Full wwPDB NMR Structure Validation Report (i)

Oct 15, 2026 – 05:47 pm BST

PDB ID	:	31DL / pdb_000031dl
BMRB ID	:	53779
Title	:	Apo form of calmodulin-like domain of human alpha-actinin-4
Authors	:	Hocevar, J.; Kovacic, M.; Plavec, J.; Djinovic-Carugo, K.; Pavsic, M.
Deposited on	:	2026-05-27

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 (i) 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 (i)) were used in the production of this report:

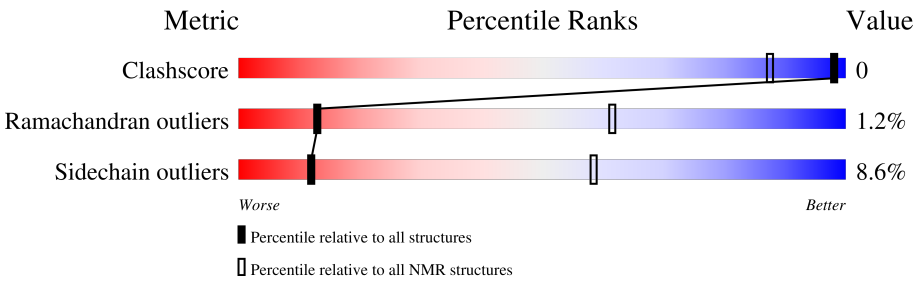
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.3.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	153	71% • 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:774-A:834 (61)	0.94	14
2	A:844-A:855 (12)	0.56	16
3	A:861-A:901 (41)	0.43	16

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2309 atoms, of which 1115 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-actinin-4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	153	2309	745	1115	198	245	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	GLY	-	expression tag	UNP O43707
A	760	SER	-	expression tag	UNP O43707
A	761	SER	-	expression tag	UNP O43707

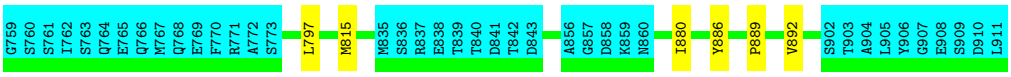
4 Residue-property plots (i)

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: Alpha-actinin-4

Chain A:



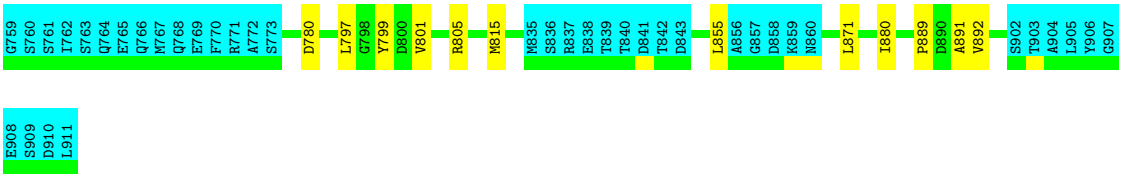
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Alpha-actinin-4

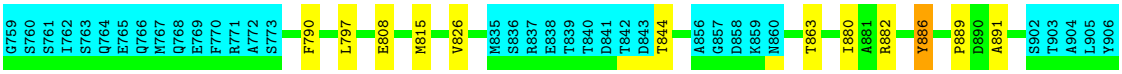
Chain A:



4.2.2 Score per residue for model 2

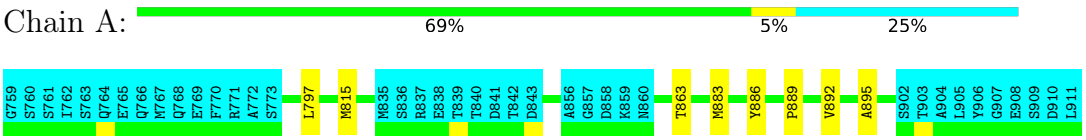
• Molecule 1: Alpha-actinin-4

Chain A:



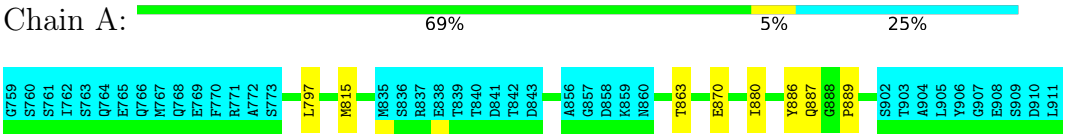
4.2.3 Score per residue for model 3

• Molecule 1: Alpha-actinin-4



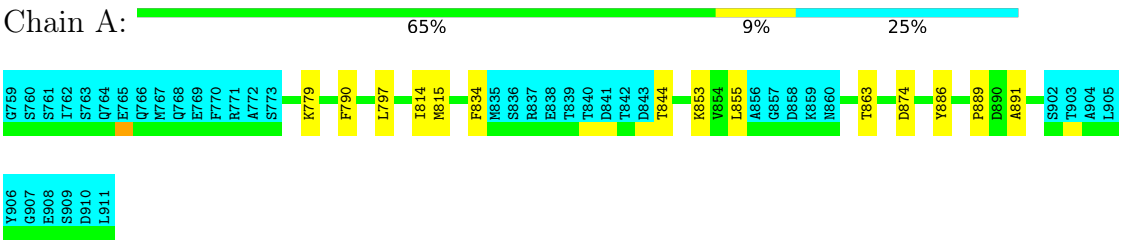
4.2.4 Score per residue for model 4

• Molecule 1: Alpha-actinin-4



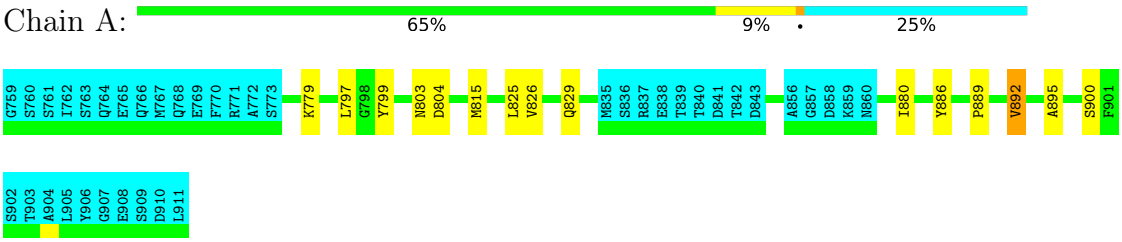
4.2.5 Score per residue for model 5

• Molecule 1: Alpha-actinin-4



4.2.6 Score per residue for model 6

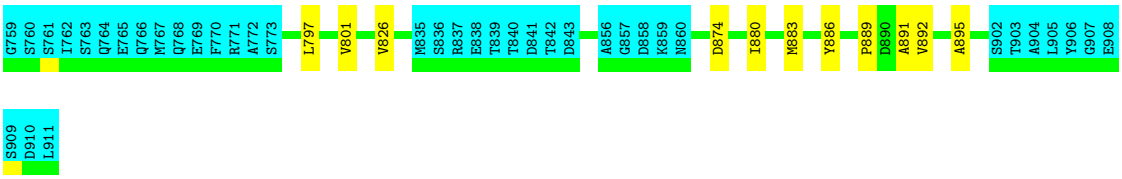
• Molecule 1: Alpha-actinin-4



4.2.7 Score per residue for model 7

- Molecule 1: Alpha-actinin-4

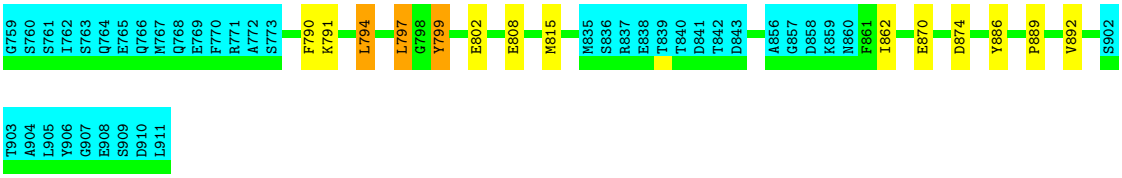
Chain A: 67% 7% 25%



4.2.8 Score per residue for model 8

- Molecule 1: Alpha-actinin-4

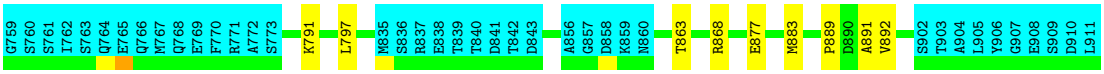
Chain A: 65% 7% • 25%



4.2.9 Score per residue for model 9

- Molecule 1: Alpha-actinin-4

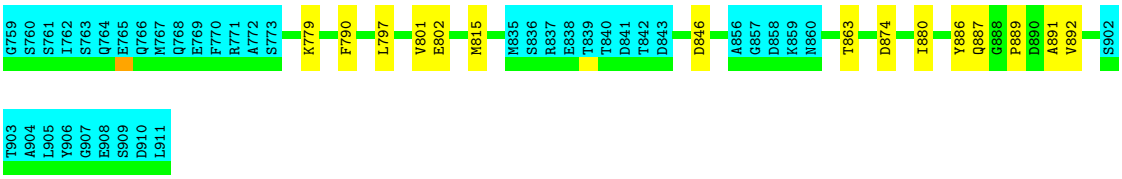
Chain A: 69% 6% 25%



4.2.10 Score per residue for model 10

- Molecule 1: Alpha-actinin-4

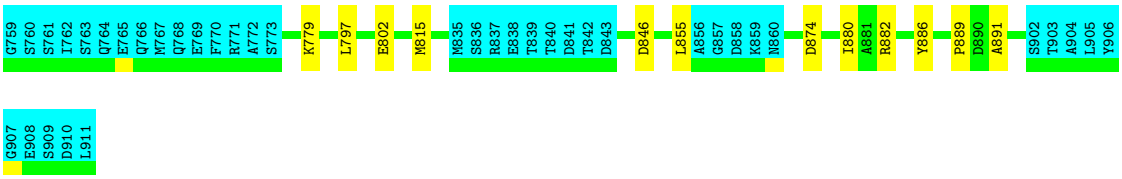
Chain A: 65% 10% 25%



4.2.11 Score per residue for model 11

- Molecule 1: Alpha-actinin-4

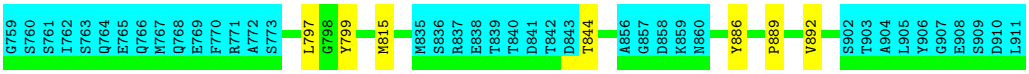
Chain A: 67% 8% 25%



4.2.12 Score per residue for model 12

- Molecule 1: Alpha-actinin-4

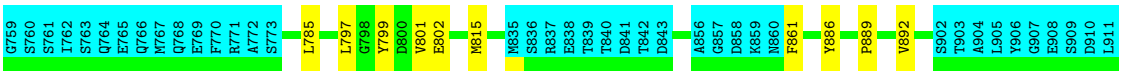
Chain A: 70% 5% 25%



4.2.13 Score per residue for model 13

- Molecule 1: Alpha-actinin-4

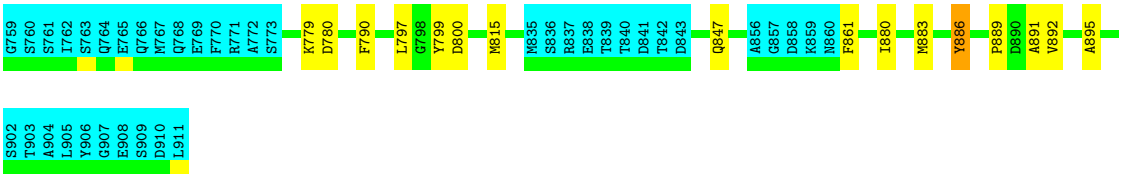
Chain A: 68% 7% 25%



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Alpha-actinin-4

Chain A: 64% 10% • 25%



4.2.15 Score per residue for model 15

- Molecule 1: Alpha-actinin-4

Chain A: 68% 7% 25%

G759 S760 S761 I762 S763 Q764 E765 Q766 M767 Q768 E769 F770 R771 A772 S773 L797 G798 Y799 E802 N812 M835 S836 R837 E838 T839 T840 D841 T842 D843 A856 G857 D858 K859 N860 T863 I880 Y886 P889 V892 S900 F901 S902 T903 A904 L905 Y906 G907 E908 S909

D910 L911

4.2.16 Score per residue for model 16

- Molecule 1: Alpha-actinin-4

Chain A: 67% 7% • 25%

G759 S760 S761 I762 S763 Q764 E765 Q766 M767 Q768 E769 F770 R771 A772 S773 L797 G798 Y799 D800 V801 E802 R805 M835 S836 R837 E838 T839 T840 D841 T842 D843 A856 G857 D858 K859 N860 F861 I880 Y886 P889 V892 A895 S900 F901 S902 T903 A904 L905 Y906 G907

E908 S909 D910 L911

4.2.17 Score per residue for model 17

- Molecule 1: Alpha-actinin-4

Chain A: 67% 8% 25%

G759 S760 S761 I762 S763 Q764 E765 Q766 M767 Q768 E769 F770 R771 A772 S773 L797 G798 Y799 D804 R805 M815 M835 S836 R837 E838 T839 T840 D841 T842 D843 D846 L855 A856 G857 D858 K859 N860 I880 Y886 P889 V892 A895 S902 T903 A904 L905 Y906 G907

E908 S909 D910 L911

4.2.18 Score per residue for model 18

- Molecule 1: Alpha-actinin-4

Chain A: 67% 7% 25%

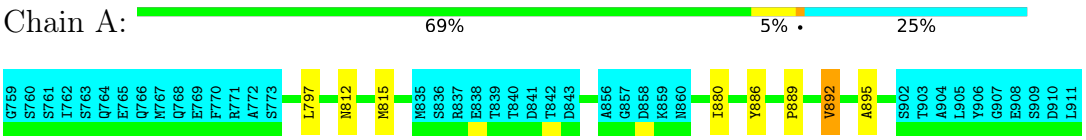
G759 S760 S761 I762 S763 Q764 E765 Q766 M767 Q768 E769 F770 R771 A772 S773 L797 M815 V826 Q829 M835 S836 R837 E838 T839 T840 D841 T842 D843 K853 V854 L855 A856 G857 D858 K859 N860 D874 Y886 P889 V892 A895 S902 T903 A904 L905 Y906 G907 E908

S909 D910 L911

4.2.19 Score per residue for model 19

- Molecule 1: Alpha-actinin-4

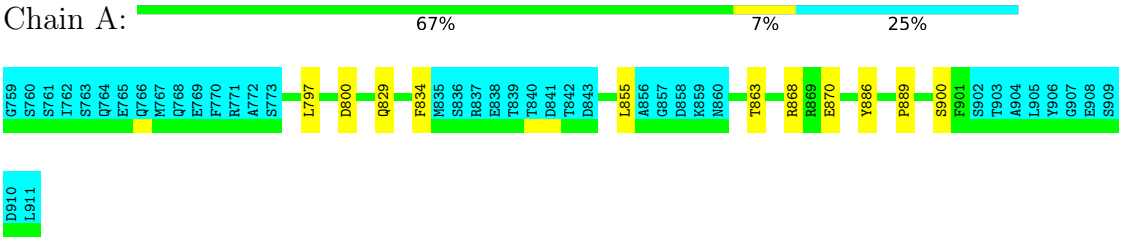
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Alpha-actinin-4

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
YASARA	refinement	14.7.17
ARTINA	structure calculation	
YASARA	structure calculation	14.7.17

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	1846
Number of shifts mapped to atoms	1845
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.75±0.03	0±0/923 (0.0± 0.0%)	0.92±0.03	2±1/1252 (0.1± 0.1%)
All	All	0.75	2/18460 (0.0%)	0.92	31/25040 (0.1%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	799	TYR	CE1-CZ	6.63	1.54	1.38	8	1
1	A	799	TYR	CG-CD1	5.70	1.51	1.39	8	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	891	ALA	N-CA-C	7.81	119.58	111.14	14	8
1	A	862	ILE	N-CA-C	-6.48	98.27	108.95	8	1
1	A	892	VAL	CA-C-N	-6.18	113.58	119.76	8	8
1	A	892	VAL	C-N-CA	-6.18	113.58	119.76	8	8
1	A	886	TYR	N-CA-C	5.94	118.43	110.35	2	2
1	A	871	LEU	CA-C-N	-5.64	115.60	119.66	1	1
1	A	871	LEU	C-N-CA	-5.64	115.60	119.66	1	1
1	A	861	PHE	N-CA-C	-5.40	100.91	108.96	16	1
1	A	799	TYR	N-CA-C	5.07	116.83	110.24	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	A	899	848	848	1±1
All	All	17980	16960	16960	14

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:A:892:VAL:HG23	1:A:895:ALA:HB2	0.55	1.76	17	8
1:A:892:VAL:CG2	1:A:895:ALA:HB2	0.51	2.36	19	2
1:A:794:LEU:HD13	1:A:799:TYR:HD1	0.49	1.68	8	1
1:A:794:LEU:HD13	1:A:799:TYR:CD1	0.49	2.43	8	1
1:A:797:LEU:HD11	1:A:799:TYR:CE2	0.43	2.49	8	1
1:A:804:ASP:CG	1:A:805:ARG:N	0.41	2.78	17	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	A	114/153 (75%)	111±1 (97±1%)	2±1 (2±1%)	1±0 (1±0%)	13 61
All	All	2280/3060 (75%)	2211 (97%)	42 (2%)	27 (1%)	13 61

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	889	PRO	20
1	A	801	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	803	ASN	1
1	A	800	ASP	1

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	94/127 (74%)	86±2 (91±2%)	8±2 (9±2%)	12 58
All	All	1880/2540 (74%)	1719 (91%)	161 (9%)	12 58

All 37 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	797	LEU	20
1	A	886	TYR	18
1	A	815	MET	15
1	A	880	ILE	12
1	A	863	THR	8
1	A	799	TYR	7
1	A	855	LEU	6
1	A	874	ASP	6
1	A	802	GLU	6
1	A	790	PHE	5
1	A	779	LYS	5
1	A	826	VAL	4
1	A	883	MET	4
1	A	900	SER	4
1	A	870	GLU	3
1	A	829	GLN	3
1	A	846	ASP	3
1	A	861	PHE	3
1	A	780	ASP	2
1	A	805	ARG	2
1	A	808	GLU	2
1	A	882	ARG	2
1	A	887	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	834	PHE	2
1	A	853	LYS	2
1	A	791	LYS	2
1	A	868	ARG	2
1	A	812	ASN	2
1	A	814	ILE	1
1	A	804	ASP	1
1	A	825	LEU	1
1	A	794	LEU	1
1	A	877	GLU	1
1	A	785	LEU	1
1	A	847	GLN	1
1	A	892	VAL	1
1	A	800	ASP	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 (i)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *flya*

7.1.1 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	1846
Number of shifts mapped to atoms	1845
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	759	GLY	H	8.497	0.010	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	153	-0.25 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	142	0.12 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	151	-0.31 ± 0.10	None needed (< 0.5 ppm)
^{15}N	145	0.33 ± 0.26	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 93%, i.e. 1411 atoms were assigned a chemical shift out of a possible 1520. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	563/564 (100%)	229/229 (100%)	227/228 (100%)	107/107 (100%)
Sidechain	727/799 (91%)	498/518 (96%)	220/253 (87%)	9/28 (32%)
Aromatic	121/157 (77%)	75/78 (96%)	43/76 (57%)	3/3 (100%)
Overall	1411/1520 (93%)	802/825 (97%)	490/557 (88%)	119/138 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1844 atoms were assigned a chemical shift out of a possible 1989. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	759/762 (100%)	310/310 (100%)	304/306 (99%)	145/146 (99%)
Sidechain	950/1051 (90%)	650/678 (96%)	287/334 (86%)	13/39 (33%)
Aromatic	135/176 (77%)	84/87 (97%)	48/86 (56%)	3/3 (100%)
Overall	1844/1989 (93%)	1044/1075 (97%)	639/726 (88%)	161/188 (86%)

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.

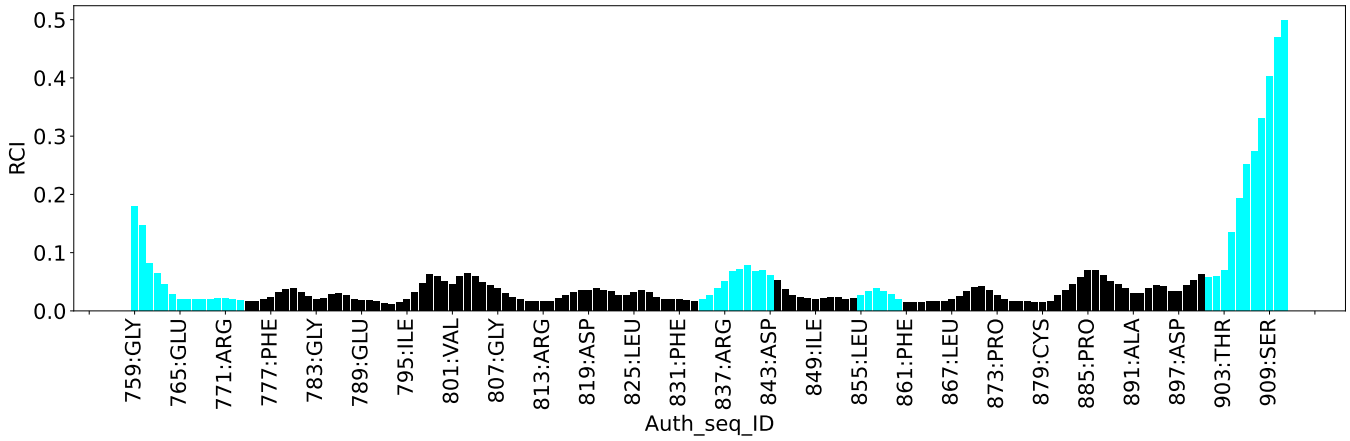
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	906	TYR	HD1	2.86	5.49 – 8.39	-14.1
1	A	770	PHE	HE1	4.97	5.56 – 8.62	-6.9
1	A	853	LYS	HD3	2.98	0.54 – 2.65	6.5
1	A	799	TYR	HE2	8.13	5.58 – 7.83	6.3
1	A	877	GLU	HB2	0.82	1.00 – 3.05	-5.9

7.1.5 Random Coil Index (RCI) plots (i)

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

bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1970
Intra-residue (|i-j|=0)	551
Sequential (|i-j|=1)	585
Medium range (|i-j|>1 and |i-j|<5)	425
Long range (|i-j|≥5)	409
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	12.9
Number of long range restraints per residue[1]	2.7

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.4	0.16
0.2-0.5 (Medium)	0.9	0.47
>0.5 (Large)	2.5	1.51

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 (i)

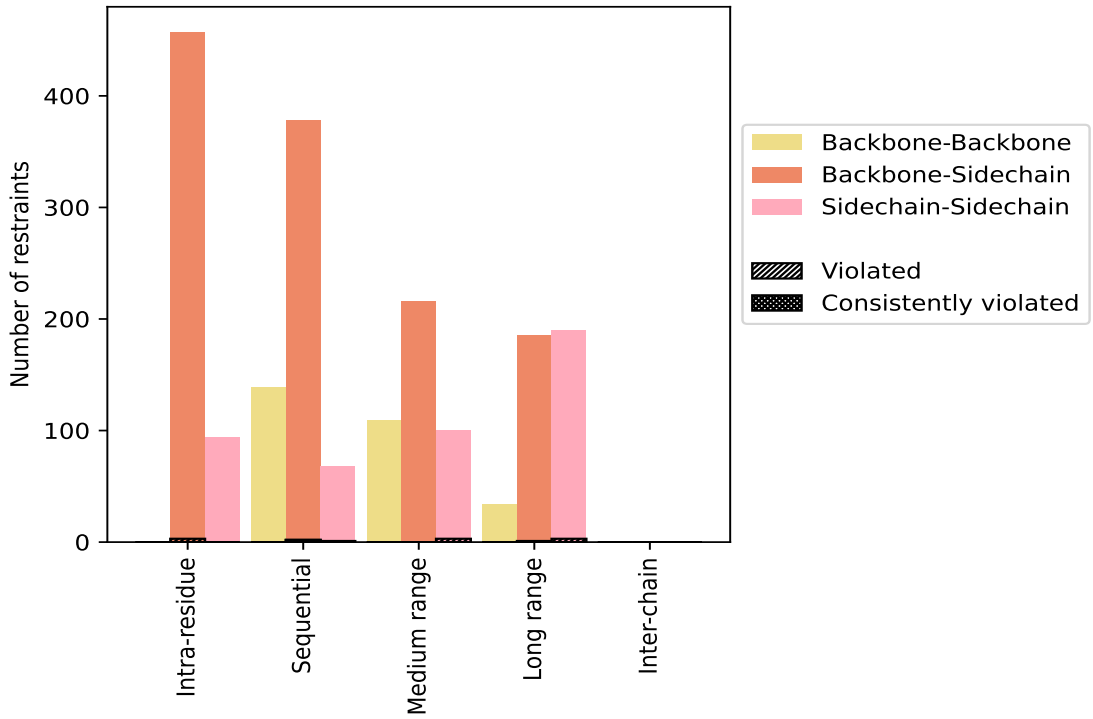
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	551	28.0	3	0.5	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	457	23.2	3	0.7	0.2	0	0.0	0.0
Sidechain-Sidechain	94	4.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	585	29.7	3	0.5	0.2	2	0.3	0.1
Backbone-Backbone	139	7.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	378	19.2	2	0.5	0.1	2	0.5	0.1
Sidechain-Sidechain	68	3.5	1	1.5	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	425	21.6	3	0.7	0.2	0	0.0	0.0
Backbone-Backbone	109	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	216	11.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	100	5.1	3	3.0	0.2	0	0.0	0.0
Long range (|i-j|≥5)	409	20.8	4	1.0	0.2	0	0.0	0.0
Backbone-Backbone	34	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	185	9.4	1	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	190	9.6	3	1.6	0.2	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	1970	100.0	13	0.7	0.7	2	0.1	0.1
Backbone-Backbone	282	14.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1236	62.7	6	0.5	0.3	2	0.2	0.1
Sidechain-Sidechain	452	22.9	7	1.5	0.4	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	1	2	0	0	0	3	0.88	1.26	0.38	1.01
2	1	2	0	0	0	3	0.9	1.28	0.4	1.08
3	1	2	0	0	0	3	0.73	1.07	0.24	0.6
4	1	2	0	0	0	3	0.83	1.15	0.32	0.96
5	1	2	0	0	0	3	0.78	1.08	0.33	0.94
6	1	2	0	0	0	3	0.82	1.08	0.26	0.93
7	1	2	0	0	0	3	0.81	1.14	0.38	1.02
8	1	2	1	2	0	6	0.57	0.98	0.28	0.55
9	1	2	1	0	0	4	0.7	1.24	0.48	0.69
10	1	2	0	0	0	3	0.77	1.06	0.3	0.89

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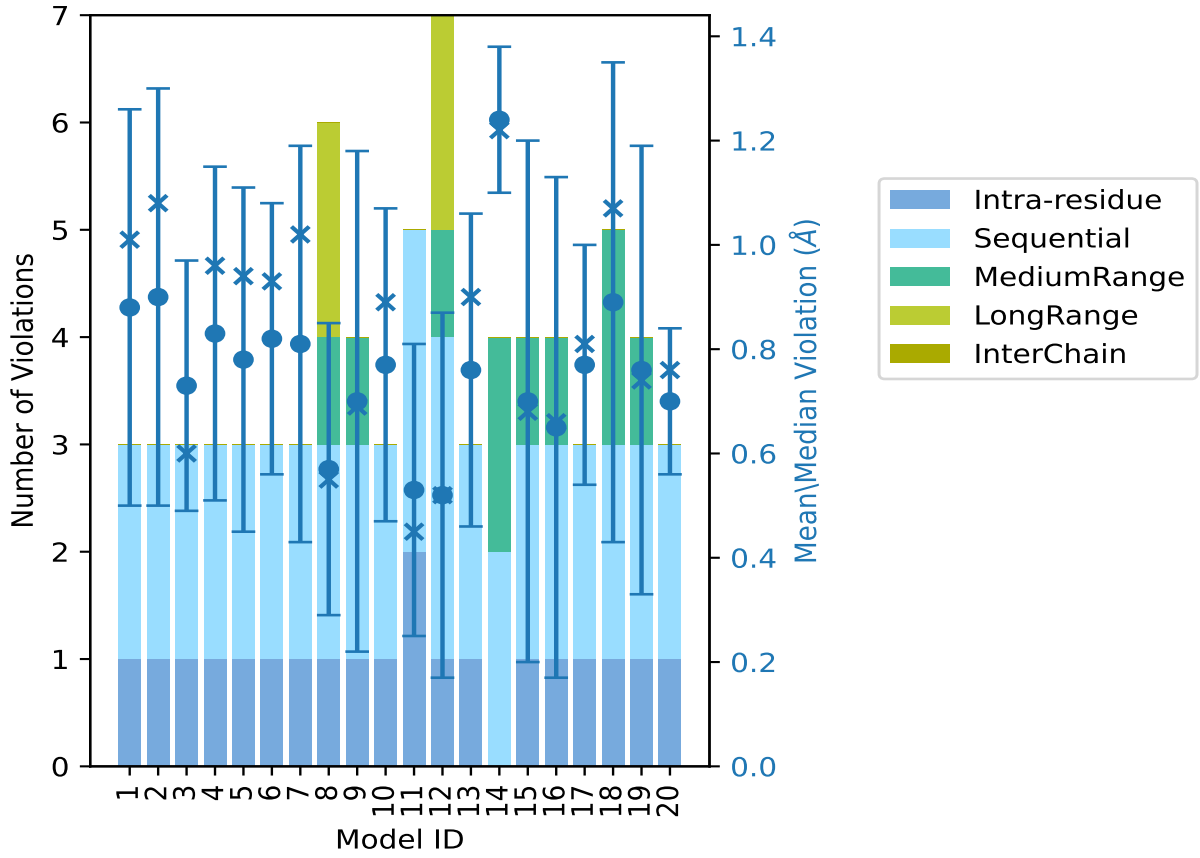
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	2	3	0	0	0	5	0.53	0.91	0.28	0.45
12	1	3	1	2	0	7	0.52	1.0	0.35	0.52
13	1	2	0	0	0	3	0.76	1.04	0.3	0.9
14	0	2	2	0	0	4	1.24	1.46	0.14	1.22
15	1	2	1	0	0	4	0.7	1.31	0.5	0.68
16	1	2	1	0	0	4	0.65	1.16	0.48	0.66
17	1	2	0	0	0	3	0.77	1.02	0.23	0.81
18	1	2	2	0	0	5	0.89	1.51	0.46	1.07
19	1	2	1	0	0	4	0.76	1.25	0.43	0.74
20	1	2	0	0	0	3	0.7	0.83	0.14	0.76

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

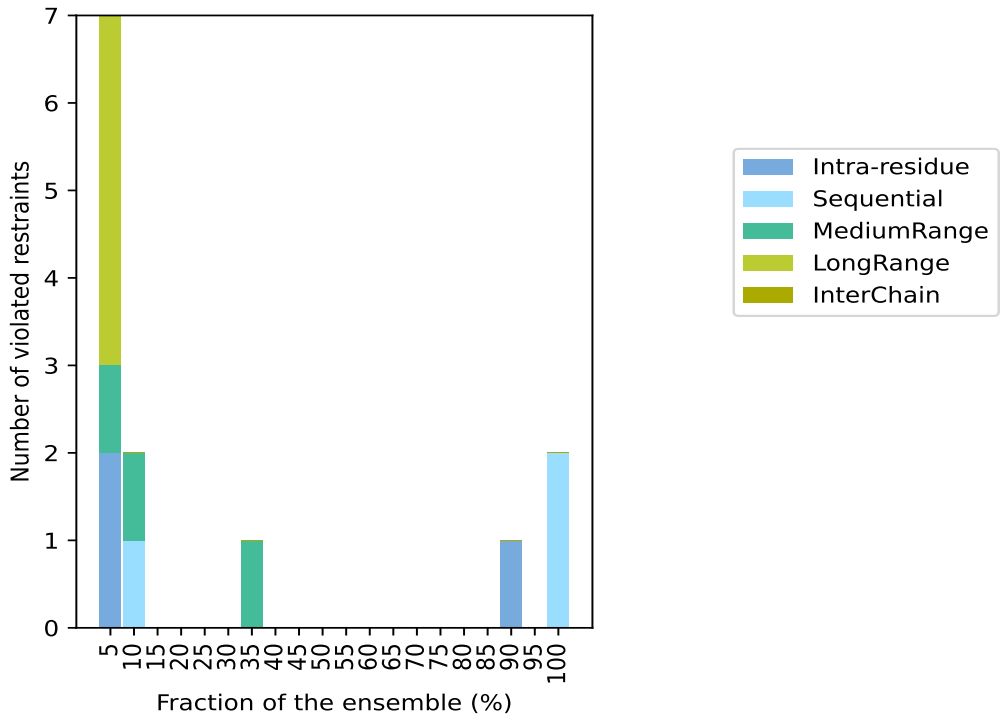
9.3 Distance violation statistics for the ensemble (i)

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, 1957(IR:548, SQ:582, MR:422, LR:405, 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]	%
2	0	1	4	0	7	1	5.0
0	1	1	0	0	2	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	1	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
1	0	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	2	0	0	0	2	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

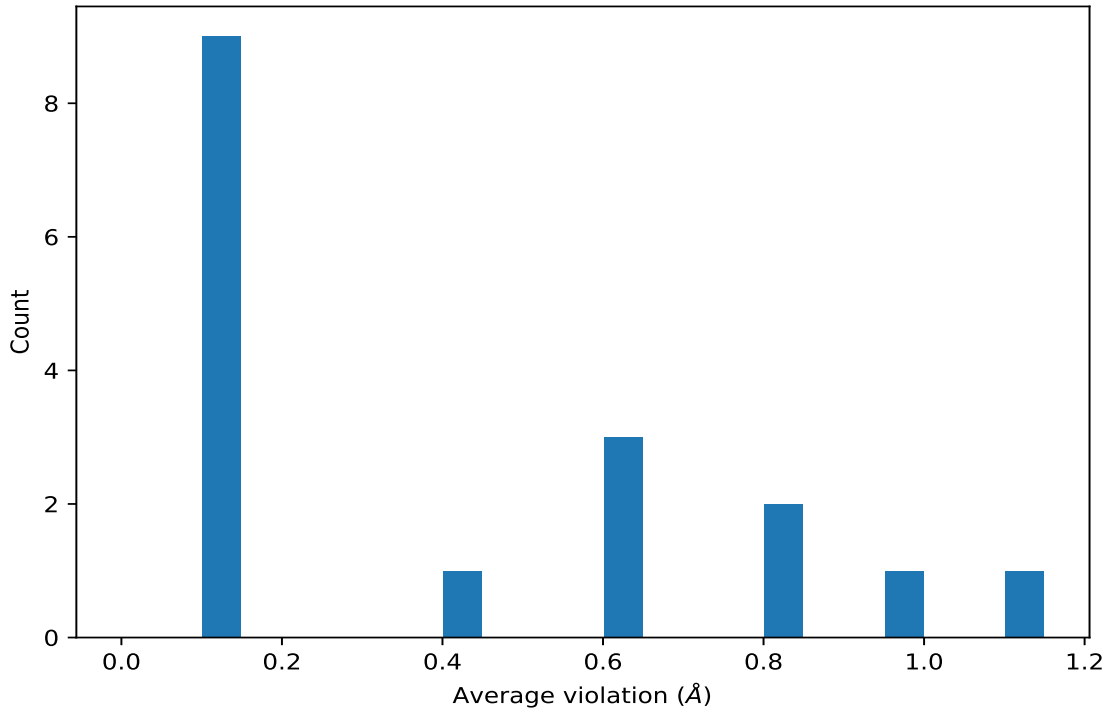
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 theviolation 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)
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	20	1.1	0.14	1.1
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	20	0.95	0.15	0.95
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	18	0.41	0.17	0.36
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	7	0.6	0.58	0.3
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	7	0.6	0.58	0.3
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	7	0.6	0.58	0.3
(1,1491)	1:763:A:SER:HB2	1:766:A:GLN:HE21	2	0.84	0.23	0.84
(1,1491)	1:763:A:SER:HB3	1:766:A:GLN:HE21	2	0.84	0.23	0.84
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB1	2	0.12	0.0	0.12
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB2	2	0.12	0.0	0.12
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB3	2	0.12	0.0	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB1	2	0.12	0.0	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB2	2	0.12	0.0	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB3	2	0.12	0.0	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB1	2	0.12	0.0	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB2	2	0.12	0.0	0.12

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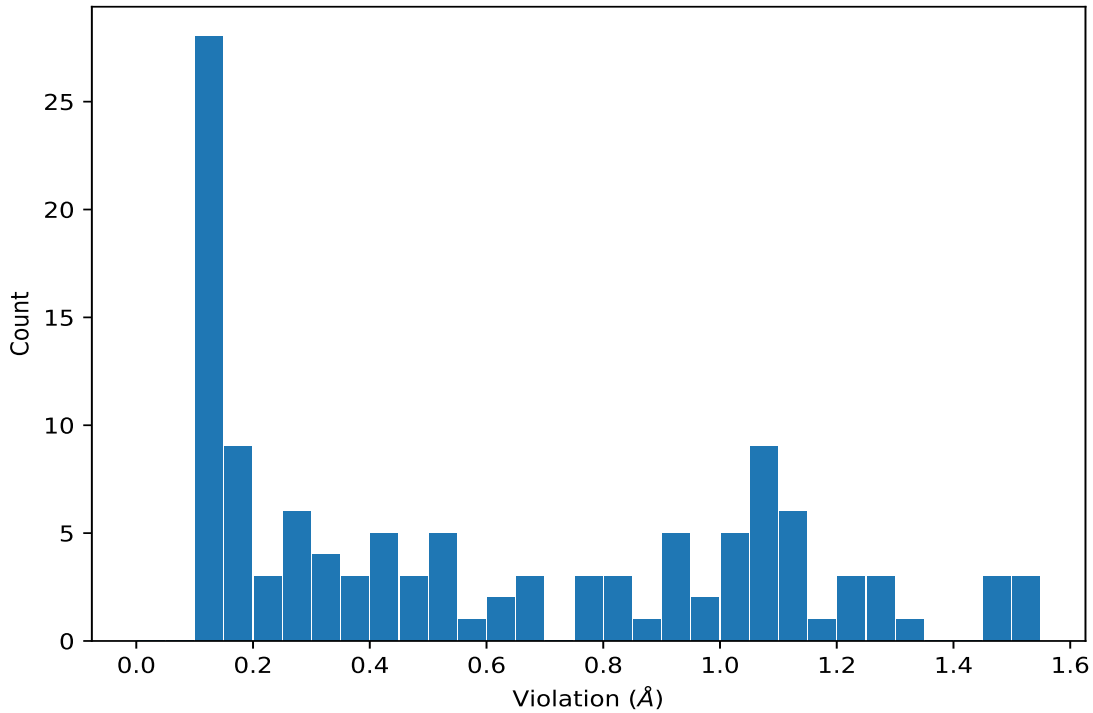
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB3	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard 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)
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	18	1.51
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	18	1.51
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	18	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	14	1.46
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	14	1.46
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	14	1.46
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	15	1.31
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	2	1.28
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	1	1.26
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	19	1.25
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	9	1.24
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	14	1.22
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	14	1.22
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	16	1.16
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	4	1.15
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	7	1.14
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	19	1.13
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	9	1.11
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	18	1.11
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	16	1.1
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	2	1.08
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	5	1.08
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	6	1.08
(1,1491)	1:763:A:SER:HB2	1:766:A:GLN:HE21	14	1.07
(1,1491)	1:763:A:SER:HB3	1:766:A:GLN:HE21	14	1.07
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	18	1.07
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	3	1.07
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	15	1.06
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	10	1.06
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	13	1.04
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	7	1.02
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	17	1.02
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	1	1.01
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	12	1.0
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	8	0.98
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	4	0.96
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	5	0.94
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	6	0.93
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	11	0.91
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	12	0.91
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	13	0.9
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	10	0.89
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	20	0.83
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	8	0.81
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	17	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	11	0.76
(1,1384)	1:766:A:GLN:HE21	1:767:A:MET:HA	20	0.76
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	12	0.75
(1,595)	1:794:A:LEU:HD21	1:799:A:TYR:HE2	8	0.65
(1,595)	1:794:A:LEU:HD22	1:799:A:TYR:HE2	8	0.65
(1,595)	1:794:A:LEU:HD23	1:799:A:TYR:HE2	8	0.65
(1,1491)	1:763:A:SER:HB2	1:766:A:GLN:HE21	18	0.62
(1,1491)	1:763:A:SER:HB3	1:766:A:GLN:HE21	18	0.62
(1,1410)	1:766:A:GLN:HE21	1:767:A:MET:H	3	0.6
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	3	0.53
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	12	0.52
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	12	0.52
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	12	0.52
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	20	0.51
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	17	0.47
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	6	0.46
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	11	0.45
(1,521)	1:794:A:LEU:HD11	1:799:A:TYR:HE2	8	0.44
(1,521)	1:794:A:LEU:HD12	1:799:A:TYR:HE2	8	0.44
(1,521)	1:794:A:LEU:HD13	1:799:A:TYR:HE2	8	0.44
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	8	0.42
(1,201)	1:906:A:TYR:HA	1:906:A:TYR:HD2	11	0.41
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	4	0.39
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	1	0.36
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	19	0.36
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	10	0.35
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	2	0.34
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	13	0.34
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	5	0.33
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	15	0.3
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	19	0.3
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	19	0.3
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	19	0.3
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	7	0.27
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	9	0.27
(1,1599)	1:791:A:LYS:HG2	1:811:A:PHE:HE2	12	0.22
(1,1599)	1:791:A:LYS:HG3	1:811:A:PHE:HE2	12	0.22
(1,1367)	1:766:A:GLN:HA	1:766:A:GLN:HE21	16	0.21
(1,1958)	1:905:A:LEU:HA	1:905:A:LEU:HD11	18	0.16
(1,1958)	1:905:A:LEU:HA	1:905:A:LEU:HD12	18	0.16
(1,1958)	1:905:A:LEU:HA	1:905:A:LEU:HD13	18	0.16
(1,1958)	1:905:A:LEU:HA	1:905:A:LEU:HD21	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1958)	1:905:A:LEU:HA	1:905:A:LEU:HD22	18	0.16
(1,1958)	1:905:A:LEU:HA	1:905:A:LEU:HD23	18	0.16
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	9	0.16
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	9	0.16
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	9	0.16
(1,591)	1:797:A:LEU:HB2	1:799:A:TYR:HE1	8	0.14
(1,591)	1:797:A:LEU:HB3	1:799:A:TYR:HE1	8	0.14
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB1	11	0.12
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB2	11	0.12
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB3	11	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB1	11	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB2	11	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB3	11	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB1	11	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB2	11	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB3	11	0.12
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB1	12	0.12
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB2	12	0.12
(1,672)	1:844:A:THR:HG21	1:845:A:ALA:HB3	12	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB1	12	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB2	12	0.12
(1,672)	1:844:A:THR:HG22	1:845:A:ALA:HB3	12	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB1	12	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB2	12	0.12
(1,672)	1:844:A:THR:HG23	1:845:A:ALA:HB3	12	0.12
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	16	0.12
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	16	0.12
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	16	0.12
(1,1842)	1:868:A:ARG:HD2	1:880:A:ILE:HA	12	0.11
(1,1842)	1:868:A:ARG:HD3	1:880:A:ILE:HA	12	0.11
(1,121)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	15	0.11
(1,121)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	15	0.11
(1,121)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	15	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found