wwPDB NMR Structure Validation Summary Report (i)

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Title	:	Insight into the molecular recognition mechanism of the coactivator NCoA1 by STAT6
Authors	:	Russo, L.; Becker, S.; Griesinger, C.
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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:

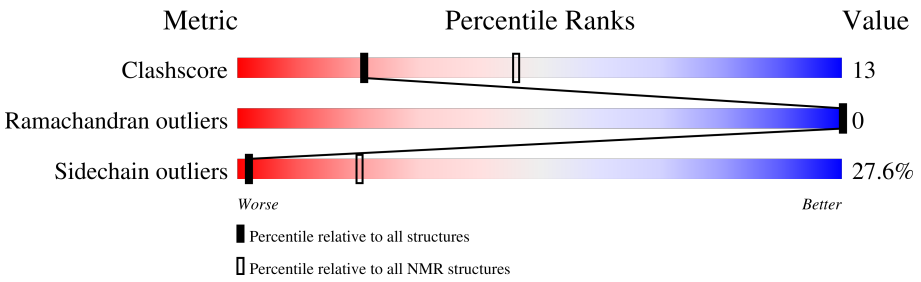
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 88%.

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	132	37% 35% • 27%
2	B	32	100%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:260-A:303, A:307-A:348, A:356-A:366 (97)	0.32	10

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2523 atoms, of which 1247 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	132	2041	641	1008	185	197	10	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q15788
A	255	HIS	-	expression tag	UNP Q15788
A	256	MET	-	expression tag	UNP Q15788
A	343	ARG	LYS	engineered mutation	UNP Q15788

- Molecule 2 is a protein called Signal transducer and activator of transcription 6.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	32	482	157	239	36	50	0

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: Nuclear receptor coactivator 1

Chain A: 37% 35% • 27%

G254 H255 M256 T257 G258 V259 M263 T264 K265 Q266 D267 T268 K271 I272 I273 S274 I275 S279 L280 R281 W288 E289 D290 L291 V292 R293 K294 Y297 A298 F299 F300 Q303 G304 R305 E306 P307 S308 Y309 Q312 L313 F314 Q315 E316 V317 M318 T322 S325 Y328 R329 F330

I331 L332 M337 L338 S339 A340 H341 T342 K345 L346 C347 Y348 P349 Q350 S351 P352 D353 M354 Q355 P356 F357 I358 I364 D365 R366 E367 H368 S369 G370 L371 S372 P373 Q374 D375 D376 T377 N378 S379 G380 M381 S382 I383 P384 R385

• Molecule 2: Signal transducer and activator of transcription 6

Chain B: 100%

G783 T784 W785 I786 G787 E788 D789 I790 F791 P792 P793 L794 L795 P796 P797 T798 E799 Q800 D801 L802 T803 K804 L805 L806 L807 E808 G809 Q810 G811 E812 S813 G814

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

The representative model is number 10. Colouring as in section 4.1 above.

• Molecule 1: Nuclear receptor coactivator 1

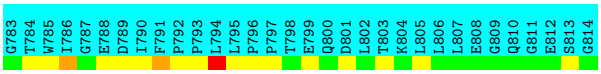
Chain A: 39% 30% 5% 27%

G254 H255 M256 T257 G258 V259 M263 T264 K265 Q266 D267 T268 T269 G270 K271 I272 I273 S274 I275 D276 T277 S278 S279 L280 R285 W288 E289 D290 L291 V292 Y297 A298 F299 F300 G304 R305 E306 P307 S308 Y309 Q312 L313 F314 V317 T322 S325 Y328 R329 L332

N333 M337 L338 S339 A340 H341 T342 K345 L346 C347 Y348 P349 Q350 S351 P352 D353 M354 Q355 P356 F357 I358 R366 E367 H368 S369 G370 L371 S372 P373 Q374 D375 D376 T377 N378 S379 G380 M381 S382 I383 P384 R385

• Molecule 2: Signal transducer and activator of transcription 6

Chain B: 100%


G783
T784
W785
I786
G787
E788
D789
I790
F791
P792
P793
L794
L795
P796
P797
T798
E799
Q800
D801
L802
T803
K804
L805
L806
L807
E808
G809
Q810
G811
E812
S813
G814

5 Refinement protocol and experimental data overview (i)

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

Of the 100 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	refinement	
CYANA	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	1881
Number of shifts mapped to atoms	1881
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

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	775	772	772	21±6
2	B	0	0	0	0±0
All	All	15500	15440	15440	413

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 13.

5 of 152 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:332:LEU:HD11	1:A:338:LEU:HD21	0.86	1.44	7	2
1:A:291:LEU:HD21	1:A:364:ILE:HD13	0.81	1.50	19	1
1:A:313:LEU:HD11	1:A:325:SER:N	0.70	2.02	18	2
1:A:299:PHE:CE1	1:A:342:THR:HG21	0.68	2.23	9	5
1:A:299:PHE:CZ	1:A:342:THR:HG21	0.67	2.24	5	5

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	97/132 (73%)	96±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100 100
2	B	0	-	-	-	-
All	All	1940/3280 (59%)	1912 (99%)	28 (1%)	0 (0%)	100 100

There are no Ramachandran outliers.

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	85/115 (74%)	62±3 (72±3%)	23±3 (28±3%)	2 20
2	B	0	-	-	-
All	All	1700/2840 (60%)	1231 (72%)	469 (28%)	2 20

5 of 62 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	297	TYR	20
1	A	345	LYS	20
1	A	279	SER	19
1	A	309	TYR	18
1	A	314	PHE	18

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 88% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CS_NCoA1_STAT6_FINAL.str*

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	1881
Number of shifts mapped to atoms	1881
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	157	0.01 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	143	0.32 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	133	0.13 ± 0.10	None needed (< 0.5 ppm)
^{15}N	145	-0.06 ± 0.25	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 88%, i.e. 1188 atoms were assigned a chemical shift out of a possible 1345. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	474/483 (98%)	196/196 (100%)	185/194 (95%)	93/93 (100%)
Sidechain	629/738 (85%)	426/481 (89%)	197/223 (88%)	6/34 (18%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	85/124 (69%)	50/60 (83%)	30/59 (51%)	5/5 (100%)
Overall	1188/1345 (88%)	672/737 (91%)	412/476 (87%)	104/132 (79%)

7.1.4 Statistically unusual chemical shifts (i)

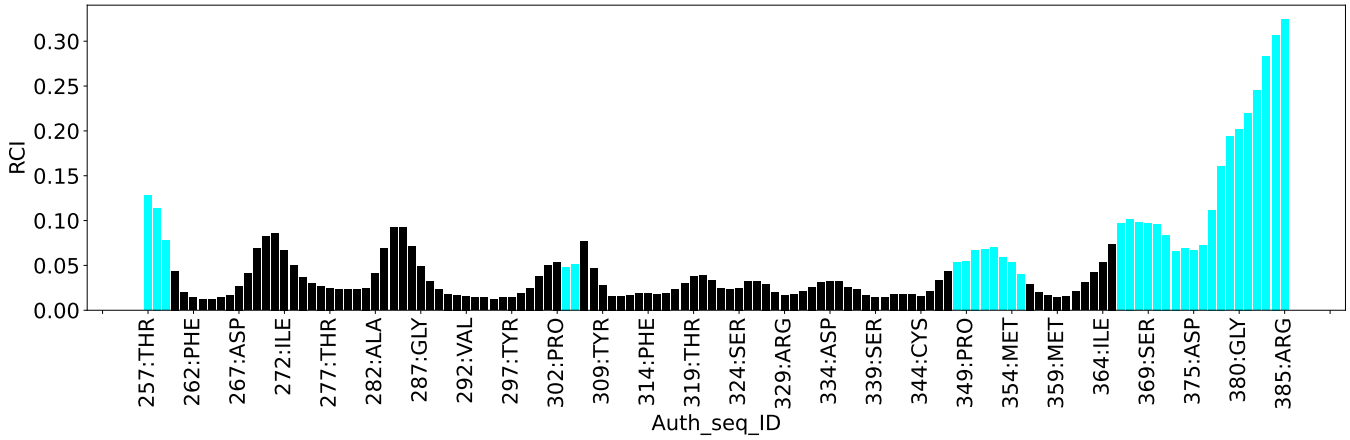
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	319	THR	HG1	-1.78	0.08 – 2.19	-13.8
1	A	377	THR	HG1	-1.71	0.08 – 2.19	-13.5
1	A	269	THR	HG1	-1.64	0.08 – 2.19	-13.2
1	A	264	THR	HG1	-1.60	0.08 – 2.19	-13.0
1	A	286	THR	HG1	-1.43	0.08 – 2.19	-12.2
1	A	271	LYS	CD	39.73	23.50 – 34.42	9.9
1	A	311	ARG	CD	35.84	38.57 – 47.75	-8.0
1	A	310	ALA	HB1	-0.43	0.14 – 2.58	-7.3
1	A	310	ALA	HB2	-0.43	0.14 – 2.58	-7.3
1	A	310	ALA	HB3	-0.43	0.14 – 2.58	-7.3
1	A	289	GLU	HG3	0.78	1.20 – 3.30	-7.0
1	A	288	TRP	CZ2	124.06	107.20 – 121.33	6.9
1	A	313	LEU	CD2	13.17	15.73 – 32.47	-6.5
1	A	288	TRP	CH2	114.99	116.19 – 131.43	-5.8

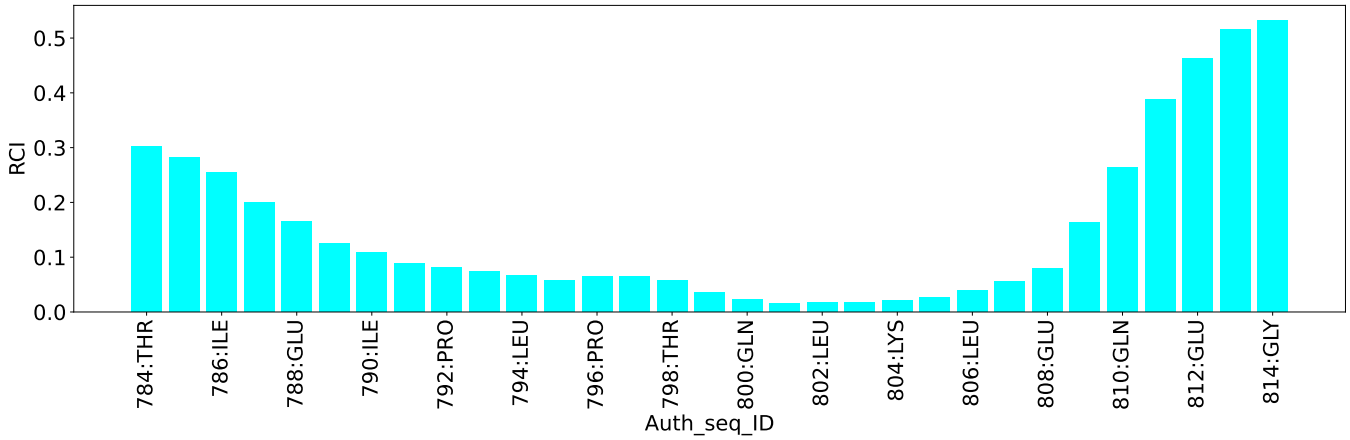
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:



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	1307
Intra-residue (|i-j|=0)	402
Sequential (|i-j|=1)	385
Medium range (|i-j|>1 and |i-j|<5)	200
Long range (|i-j|≥5)	159
Inter-chain	81
Hydrogen bond restraints	80
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	8.0
Number of long range restraints per residue[1]	1.2

[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 (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)	25.1	0.2
0.2-0.5 (Medium)	24.5	0.5
>0.5 (Large)	40.0	4.19

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)

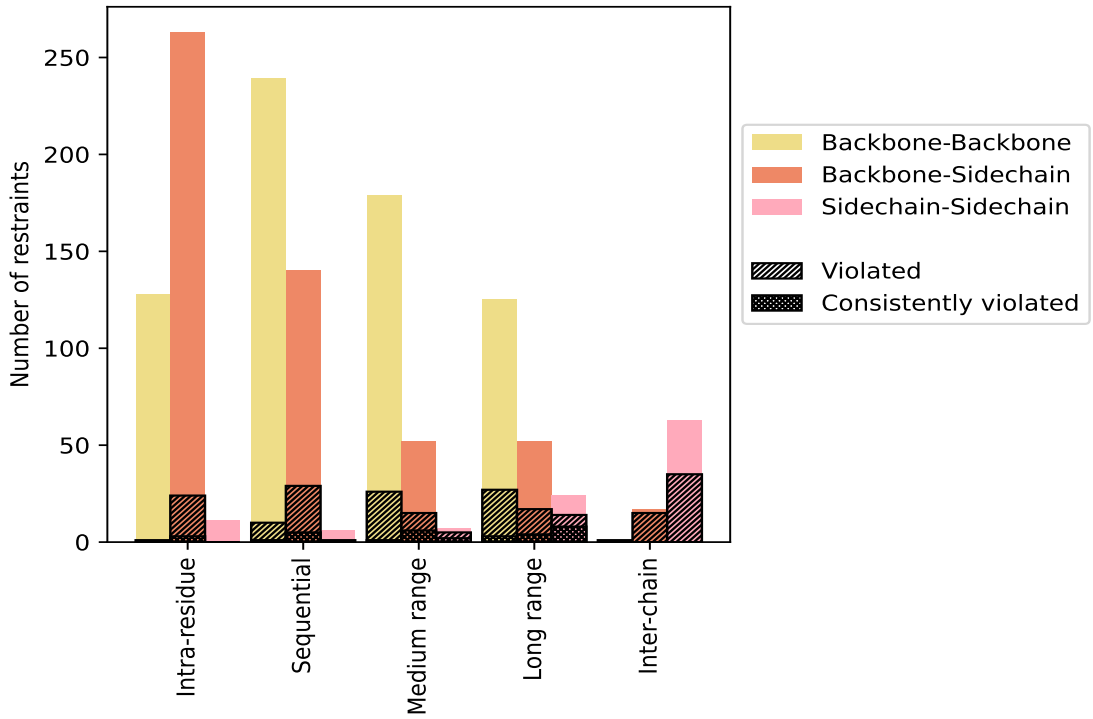
9.1 Summary of distance violations (i)

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)	402	30.8	25	6.2	1.9	3	0.7	0.2
Backbone-Backbone	128	9.8	1	0.8	0.1	0	0.0	0.0
Backbone-Sidechain	263	20.1	24	9.1	1.8	3	1.1	0.2
Sidechain-Sidechain	11	0.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	385	29.5	40	10.4	3.1	6	1.6	0.5
Backbone-Backbone	239	18.3	10	4.2	0.8	1	0.4	0.1
Backbone-Sidechain	140	10.7	29	20.7	2.2	5	3.6	0.4
Sidechain-Sidechain	6	0.5	1	16.7	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	200	15.3	39	19.5	3.0	8	4.0	0.6
Backbone-Backbone	141	10.8	19	13.5	1.5	0	0.0	0.0
Backbone-Sidechain	52	4.0	15	28.8	1.1	6	11.5	0.5
Sidechain-Sidechain	7	0.5	5	71.4	0.4	2	28.6	0.2
Long range (|i-j|≥5)	159	12.2	52	32.7	4.0	13	8.2	1.0
Backbone-Backbone	83	6.4	21	25.3	1.6	1	1.2	0.1
Backbone-Sidechain	52	4.0	17	32.7	1.3	4	7.7	0.3
Sidechain-Sidechain	24	1.8	14	58.3	1.1	8	33.3	0.6
Inter-chain	81	6.2	51	63.0	3.9	0	0.0	0.0
Backbone-Backbone	1	0.1	1	100.0	0.1	0	0.0	0.0
Backbone-Sidechain	17	1.3	15	88.2	1.1	0	0.0	0.0
Sidechain-Sidechain	63	4.8	35	55.6	2.7	0	0.0	0.0
Hydrogen bond	80	6.1	13	16.2	1.0	3	3.8	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1307	100.0	220	16.8	16.8	33	2.5	2.5
Backbone-Backbone	672	51.4	65	9.7	5.0	5	0.7	0.4
Backbone-Sidechain	524	40.1	100	19.1	7.7	18	3.4	1.4
Sidechain-Sidechain	111	8.5	55	49.5	4.2	10	9.0	0.8

[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	6	18	19	23	14	80	0.74	3.65	0.8	0.4
2	5	18	18	33	12	86	0.7	3.45	0.76	0.33
3	6	15	22	22	20	85	0.66	3.38	0.68	0.4
4	9	22	18	28	27	104	0.72	3.68	0.74	0.44
5	9	16	24	35	23	107	0.63	3.91	0.75	0.33
6	7	17	18	30	13	85	0.81	3.48	0.74	0.52
7	7	19	19	28	13	86	0.72	3.34	0.74	0.38
8	5	21	19	27	31	103	0.77	3.56	0.74	0.48
9	8	16	18	28	20	90	0.71	3.42	0.7	0.45
10	10	19	19	24	22	94	0.82	3.6	0.81	0.54
11	7	19	18	24	24	92	0.72	3.41	0.7	0.44

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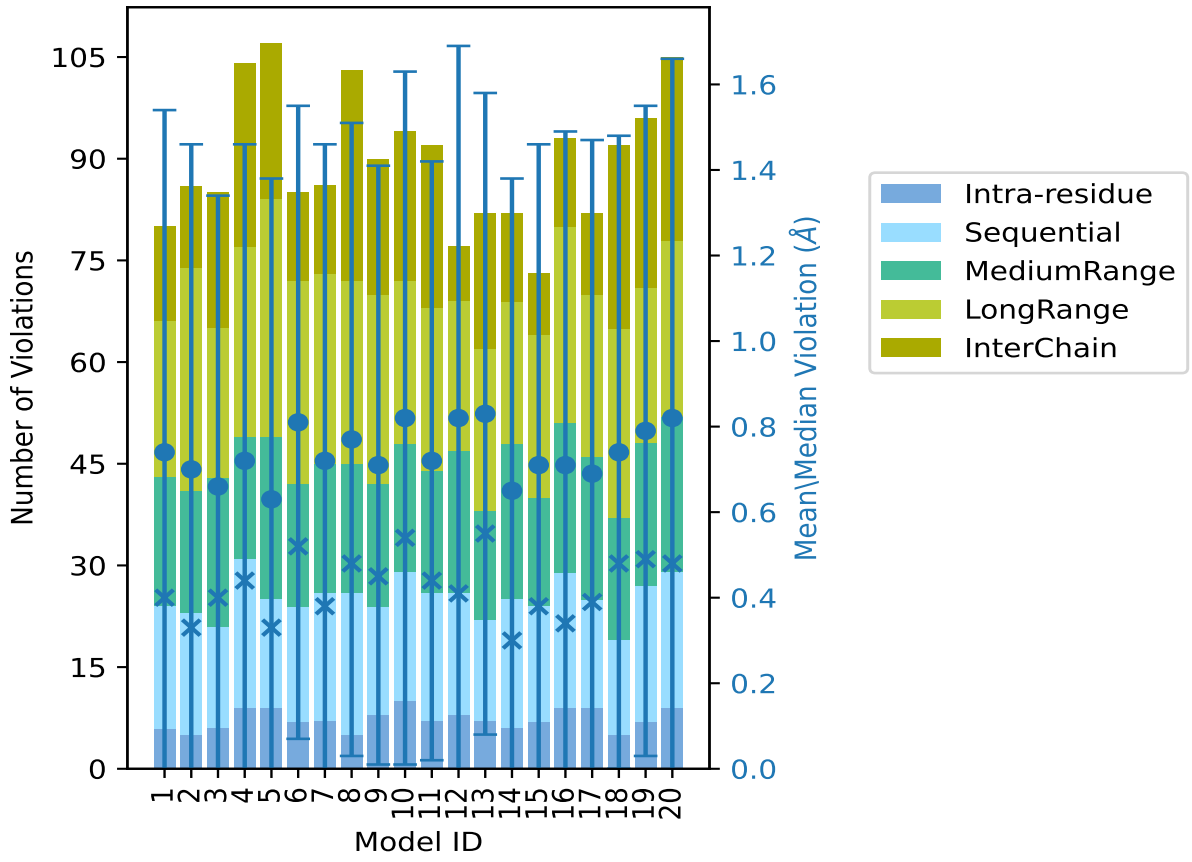
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	8	18	21	22	8	77	0.82	3.46	0.87	0.41
13	7	15	16	24	20	82	0.83	3.27	0.75	0.55
14	6	19	23	21	13	82	0.65	3.31	0.73	0.3
15	7	17	16	24	9	73	0.71	3.53	0.75	0.38
16	9	20	22	29	13	93	0.71	3.8	0.78	0.34
17	9	16	21	24	12	82	0.69	3.72	0.78	0.39
18	5	14	18	28	27	92	0.74	4.01	0.74	0.48
19	7	20	21	23	25	96	0.79	3.36	0.76	0.49
20	9	20	23	26	27	105	0.82	4.19	0.84	0.48

[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

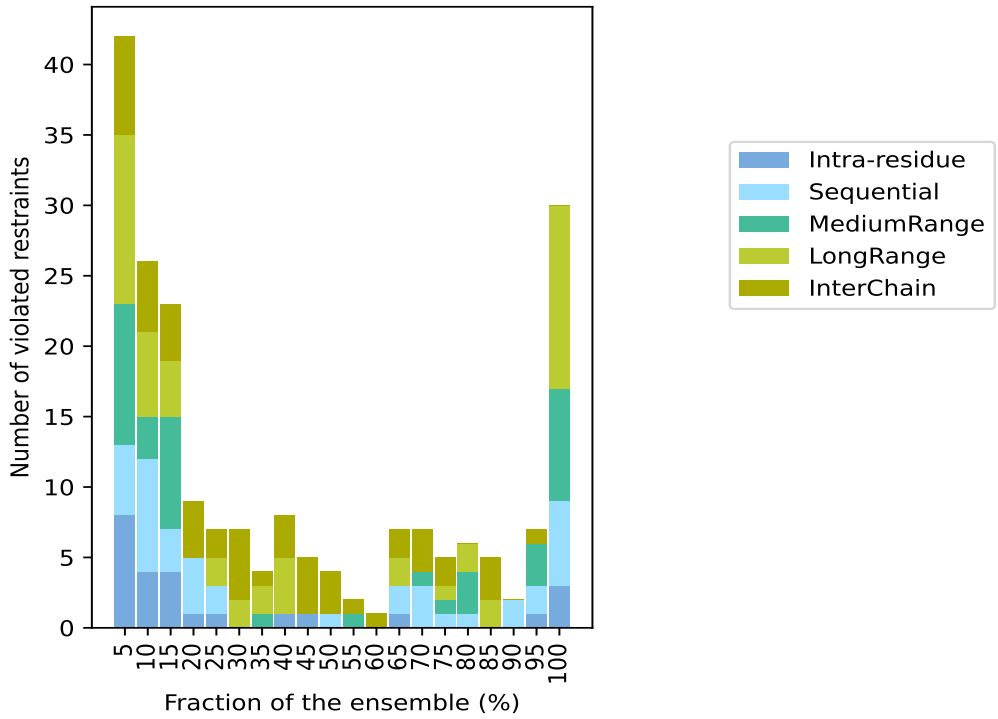
9.3 Distance violation statistics for the ensemble (i)

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, 1020(IR:377, SQ:345, MR:161, LR:107, IC:30) 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]	%
8	5	10	12	7	42	1	5.0
4	8	3	6	5	26	2	10.0
4	3	8	4	4	23	3	15.0
1	4	0	0	4	9	4	20.0
1	2	0	2	2	7	5	25.0
0	0	0	2	5	7	6	30.0
0	0	1	2	1	4	7	35.0
1	0	0	4	3	8	8	40.0
1	0	0	0	4	5	9	45.0
0	1	0	0	3	4	10	50.0
0	0	1	0	1	2	11	55.0
0	0	0	0	1	1	12	60.0
1	2	0	2	2	7	13	65.0
0	3	1	0	3	7	14	70.0
0	1	1	1	2	5	15	75.0
0	1	3	2	0	6	16	80.0
0	0	0	2	3	5	17	85.0
0	2	0	0	0	2	18	90.0
1	2	3	0	1	7	19	95.0
3	6	8	13	0	30	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

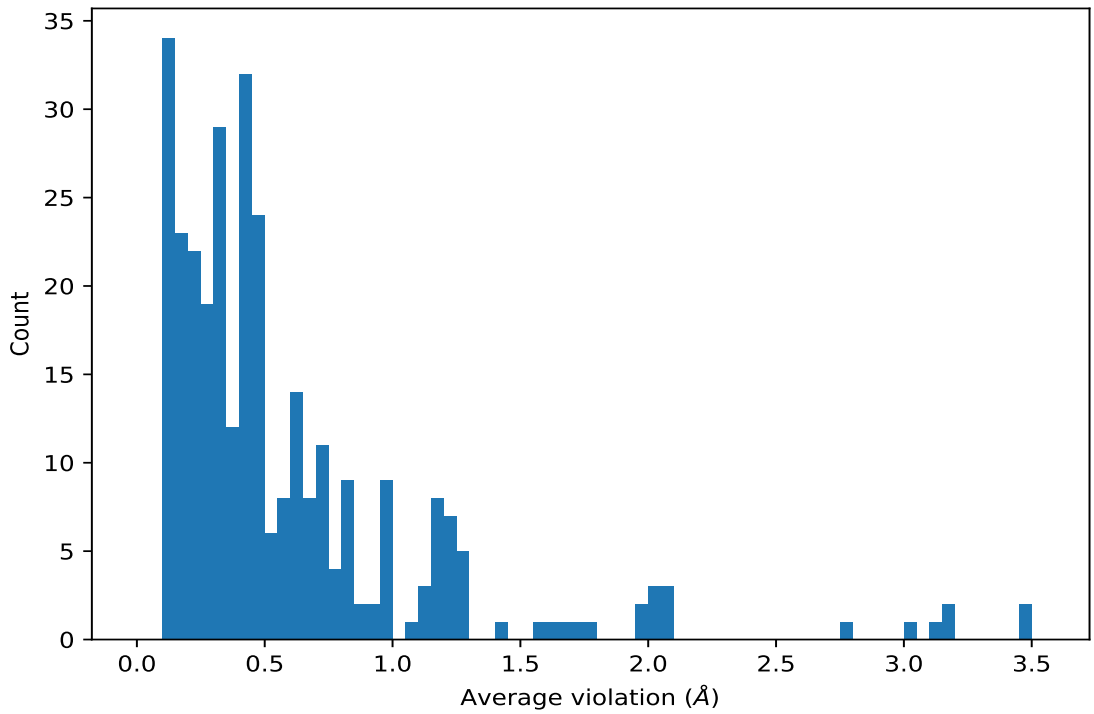
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

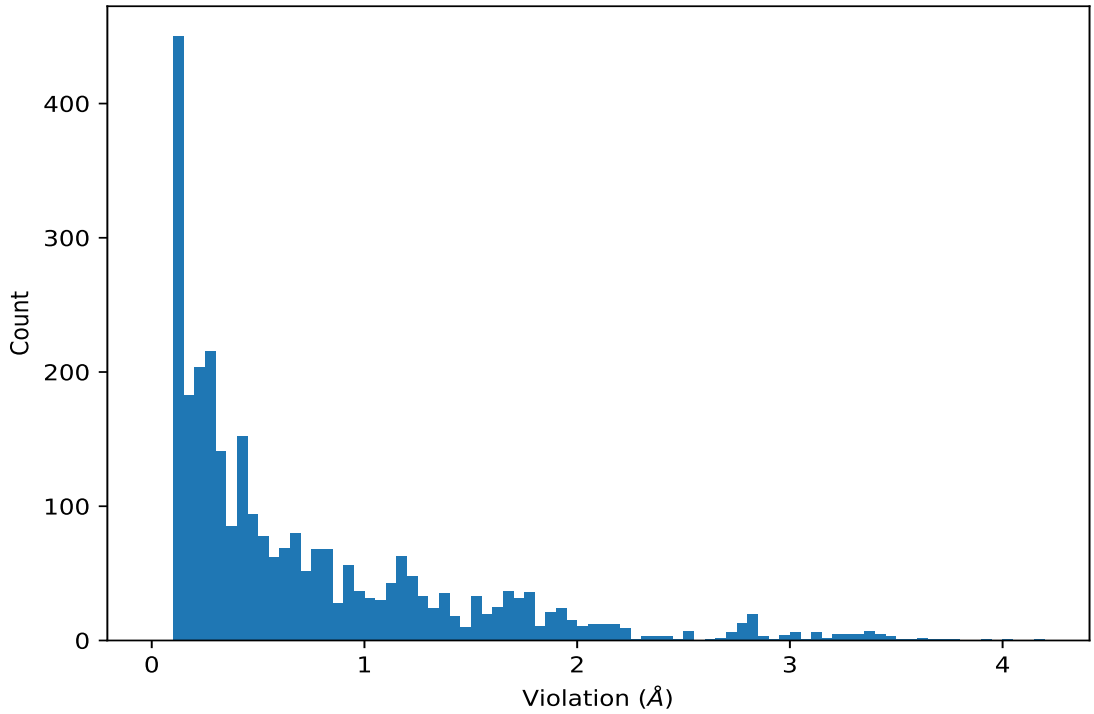
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	20	3.46	0.28	3.38
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	20	3.12	0.24	3.15
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	20	2.78	0.06	2.8
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	20	2.04	0.22	2.02
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	20	2.04	0.22	2.02
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	20	2.04	0.22	2.02
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	20	1.77	0.03	1.78
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	20	1.67	0.39	1.65
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	20	1.6	0.04	1.59
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	20	1.57	0.27	1.57
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	20	1.26	0.49	1.67
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	20	1.26	0.49	1.67
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	20	1.26	0.49	1.67
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	20	1.26	0.25	1.19

[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)
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	20	4.19
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	18	4.01
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	5	3.91
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	16	3.8
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	17	3.72
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	4	3.68
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	1	3.65
(1,825)	1:A:357:PHE:HD1	1:A:359:MET:H	10	3.6
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	8	3.56
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	15	3.53

10 Dihedral-angle violation analysis (i)

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