wwPDB NMR Structure Validation Summary Report (i)

Jun 3, 2023 – 10:02 PM EDT

PDB ID	:	2KNC
BMRB ID	:	16496
Title	:	Platelet integrin ALFAIIB-BETA3 transmembrane-cytoplasmic heterocomplex
Authors	:	Yang, J.; Ma, Y.; Page, R.C.; Misra, S.; Plow, E.F.; Qin, J.
Deposited on	:	2009-08-20

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:

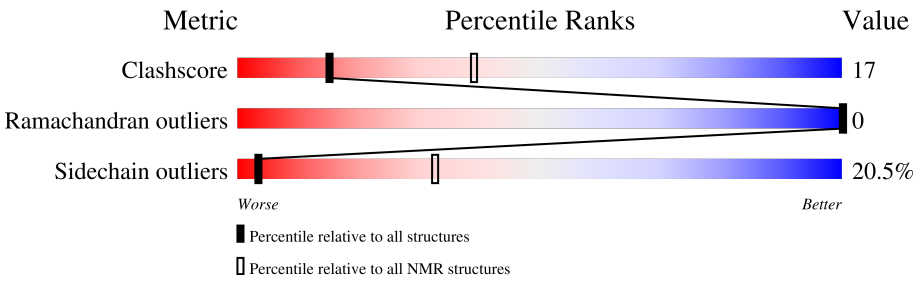
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 86%.

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	54	28% • • 65%
2	B	79	19% 6% • 73%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 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:970-A:988, B:700-B:720 (40)	0.34	5

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 4 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2128 atoms, of which 1083 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	54	862	280	435	69	76	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	955	GLY	-	expression tag	UNP P08514
A	956	ALA	-	expression tag	UNP P08514
A	957	MET	-	expression tag	UNP P08514
A	958	GLY	-	expression tag	UNP P08514
A	959	SER	-	expression tag	UNP P08514

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	79	1266	401	648	104	111	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	684	GLY	-	expression tag	UNP P05106
B	685	ALA	-	expression tag	UNP P05106
B	686	MET	-	expression tag	UNP P05106
B	687	GLY	-	expression tag	UNP P05106
B	688	SER	-	expression tag	UNP P05106

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: Integrin alpha-IIb

Chain A: 28% • • 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 L974 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

• Molecule 2: Integrin beta-3

Chain B: 19% 6% • 73%

G684 A685 M686 G687 S688 K689 G690 P691 D692 I693 L694 V695 V696 L697 L698 S699 V700 M701 L705 L709 K716 L717 L718 I719 T720 I721 H722 D723 R724 K725 E726 F727 A728 K729 F730 E731 E732 E733 R734 A735 R736 A737 K738 W739 D740 T741 A742 N743 N744 P745 L746 Y747 K748 E749 A750 T751 S752

T753 F754 T755 N756 I757 T758 Y759 R760 G761 T762

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

The representative model is number 5. Colouring as in section 4.1 above.

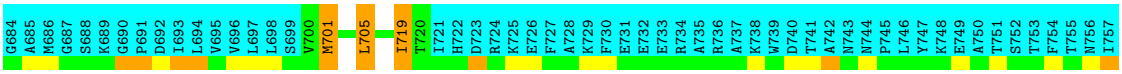
• Molecule 1: Integrin alpha-IIb

Chain A: 28% • • 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 L974 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

• Molecule 2: Integrin beta-3

Chain B: 23% • 73%


G684
A685
M686
G687
S688
K689
G690
P691
D692
I693
L694
V695
V696
L697
L698
S699
V700
M701
L705
I719
T720
I721
H722
D723
R724
K725
E726
F727
A728
K729
F730
E731
E732
E733
R734
A735
R736
A737
K738
W739
D740
T741
A742
N743
N744
P745
L746
Y747
K748
E749
A750
T751
S752
T753
F754
T755
N756
I757

T758
Y759
R760
G761
T762

5 Refinement protocol and experimental data overview (i)

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

Of the 98 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
X-PLOR NIH	refinement	2.15.0
X-PLOR NIH	structure solution	2.15.0

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	1528
Number of shifts mapped to atoms	1528
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	139	166	166	8±3
2	B	156	190	190	7±3
All	All	5900	7120	7120	216

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 17.

5 of 67 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:987:MET:SD	2:B:719:ILE:HD11	0.81	2.15	3	1
1:A:988:TRP:NE1	2:B:719:ILE:HD11	0.76	1.95	12	8
1:A:972:GLY:C	2:B:704:ILE:HD11	0.69	2.07	8	3
1:A:988:TRP:CD1	2:B:719:ILE:HD11	0.66	2.25	15	5
1:A:972:GLY:O	2:B:704:ILE:HD11	0.65	1.91	8	4

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	19/54 (35%)	19±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	21/79 (27%)	21±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	800/2660 (30%)	800 (100%)	0 (0%)	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	15/44 (34%)	12±1 (79±7%)	3±1 (21±7%)	3	32
2	B	16/64 (25%)	13±1 (80±7%)	3±1 (20±7%)	3	33
All	All	620/2160 (29%)	493 (80%)	127 (20%)	3	33

5 of 19 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	988	TRP	20
2	B	719	ILE	15
2	B	701	MET	13
1	A	987	MET	13
2	B	716	LYS	10

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 86% for the well-defined parts and 82% 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	1528
Number of shifts mapped to atoms	1528
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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	132	0.10 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	119	0.57 ± 0.04	Should be checked
$^{13}C'$	131	0.29 ± 0.05	None needed (< 0.5 ppm)
^{15}N	126	0.89 ± 0.09	Should be applied

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 86%, i.e. 511 atoms were assigned a chemical shift out of a possible 596. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	202/205 (99%)	82/85 (96%)	80/80 (100%)	40/40 (100%)
Sidechain	295/367 (80%)	207/254 (81%)	88/112 (79%)	0/1 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	14/24 (58%)	12/12 (100%)	0/10 (0%)	2/2 (100%)
Overall	511/596 (86%)	301/351 (86%)	168/202 (83%)	42/43 (98%)

7.1.4 Statistically unusual chemical shifts (i)

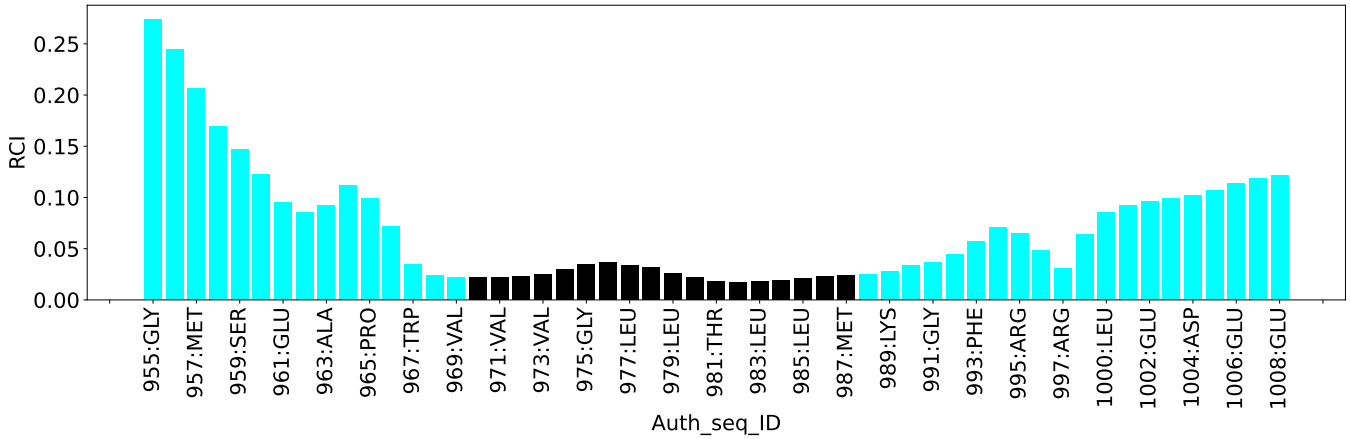
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	962	ARG	NE	110.62	76.53 – 92.65	16.1
1	A	995	ARG	NE	110.62	76.53 – 92.65	16.1
1	B	736	ARG	NE	110.44	76.53 – 92.65	16.0
1	B	734	ARG	NE	110.30	76.53 – 92.65	15.9
1	B	724	ARG	NE	110.26	76.53 – 92.65	15.9
1	A	997	ARG	CD	50.23	38.57 – 47.75	7.7

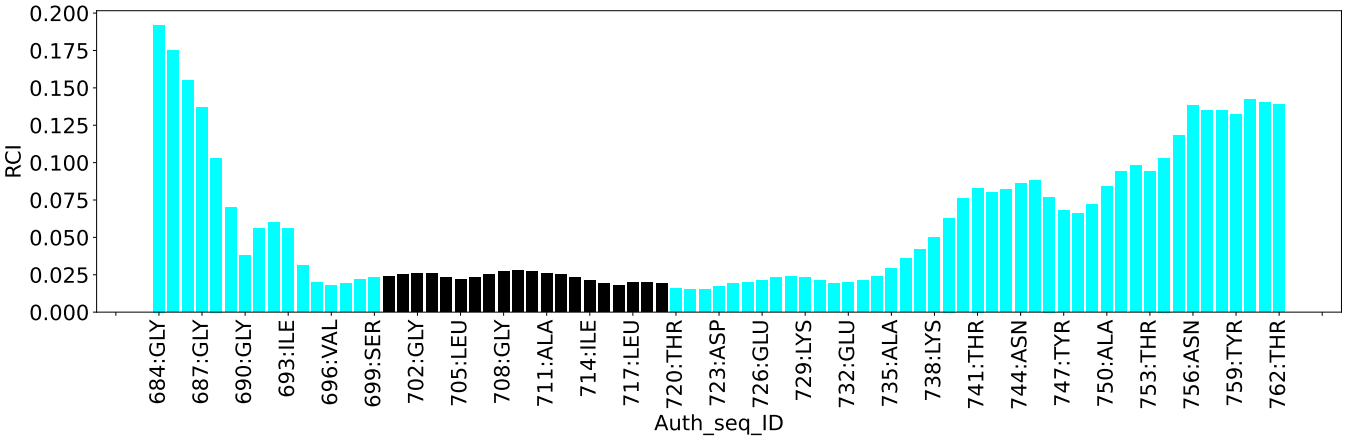
7.1.5 Random Coil Index (RCI) plots (i)

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:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
684:GLY
687:GLY
690:GLY
693:ILE
696:VAL
699:SER
702:GLY
705:LEU
708:GLY
711:ALA
714:ILE
717:LEU
720:THR
723:ASP
726:GLU
729:LYS
732:GLU
735:ALA
738:LYS
741:THR
744:ASN
747:TYR
750:ALA
753:THR
756:ASN
759:TYR
762:THR
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	4592
Intra-residue (|i-j|=0)	1320
Sequential (|i-j|=1)	1306
Medium range (|i-j|>1 and |i-j|<5)	1376
Long range (|i-j|≥5)	0
Inter-chain	164
Hydrogen bond restraints	426
Disulfide bond restraints	0
Total dihedral-angle restraints	148
Number of unmapped restraints	0
Number of restraints per residue	35.6
Number of long range restraints per residue[1]	0.0

[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)	127.8	0.2
0.2-0.5 (Medium)	129.1	0.5
>0.5 (Large)	8.1	2.12

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	10.1	9.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

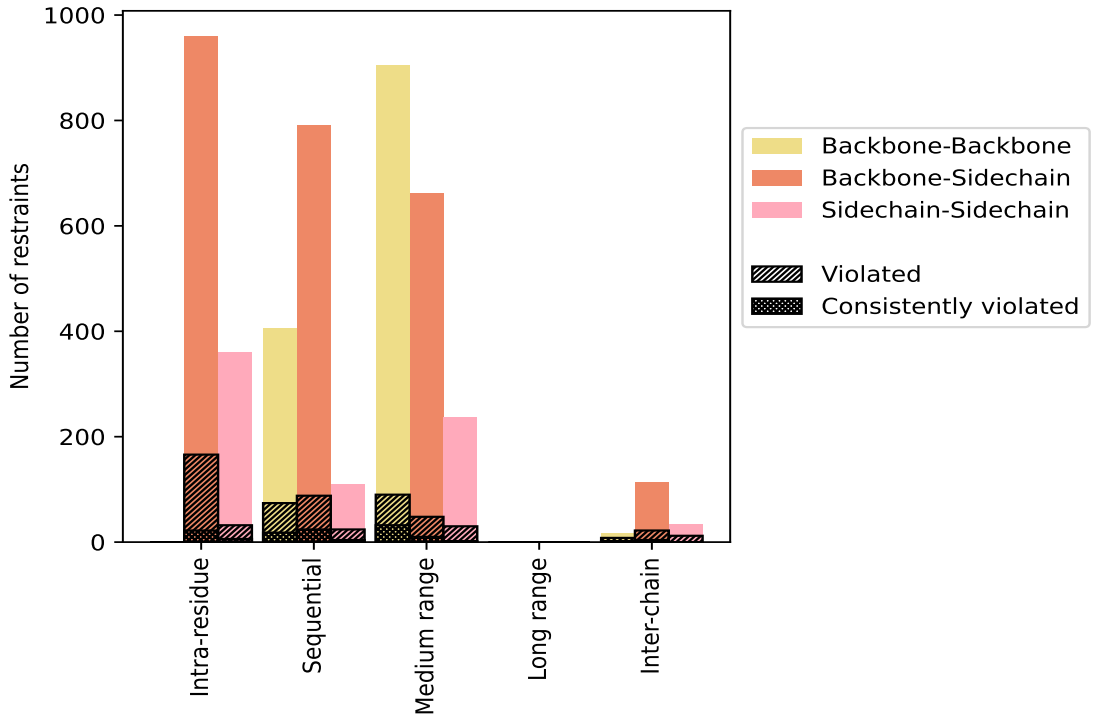
9.1 Summary of distance violations (i)

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)	1320	28.7	198	15.0	4.3	28	2.1	0.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	960	20.9	166	17.3	3.6	22	2.3	0.5
Sidechain-Sidechain	360	7.8	32	8.9	0.7	6	1.7	0.1
Sequential (|i-j|=1)	1306	28.4	186	14.2	4.1	46	3.5	1.0
Backbone-Backbone	406	8.8	74	18.2	1.6	18	4.4	0.4
Backbone-Sidechain	790	17.2	88	11.1	1.9	24	3.0	0.5
Sidechain-Sidechain	110	2.4	24	21.8	0.5	4	3.6	0.1
Medium range (|i-j|>1 & |i-j|<5)	1376	30.0	154	11.2	3.4	44	3.2	1.0
Backbone-Backbone	478	10.4	76	15.9	1.7	32	6.7	0.7
Backbone-Sidechain	662	14.4	48	7.3	1.0	10	1.5	0.2
Sidechain-Sidechain	236	5.1	30	12.7	0.7	2	0.8	0.0
Long range (|i-j|≥5)	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
Inter-chain	164	3.6	42	25.6	0.9	6	3.7	0.1
Backbone-Backbone	16	0.3	8	50.0	0.2	2	12.5	0.0
Backbone-Sidechain	114	2.5	22	19.3	0.5	4	3.5	0.1
Sidechain-Sidechain	34	0.7	12	35.3	0.3	0	0.0	0.0
Hydrogen bond	426	9.3	14	3.3	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4592	100.0	594	12.9	12.9	124	2.7	2.7
Backbone-Backbone	1326	28.9	172	13.0	3.7	52	3.9	1.1
Backbone-Sidechain	2526	55.0	324	12.8	7.1	60	2.4	1.3
Sidechain-Sidechain	740	16.1	98	13.2	2.1	12	1.6	0.3

[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	86	84	92	0	16	278	0.25	1.05	0.13	0.23
2	84	92	84	0	18	278	0.22	0.55	0.11	0.19
3	66	78	80	0	10	234	0.25	0.76	0.13	0.21
4	76	88	78	0	16	258	0.24	0.53	0.11	0.2
5	72	92	84	0	16	264	0.24	0.79	0.12	0.2
6	70	94	80	0	20	264	0.23	0.51	0.11	0.2
7	80	84	88	0	14	266	0.26	2.12	0.2	0.21
8	74	84	90	0	18	266	0.25	1.63	0.16	0.22
9	88	88	86	0	20	282	0.23	0.58	0.11	0.2
10	70	96	78	0	18	262	0.24	0.61	0.12	0.21
11	64	100	80	0	20	264	0.24	0.57	0.11	0.21

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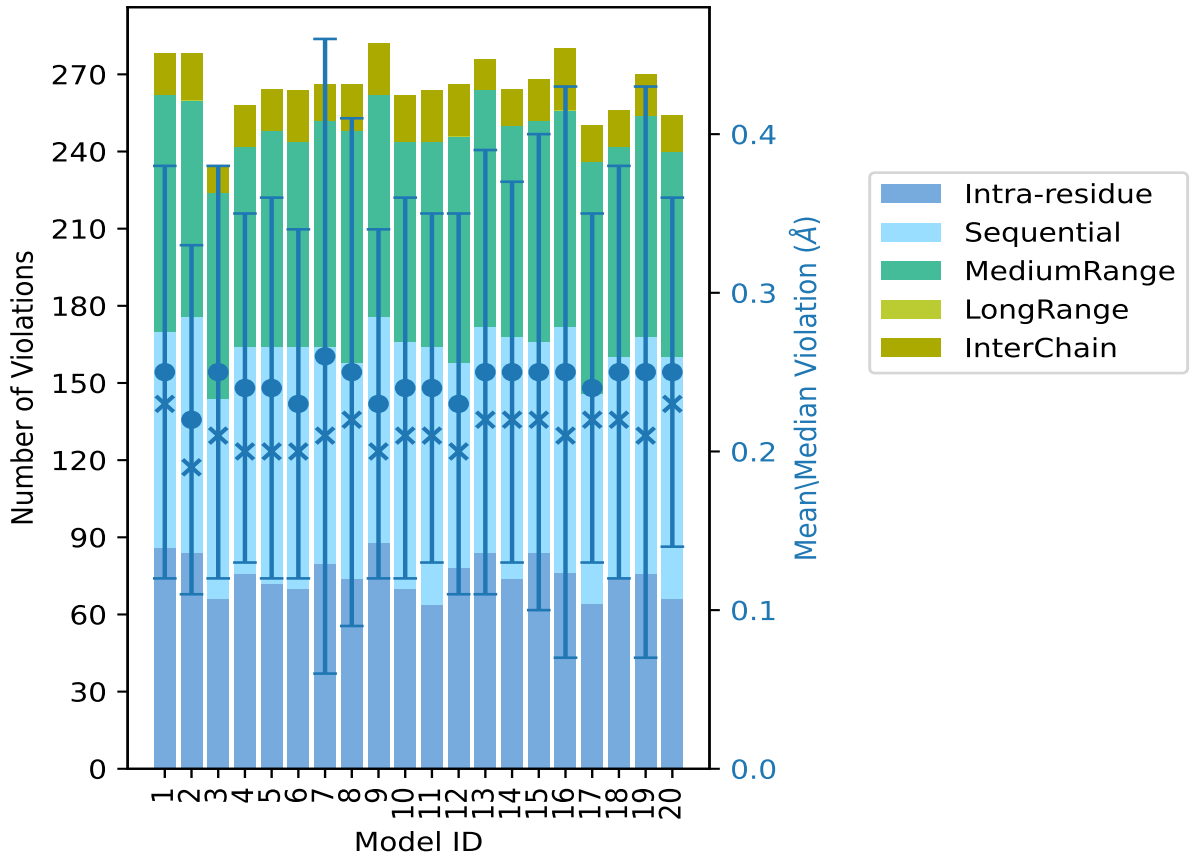
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	78	80	88	0	20	266	0.23	0.53	0.12	0.2
13	84	88	92	0	12	276	0.25	1.14	0.14	0.22
14	74	94	82	0	14	264	0.25	0.95	0.12	0.22
15	84	82	86	0	16	268	0.25	1.34	0.15	0.22
16	76	96	84	0	24	280	0.25	1.91	0.18	0.21
17	64	82	90	0	14	250	0.24	0.56	0.11	0.22
18	74	86	82	0	14	256	0.25	0.98	0.13	0.22
19	76	92	86	0	16	270	0.25	1.83	0.18	0.21
20	66	94	80	0	14	254	0.25	0.59	0.11	0.23

[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

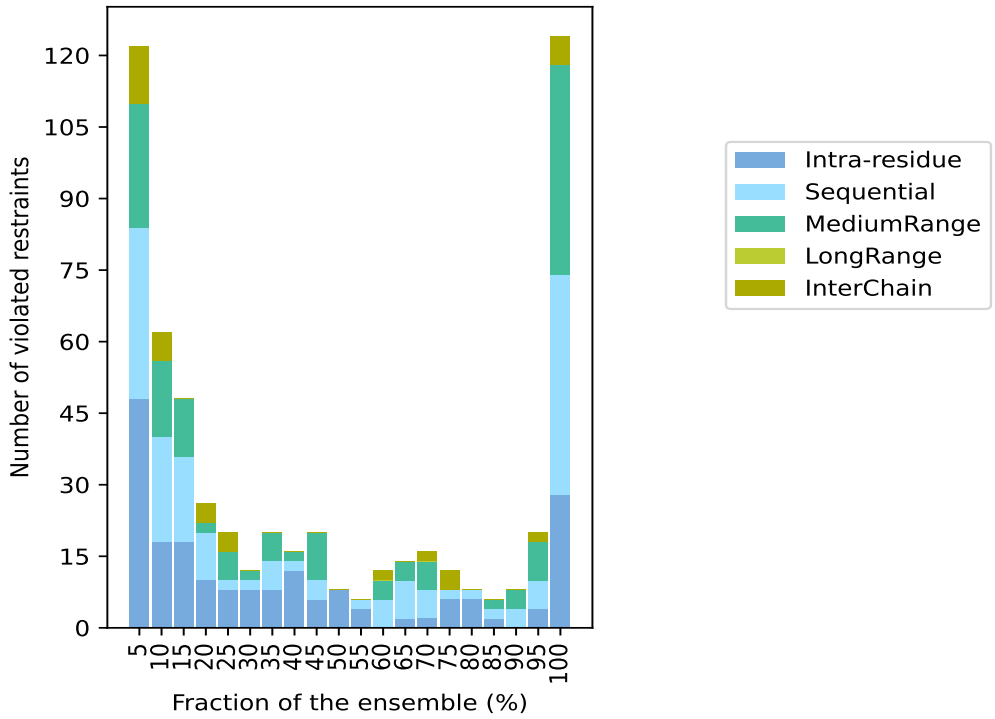
9.3 Distance violation statistics for the ensemble (i)

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, 3586(IR:1122, SQ:1120, MR:1222, LR:0, IC:122) 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]	%
48	36	26	0	12	122	1	5.0
18	22	16	0	6	62	2	10.0
18	18	12	0	0	48	3	15.0
10	10	2	0	4	26	4	20.0
8	2	6	0	4	20	5	25.0
8	2	2	0	0	12	6	30.0
8	6	6	0	0	20	7	35.0
12	2	2	0	0	16	8	40.0
6	4	10	0	0	20	9	45.0
8	0	0	0	0	8	10	50.0
4	2	0	0	0	6	11	55.0
0	6	4	0	2	12	12	60.0
2	8	4	0	0	14	13	65.0
2	6	6	0	2	16	14	70.0
6	2	0	0	4	12	15	75.0
6	2	0	0	0	8	16	80.0
2	2	2	0	0	6	17	85.0
0	4	4	0	0	8	18	90.0
4	6	8	0	2	20	19	95.0
28	46	44	0	6	124	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

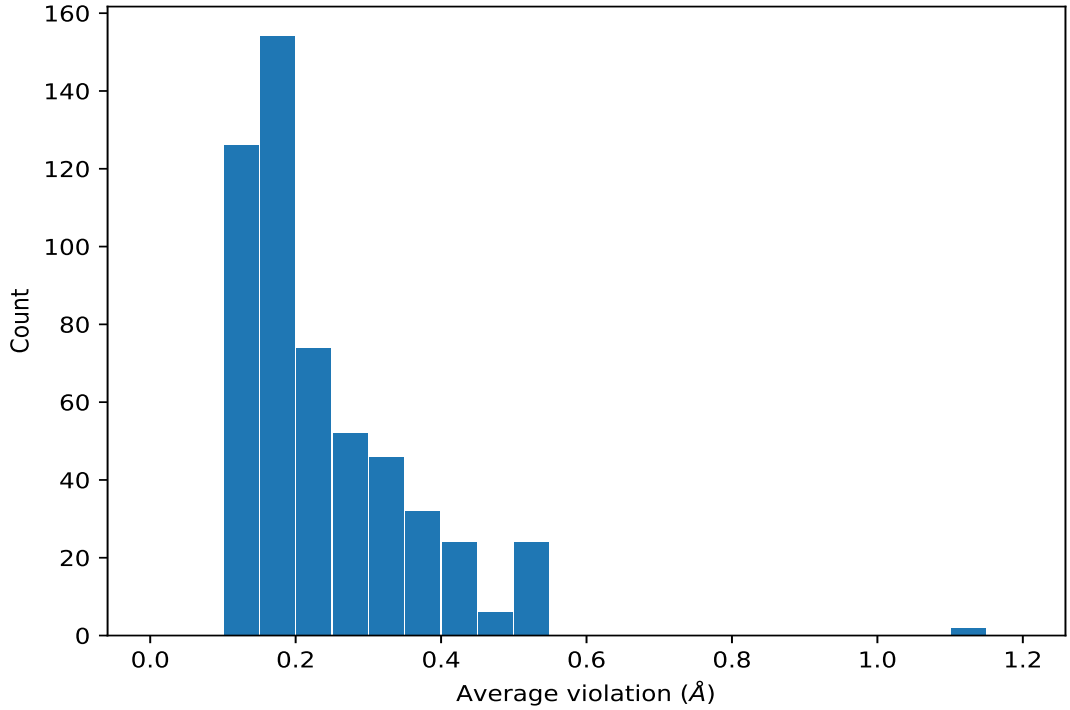
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

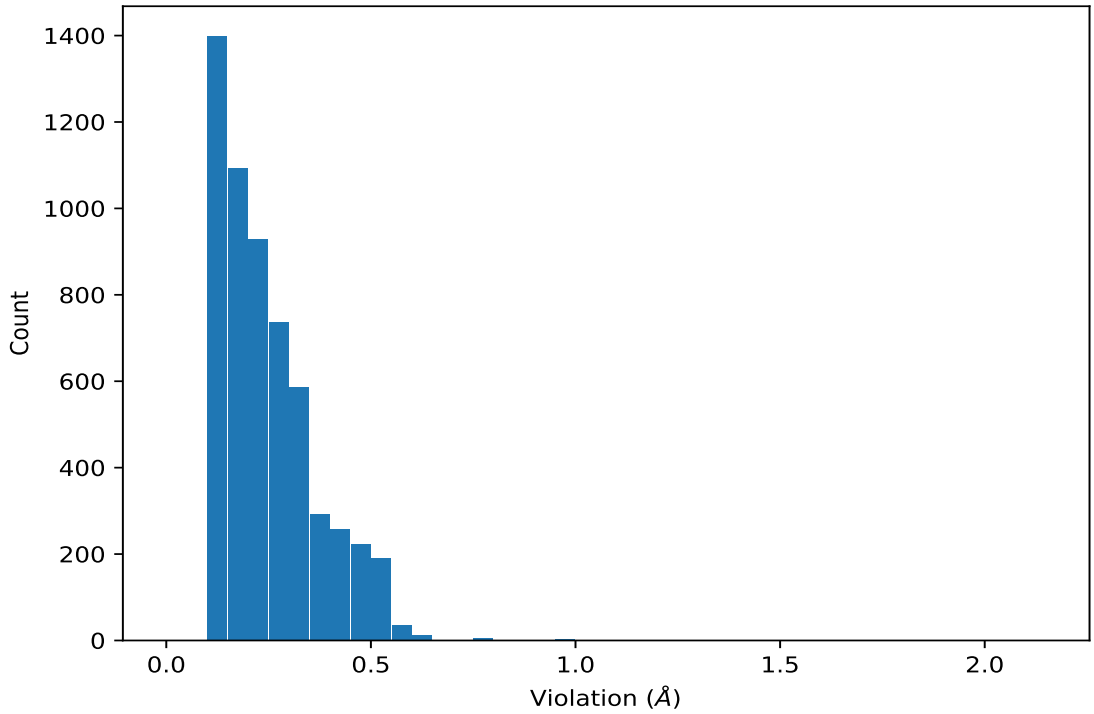
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	20	0.51	0.04	0.52
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	20	0.51	0.04	0.52
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	20	0.5	0.01	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	20	0.5	0.01	0.5
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	20	0.47	0.01	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	20	0.47	0.01	0.47
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	20	0.47	0.02	0.47
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	20	0.47	0.02	0.47
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	20	0.47	0.01	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	20	0.47	0.01	0.48

[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)
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	7	2.12
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	7	2.12
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	16	1.91
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	16	1.91
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	19	1.83
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	19	1.83
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	8	1.63
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	8	1.63
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	15	1.34
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	15	1.34

10 Dihedral-angle violation analysis (i)

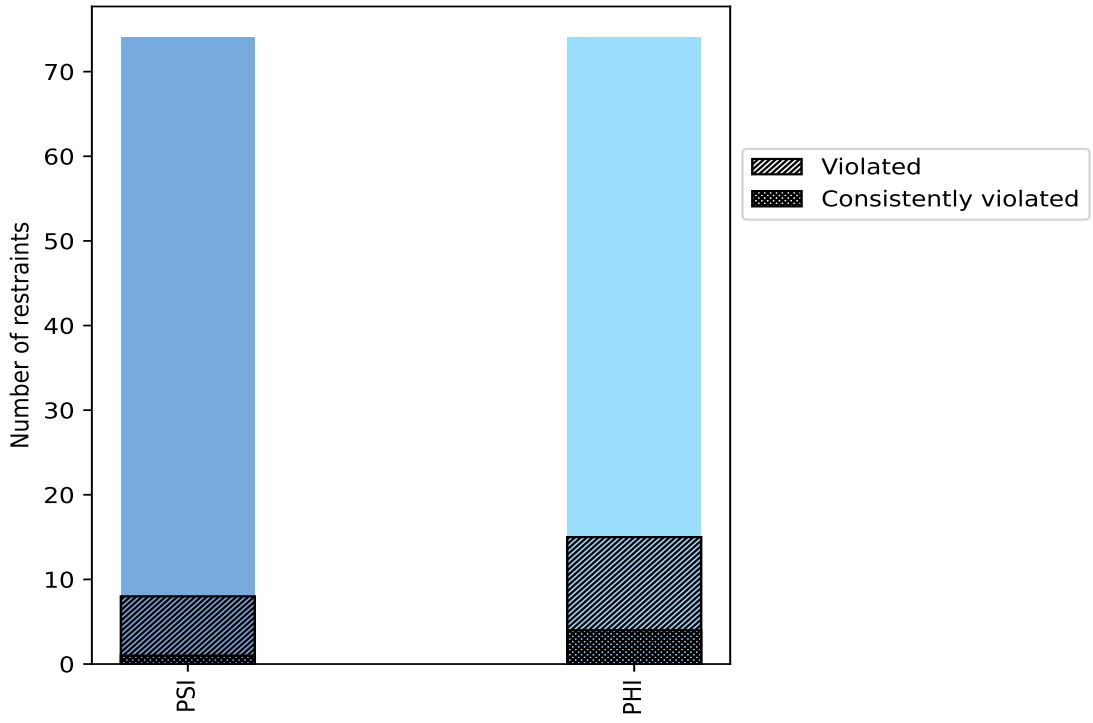
10.1 Summary of dihedral-angle violations (i)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	74	50.0	8	10.8	5.4	1	1.4	0.7
PHI	74	50.0	15	20.3	10.1	4	5.4	2.7
Total	148	100.0	23	15.5	15.5	5	3.4	3.4

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



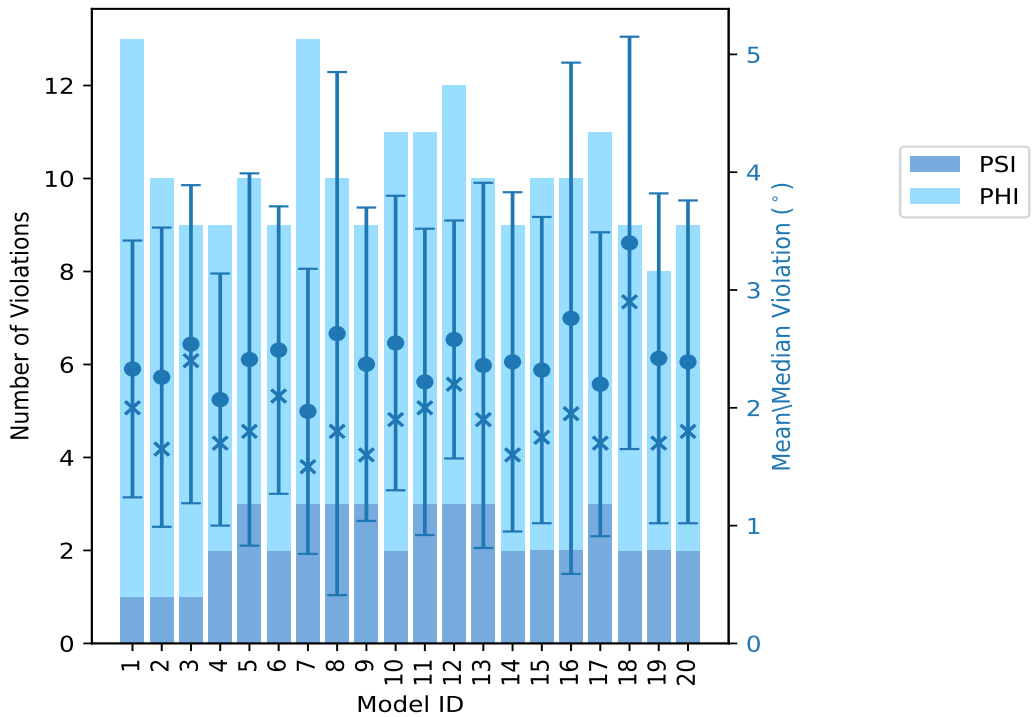
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	12	13	2.33	5.0	1.09	2.0
2	1	9	10	2.26	5.6	1.27	1.65
3	1	8	9	2.54	6.0	1.35	2.4
4	2	7	9	2.07	4.9	1.07	1.7
5	3	7	10	2.41	6.3	1.58	1.8
6	2	7	9	2.49	5.3	1.22	2.1
7	3	10	13	1.97	5.6	1.21	1.5
8	3	7	10	2.63	9.1	2.22	1.8
9	3	6	9	2.37	5.5	1.33	1.6
10	2	9	11	2.55	5.4	1.25	1.9
11	3	8	11	2.22	5.8	1.3	2.0
12	3	9	12	2.58	5.1	1.01	2.2
13	3	7	10	2.36	6.8	1.55	1.9
14	2	7	9	2.39	6.0	1.44	1.6
15	2	8	10	2.32	5.8	1.3	1.75
16	2	8	10	2.76	8.8	2.17	1.95
17	3	8	11	2.2	5.8	1.29	1.7
18	2	7	9	3.4	7.9	1.75	2.9
19	2	6	8	2.42	5.9	1.4	1.7
20	2	7	9	2.39	5.9	1.37	1.8

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
2	4	6	1	5.0
2	1	3	2	10.0
0	0	0	3	15.0
0	1	1	4	20.0
1	0	1	5	25.0
0	0	0	6	30.0
2	0	2	7	35.0
0	0	0	8	40.0
0	1	1	9	45.0
0	0	0	10	50.0
0	1	1	11	55.0

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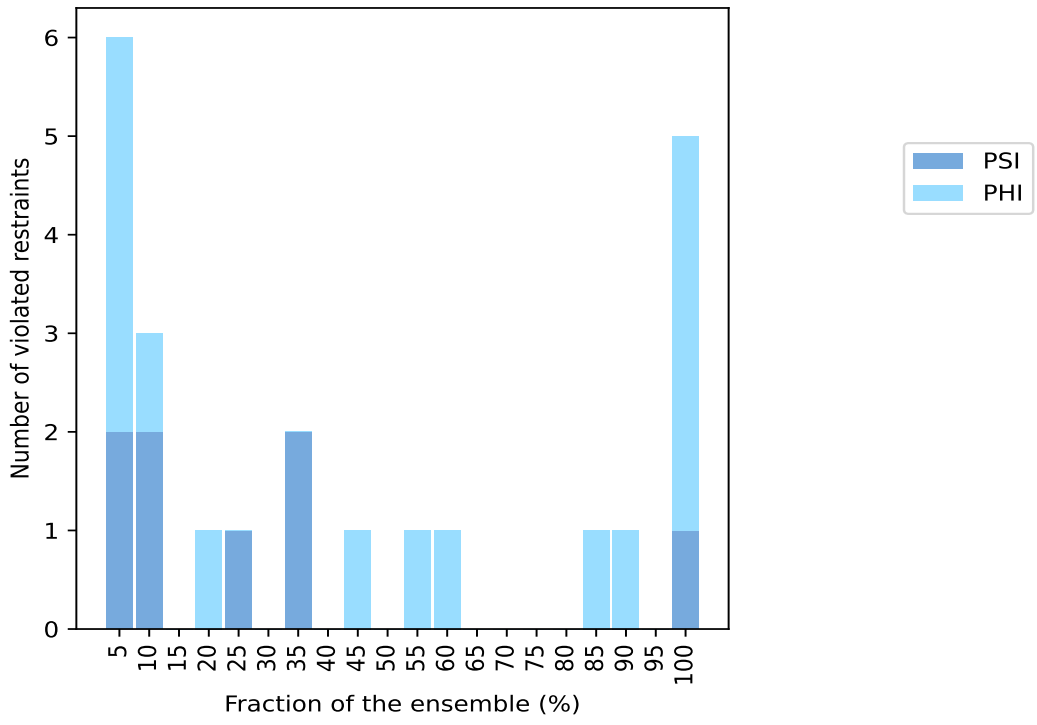
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	1	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	1	1	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
1	4	5	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)

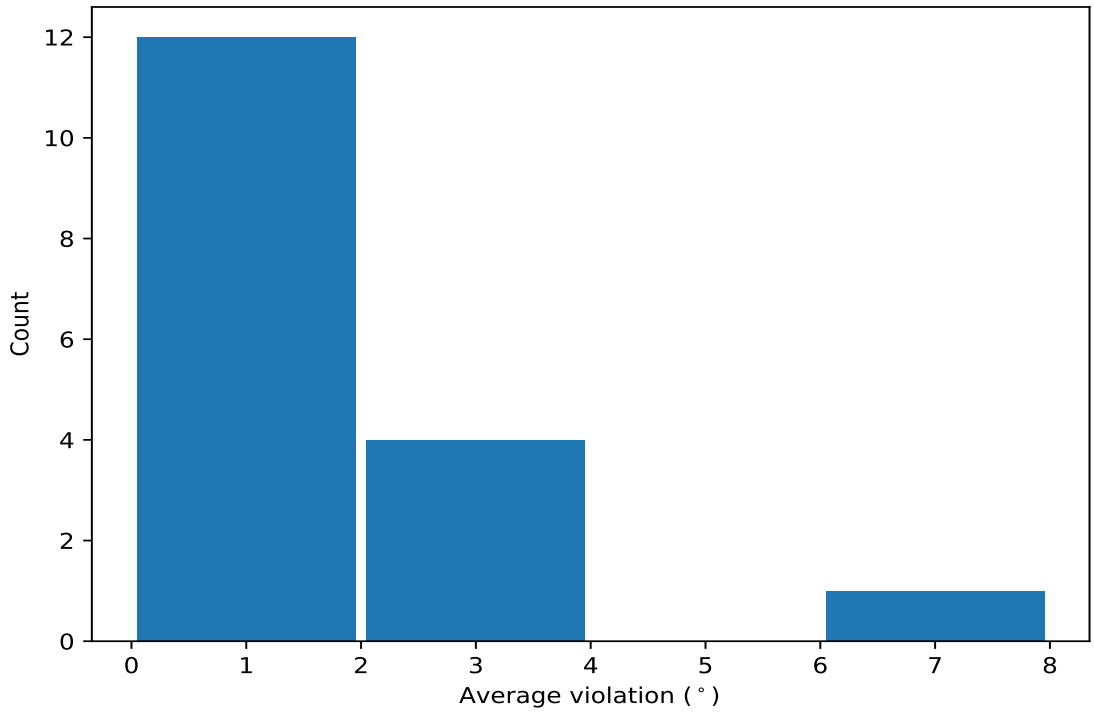


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

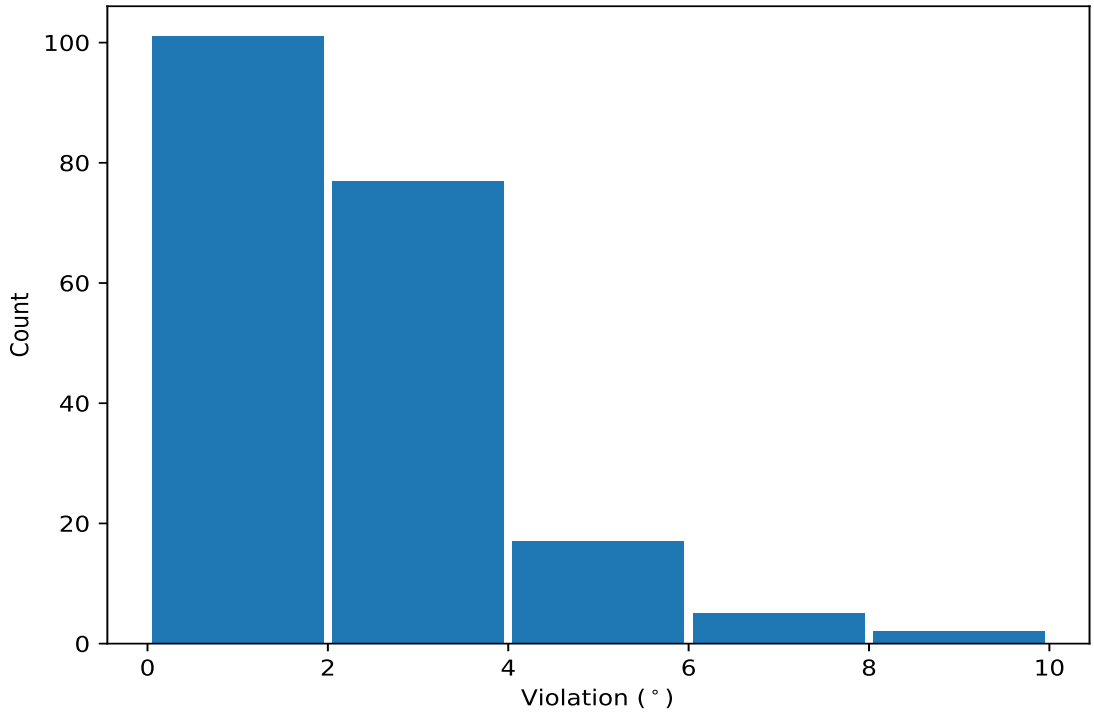
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	20	6.13	1.14	5.8
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	20	2.98	0.49	3.05
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	20	2.55	0.47	2.6
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	20	2.52	0.36	2.55
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	20	1.64	0.25	1.6
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	18	1.83	0.7	1.7
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	17	1.92	0.47	1.9
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	12	2.27	0.97	2.0
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	11	1.5	0.34	1.4
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	9	1.41	0.32	1.3

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table provides the list of violationsfor 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	8	9.1
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	16	8.8
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	18	7.9
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	13	6.8
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	5	6.3
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	3	6.0
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	14	6.0
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	19	5.9
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	20	5.9
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	11	5.8