wwPDB NMR Structure Validation Summary Report

Jul 2, 2020 – 12:14 AM CDT

PDB ID	:	2PNG
Title	:	Type I rat fatty acid synthase acyl carrier protein (ACP) domain
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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 following versions of software and data (see references (i)) were used in the production of this report:

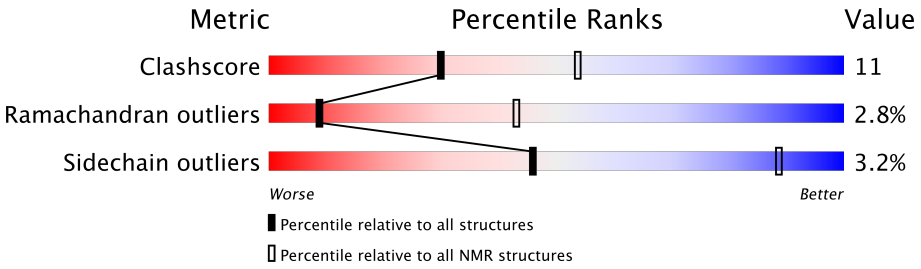
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.6.dev1
BMRB Restraints Analalysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.6.dev1

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 53%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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	89	60% 16% 25%

2 Ensemble composition and analysis

This entry contains 30 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:8-A:74 (67)	0.52	1

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 8, 9, 10, 12, 17, 19, 20, 21, 22, 25, 26, 27, 28, 29
2	7, 11, 13, 16, 24, 30
3	14, 15, 23
Single-model clusters	18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1386 atoms, of which 708 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fatty acid synthase (EC 2.3.1.85).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1386	416	708	125	135	2	0

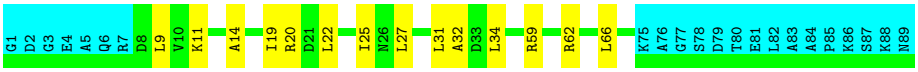
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Fatty acid synthase (EC 2.3.1.85)

Chain A:

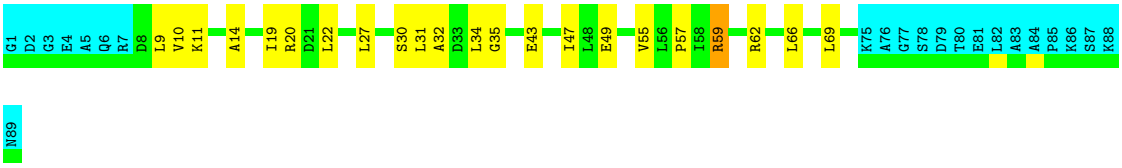


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Fatty acid synthase (EC 2.3.1.85)

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 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
CNS	refinement	1.1
Aria	structure solution	1.2

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)	2png_nmr.cif
Number of chemical shift lists	1
Total number of shifts	980
Number of shifts mapped to atoms	558
Number of unparsed shifts	156
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	266
Assignment completeness (well-defined parts)	53%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

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	0.6±0.7
All	All	0	19

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All 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	45	ARG	Sidechain	6
1	A	67	ARG	Sidechain	5
1	A	59	ARG	Sidechain	5
1	A	20	ARG	Sidechain	2
1	A	62	ARG	Sidechain	1

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	522	556	554	12±3
All	All	15660	16680	16620	352

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 11.

5 of 122 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ASP:HB2	1:A:11:LYS:HG2	0.89	1.45	13	6
1:A:31:LEU:HD12	1:A:34:LEU:HD12	0.79	1.54	4	9
1:A:32:ALA:HB2	1:A:62:ARG:HG2	0.79	1.53	24	8
1:A:27:LEU:HD22	1:A:67:ARG:HG2	0.72	1.62	10	2
1:A:22:LEU:HG	1:A:27:LEU:HD21	0.72	1.62	14	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	67/89 (75%)	56±2 (84±3%)	9±2 (13±3%)	2±1 (3±2%)	9	43
All	All	2010/2670 (75%)	1687 (84%)	266 (13%)	57 (3%)	9	43

5 of 13 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	20	ARG	22
1	A	35	GLY	10
1	A	38	SER	8
1	A	37	ASP	5
1	A	41	GLY	2

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	59/74 (80%)	57±1 (97±2%)	2±1 (3±2%)	46	89
All	All	1770/2220 (80%)	1713 (97%)	57 (3%)	46	89

5 of 12 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	59	ARG	18
1	A	11	LYS	10
1	A	63	GLN	9
1	A	66	LEU	8
1	A	34	LEU	3

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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: 2png_nmr.cif

Chemical shift list name: *nef_chemical_shift_list_*

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	980
Number of shifts mapped to atoms	558
Number of unparsed shifts	156
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	266
Number of shift outliers (ShiftChecker)	0

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

- Chemical shift has been reported more than once. First 5 (of 156) occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
9	A	4	GLU	HG%	2.208	0.000	1
17	A	5	ALA	HB%	1.348	0.000	1
18	A	5	ALA	HB%	1.348	0.000	1
40	A	7	ARG	HD%	3.121	0.000	1
42	A	7	ARG	HG%	1.599	0.000	1

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

- No matching atoms found in structure. First 5 (of 266) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	9	LEU	HD1%	0.577	0.0	1
A	13	VAL	HG2%	0.986	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	60	GLU	HBy	1.915	0.0	2
A	86	LYS	HG%	1.457	0.0	1
A	16	ILE	HG1y	1.224	0.0	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	-0.36 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	80	-0.10 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	84	-0.18 ± 0.37	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 53%, i.e. 444 atoms were assigned a chemical shift out of a possible 844. 16 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	260/333 (78%)	128/133 (96%)	67/134 (50%)	65/66 (98%)
Sidechain	184/495 (37%)	29/285 (10%)	152/186 (82%)	3/24 (12%)
Aromatic	0/16 (0%)	0/8 (0%)	0/4 (0%)	0/4 (0%)
Overall	444/844 (53%)	157/426 (37%)	219/324 (68%)	68/94 (72%)

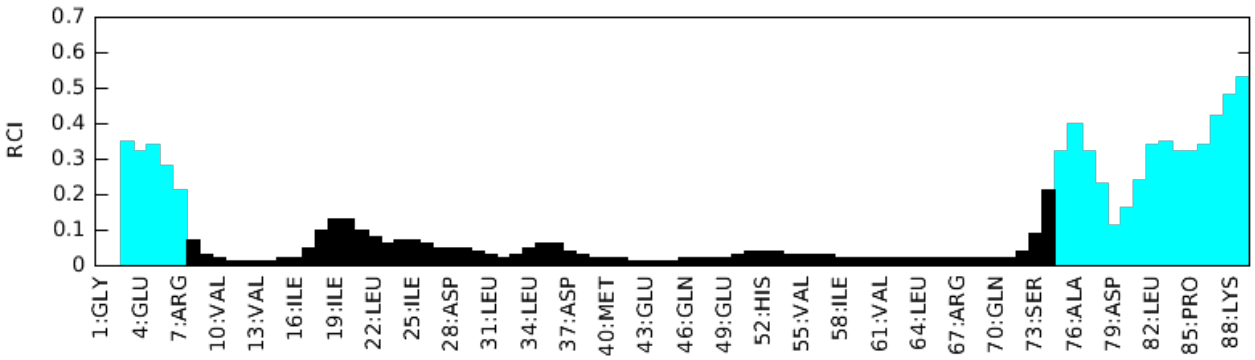
7.1.4 Statistically unusual chemical shifts (i)

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.

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	1732
Intra-residue (|i-j|=0)	697
Sequential (|i-j|=1)	396
Medium range (|i-j|>1 and |i-j|<5)	425
Long range (|i-j|≥5)	214
Inter-chain	0
Total dihedral-anlge restraints	0
Total hydrogen bond restraints	0
Total disulfide bond restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.8
Number of long range restraints per residue	0.1

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)	8.8	0.2
0.2-0.5 (Medium)	7.7	0.5
>0.5 (Large)	11.5	3.01

8.2.2 Average number of dihedral-anlge violations per model

Dihedral-anlge violations less than 1° are not included in the calculation.There are no dihedral-anlge violations

9 Distance violation analysis

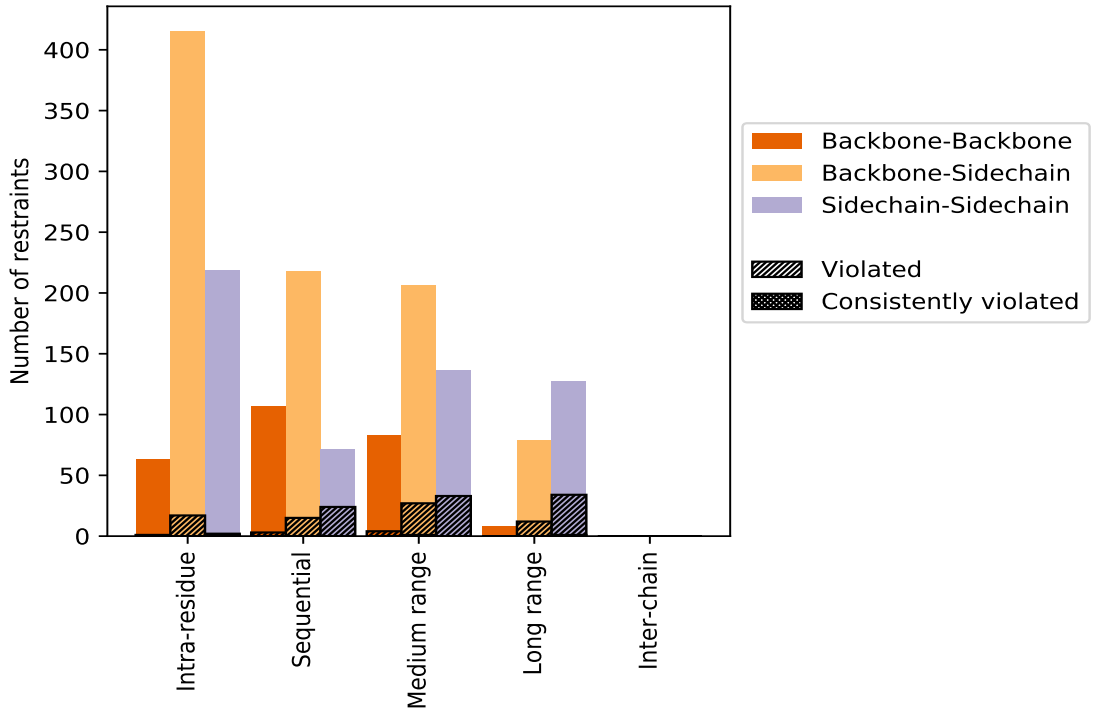
9.1 Summary of distance violations

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	697	40.2	20	2.9	1.2	1	0.1	0.1
Backbone-Backbone	63	3.6	1	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	415	24.0	17	4.1	1.0	0	0.0	0.0
Sidechain-Sidechain	219	12.6	2	0.9	0.1	1	0.5	0.1
Sequential (|i-j|=1)	396	22.9	42	10.6	2.4	0	0.0	0.0
Backbone-Backbone	107	6.2	3	2.8	0.2	0	0.0	0.0
Backbone-Sidechain	218	12.6	15	6.9	0.9	0	0.0	0.0
Sidechain-Sidechain	71	4.1	24	33.8	1.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	425	24.5	64	15.1	3.7	1	0.2	0.1
Backbone-Backbone	83	4.8	4	4.8	0.2	0	0.0	0.0
Backbone-Sidechain	206	11.9	27	13.1	1.6	1	0.5	0.1
Sidechain-Sidechain	136	7.9	33	24.3	1.9	0	0.0	0.0
Long range (|i-j|≥5)	214	12.4	46	21.5	2.7	1	0.5	0.1
Backbone-Backbone	8	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	79	4.6	12	15.2	0.7	0	0.0	0.0
Sidechain-Sidechain	127	7.3	34	26.8	2.0	1	0.8	0.1
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
Total	1732	100.0	172	9.9	9.9	3	0.2	0.2
Backbone-Backbone	261	15.1	8	3.1	0.5	0	0.0	0.0
Backbone-Sidechain	918	53.0	71	7.7	4.1	1	0.1	0.1
Sidechain-Sidechain	553	31.9	93	16.8	5.4	2	0.4	0.1

[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

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)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total			
1	2	7	12	8	0	29	0.6	1.58	0.41
2	2	5	15	6	0	28	0.71	3.01	0.64
3	3	6	10	12	0	31	0.5	1.56	0.41
4	1	2	4	7	0	14	0.49	1.72	0.52
5	4	4	11	13	0	32	0.52	1.62	0.36
6	3	1	12	9	0	25	0.43	1.56	0.41
7	3	5	10	11	0	29	0.4	1.39	0.33
8	4	7	9	5	0	25	0.47	1.62	0.38
9	2	4	6	6	0	18	0.41	1.64	0.46
10	2	1	9	4	0	16	0.58	1.51	0.43
11	2	3	9	9	0	23	0.52	1.62	0.35
12	4	6	9	7	0	26	0.4	1.52	0.34

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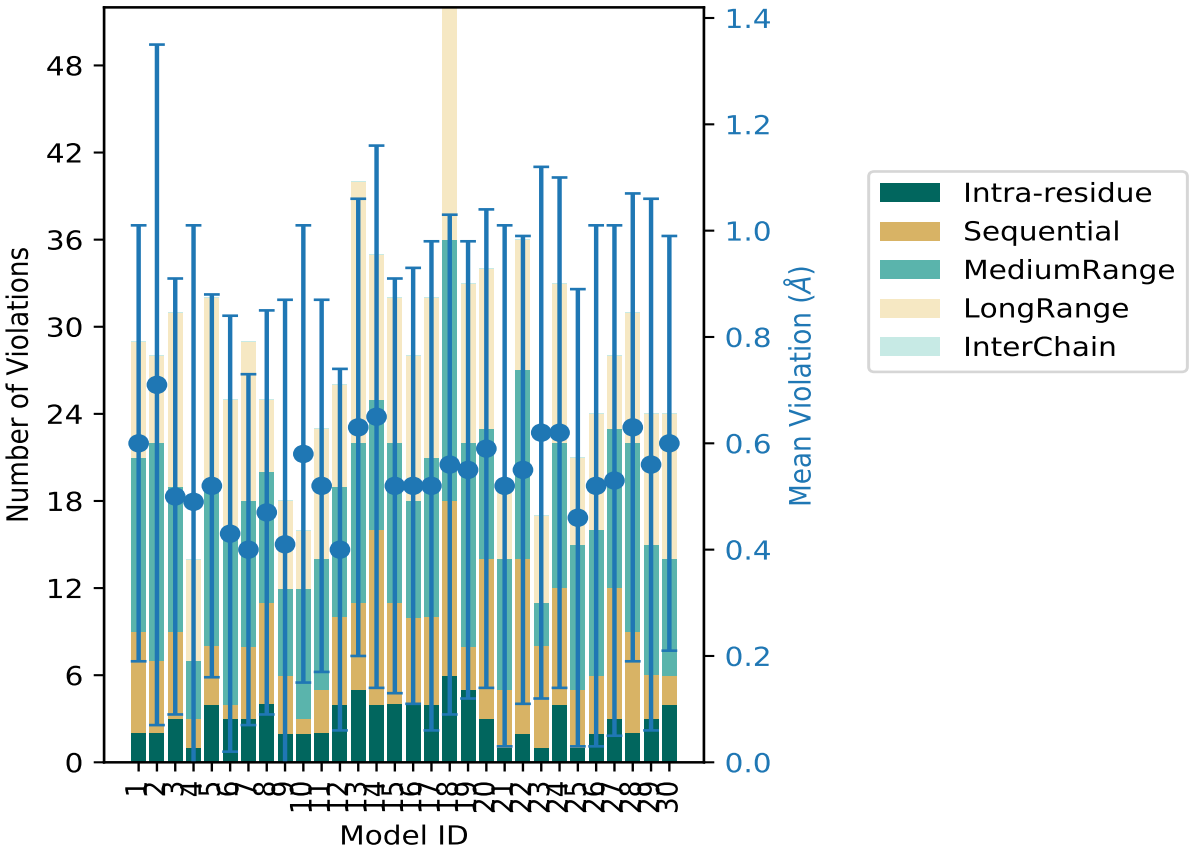
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total			
13	5	6	11	18	0	40	0.63	1.87	0.43
14	4	12	9	10	0	35	0.65	2.01	0.51
15	4	7	11	10	0	32	0.52	1.65	0.39
16	4	6	8	10	0	28	0.52	1.66	0.41
17	4	6	11	11	0	32	0.52	1.89	0.46
18	6	12	18	16	0	52	0.56	1.88	0.47
19	5	3	14	11	0	33	0.55	1.72	0.43
20	3	11	9	11	0	34	0.59	1.51	0.45
21	1	4	9	5	0	19	0.52	1.82	0.49
22	2	12	13	9	0	36	0.55	1.67	0.44
23	1	7	3	6	0	17	0.62	1.71	0.5
24	4	8	10	11	0	33	0.62	2.1	0.48
25	1	4	10	6	0	21	0.46	1.59	0.43
26	2	4	10	8	0	24	0.52	1.96	0.49
27	3	9	11	5	0	28	0.53	1.98	0.48
28	2	7	13	9	0	31	0.63	1.72	0.44
29	3	3	9	9	0	24	0.56	1.72	0.5
30	4	2	8	10	0	24	0.6	1.57	0.39

[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 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

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, 1560(IR:677, SQ:354, MR:361, LR:168, 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]	%
7	14	25	12	0	58	1	3.3
4	7	9	6	0	26	2	6.7
3	7	7	5	0	22	3	10.0
0	5	2	3	0	10	4	13.3
1	0	4	0	0	5	5	16.7
2	1	0	6	0	9	6	20.0
1	1	2	1	0	5	7	23.3
0	1	4	1	0	6	8	26.7

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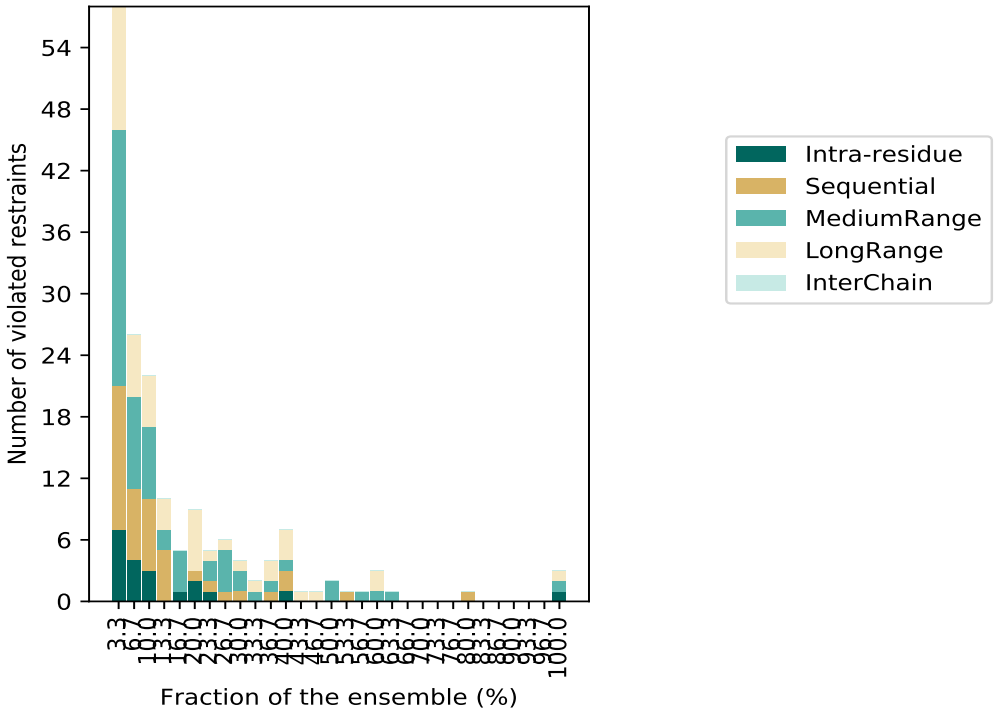
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	2	1	0	4	9	30.0
0	0	1	1	0	2	10	33.3
0	1	1	2	0	4	11	36.7
1	2	1	3	0	7	12	40.0
0	0	0	1	0	1	13	43.3
0	0	0	1	0	1	14	46.7
0	0	2	0	0	2	15	50.0
0	1	0	0	0	1	16	53.3
0	0	1	0	0	1	17	56.7
0	0	1	2	0	3	18	60.0
0	0	1	0	0	1	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	1	0	0	0	1	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
1	0	1	1	0	3	30	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

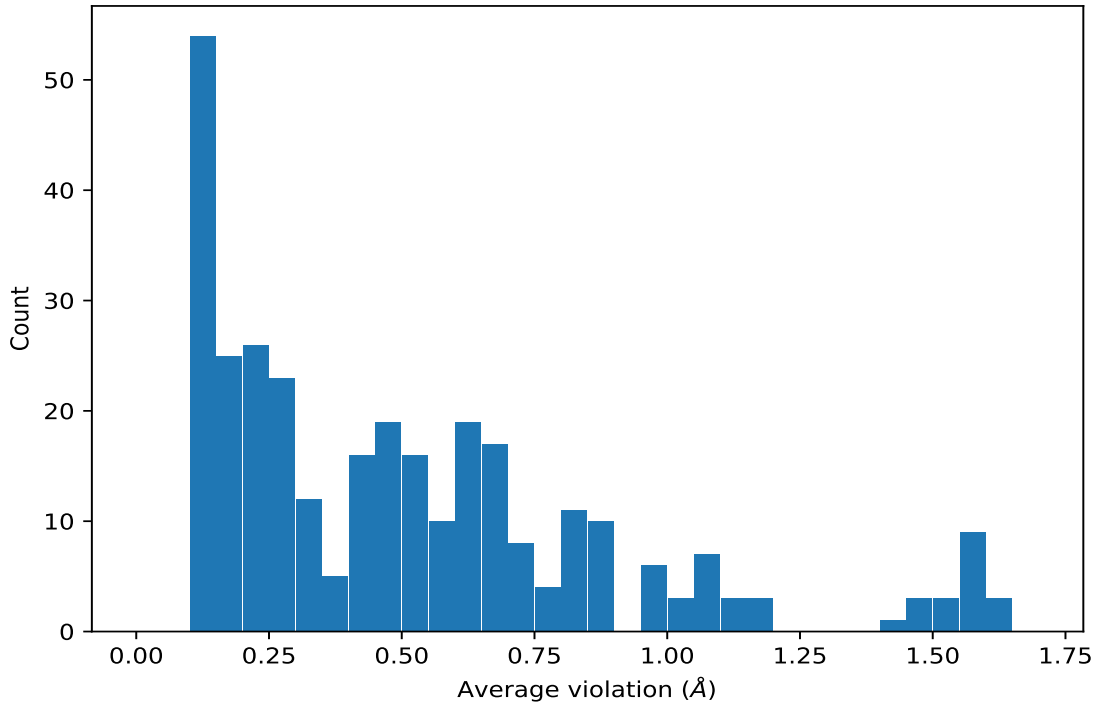
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 top ten absolute value of the violation 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)
(1,323)	1:A:45:ARG:HB2	1:A:45:ARG:HG2	30	0.2	0.01
(1,1581)	1:A:14:ALA:HB1	1:A:70:GLN:HG3	30	1.46	0.35
(1,1581)	1:A:14:ALA:HB2	1:A:70:GLN:HG3	30	1.46	0.35
(1,1581)	1:A:14:ALA:HB3	1:A:70:GLN:HG3	30	1.46	0.35
(1,1271)	1:A:62:ARG:HA	1:A:58:ILE:HG12	30	0.86	0.32
(1,1020)	1:A:34:LEU:HD21	1:A:33:ASP:HB2	24	1.01	0.59
(1,1020)	1:A:34:LEU:HD22	1:A:33:ASP:HB2	24	1.01	0.59
(1,1020)	1:A:34:LEU:HD23	1:A:33:ASP:HB2	24	1.01	0.59
(1,1595)	1:A:68:LYS:HB2	1:A:64:LEU:H	19	0.42	0.17
(1,1595)	1:A:68:LYS:HB3	1:A:64:LEU:H	19	0.42	0.17
(1,778)	1:A:52:HIS:HB3	1:A:6:GLN:HE21	18	0.84	0.41
(1,264)	1:A:32:ALA:HA	1:A:34:LEU:HD11	18	0.23	0.2
(1,264)	1:A:32:ALA:HA	1:A:34:LEU:HD12	18	0.23	0.2
(1,264)	1:A:32:ALA:HA	1:A:34:LEU:HD13	18	0.23	0.2
(1,1589)	1:A:20:ARG:HG3	1:A:67:ARG:HE	18	1.05	0.42
(1,475)	1:A:22:LEU:HD21	1:A:20:ARG:HB2	17	0.23	0.09

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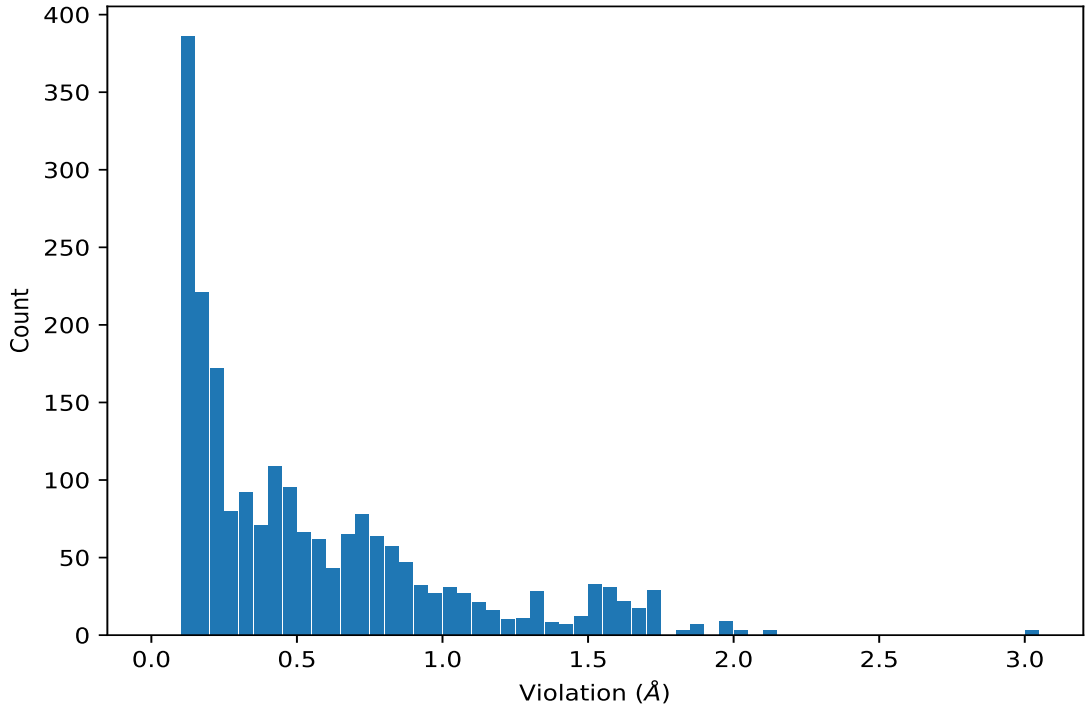
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)
(1,475)	1:A:22:LEU:HD22	1:A:20:ARG:HB2	17	0.23	0.09
(1,475)	1:A:22:LEU:HD23	1:A:20:ARG:HB2	17	0.23	0.09
(1,1248)	1:A:61:VAL:HA	1:A:62:ARG:HB3	16	0.56	0.05

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

9.5 All distance violations

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 lists the top ten 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)
(1,1123)	1:A:48:LEU:HD11	1:A:52:HIS:HB2	2	3.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:A:48:LEU:HD12	1:A:52:HIS:HB2	2	3.01
(1,1123)	1:A:48:LEU:HD13	1:A:52:HIS:HB2	2	3.01
(1,1020)	1:A:34:LEU:HD21	1:A:33:ASP:HB2	24	2.1
(1,1020)	1:A:34:LEU:HD22	1:A:33:ASP:HB2	24	2.1
(1,1020)	1:A:34:LEU:HD23	1:A:33:ASP:HB2	24	2.1
(1,1020)	1:A:34:LEU:HD21	1:A:33:ASP:HB2	14	2.01
(1,1020)	1:A:34:LEU:HD22	1:A:33:ASP:HB2	14	2.01
(1,1020)	1:A:34:LEU:HD23	1:A:33:ASP:HB2	14	2.01
(1,1163)	1:A:54:LEU:HD11	1:A:51:GLU:HB2	24	1.99
(1,1163)	1:A:54:LEU:HD12	1:A:51:GLU:HB2	24	1.99
(1,1163)	1:A:54:LEU:HD13	1:A:51:GLU:HB2	24	1.99
(1,1020)	1:A:34:LEU:HD21	1:A:33:ASP:HB2	27	1.98
(1,1020)	1:A:34:LEU:HD22	1:A:33:ASP:HB2	27	1.98
(1,1020)	1:A:34:LEU:HD23	1:A:33:ASP:HB2	27	1.98
(1,1020)	1:A:34:LEU:HD21	1:A:33:ASP:HB2	26	1.96
(1,1020)	1:A:34:LEU:HD22	1:A:33:ASP:HB2	26	1.96
(1,1020)	1:A:34:LEU:HD23	1:A:33:ASP:HB2	26	1.96
(1,1020)	1:A:34:LEU:HD21	1:A:33:ASP:HB2	17	1.89
(1,1020)	1:A:34:LEU:HD22	1:A:33:ASP:HB2	17	1.89
(1,1020)	1:A:34:LEU:HD23	1:A:33:ASP:HB2	17	1.89
(1,1589)	1:A:20:ARG:HG3	1:A:67:ARG:HE	18	1.88
(1,1020)	1:A:34:LEU:HD21	1:A:33:ASP:HB2	13	1.87
(1,1020)	1:A:34:LEU:HD22	1:A:33:ASP:HB2	13	1.87
(1,1020)	1:A:34:LEU:HD23	1:A:33:ASP:HB2	13	1.87
(1,1163)	1:A:54:LEU:HD11	1:A:51:GLU:HB2	21	1.82

10 Dihedral-anlge violation analysis

No dihedral-anlge restraints found