wwPDB NMR Structure Validation Summary Report (i)

Jun 6, 2023 – 05:39 pm BST

PDB ID	:	5A4G
BMRB ID	:	25658
Title	:	NMR structure of a 180 residue construct encompassing the N-terminal metal-binding site and the membrane proximal domain of SilB from Cupriavidus metallidurans CH34
Authors	:	Bersch, B.; Urbina Fernandez, P.; Vandenbussche, G.
Deposited on	:	2015-06-09

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

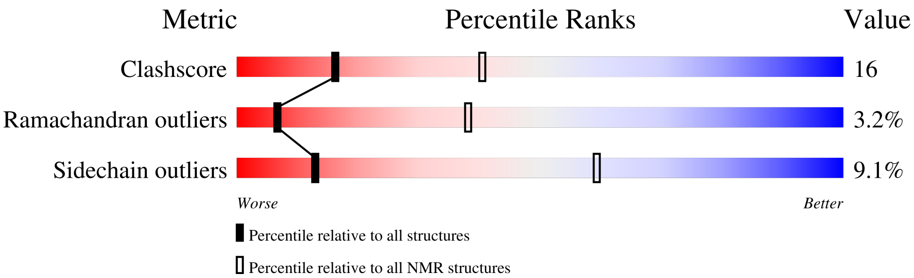
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

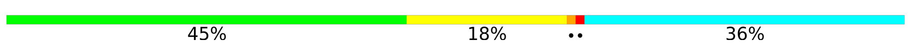
The overall completeness of chemical shifts assignment is 82%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	180	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:25-A:59 (35)	0.44	14
2	A:80-A:87, A:93-A:149 (65)	0.63	2
3	A:152-A:166 (15)	2.64	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 4 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2684 atoms, of which 1347 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SILB, SILVER EFFLUX PROTEIN, MFP COMPONENT OF THE THREE COMPONENTS PROTON ANTIPORTER METAL EFFLUX SYSTEM.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	180	2683	829	1347	240	261	6	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q58AF3
A	175	LEU	-	expression tag	UNP Q58AF3
A	176	GLU	-	expression tag	UNP Q58AF3
A	177	VAL	-	expression tag	UNP Q58AF3
A	178	LEU	-	expression tag	UNP Q58AF3
A	179	PHE	-	expression tag	UNP Q58AF3
A	180	GLN	-	expression tag	UNP Q58AF3
A	90	GLY	-	linker	UNP Q58AF3
A	91	SER	-	linker	UNP Q58AF3

- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

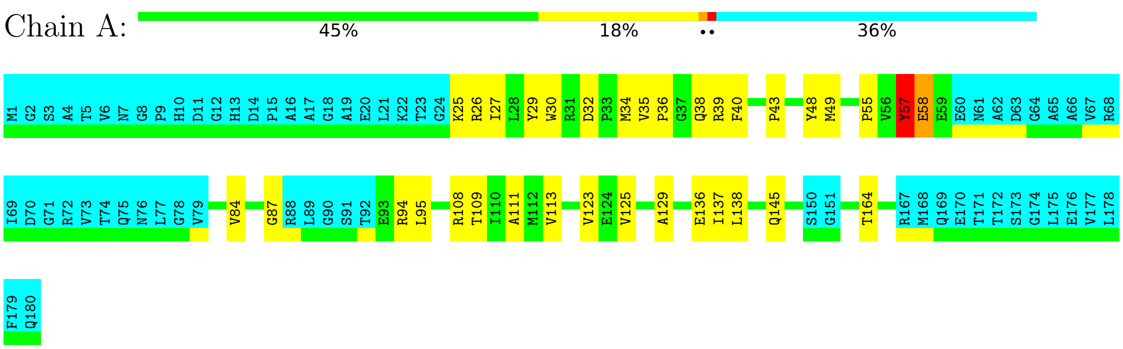
Mol	Chain	Residues	Atoms	
			Total	Ag
2	A	1	1	1

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.

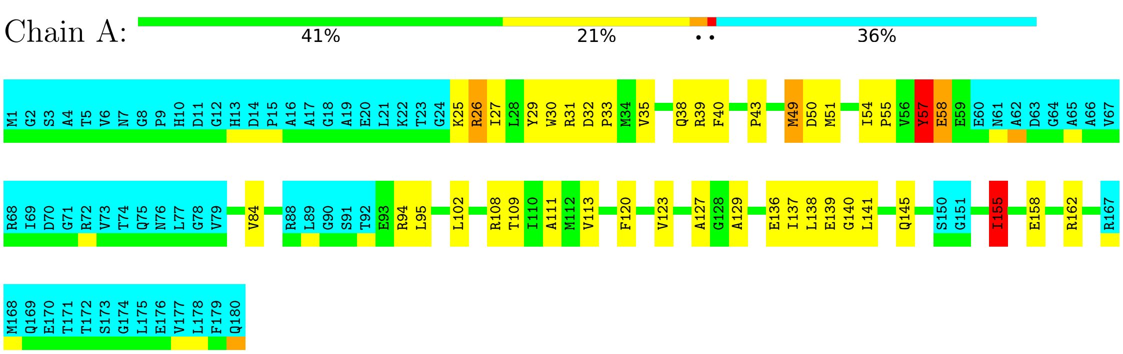
• Molecule 1: SILB, SILVER EFFLUX PROTEIN, MFP COMPONENT OF THE THREE COMPONENTS PROTON ANTIPORTER METAL EFFLUX SYSTEM



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

The representative model is number 2. Colouring as in section 4.1 above.

• Molecule 1: SILB, SILVER EFFLUX PROTEIN, MFP COMPONENT OF THE THREE COMPONENTS PROTON ANTIPORTER METAL EFFLUX SYSTEM



5 Refinement protocol and experimental data overview (i)

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

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	1.1
NMRDraw	structure solution	ANY
NMRPipe	structure solution	ANY
CcpNmr Analysis	structure solution	2.3
CcpNmr Analysis	structure solution	2.4
NMRView	structure solution	ANY
CYANA	structure solution	ANY

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	1807
Number of shifts mapped to atoms	1807
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AG

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	0.42±0.03	0±0/890 (0.0± 0.0%)	0.54±0.02	0±0/1203 (0.0± 0.0%)
All	All	0.42	2/17800 (0.0%)	0.54	0/24060 (0.0%)

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	29	TYR	CE1-CZ	-8.38	1.27	1.38	10	1
1	A	29	TYR	CE2-CZ	7.08	1.47	1.38	10	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	874	900	900	28±4
All	All	17500	18000	18000	564

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 16.

5 of 192 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASP:HB3	1:A:34:MET:SD	0.91	2.06	19	1
1:A:129:ALA:HB3	1:A:136:GLU:HB2	0.91	1.42	13	18
1:A:84:VAL:HG23	1:A:143:ALA:HA	0.88	1.42	18	1
1:A:32:ASP:HB3	1:A:35:VAL:HG22	0.80	1.53	10	16
1:A:27:ILE:HG12	1:A:58:GLU:OE2	0.76	1.80	10	11

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	115/180 (64%)	99±3 (86±2%)	13±3 (11±2%)	4±1 (3±1%)	7	38
All	All	2300/3600 (64%)	1976 (86%)	251 (11%)	73 (3%)	7	38

5 of 15 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	57	TYR	20
1	A	87	GLY	11
1	A	164	THR	9
1	A	155	ILE	6
1	A	43	PRO	5

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	91/138 (66%)	83±2 (91±2%)	8±2 (9±2%)	13	59
All	All	1820/2760 (66%)	1655 (91%)	165 (9%)	13	59

5 of 35 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	57	TYR	20
1	A	34	MET	16
1	A	58	GLU	13
1	A	125	VAL	12
1	A	25	LYS	11

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 82% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1807
Number of shifts mapped to atoms	1807
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	167	-0.04 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	145	-0.01 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	151	-0.10 ± 0.11	None needed (< 0.5 ppm)
^{15}N	157	-0.23 ± 0.42	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 82%, i.e. 1283 atoms were assigned a chemical shift out of a possible 1556. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	534/572 (93%)	223/235 (95%)	210/230 (91%)	101/107 (94%)
Sidechain	701/915 (77%)	469/598 (78%)	231/281 (82%)	1/36 (3%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	48/69 (70%)	24/33 (73%)	23/35 (66%)	1/1 (100%)
Overall	1283/1556 (82%)	716/866 (83%)	464/546 (85%)	103/144 (72%)

7.1.4 Statistically unusual chemical shifts (i)

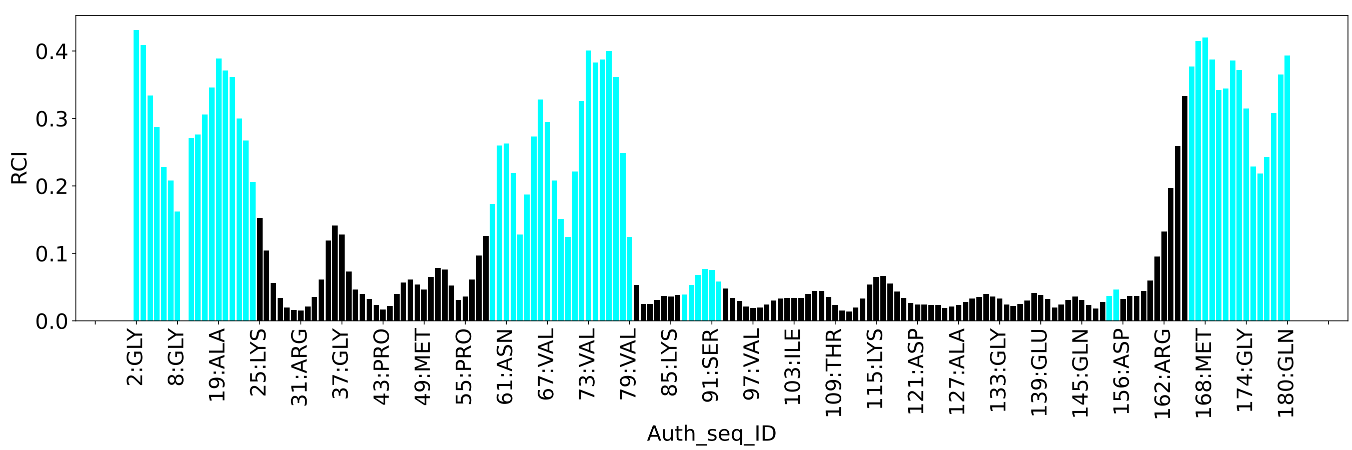
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	27	ILE	HG21	-0.79	-0.56 – 2.11	-5.8
1	A	27	ILE	HG22	-0.79	-0.56 – 2.11	-5.8
1	A	27	ILE	HG23	-0.79	-0.56 – 2.11	-5.8
1	A	39	ARG	HD2	1.85	1.97 – 4.26	-5.5

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	4633
Intra-residue (|i-j|=0)	1754
Sequential (|i-j|=1)	1306
Medium range (|i-j|>1 and |i-j|<5)	454
Long range (|i-j|≥5)	1119
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	25.7
Number of long range restraints per residue[1]	6.2

[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 ⓘ

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)	128.0	0.2
0.2-0.5 (Medium)	183.8	0.5
>0.5 (Large)	543.8	45.09

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)

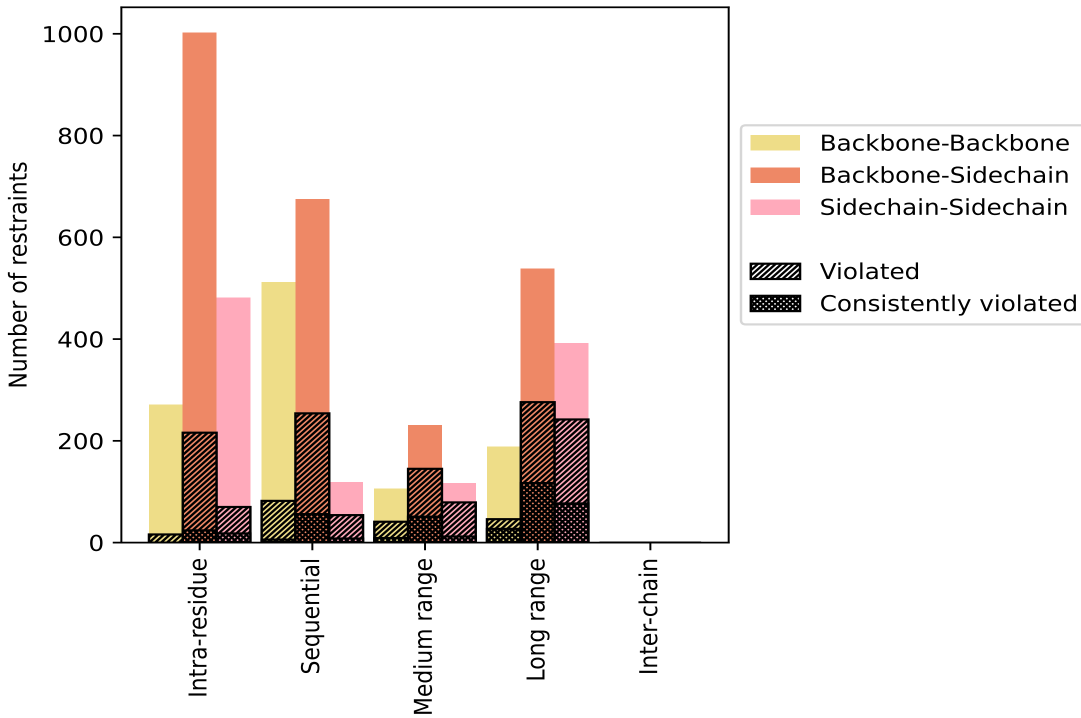
9.1 Summary of distance violations (i)

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)	1754	37.9	302	17.2	6.5	42	2.4	0.9
Backbone-Backbone	271	5.8	16	5.9	0.3	0	0.0	0.0
Backbone-Sidechain	1002	21.6	216	21.6	4.7	24	2.4	0.5
Sidechain-Sidechain	481	10.4	70	14.6	1.5	18	3.7	0.4
Sequential (|i-j|=1)	1306	28.2	390	29.9	8.4	70	5.4	1.5
Backbone-Backbone	512	11.1	82	16.0	1.8	6	1.2	0.1
Backbone-Sidechain	675	14.6	254	37.6	5.5	56	8.3	1.2
Sidechain-Sidechain	119	2.6	54	45.4	1.2	8	6.7	0.2
Medium range (|i-j|>1 & |i-j|<5)	454	9.8	265	58.4	5.7	72	15.9	1.6
Backbone-Backbone	106	2.3	41	38.7	0.9	9	8.5	0.2
Backbone-Sidechain	231	5.0	145	62.8	3.1	51	22.1	1.1
Sidechain-Sidechain	117	2.5	79	67.5	1.7	12	10.3	0.3
Long range (|i-j|≥5)	1119	24.2	564	50.4	12.2	221	19.7	4.8
Backbone-Backbone	189	4.1	46	24.3	1.0	27	14.3	0.6
Backbone-Sidechain	538	11.6	276	51.3	6.0	117	21.7	2.5
Sidechain-Sidechain	392	8.5	242	61.7	5.2	77	19.6	1.7
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	4633	100.0	1521	32.8	32.8	405	8.7	8.7
Backbone-Backbone	1078	23.3	185	17.2	4.0	42	3.9	0.9
Backbone-Sidechain	2446	52.8	891	36.4	19.2	248	10.1	5.4
Sidechain-Sidechain	1109	23.9	445	40.1	9.6	115	10.4	2.5

[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 ⓘ



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 ⓘ

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	135	198	160	370	0	863	1.95	29.85	3.36	0.75
2	145	190	157	372	0	864	1.99	30.77	3.52	0.77
3	141	191	162	367	0	861	1.95	38.02	3.43	0.78
4	138	194	160	367	0	859	2.04	29.05	3.61	0.76
5	137	205	154	368	0	864	1.97	31.26	3.58	0.71
6	151	197	162	376	0	886	1.92	38.61	3.38	0.79
7	126	193	158	355	0	832	2.05	34.14	3.59	0.83
8	135	206	164	357	0	862	2.0	29.33	3.53	0.78
9	145	207	163	355	0	870	1.88	27.12	3.03	0.77
10	141	198	156	366	0	861	1.93	30.11	3.34	0.73
11	135	190	155	349	0	829	2.05	36.46	3.76	0.74

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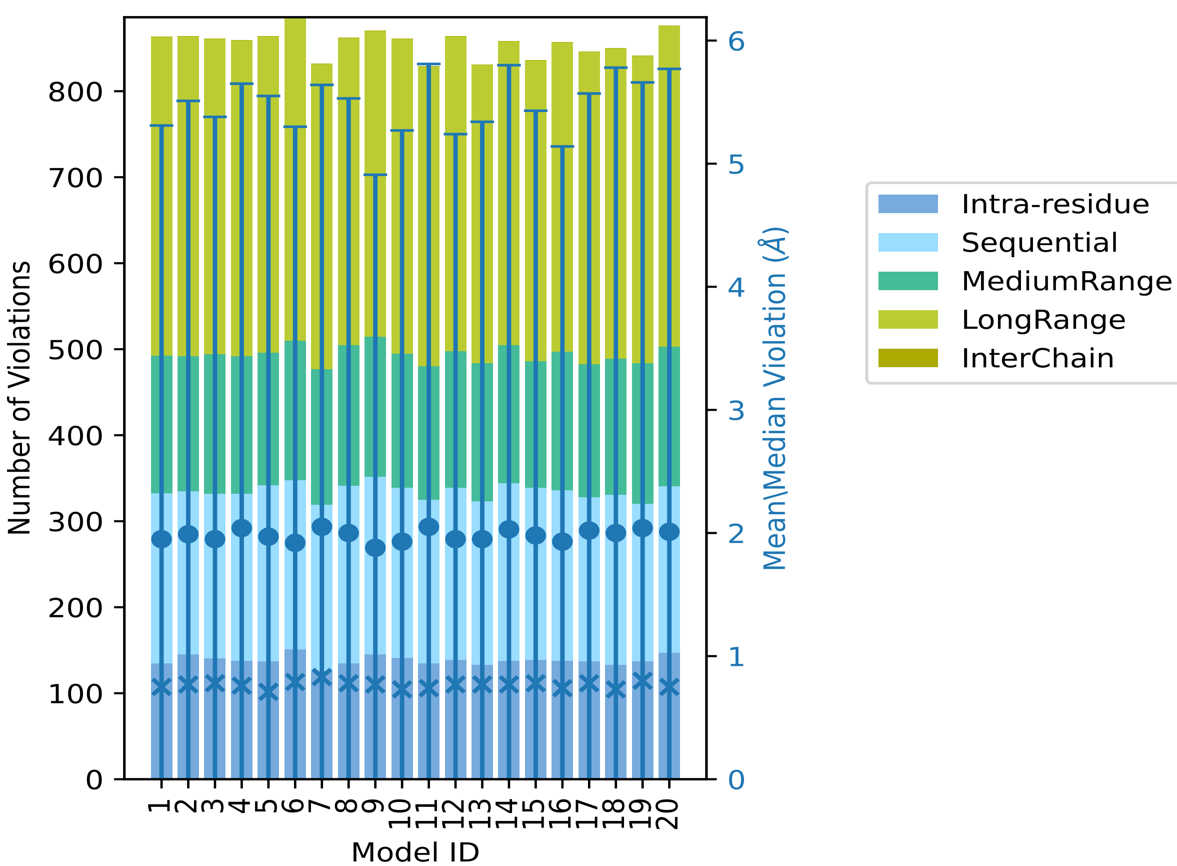
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	139	200	159	366	0	864	1.95	26.19	3.29	0.77
13	133	190	161	347	0	831	1.95	32.01	3.39	0.77
14	138	206	161	353	0	858	2.03	38.61	3.77	0.77
15	139	200	147	350	0	836	1.98	42.08	3.45	0.78
16	138	198	161	360	0	857	1.93	23.63	3.21	0.74
17	137	191	155	363	0	846	2.02	29.57	3.55	0.78
18	133	198	158	361	0	850	2.0	37.46	3.78	0.73
19	137	183	164	357	0	841	2.04	28.59	3.62	0.8
20	147	194	162	373	0	876	2.01	45.09	3.76	0.75

[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

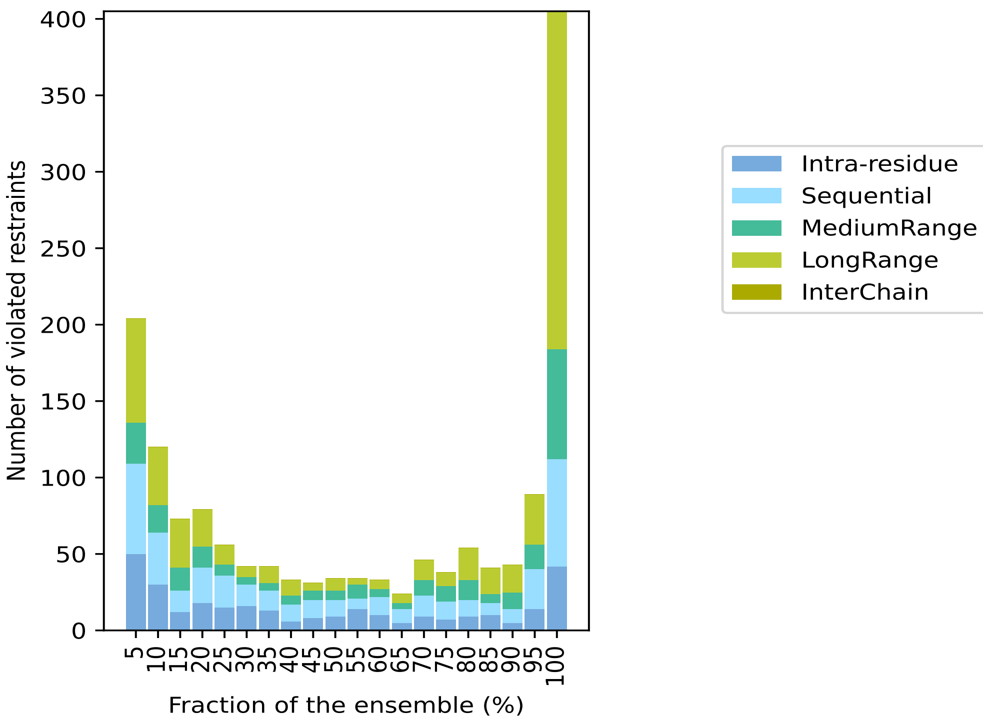
9.3 Distance violation statistics for the ensemble (i)

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, 3112(IR:1452, SQ:916, MR:189, LR:555, 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]	%
50	59	27	68	0	204	1	5.0
30	34	18	38	0	120	2	10.0
12	14	15	32	0	73	3	15.0
18	23	14	24	0	79	4	20.0
15	21	7	13	0	56	5	25.0
16	14	5	7	0	42	6	30.0
13	13	5	11	0	42	7	35.0
6	11	6	10	0	33	8	40.0
8	12	6	5	0	31	9	45.0
9	11	6	8	0	34	10	50.0
14	7	9	4	0	34	11	55.0
10	12	5	6	0	33	12	60.0
5	9	4	6	0	24	13	65.0
9	14	10	13	0	46	14	70.0
7	12	10	9	0	38	15	75.0
9	11	13	21	0	54	16	80.0
10	8	6	17	0	41	17	85.0
5	9	11	18	0	43	18	90.0
14	26	16	33	0	89	19	95.0
42	70	72	221	0	405	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

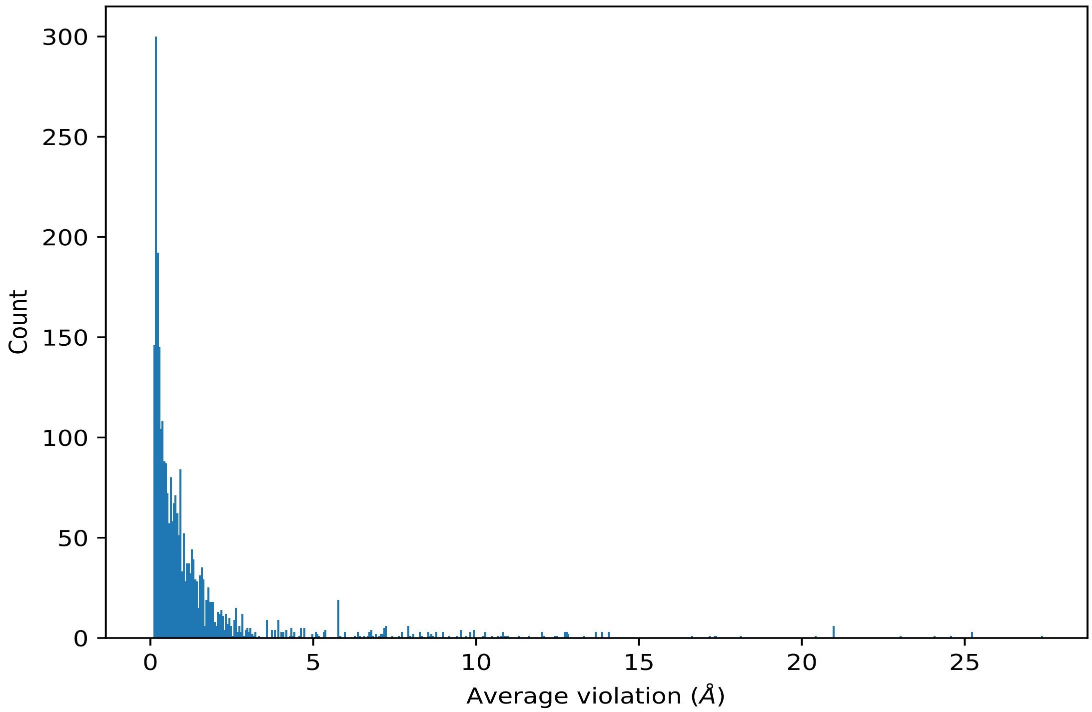
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 ⓘ

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)
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	20	27.35	10.52	27.7
(4,68)	1:A:35:VAL:HG11	1:A:81:THR:HA	20	25.21	6.75	26.19
(4,68)	1:A:35:VAL:HG12	1:A:81:THR:HA	20	25.21	6.75	26.19
(4,68)	1:A:35:VAL:HG13	1:A:81:THR:HA	20	25.21	6.75	26.19
(4,23)	1:A:87:GLY:HA3	1:A:75:GLN:H	20	24.57	3.87	25.54
(4,89)	1:A:17:ALA:HA	1:A:32:ASP:HB3	20	24.05	4.37	23.54
(4,20)	1:A:69:ILE:H	1:A:133:GLY:HA2	20	23.03	6.33	24.07
(4,95)	1:A:120:PHE:HB2	1:A:35:VAL:HG11	20	20.97	6.38	19.57
(4,95)	1:A:120:PHE:HB2	1:A:35:VAL:HG12	20	20.97	6.38	19.57
(4,95)	1:A:120:PHE:HB2	1:A:35:VAL:HG13	20	20.97	6.38	19.57
(4,95)	1:A:120:PHE:HB3	1:A:35:VAL:HG11	20	20.97	6.38	19.57
(4,95)	1:A:120:PHE:HB3	1:A:35:VAL:HG12	20	20.97	6.38	19.57
(4,95)	1:A:120:PHE:HB3	1:A:35:VAL:HG13	20	20.97	6.38	19.57
(4,21)	1:A:75:GLN:H	1:A:133:GLY:HA2	20	20.42	4.81	20.98
(4,19)	1:A:69:ILE:H	1:A:52:PRO:HD2	20	18.1	3.74	18.87
(4,22)	1:A:75:GLN:H	1:A:122:PRO:HD2	20	17.36	3.88	16.98

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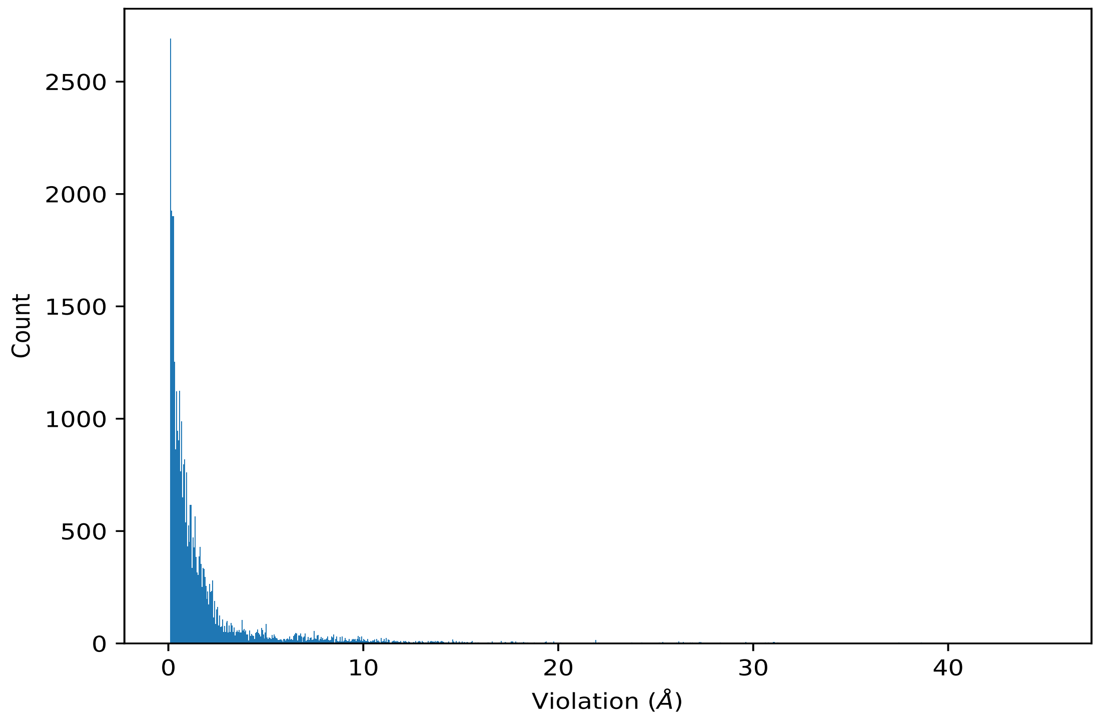
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,57)	1:A:68:ARG:HA	1:A:172:THR:HB	20	17.34	3.08	17.56

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

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)
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	20	45.09
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	15	42.08
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	6	38.61
(4,68)	1:A:35:VAL:HG11	1:A:81:THR:HA	14	38.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,68)	1:A:35:VAL:HG12	1:A:81:THR:HA	14	38.61
(4,68)	1:A:35:VAL:HG13	1:A:81:THR:HA	14	38.61
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	3	38.02
(4,68)	1:A:35:VAL:HG11	1:A:81:THR:HA	18	37.46
(4,68)	1:A:35:VAL:HG12	1:A:81:THR:HA	18	37.46
(4,68)	1:A:35:VAL:HG13	1:A:81:THR:HA	18	37.46
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	11	36.46
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	7	34.14
(4,20)	1:A:69:ILE:H	1:A:133:GLY:HA2	20	34.0
(4,88)	1:A:17:ALA:HA	1:A:98:PRO:HB3	18	33.96

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value