wwPDB NMR Structure Validation Summary Report (i)

Jun 5, 2023 – 08:16 PM EDT

PDB ID	:	2MBS
BMRB ID	:	19413
Title	:	NMR solution structure of oxidized KpDsbA
Authors	:	Kurth, F.; Rimmer, K.; Premkumar, L.; Mohanty, B.; Duprez, W.; Halili, M.A.; Shouldice, S.R.; Heras, B.; Fairlie, D.P.; Scanlon, M.J.; Martin, J.L.
Deposited on	:	2013-08-03

This is a wwPDB NMR Structure Validation Summary 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 (1)) were used in the production of this report:

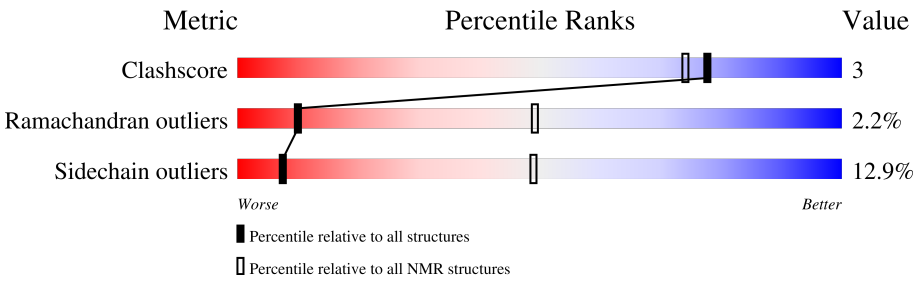
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 80%.

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	190	85% 11% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:15, A:22-A:188 (182)	0.82	9

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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2955 atoms, of which 1467 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thiol:disulfide interchange protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	190	2955	952	1467	243	286	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP B5XZJ6
A	0	ASN	-	expression tag	UNP B5XZJ6

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: Thiol:disulfide interchange protein

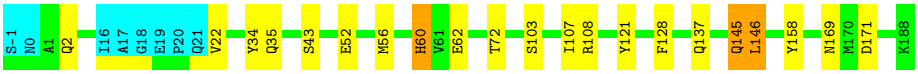
Chain A:

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

The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: Thiol:disulfide interchange protein

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *water refinement*.

Of the 40 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 solution	3.0
OPALp	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	2032
Number of shifts mapped to atoms	2032
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	0.60±0.09	0±0/1462 (0.0± 0.0%)	0.98±0.15	2±1/1982 (0.1± 0.1%)
All	All	0.61	0/29240 (0.0%)	0.99	34/39640 (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	1.9±1.1
All	All	0	37

There are no bond-length outliers.

5 of 19 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	154	VAL	CA-CB-CG1	14.40	132.49	110.90	14	1
1	A	28	PHE	CB-CG-CD2	-7.31	115.69	120.80	16	7
1	A	25	PHE	CB-CG-CD1	-7.06	115.86	120.80	3	1
1	A	28	PHE	CB-CG-CD1	6.50	125.35	120.80	11	4
1	A	108	ARG	NE-CZ-NH2	-6.39	117.11	120.30	2	1

There are no chirality outliers.

5 of 12 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	34	TYR	Sidechain	15
1	A	29	TYR	Sidechain	6
1	A	153	TYR	Sidechain	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	121	TYR	Sidechain	2
1	A	25	PHE	Sidechain	2

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	1432	1416	1416	8±8
All	All	28640	28320	28320	167

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 3.

5 of 109 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PHE:CD1	1:A:71:LEU:HD11	0.76	2.16	4	6
1:A:25:PHE:CE1	1:A:149:VAL:HG13	0.75	2.17	3	1
1:A:28:PHE:CD2	1:A:95:VAL:HG21	0.75	2.16	4	6
1:A:28:PHE:CZ	1:A:71:LEU:HD21	0.74	2.16	11	4
1:A:60:HIS:CE1	1:A:72:THR:HG22	0.74	2.17	7	6

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	181/190 (95%)	154±4 (85±2%)	23±3 (13±2%)	4±2 (2±1%)	10	49
All	All	3620/3800 (95%)	3081 (85%)	458 (13%)	81 (2%)	10	49

5 of 24 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	55	LYS	12
1	A	144	LEU	10
1	A	143	ASP	9
1	A	22	VAL	9
1	A	53	GLY	8

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	154/160 (96%)	134±4 (87±3%)	20±4 (13±3%)	7 49
All	All	3080/3200 (96%)	2683 (87%)	397 (13%)	7 49

5 of 79 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	145	GLN	19
1	A	169	ASN	18
1	A	62	GLU	16
1	A	103	SER	16
1	A	171	ASP	15

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)

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 80% for the well-defined parts and 79% 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 (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	2032
Number of shifts mapped to atoms	2032
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	LEU	HD11	0.980	0.020	.
1	A	133	LEU	HD12	0.980	0.020	.
1	A	133	LEU	HD13	0.980	0.020	.
1	A	184	LEU	HD11	-1.059	0.020	.
1	A	184	LEU	HD12	-1.059	0.020	.
1	A	184	LEU	HD13	-1.059	0.020	.
1	A	40	LEU	HD11	0.804	0.020	.
1	A	40	LEU	HD12	0.804	0.020	.
1	A	40	LEU	HD13	0.804	0.020	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	185	-0.32 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	175	0.21 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	169	-0.06 ± 0.30	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 80%, i.e. 1981 atoms were assigned a chemical shift out of a possible 2463. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	706/906 (78%)	358/367 (98%)	180/364 (49%)	168/175 (96%)
Sidechain	1165/1350 (86%)	796/879 (91%)	355/428 (83%)	14/43 (33%)
Aromatic	110/207 (53%)	61/101 (60%)	47/101 (47%)	2/5 (40%)
Overall	1981/2463 (80%)	1215/1347 (90%)	582/893 (65%)	184/223 (83%)

7.1.4 Statistically unusual chemical shifts (i)

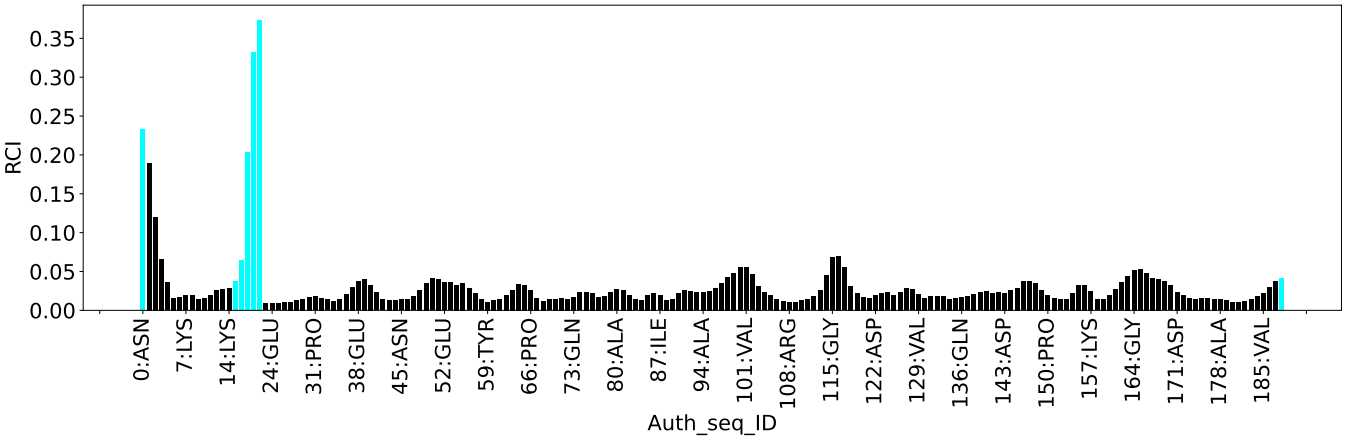
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	73	GLN	HG2	0.43	1.01 – 3.62	-7.2
1	A	16	ILE	CG2	26.89	10.93 – 24.12	7.1
1	A	184	LEU	HD21	-1.06	-0.65 – 2.13	-6.5
1	A	184	LEU	HD22	-1.06	-0.65 – 2.13	-6.5
1	A	184	LEU	HD23	-1.06	-0.65 – 2.13	-6.5
1	A	16	ILE	CG1	17.50	19.24 – 36.26	-6.0

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:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0:ASN
7:LYS
14:LYS
24:GLU
31:PRO
38:GLU
45:ASN
52:GLU
59:TYR
66:PRO
73:GLN
80:ALA
87:ILE
94:ALA
101:VAL
108:ARG
115:GLY
122:ASP
129:VAL
136:GLN
143:ASP
150:PRO
157:LYS
164:GLY
171:ASP
178:ALA
185:VAL
Auth_seq_ID

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	3531
Intra-residue (|i-j|=0)	733
Sequential (|i-j|=1)	991
Medium range (|i-j|>1 and |i-j|<5)	901
Long range (|i-j|≥5)	906
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	18.6
Number of long range restraints per residue[1]	4.8

[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)	90.8	0.2
0.2-0.5 (Medium)	147.9	0.5
>0.5 (Large)	287.4	5.36

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)

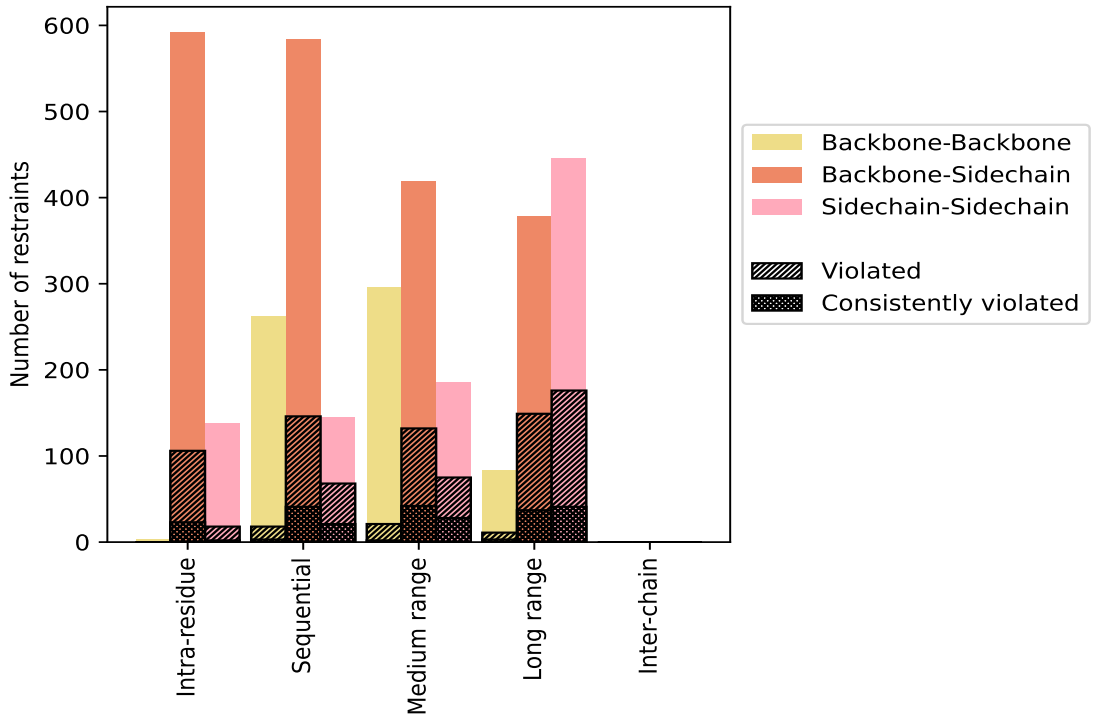
9.1 Summary of distance violations (i)

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)	733	20.8	124	16.9	3.5	25	3.4	0.7
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	592	16.8	106	17.9	3.0	23	3.9	0.7
Sidechain-Sidechain	138	3.9	18	13.0	0.5	2	1.4	0.1
Sequential (|i-j|=1)	991	28.1	232	23.4	6.6	65	6.6	1.8
Backbone-Backbone	262	7.4	18	6.9	0.5	3	1.1	0.1
Backbone-Sidechain	584	16.5	146	25.0	4.1	41	7.0	1.2
Sidechain-Sidechain	145	4.1	68	46.9	1.9	21	14.5	0.6
Medium range (|i-j|>1 & |i-j|<5)	901	25.5	228	25.3	6.5	72	8.0	2.0
Backbone-Backbone	296	8.4	21	7.1	0.6	2	0.7	0.1
Backbone-Sidechain	419	11.9	132	31.5	3.7	42	10.0	1.2
Sidechain-Sidechain	186	5.3	75	40.3	2.1	28	15.1	0.8
Long range (|i-j|≥5)	906	25.7	336	37.1	9.5	81	8.9	2.3
Backbone-Backbone	83	2.4	11	13.3	0.3	3	3.6	0.1
Backbone-Sidechain	378	10.7	149	39.4	4.2	37	9.8	1.0
Sidechain-Sidechain	445	12.6	176	39.6	5.0	41	9.2	1.2
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	3531	100.0	920	26.1	26.1	243	6.9	6.9
Backbone-Backbone	644	18.2	50	7.8	1.4	8	1.2	0.2
Backbone-Sidechain	1973	55.9	533	27.0	15.1	143	7.2	4.0
Sidechain-Sidechain	914	25.9	337	36.9	9.5	92	10.1	2.6

[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	71	141	133	192	0	537	0.76	4.81	0.68	0.54
2	76	133	130	183	0	522	0.77	4.79	0.67	0.56
3	73	137	140	185	0	535	0.73	4.31	0.61	0.56
4	70	133	140	174	0	517	0.75	4.89	0.66	0.56
5	66	143	143	191	0	543	0.76	4.55	0.65	0.53
6	70	134	134	182	0	520	0.76	4.31	0.66	0.59
7	65	122	134	183	0	504	0.78	5.12	0.67	0.57
8	74	142	131	175	0	522	0.78	4.92	0.69	0.56
9	72	143	140	181	0	536	0.78	5.36	0.71	0.58
10	64	146	138	193	0	541	0.74	3.65	0.64	0.54
11	64	133	129	180	0	506	0.77	5.36	0.7	0.56

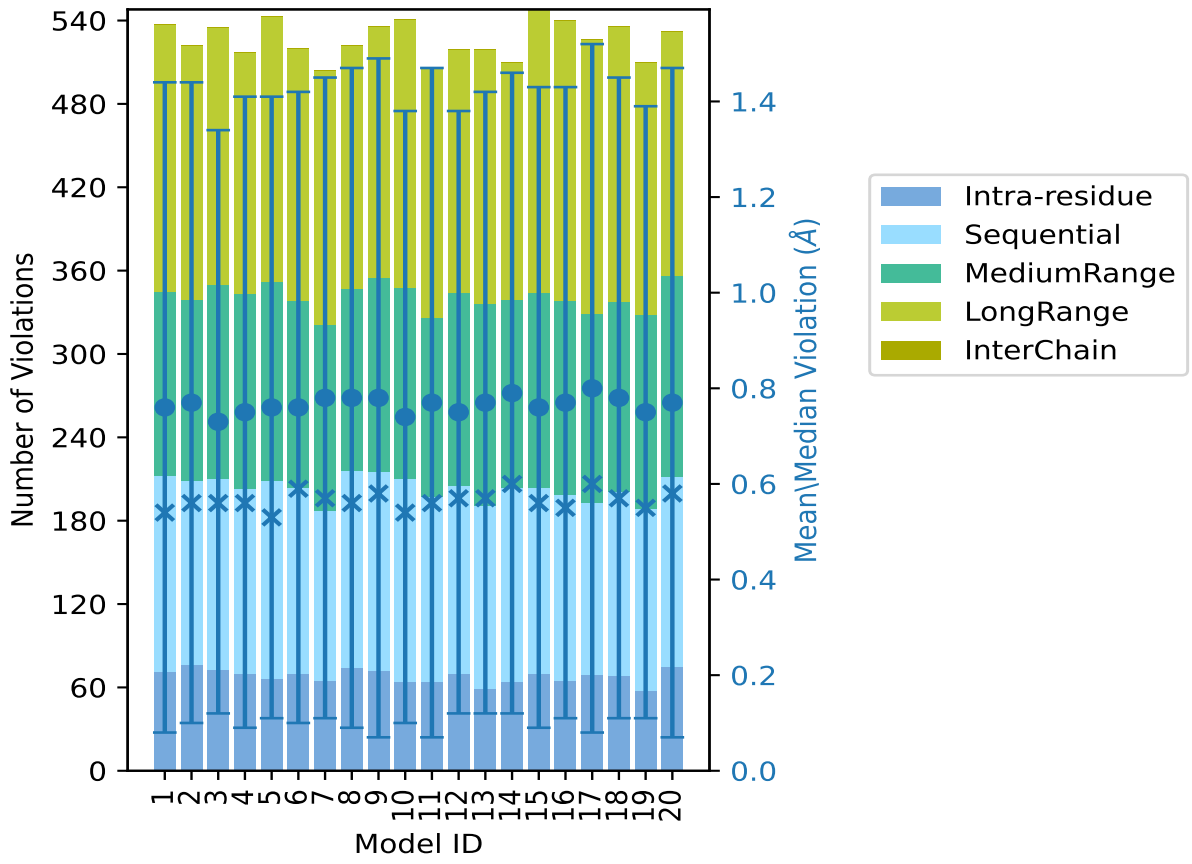
Continued on next page...

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				
12	70	135	139	175	0	519	0.75	4.44	0.63	0.57
13	59	132	145	183	0	519	0.77	4.42	0.65	0.57
14	64	140	135	171	0	510	0.79	4.67	0.67	0.6
15	70	134	140	204	0	548	0.76	5.18	0.67	0.56
16	65	134	139	202	0	540	0.77	3.77	0.66	0.55
17	69	124	136	197	0	526	0.8	5.14	0.72	0.6
18	68	133	137	198	0	536	0.78	4.31	0.67	0.57
19	58	131	139	182	0	510	0.75	4.01	0.64	0.55
20	75	137	144	176	0	532	0.77	4.34	0.7	0.58

[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

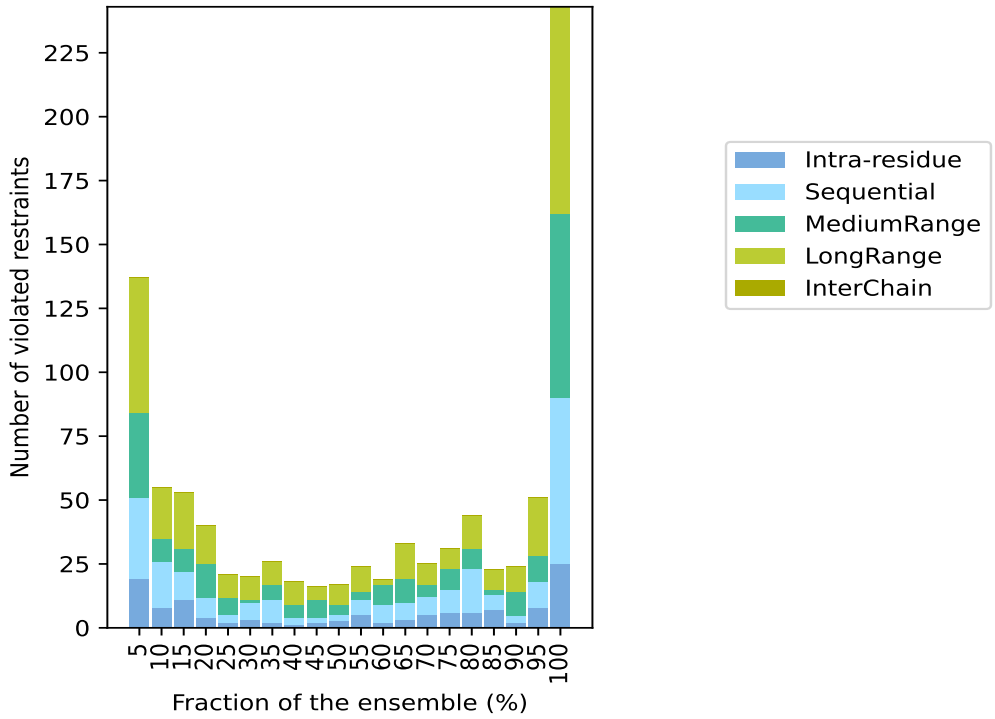
9.3 Distance violation statistics for the ensemble (i)

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, 2611(IR:609, SQ:759, MR:673, LR:570, 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]	%
19	32	33	53	0	137	1	5.0
8	18	9	20	0	55	2	10.0
11	11	9	22	0	53	3	15.0
4	8	13	15	0	40	4	20.0
2	3	7	9	0	21	5	25.0
3	7	1	9	0	20	6	30.0
2	9	6	9	0	26	7	35.0
1	3	5	9	0	18	8	40.0
2	2	7	5	0	16	9	45.0
3	2	4	8	0	17	10	50.0
5	6	3	10	0	24	11	55.0
2	7	8	2	0	19	12	60.0
3	7	9	14	0	33	13	65.0
5	7	5	8	0	25	14	70.0
6	9	8	8	0	31	15	75.0
6	17	8	13	0	44	16	80.0
7	6	2	8	0	23	17	85.0
2	3	9	10	0	24	18	90.0
8	10	10	23	0	51	19	95.0
25	65	72	81	0	243	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

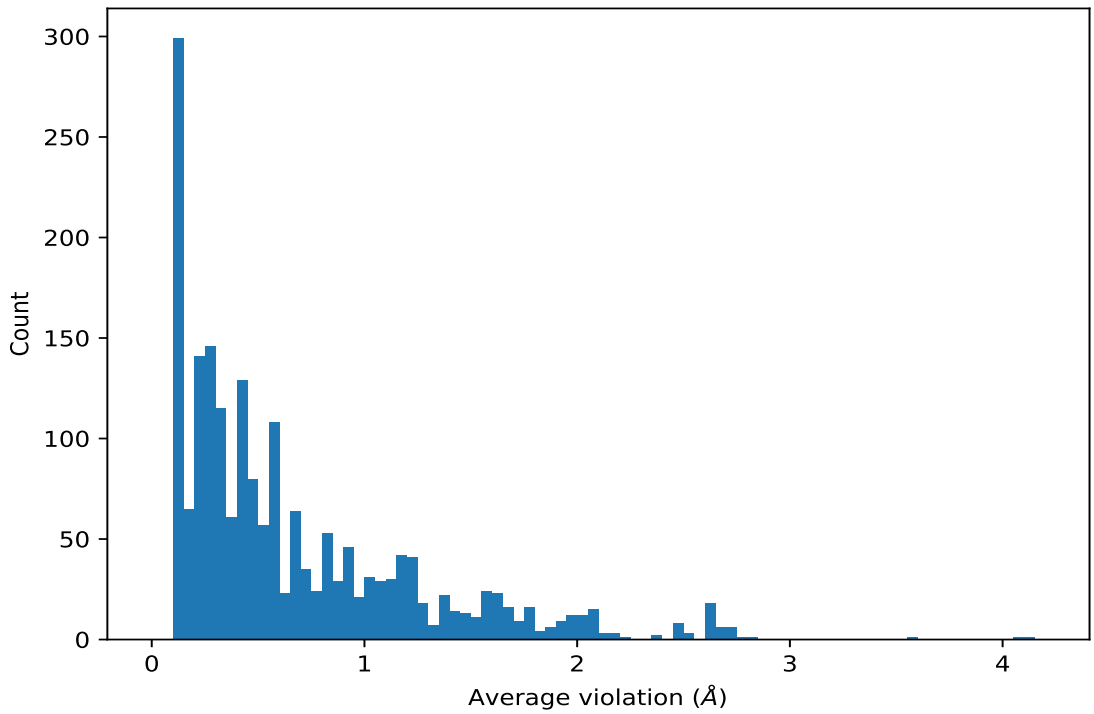
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 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)
(1,3293)	1:A:16:ILE:HB	1:A:156:GLY:HA2	20	4.14	0.97	4.35
(1,1772)	1:A:11:THR:HB	1:A:157:LYS:HG2	20	4.06	0.6	4.11
(1,1509)	1:A:16:ILE:HB	1:A:156:GLY:HA3	20	3.58	1.11	3.76
(1,2370)	1:A:12:LEU:H	1:A:157:LYS:HG2	20	2.83	0.36	2.84
(1,2019)	1:A:86:LYS:HD2	1:A:115:GLY:H	20	2.77	0.84	2.64
(1,3073)	1:A:43:SER:HB2	1:A:56:MET:HE1	20	2.7	1.27	2.77
(1,3073)	1:A:43:SER:HB2	1:A:56:MET:HE2	20	2.7	1.27	2.77
(1,3073)	1:A:43:SER:HB2	1:A:56:MET:HE3	20	2.7	1.27	2.77
(1,3073)	1:A:43:SER:HB3	1:A:56:MET:HE1	20	2.7	1.27	2.77
(1,3073)	1:A:43:SER:HB3	1:A:56:MET:HE2	20	2.7	1.27	2.77
(1,3073)	1:A:43:SER:HB3	1:A:56:MET:HE3	20	2.7	1.27	2.77
(1,3294)	1:A:16:ILE:HG21	1:A:156:GLY:HA2	20	2.68	0.72	2.65
(1,3294)	1:A:16:ILE:HG22	1:A:156:GLY:HA2	20	2.68	0.72	2.65
(1,3294)	1:A:16:ILE:HG23	1:A:156:GLY:HA2	20	2.68	0.72	2.65
(1,2473)	1:A:42:VAL:HG21	1:A:46:VAL:HG11	20	2.64	0.17	2.7
(1,2473)	1:A:42:VAL:HG21	1:A:46:VAL:HG12	20	2.64	0.17	2.7

Continued on next page...

Continued from previous page...

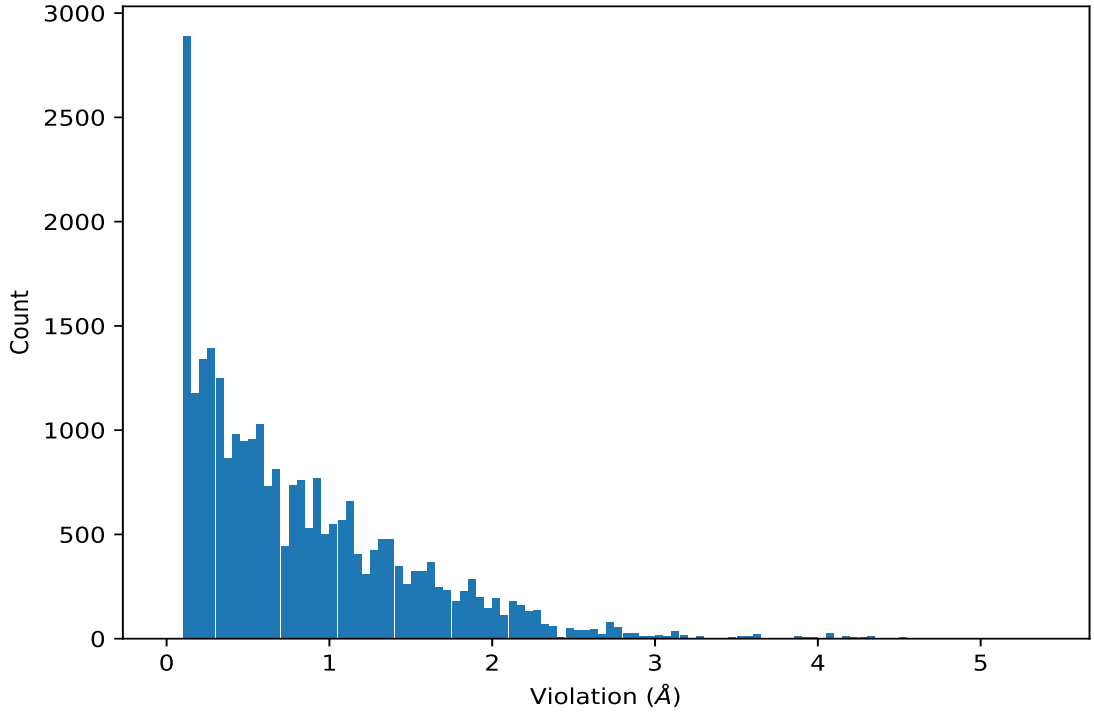
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2473)	1:A:42:VAL:HG21	1:A:46:VAL:HG13	20	2.64	0.17	2.7
(1,2473)	1:A:42:VAL:HG22	1:A:46:VAL:HG11	20	2.64	0.17	2.7
(1,2473)	1:A:42:VAL:HG22	1:A:46:VAL:HG12	20	2.64	0.17	2.7
(1,2473)	1:A:42:VAL:HG22	1:A:46:VAL:HG13	20	2.64	0.17	2.7
(1,2473)	1:A:42:VAL:HG23	1:A:46:VAL:HG11	20	2.64	0.17	2.7
(1,2473)	1:A:42:VAL:HG23	1:A:46:VAL:HG12	20	2.64	0.17	2.7
(1,2473)	1:A:42:VAL:HG23	1:A:46:VAL:HG13	20	2.64	0.17	2.7
(1,3078)	1:A:46:VAL:HG21	1:A:56:MET:HE1	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG21	1:A:56:MET:HE2	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG21	1:A:56:MET:HE3	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG22	1:A:56:MET:HE1	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG22	1:A:56:MET:HE2	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG22	1:A:56:MET:HE3	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG23	1:A:56:MET:HE1	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG23	1:A:56:MET:HE2	20	2.62	0.9	2.54
(1,3078)	1:A:46:VAL:HG23	1:A:56:MET:HE3	20	2.62	0.9	2.54
(1,1782)	1:A:46:VAL:HG21	1:A:56:MET:HG3	20	2.52	1.07	2.55

[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 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)
(1,3293)	1:A:16:ILE:HB	1:A:156:GLY:HA2	9	5.36
(1,3293)	1:A:16:ILE:HB	1:A:156:GLY:HA2	11	5.36
(1,3293)	1:A:16:ILE:HB	1:A:156:GLY:HA2	15	5.18
(1,3293)	1:A:16:ILE:HB	1:A:156:GLY:HA2	17	5.14
(1,3293)	1:A:16:ILE:HB	1:A:156:GLY:HA2	7	5.12
(1,1509)	1:A:16:ILE:HB	1:A:156:GLY:HA3	11	5.07
(1,1772)	1:A:11:THR:HB	1:A:157:LYS:HG2	15	5.02
(1,1772)	1:A:11:THR:HB	1:A:157:LYS:HG2	8	4.92
(1,1772)	1:A:11:THR:HB	1:A:157:LYS:HG2	4	4.89
(1,3293)	1:A:16:ILE:HB	1:A:156:GLY:HA2	1	4.81

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found