wwPDB NMR Structure Validation Summary Report

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Authors	:	Moretto, L.; Heylen, R.; Holroyd, N.; Vance, S.; Broadhurst, R.W.
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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:

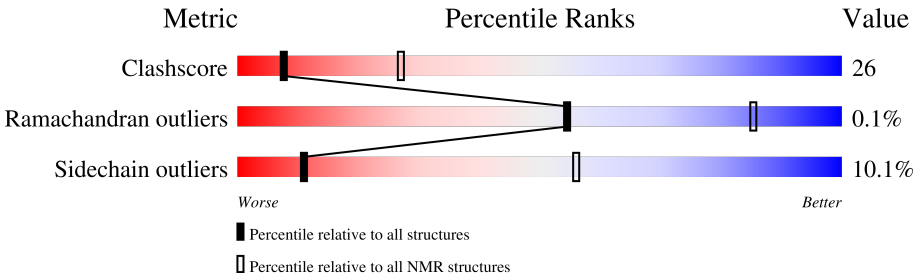
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 92%.

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	100	46% 45% · 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:6-A:100 (95)	0.17	4

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

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

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

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1501 atoms, of which 754 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Type I modular polyketide synthase.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	100	1501	467	754	127	153	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q6MZA4

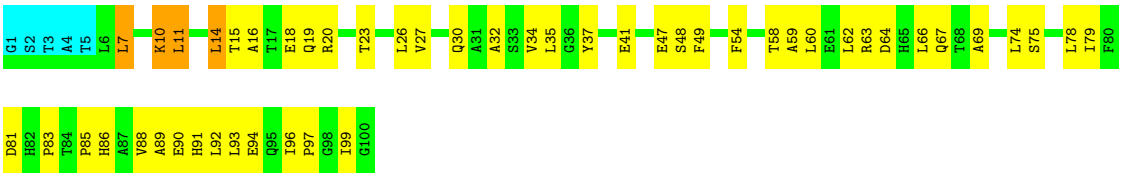
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Type I modular polyketide synthase

Chain A:

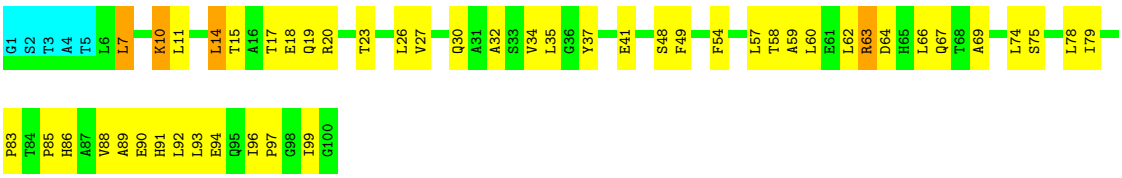


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: Type I modular polyketide synthase

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
ARIA	structure calculation	

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	1182
Number of shifts mapped to atoms	1182
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality

6.1 Standard geometry

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	0.50±0.05	1±1/729 (0.1± 0.1%)	0.61±0.01	0±0/991 (0.0± 0.0%)
All	All	0.50	13/14580 (0.1%)	0.61	0/19820 (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	37	TYR	CE1-CZ	-6.74	1.29	1.38	19	7
1	A	37	TYR	CE2-CZ	6.61	1.47	1.38	19	6

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	718	725	720	37±3
All	All	14360	14500	14400	736

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 26.

5 of 81 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:THR:O	1:A:27:VAL:HG12	0.79	1.78	11	20
1:A:49:PHE:CD2	1:A:79:ILE:HB	0.77	2.15	12	20
1:A:74:LEU:HD21	1:A:92:LEU:HD11	0.74	1.60	5	19
1:A:16:ALA:O	1:A:20:ARG:HG3	0.66	1.89	5	14
1:A:92:LEU:O	1:A:96:ILE:HG12	0.66	1.90	11	20

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	94/100 (94%)	85±1 (91±1%)	9±1 (9±1%)	0±0 (0±0%)	54	85
All	All	1880/2000 (94%)	1705 (91%)	173 (9%)	2 (0%)	54	85

All 2 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	41	GLU	1
1	A	99	ILE	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	79/82 (96%)	71±1 (90±1%)	8±1 (10±1%)	11	56
All	All	1580/1640 (96%)	1421 (90%)	159 (10%)	11	56

5 of 16 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	7	LEU	20
1	A	10	LYS	20
1	A	14	LEU	20
1	A	35	LEU	20
1	A	99	ILE	18

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *mH0ACPa_180709b.csdep*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1182
Number of shifts mapped to atoms	1182
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	99	-0.37 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	92	0.37 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	92	-0.43 ± 0.13	None needed (< 0.5 ppm)
^{15}N	93	0.12 ± 0.25	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1151 atoms were assigned a chemical shift out of a possible 1257. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	467/475 (98%)	191/193 (99%)	185/190 (97%)	91/92 (99%)
Sidechain	626/703 (89%)	419/464 (90%)	199/222 (90%)	8/17 (47%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	58/79 (73%)	29/39 (74%)	29/30 (97%)	0/10 (0%)
Overall	1151/1257 (92%)	639/696 (92%)	413/442 (93%)	99/119 (83%)

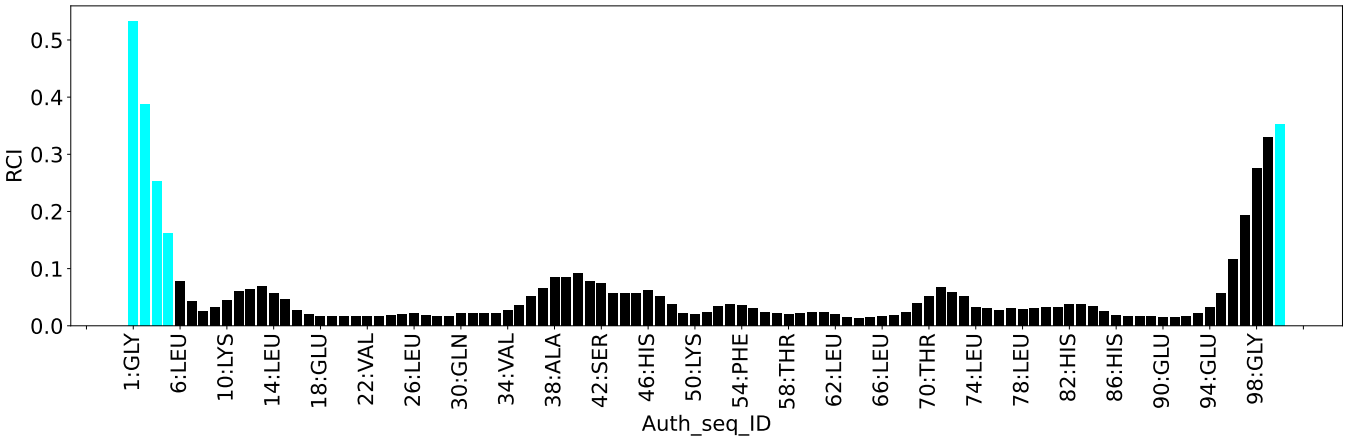
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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	3700
Intra-residue (|i-j|=0)	1087
Sequential (|i-j|=1)	938
Medium range (|i-j|>1 and |i-j|<5)	990
Long range (|i-j|≥5)	685
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	37.0
Number of long range restraints per residue[1]	6.8

[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

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)	169.8	0.2
0.2-0.5 (Medium)	352.9	0.5
>0.5 (Large)	399.0	3.28

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)

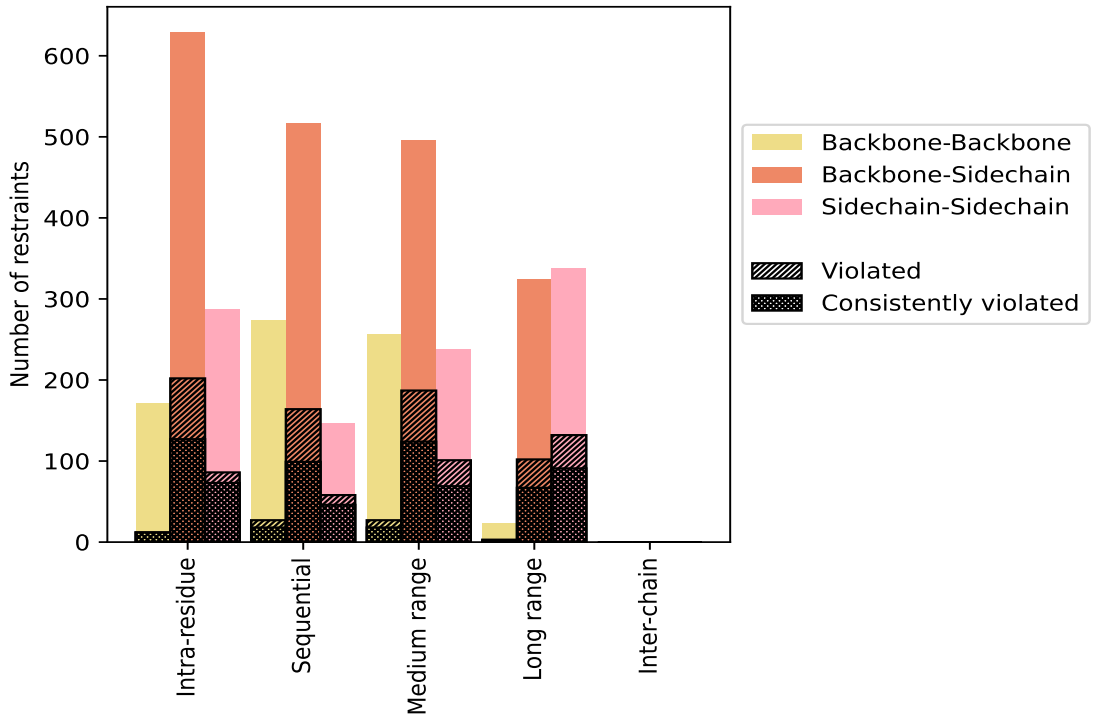
9.1 Summary of distance violations (i)

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)	1087	29.4	300	27.6	8.1	212	19.5	5.7
Backbone-Backbone	171	4.6	12	7.0	0.3	12	7.0	0.3
Backbone-Sidechain	629	17.0	202	32.1	5.5	127	20.2	3.4
Sidechain-Sidechain	287	7.8	86	30.0	2.3	73	25.4	2.0
Sequential (|i-j|=1)	938	25.4	249	26.5	6.7	163	17.4	4.4
Backbone-Backbone	274	7.4	27	9.9	0.7	18	6.6	0.5
Backbone-Sidechain	517	14.0	164	31.7	4.4	99	19.1	2.7
Sidechain-Sidechain	147	4.0	58	39.5	1.6	46	31.3	1.2
Medium range (|i-j|>1 & |i-j|<5)	990	26.8	315	31.8	8.5	211	21.3	5.7
Backbone-Backbone	256	6.9	27	10.5	0.7	18	7.0	0.5
Backbone-Sidechain	496	13.4	187	37.7	5.1	124	25.0	3.4
Sidechain-Sidechain	238	6.4	101	42.4	2.7	69	29.0	1.9
Long range (|i-j|≥5)	685	18.5	237	34.6	6.4	160	23.4	4.3
Backbone-Backbone	23	0.6	3	13.0	0.1	2	8.7	0.1
Backbone-Sidechain	324	8.8	102	31.5	2.8	67	20.7	1.8
Sidechain-Sidechain	338	9.1	132	39.1	3.6	91	26.9	2.5
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	3700	100.0	1101	29.8	29.8	746	20.2	20.2
Backbone-Backbone	724	19.6	69	9.5	1.9	50	6.9	1.4
Backbone-Sidechain	1966	53.1	655	33.3	17.7	417	21.2	11.3
Sidechain-Sidechain	1010	27.3	377	37.3	10.2	279	27.6	7.5

[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	252	199	266	202	0	919	0.57	2.9	0.45	0.44
2	248	202	264	202	0	916	0.57	2.93	0.45	0.44
3	252	198	266	201	0	917	0.58	2.89	0.44	0.44
4	260	201	261	206	0	928	0.57	3.28	0.45	0.45
5	252	198	266	200	0	916	0.57	2.87	0.44	0.44
6	251	198	263	197	0	909	0.58	2.88	0.44	0.45
7	253	197	265	203	0	918	0.57	2.88	0.45	0.44
8	259	204	266	205	0	934	0.57	2.91	0.44	0.44
9	254	202	264	201	0	921	0.57	2.92	0.44	0.44
10	261	198	260	196	0	915	0.57	2.91	0.44	0.44
11	259	195	265	201	0	920	0.57	2.84	0.44	0.44

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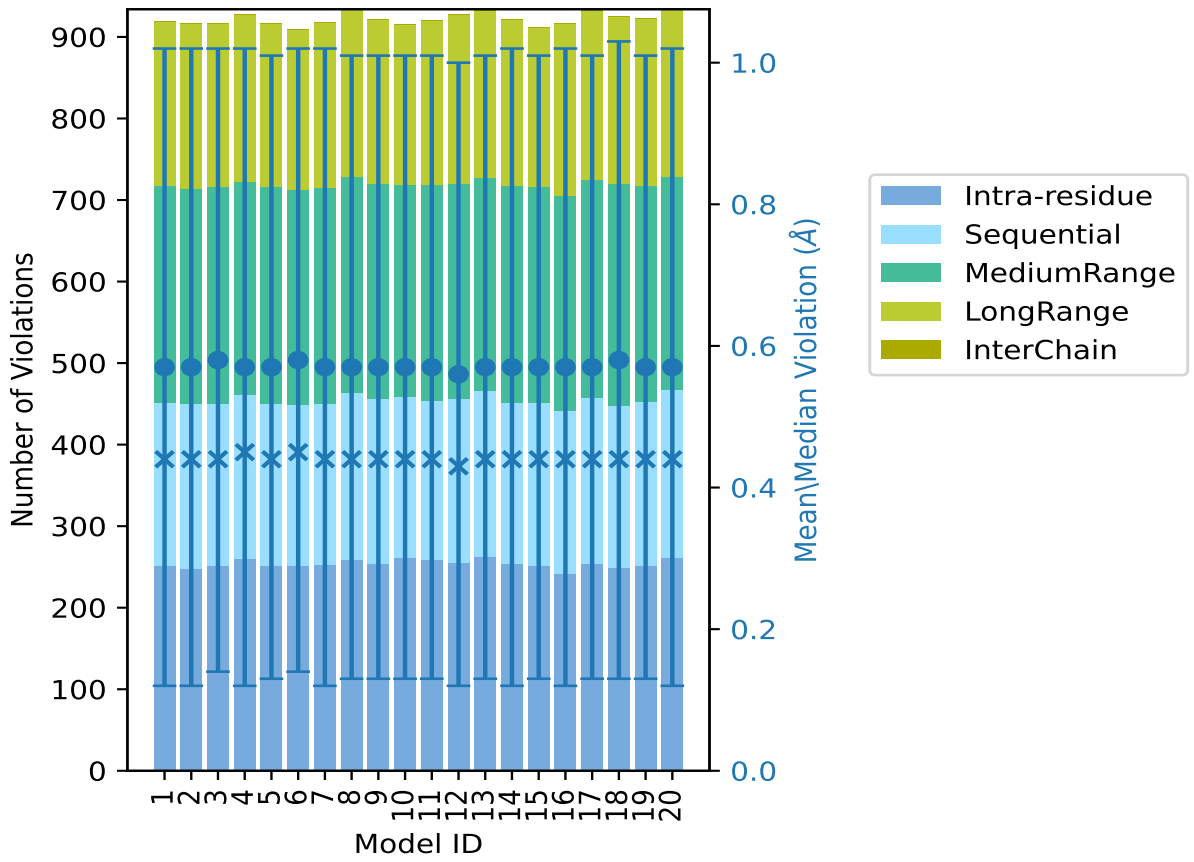
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	255	201	264	207	0	927	0.56	2.88	0.44	0.43
13	262	204	262	204	0	932	0.57	2.91	0.44	0.44
14	254	197	266	204	0	921	0.57	2.86	0.45	0.44
15	251	201	264	196	0	912	0.57	2.87	0.44	0.44
16	242	200	264	210	0	916	0.57	2.91	0.45	0.44
17	254	203	268	208	0	933	0.57	2.87	0.44	0.44
18	249	199	272	205	0	925	0.58	2.92	0.45	0.44
19	251	201	266	205	0	923	0.57	2.94	0.44	0.44
20	261	206	261	206	0	934	0.57	3.24	0.45	0.44

[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



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

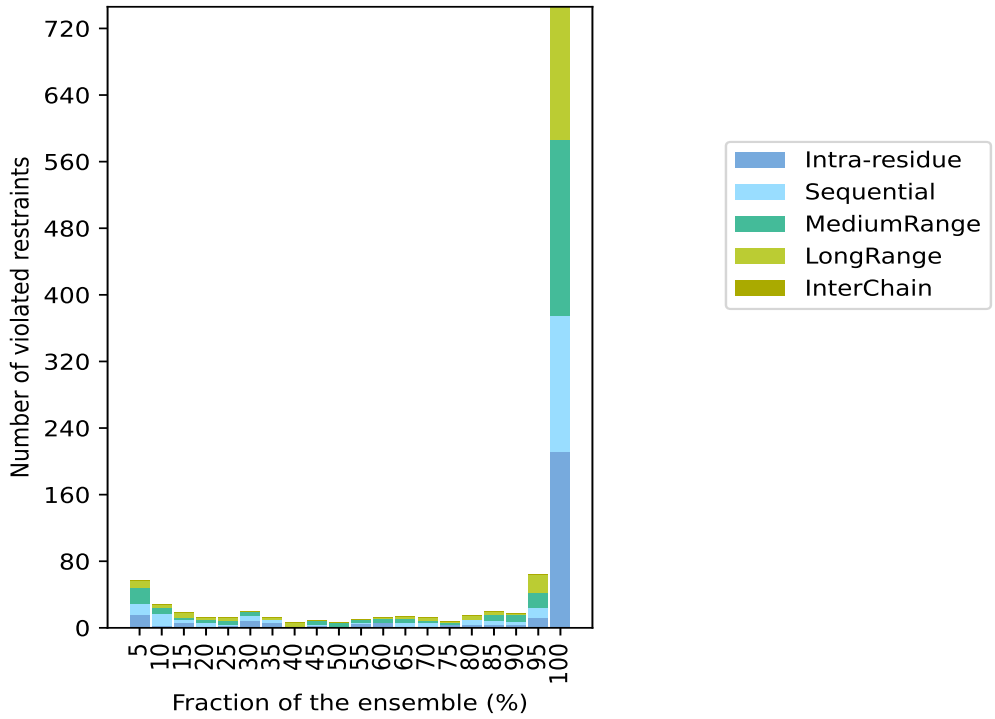
9.3 Distance violation statistics for the ensemble (i)

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, 2599(IR:787, SQ:689, MR:675, LR:448, 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]	%
16	13	19	9	0	57	1	5.0
3	14	7	4	0	28	2	10.0
6	4	2	7	0	19	3	15.0
1	5	4	2	0	12	4	20.0
2	2	5	3	0	12	5	25.0
8	7	4	1	0	20	6	30.0
6	3	1	3	0	13	7	35.0
1	1	0	4	0	6	8	40.0
2	2	4	1	0	9	9	45.0
1	1	4	0	0	6	10	50.0
5	1	3	1	0	10	11	55.0
6	0	5	2	0	13	12	60.0
1	5	5	3	0	14	13	65.0
2	4	3	3	0	12	14	70.0
4	0	2	2	0	8	15	75.0
4	5	1	5	0	15	16	80.0
4	4	8	4	0	20	17	85.0
4	3	9	1	0	17	18	90.0
12	12	18	22	0	64	19	95.0
212	163	211	160	0	746	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

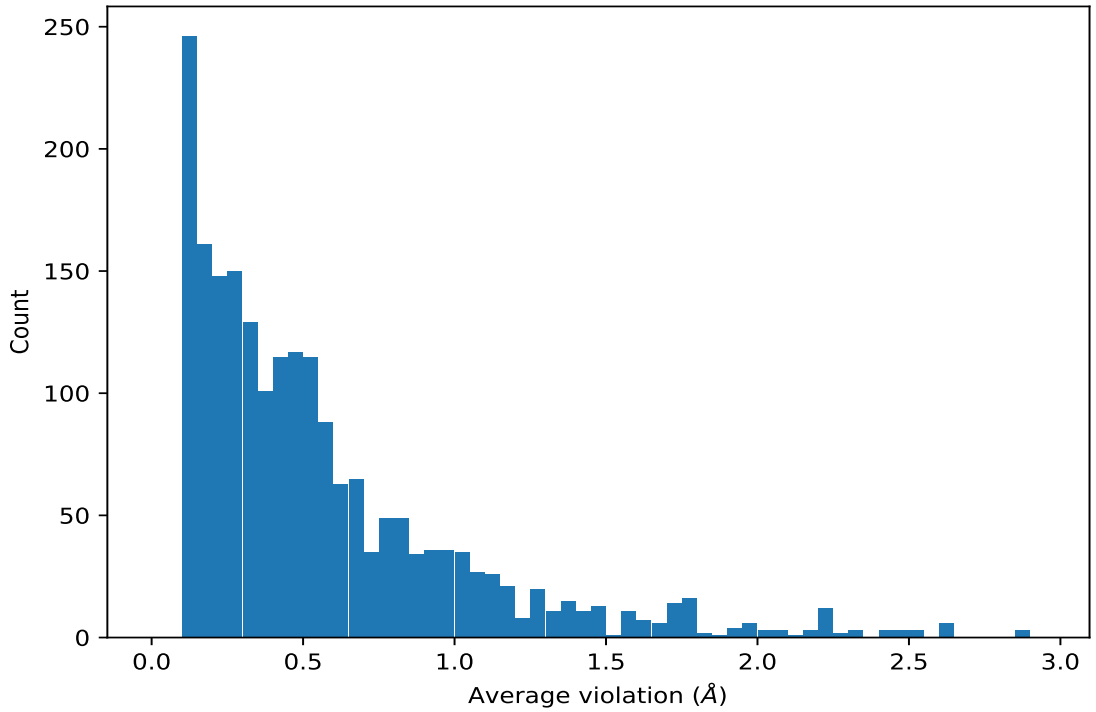
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	20	2.89	0.03	2.9
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	20	2.89	0.03	2.9
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	20	2.89	0.03	2.9
(2,15)	1:A:95:GLN:HE22	1:A:92:LEU:HD21	20	2.65	0.03	2.65
(2,15)	1:A:95:GLN:HE22	1:A:92:LEU:HD22	20	2.65	0.03	2.65
(2,15)	1:A:95:GLN:HE22	1:A:92:LEU:HD23	20	2.65	0.03	2.65
(1,1940)	1:A:66:LEU:HD21	1:A:30:GLN:HG2	20	2.63	0.52	2.74
(1,1940)	1:A:66:LEU:HD22	1:A:30:GLN:HG2	20	2.63	0.52	2.74
(1,1940)	1:A:66:LEU:HD23	1:A:30:GLN:HG2	20	2.63	0.52	2.74
(1,1808)	1:A:93:LEU:HD21	1:A:96:ILE:HG12	20	2.53	0.04	2.52
(1,1808)	1:A:93:LEU:HD22	1:A:96:ILE:HG12	20	2.53	0.04	2.52
(1,1808)	1:A:93:LEU:HD23	1:A:96:ILE:HG12	20	2.53	0.04	2.52
(1,1835)	1:A:34:VAL:HG11	1:A:65:HIS:HB3	20	2.47	0.01	2.47
(1,1835)	1:A:34:VAL:HG12	1:A:65:HIS:HB3	20	2.47	0.01	2.47
(1,1835)	1:A:34:VAL:HG13	1:A:65:HIS:HB3	20	2.47	0.01	2.47
(1,2105)	1:A:33:SER:HB2	1:A:34:VAL:HG11	20	2.42	0.46	2.61

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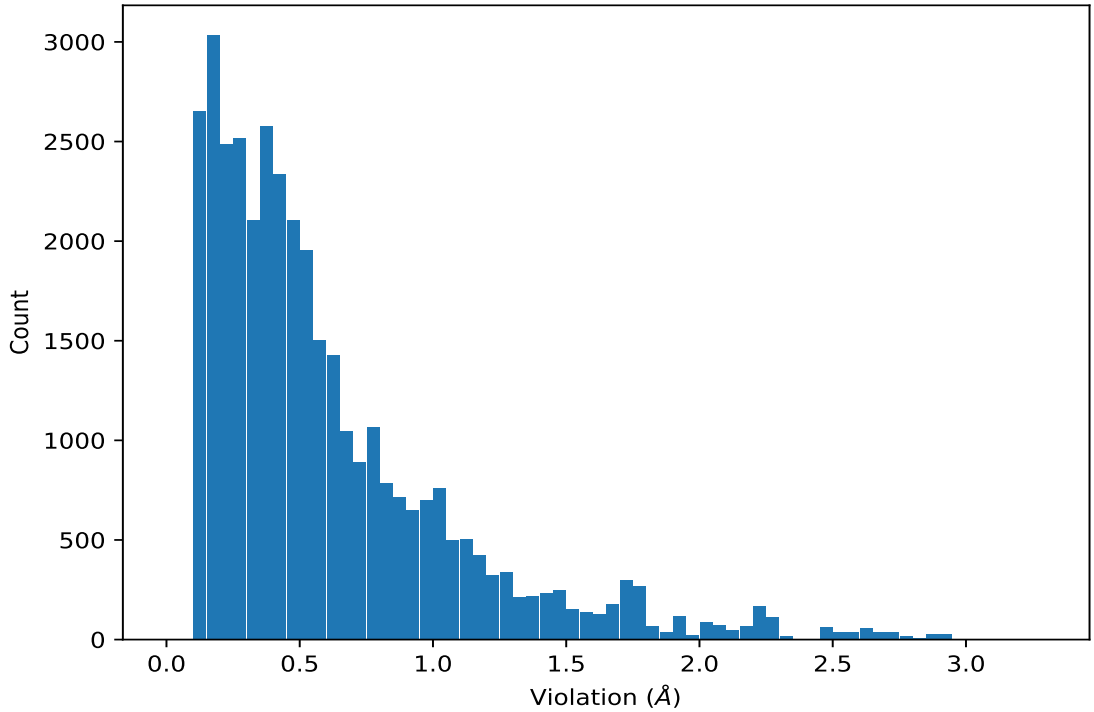
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2105)	1:A:33:SER:HB2	1:A:34:VAL:HG12	20	2.42	0.46	2.61
(1,2105)	1:A:33:SER:HB2	1:A:34:VAL:HG13	20	2.42	0.46	2.61
(1,1308)	1:A:86:HIS:HE1	1:A:46:HIS:HD2	20	2.29	0.24	2.34
(1,2029)	1:A:17:THR:HB	1:A:14:LEU:HB2	20	2.27	0.09	2.28
(1,2422)	1:A:43:LEU:HD21	1:A:28:LEU:HD21	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD21	1:A:28:LEU:HD22	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD21	1:A:28:LEU:HD23	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD22	1:A:28:LEU:HD21	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD22	1:A:28:LEU:HD22	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD22	1:A:28:LEU:HD23	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD23	1:A:28:LEU:HD21	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD23	1:A:28:LEU:HD22	20	2.24	0.04	2.24
(1,2422)	1:A:43:LEU:HD23	1:A:28:LEU:HD23	20	2.24	0.04	2.24
(1,2359)	1:A:52:LEU:HD11	1:A:31:ALA:H	20	2.23	0.04	2.24

[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)
(1,2346)	1:A:60:LEU:HD11	1:A:55:ASP:HB3	4	3.28
(1,2346)	1:A:60:LEU:HD12	1:A:55:ASP:HB3	4	3.28
(1,2346)	1:A:60:LEU:HD13	1:A:55:ASP:HB3	4	3.28
(1,2346)	1:A:60:LEU:HD11	1:A:55:ASP:HB3	20	3.24
(1,2346)	1:A:60:LEU:HD12	1:A:55:ASP:HB3	20	3.24
(1,2346)	1:A:60:LEU:HD13	1:A:55:ASP:HB3	20	3.24
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	19	2.94
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	19	2.94
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	19	2.94
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	2	2.93
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	2	2.93
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	2	2.93
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	9	2.92
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	9	2.92
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	9	2.92
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	18	2.92
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	18	2.92
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	18	2.92
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	4	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	4	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	4	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	8	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	8	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	8	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	10	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD22	10	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD23	10	2.91
(2,231)	1:A:19:GLN:H	1:A:11:LEU:HD21	13	2.91

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found