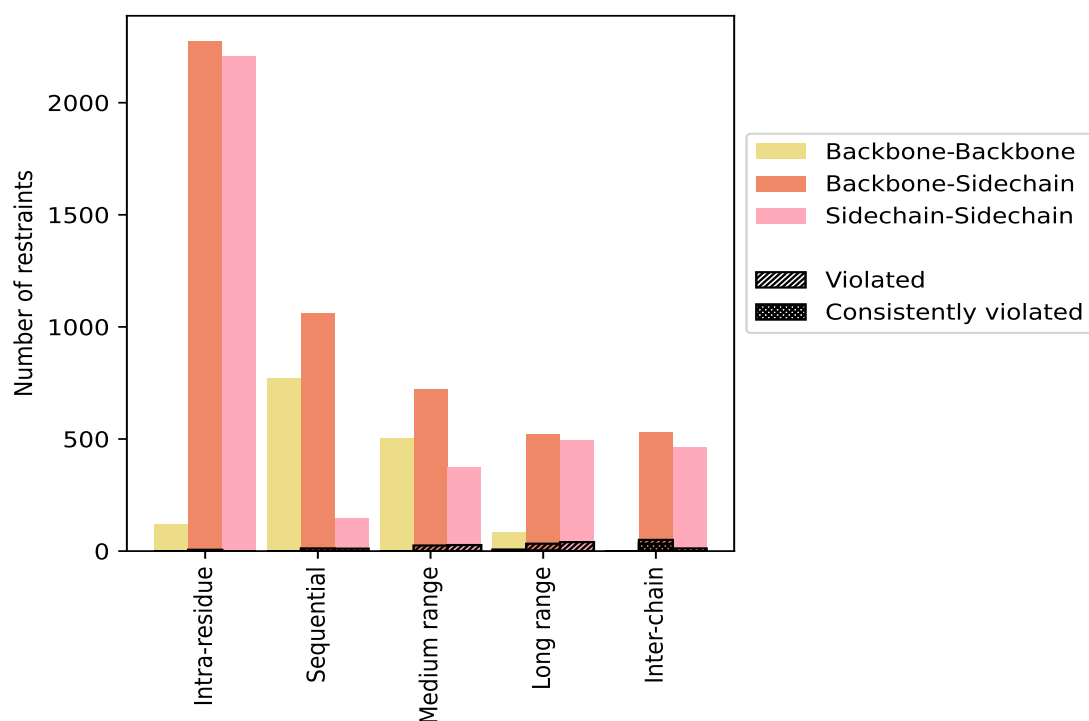
9.1 Summary of distance violations

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 ($i-j =0$)	4599	44.8	6	0.1	0.1	4	0.1	0.0
Backbone-Backbone	120	1.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2274	22.2	6	0.3	0.1	4	0.2	0.0
Sidechain-Sidechain	2205	21.5	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	1980	19.3	23	1.2	0.2	1	0.1	0.0
Backbone-Backbone	771	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1062	10.3	12	1.1	0.1	1	0.1	0.0
Sidechain-Sidechain	147	1.4	11	7.5	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	1599	15.6	52	3.3	0.5	0	0.0	0.0
Backbone-Backbone	501	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	723	7.0	25	3.5	0.2	0	0.0	0.0
Sidechain-Sidechain	375	3.7	27	7.2	0.3	0	0.0	0.0
Long range ($i-j \geq 5$)	1098	10.7	80	7.3	0.8	3	0.3	0.0
Backbone-Backbone	84	0.8	7	8.3	0.1	0	0.0	0.0
Backbone-Sidechain	519	5.1	33	6.4	0.3	3	0.6	0.0
Sidechain-Sidechain	495	4.8	40	8.1	0.4	0	0.0	0.0
Inter-chain	990	9.6	62	6.3	0.6	33	3.3	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	528	5.1	50	9.5	0.5	33	6.2	0.3
Sidechain-Sidechain	462	4.5	12	2.6	0.1	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	10266	100.0	223	2.2	2.2	41	0.4	0.4
Backbone-Backbone	1476	14.4	7	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	5106	49.7	126	2.5	1.2	41	0.8	0.4
Sidechain-Sidechain	3684	35.9	90	2.4	0.9	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

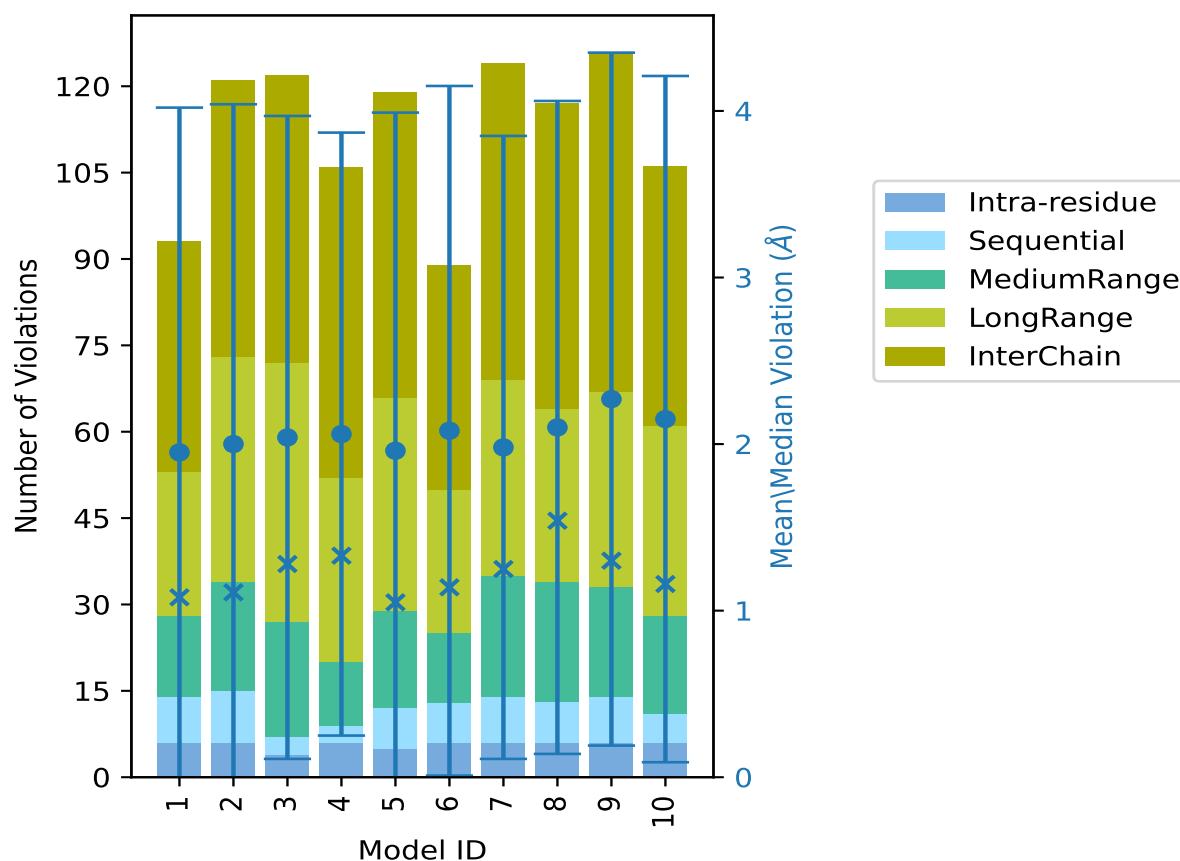
9.2 Distance violation statistics for each model [i](#)

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	6	8	14	25	40	93	1.95	8.96	2.07	1.08
2	6	9	19	39	48	121	2.0	9.14	2.04	1.11
3	4	3	20	45	50	122	2.04	7.85	1.93	1.28
4	6	3	11	32	54	106	2.06	7.91	1.81	1.33
5	5	7	17	37	53	119	1.96	7.97	2.03	1.05
6	6	7	12	25	39	89	2.08	8.94	2.07	1.14
7	6	8	21	34	55	124	1.98	9.07	1.87	1.25
8	6	7	21	30	53	117	2.1	7.88	1.96	1.54
9	6	8	19	34	59	126	2.27	9.13	2.08	1.3
10	6	5	17	33	45	106	2.15	8.9	2.06	1.16

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 10043(IR:4593, SQ:1957, MR:1547, LR:1018, IC:928) 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	13	20	20	5	58	1	10.0
0	4	7	3	0	14	2	20.0
0	1	8	12	2	23	3	30.0

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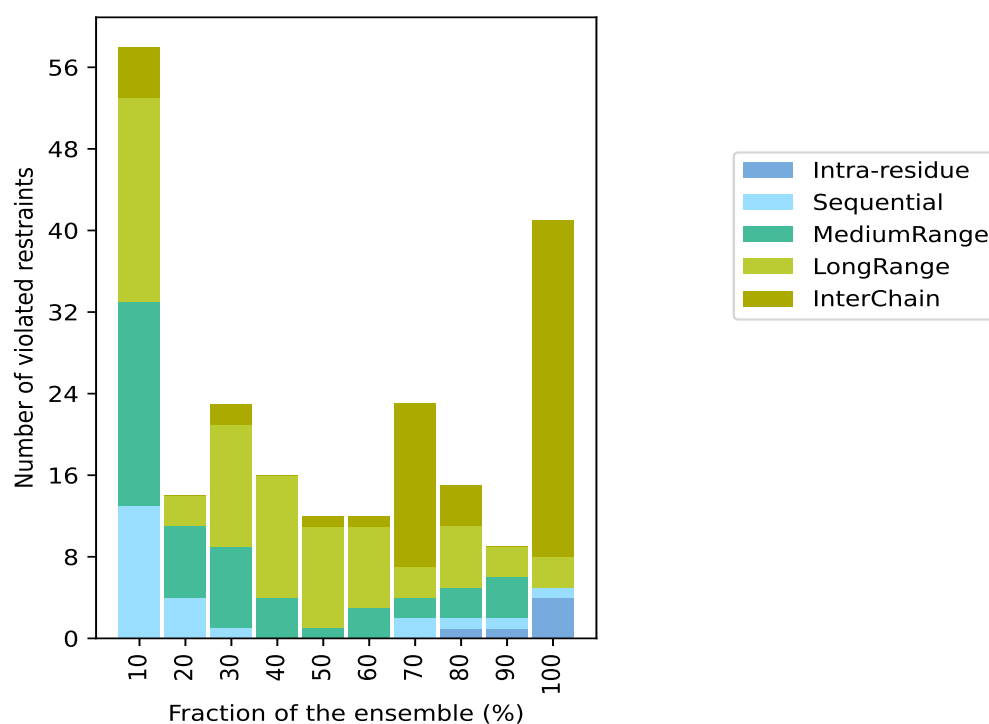
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	4	12	0	16	4	40.0
0	0	1	10	1	12	5	50.0
0	0	3	8	1	12	6	60.0
0	2	2	3	16	23	7	70.0
1	1	3	6	4	15	8	80.0
1	1	4	3	0	9	9	90.0
4	1	0	3	33	41	10	100.0

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 ⓘ

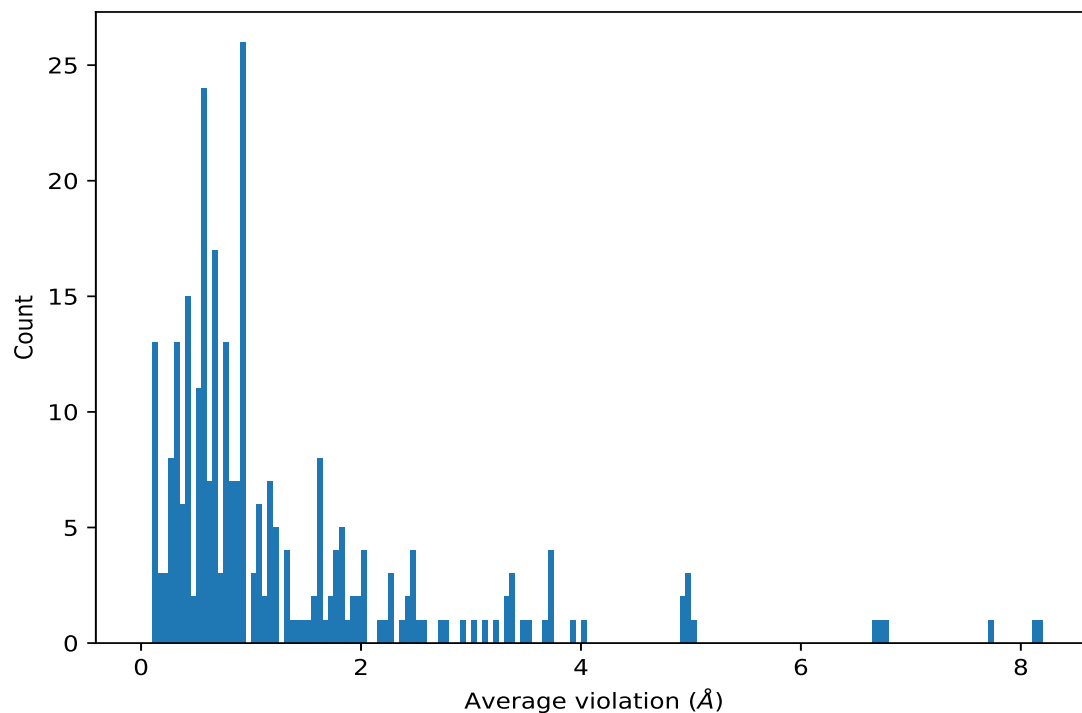


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

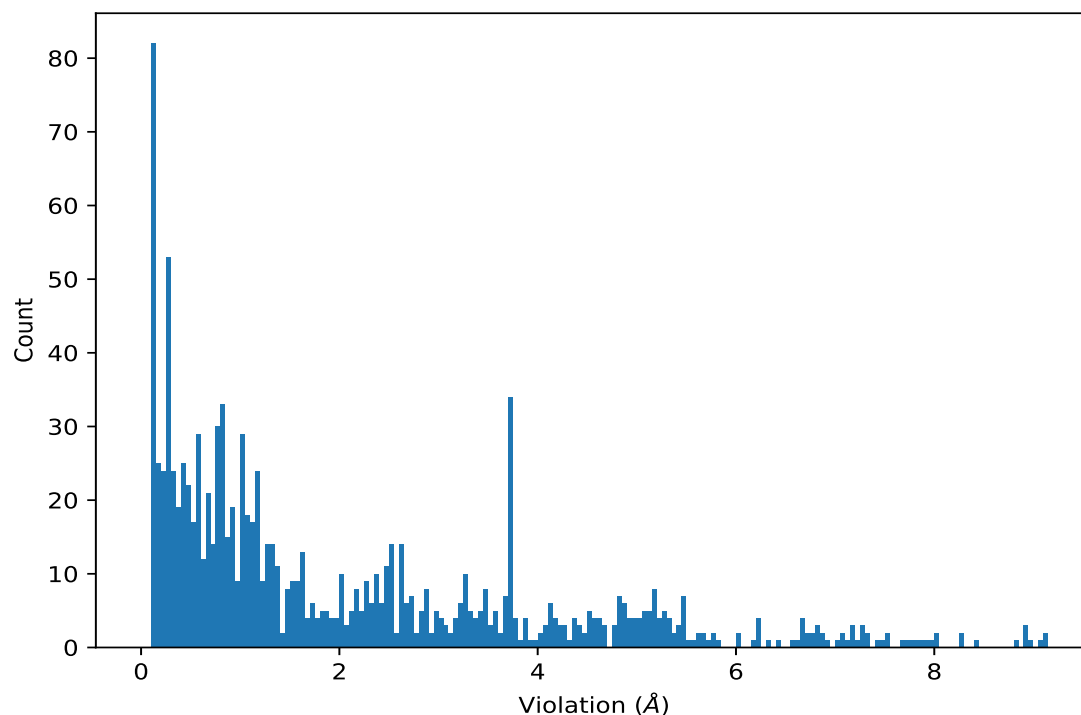
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3387)	2:301:B:RET:C4	1:83:B:LEU:CD1	10	8.2	0.69	8.09
(2,6321)	2:301:C:RET:C4	1:83:C:LEU:CD1	10	8.1	0.72	7.94
(2,453)	2:301:A:RET:C4	1:83:A:LEU:CD1	10	7.7	0.61	7.65
(2,6673)	2:301:C:RET:C4	1:209:C:SER:CB	10	6.76	0.44	6.8
(2,3739)	2:301:B:RET:C4	1:209:B:SER:CB	10	6.71	0.5	6.74
(2,805)	2:301:A:RET:C4	1:209:A:SER:CB	10	6.66	0.47	6.7
(2,5868)	2:301:B:RET:C4	1:80:B:THR:CG2	10	5.02	0.45	5.0
(2,2933)	2:301:A:RET:C4	1:179:A:TYR:CZ	10	4.96	0.43	5.06
(2,2934)	2:301:A:RET:C4	1:80:A:THR:CG2	10	4.96	0.54	5.0
(2,8801)	2:301:C:RET:C4	1:179:C:TYR:CZ	10	4.95	0.48	5.15

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6321)	2:301:C:RET:C4	1:83:C:LEU:CD1	2	9.14
(2,6321)	2:301:C:RET:C4	1:83:C:LEU:CD1	9	9.13
(2,3387)	2:301:B:RET:C4	1:83:B:LEU:CD1	7	9.07
(2,3387)	2:301:B:RET:C4	1:83:B:LEU:CD1	1	8.96
(2,3387)	2:301:B:RET:C4	1:83:B:LEU:CD1	6	8.94
(2,453)	2:301:A:RET:C4	1:83:A:LEU:CD1	1	8.94
(2,3387)	2:301:B:RET:C4	1:83:B:LEU:CD1	10	8.9
(2,6321)	2:301:C:RET:C4	1:83:C:LEU:CD1	6	8.83
(2,6321)	2:301:C:RET:C4	1:83:C:LEU:CD1	10	8.4
(2,3387)	2:301:B:RET:C4	1:83:B:LEU:CD1	9	8.27

10 Dihedral-angle violation analysis

No dihedral-angle restraints found