Full wwPDB NMR Structure Validation Report (i)

Dec 25, 2024 – 07:06 PM EST

PDB ID	:	7ZEY
BMRB ID	:	34727
Title	:	Complex Cyp33-RRM : MLL1-PHD3
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Deposited on	:	2022-03-31

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

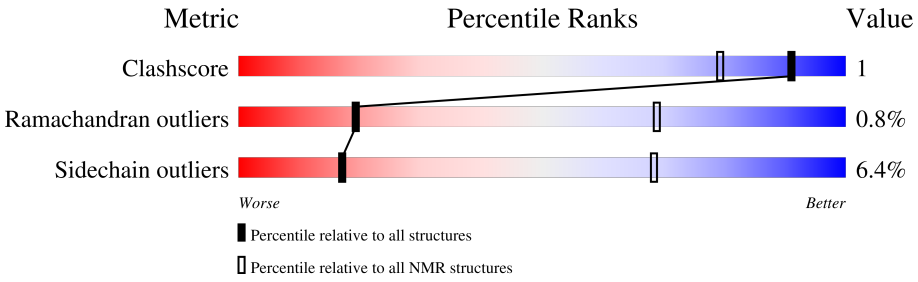
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 79%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	117	76% 11% 13%
2	B	64	91% · 6%

2 Ensemble composition and analysis (i)

This entry contains 20 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:3-A:88, A:92-A:107, B:1568-B:1627 (162)	0.62	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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2808 atoms, of which 1368 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	117	1836	589	908	157	179	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q9UNP9
A	-2	GLY	-	expression tag	UNP Q9UNP9
A	-1	HIS	-	expression tag	UNP Q9UNP9

- Molecule 2 is a protein called MLL cleavage product N320.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	64	970	310	460	83	106	11	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	B	2	2	2

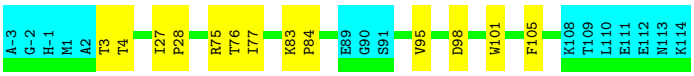
4 Residue-property plots (i)

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.

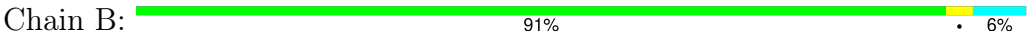
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

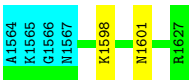
Chain A:



• Molecule 2: MLL cleavage product N320

Chain B:





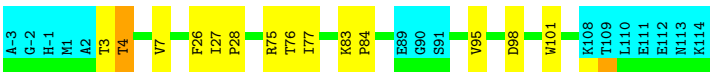
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

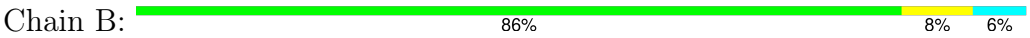
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

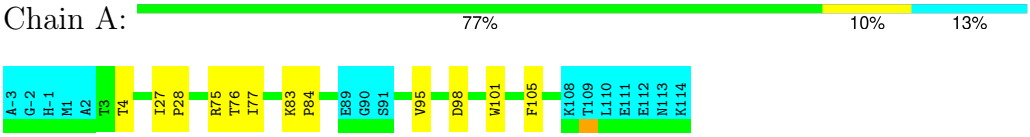
Chain B:



4.2.2 Score per residue for model 2

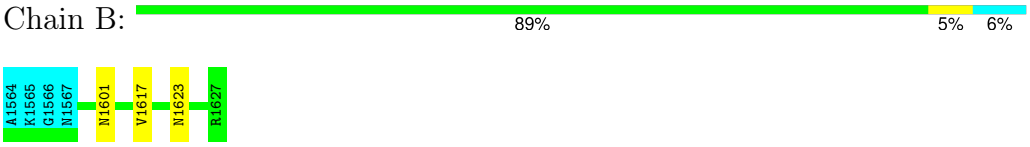
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

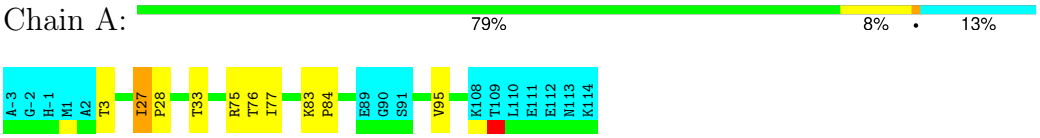
Chain B:



4.2.3 Score per residue for model 3

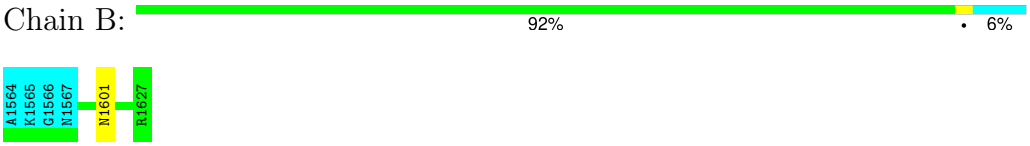
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

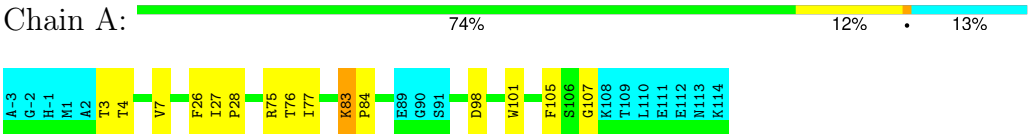
Chain B:



4.2.4 Score per residue for model 4

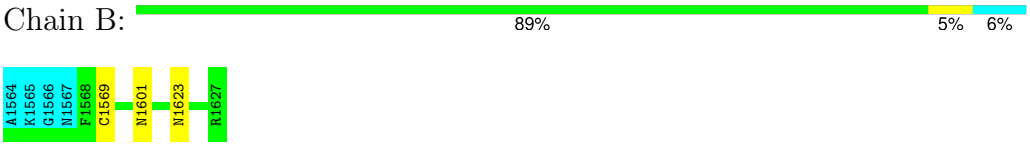
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

Chain B:



4.2.5 Score per residue for model 5

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:

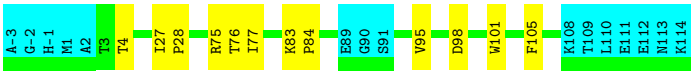
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.6 Score per residue for model 6

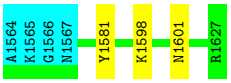
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

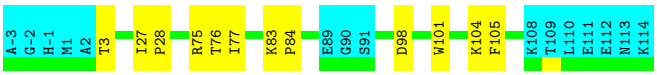
Chain B:



4.2.7 Score per residue for model 7

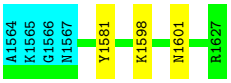
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

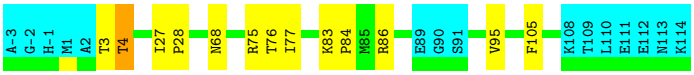
Chain B:



4.2.8 Score per residue for model 8

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



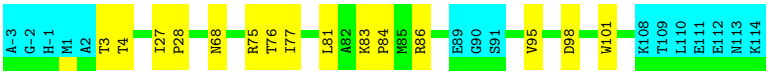
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.9 Score per residue for model 9

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



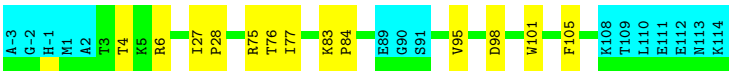
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.10 Score per residue for model 10

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

Chain B:

4.2.11 Score per residue for model 11

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:

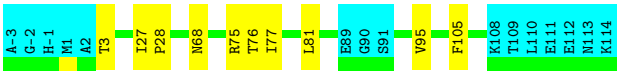
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



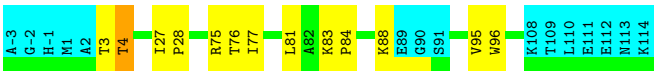
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.13 Score per residue for model 13

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



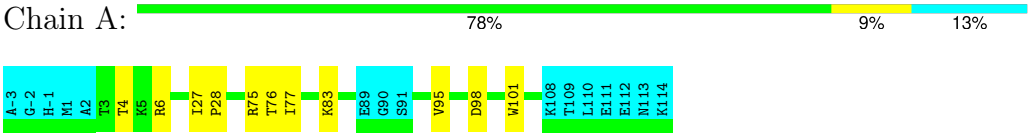
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.14 Score per residue for model 14

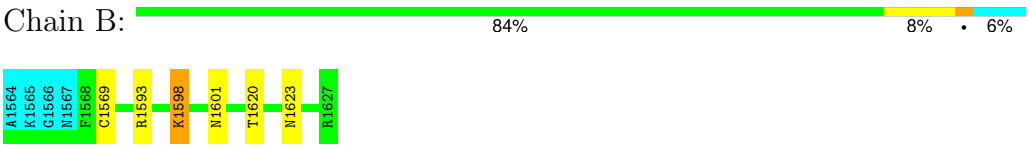
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

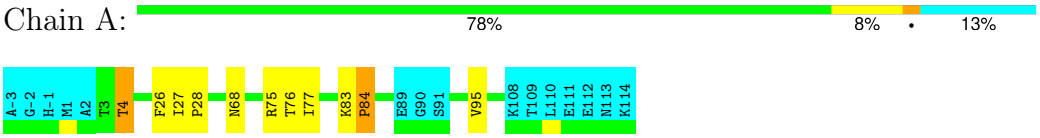
Chain B:



4.2.15 Score per residue for model 15

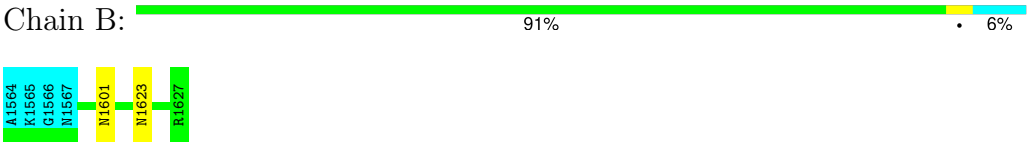
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

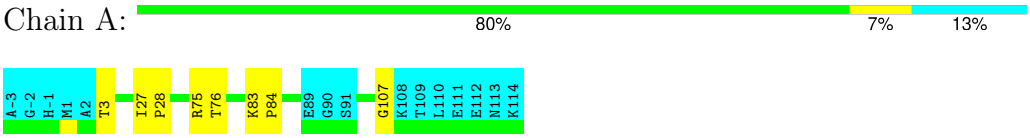
Chain B:



4.2.16 Score per residue for model 16

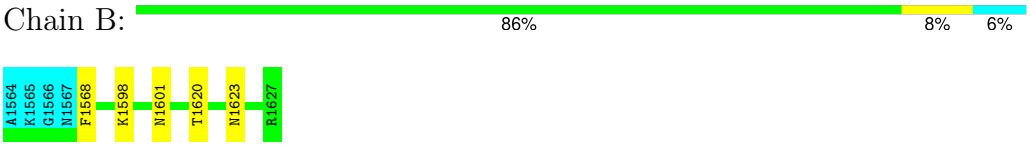
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

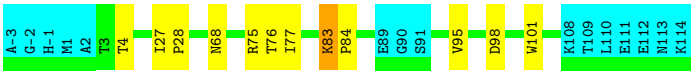
Chain B:



4.2.17 Score per residue for model 17

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



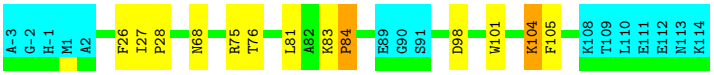
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.18 Score per residue for model 18

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

Chain B:

4.2.19 Score per residue for model 19

• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:

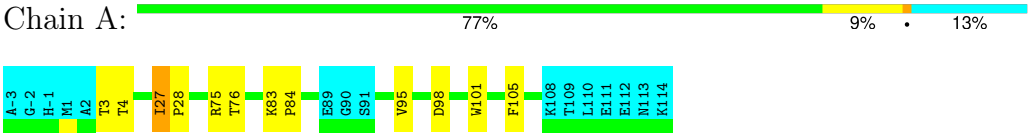
• Molecule 2: MLL cleavage product N320

Chain B:

4.2.20 Score per residue for model 20

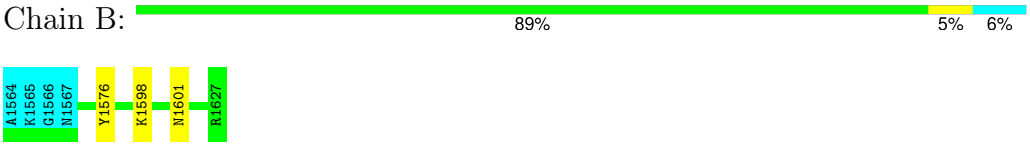
• Molecule 1: Peptidyl-prolyl cis-trans isomerase E

Chain A:



• Molecule 2: MLL cleavage product N320

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 250 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
Amber	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	2
Total number of shifts	1872
Number of shifts mapped to atoms	1872
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

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	818	801	801	3±1
2	B	484	433	433	1±1
All	All	26080	24680	24680	74

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:LYS:N	1:A:84:PRO:CD	0.52	2.72	16	14
1:A:27:ILE:N	1:A:28:PRO:CD	0.50	2.75	4	20
2:B:1585:MET:SD	2:B:1596:HIS:CD2	0.48	3.06	17	2
2:B:1584:LYS:HE3	2:B:1607:TYR:CE2	0.47	2.44	11	1
1:A:98:ASP:HA	1:A:101:TRP:CD1	0.46	2.45	7	8
1:A:88:LYS:HE2	1:A:96:TRP:CZ2	0.44	2.47	13	1
1:A:83:LYS:N	1:A:84:PRO:HD2	0.44	2.27	5	6
2:B:1598:LYS:HE2	2:B:1598:LYS:N	0.44	2.28	6	3
2:B:1598:LYS:CA	2:B:1598:LYS:HE2	0.44	2.43	16	1
1:A:81:LEU:H	1:A:81:LEU:HD22	0.44	1.73	13	3
1:A:98:ASP:O	1:A:101:TRP:CD1	0.42	2.72	6	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:PHE:C	1:A:28:PRO:HD2	0.42	2.35	1	4
2:B:1598:LYS:HE2	2:B:1598:LYS:HA	0.42	1.91	16	1
2:B:1596:HIS:HB2	2:B:1599:CYS:SG	0.41	2.56	1	1
1:A:104:LYS:HA	1:A:104:LYS:HE3	0.41	1.92	18	1
2:B:1598:LYS:N	2:B:1598:LYS:HE2	0.41	2.31	5	3
2:B:1598:LYS:HE2	2:B:1598:LYS:CA	0.40	2.46	7	1
1:A:81:LEU:HD22	1:A:81:LEU:H	0.40	1.77	9	1

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	102/117 (87%)	91±2 (89±2%)	10±2 (10±2%)	1±1 (1±1%)	15	64
2	B	59/64 (92%)	55±2 (94±3%)	4±2 (6±3%)	0±0 (0±1%)	45	81
All	All	3220/3620 (89%)	2922 (91%)	273 (8%)	25 (1%)	19	69

All 5 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	95	VAL	14
1	A	4	THR	4
1	A	107	GLY	3
2	B	1576	TYR	2
1	A	84	PRO	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	86/97 (89%)	80±1 (93±2%)	6±1 (7±2%)	16	67
2	B	58/60 (97%)	55±2 (94±3%)	3±2 (6±3%)	19	71
All	All	2880/3140 (92%)	2696 (94%)	184 (6%)	17	68

All 32 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	75	ARG	20
1	A	76	THR	20
2	B	1601	ASN	19
1	A	4	THR	14
1	A	77	ILE	14
1	A	3	THR	11
1	A	105	PHE	11
2	B	1623	ASN	10
1	A	68	ASN	8
2	B	1569	CYS	7
2	B	1620	THR	6
2	B	1581	TYR	6
1	A	86	ARG	4
2	B	1598	LYS	4
1	A	83	LYS	3
2	B	1610	LEU	3
1	A	7	VAL	2
2	B	1617	VAL	2
1	A	27	ILE	2
2	B	1591	CYS	2
1	A	104	LYS	2
1	A	6	ARG	2
2	B	1593	ARG	2
2	B	1568	PHE	2
1	A	33	THR	1
2	B	1622	VAL	1
2	B	1574	LYS	1
2	B	1584	LYS	1
2	B	1619	TYR	1
1	A	40	ASP	1
2	B	1595	VAL	1
2	B	1576	TYR	1

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 oligosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 79% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *shift_set_1*

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	1243
Number of shifts mapped to atoms	1243
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
$^{13}C_{\alpha}$	100	-0.36 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	102	-0.01 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	106	0.44 ± 0.35	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 52%, i.e. 1124 atoms were assigned a chemical shift out of a possible 2179. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	380/805 (47%)	193/325 (59%)	92/324 (28%)	95/156 (61%)
Sidechain	650/1183 (55%)	444/762 (58%)	202/378 (53%)	4/43 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	94/191 (49%)	56/94 (60%)	36/91 (40%)	2/6 (33%)
Overall	1124/2179 (52%)	693/1181 (59%)	330/793 (42%)	101/205 (49%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 1243 atoms were assigned a chemical shift out of a possible 2405. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	420/903 (47%)	214/366 (58%)	100/362 (28%)	106/175 (61%)
Sidechain	725/1304 (56%)	496/839 (59%)	224/417 (54%)	5/48 (10%)
Aromatic	98/198 (49%)	58/98 (59%)	38/93 (41%)	2/7 (29%)
Overall	1243/2405 (52%)	768/1303 (59%)	362/872 (42%)	113/230 (49%)

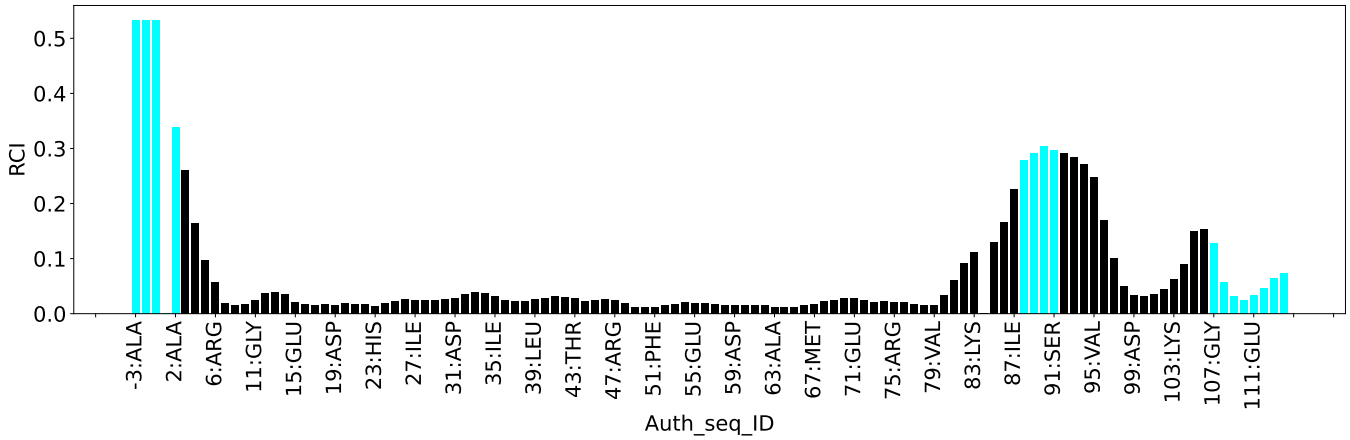
7.1.4 Statistically unusual chemical shifts (i)

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *MLL_renumb.str*

7.2.1 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	629
Number of shifts mapped to atoms	629
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	58	-0.54 ± 0.17	Should be checked
$^{13}C_{\beta}$	57	0.08 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	54	-0.42 ± 0.37	None needed (< 0.5 ppm)

7.2.3 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 27%, i.e. 592 atoms were assigned a chemical shift out of a possible 2179. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	211/805 (26%)	106/325 (33%)	54/324 (17%)	51/156 (33%)
Sidechain	333/1183 (28%)	226/762 (30%)	103/378 (27%)	4/43 (9%)
Aromatic	48/191 (25%)	29/94 (31%)	18/91 (20%)	1/6 (17%)
Overall	592/2179 (27%)	361/1181 (31%)	175/793 (22%)	56/205 (27%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 26%, i.e. 629 atoms were assigned a chemical shift out of a possible 2405. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	226/903 (25%)	114/366 (31%)	58/362 (16%)	54/175 (31%)
Sidechain	355/1304 (27%)	241/839 (29%)	109/417 (26%)	5/48 (10%)
Aromatic	48/198 (24%)	29/98 (30%)	18/93 (19%)	1/7 (14%)
Overall	629/2405 (26%)	384/1303 (29%)	185/872 (21%)	60/230 (26%)

7.2.4 Statistically unusual chemical shifts (i)

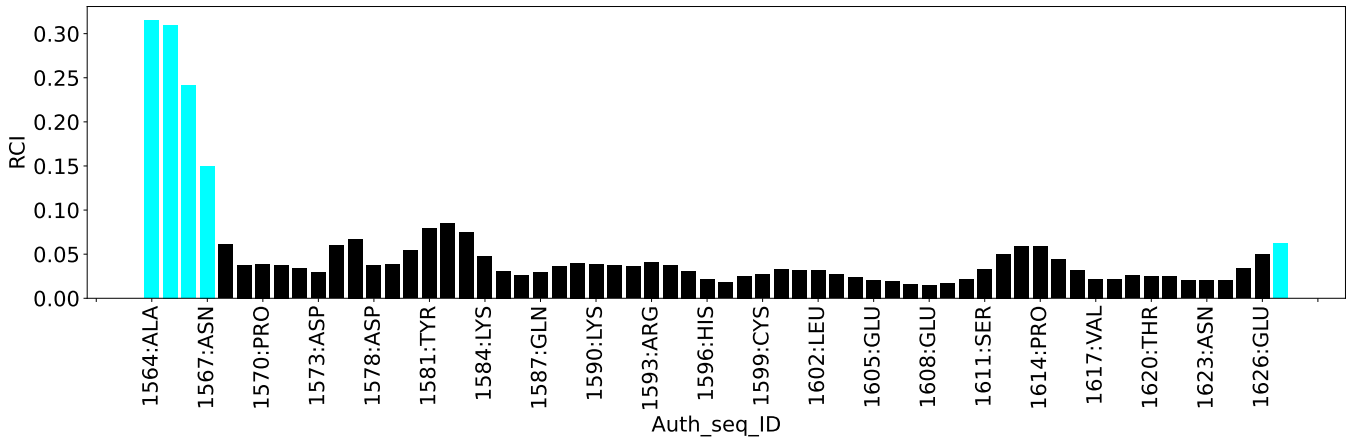
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	1594	TRP	NE1	114.59	118.53 – 139.98	-6.8
2	B	1587	GLN	HG3	0.79	0.91 – 3.68	-5.5

7.2.5 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 B:



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	4022
Intra-residue (|i-j|=0)	597
Sequential (|i-j|=1)	1057
Medium range (|i-j|>1 and |i-j|<5)	778
Long range (|i-j|≥5)	1397
Inter-chain	193
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	176
Number of unmapped restraints	0
Number of restraints per residue	22.9
Number of long range restraints per residue[1]	7.6

[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)	4.5	0.19
0.2-0.5 (Medium)	0.5	0.33
>0.5 (Large)	0.5	0.76

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)	0.1	1.22
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

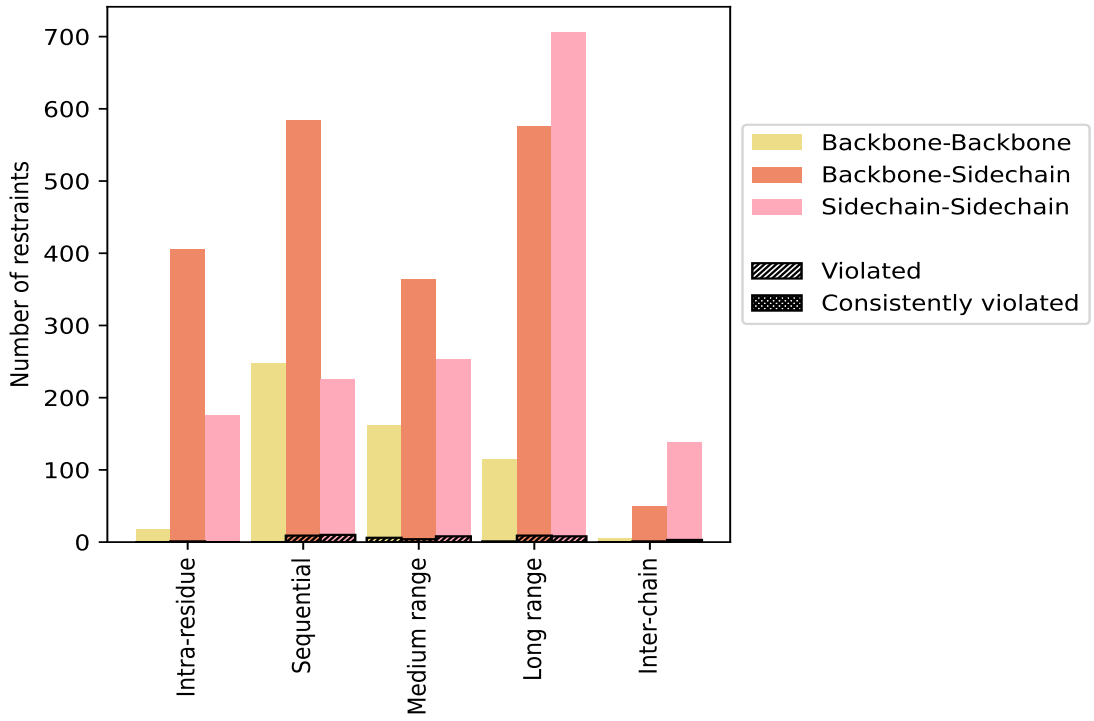
9.1 Summary of distance violations (i)

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)	597	14.8	1	0.2	0.0	0	0.0	0.0
Backbone-Backbone	17	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	405	10.1	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	175	4.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1057	26.3	19	1.8	0.5	0	0.0	0.0
Backbone-Backbone	247	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	584	14.5	9	1.5	0.2	0	0.0	0.0
Sidechain-Sidechain	226	5.6	10	4.4	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	778	19.3	18	2.3	0.4	0	0.0	0.0
Backbone-Backbone	161	4.0	6	3.7	0.1	0	0.0	0.0
Backbone-Sidechain	364	9.1	4	1.1	0.1	0	0.0	0.0
Sidechain-Sidechain	253	6.3	8	3.2	0.2	0	0.0	0.0
Long range (|i-j|≥5)	1397	34.7	18	1.3	0.4	0	0.0	0.0
Backbone-Backbone	115	2.9	1	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	576	14.3	9	1.6	0.2	0	0.0	0.0
Sidechain-Sidechain	706	17.6	8	1.1	0.2	0	0.0	0.0
Inter-chain	193	4.8	4	2.1	0.1	0	0.0	0.0
Backbone-Backbone	5	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	50	1.2	1	2.0	0.0	0	0.0	0.0
Sidechain-Sidechain	138	3.4	3	2.2	0.1	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	4022	100.0	60	1.5	1.5	0	0.0	0.0
Backbone-Backbone	545	13.6	7	1.3	0.2	0	0.0	0.0
Backbone-Sidechain	1979	49.2	24	1.2	0.6	0	0.0	0.0
Sidechain-Sidechain	1498	37.2	29	1.9	0.7	0	0.0	0.0

[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	0	2	2	1	1	6	0.24	0.71	0.21	0.16
2	0	2	2	2	2	8	0.22	0.76	0.21	0.15
3	1	2	1	1	2	7	0.22	0.74	0.21	0.15
4	0	2	3	0	1	6	0.23	0.73	0.23	0.13
5	0	0	1	1	0	2	0.12	0.13	0.01	0.12
6	0	0	1	0	1	2	0.11	0.11	0.0	0.11
7	0	4	1	1	1	7	0.17	0.33	0.07	0.14
8	0	1	2	4	0	7	0.11	0.14	0.01	0.11
9	1	3	0	1	1	6	0.16	0.22	0.03	0.15
10	0	3	2	2	2	9	0.19	0.69	0.18	0.13

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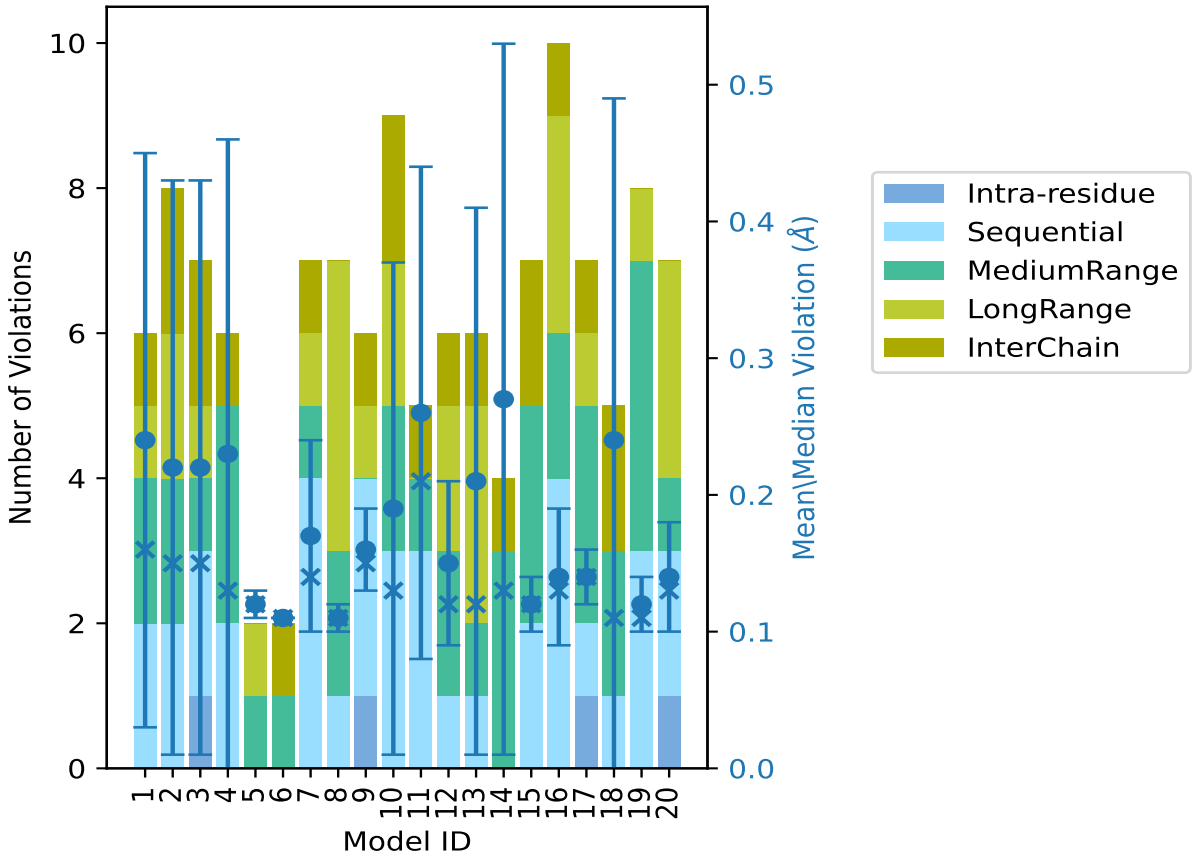
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	3	1	0	1	5	0.26	0.6	0.18	0.21
12	0	1	2	2	1	6	0.15	0.24	0.06	0.12
13	0	1	1	3	1	6	0.21	0.66	0.2	0.12
14	0	0	3	0	1	4	0.27	0.72	0.26	0.13
15	0	2	3	0	2	7	0.12	0.15	0.02	0.12
16	0	4	2	3	1	10	0.14	0.27	0.05	0.13
17	1	1	3	1	1	7	0.14	0.16	0.02	0.14
18	0	1	2	0	2	5	0.24	0.73	0.25	0.11
19	0	3	4	1	0	8	0.12	0.16	0.02	0.11
20	1	2	1	3	0	7	0.14	0.21	0.04	0.13

[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

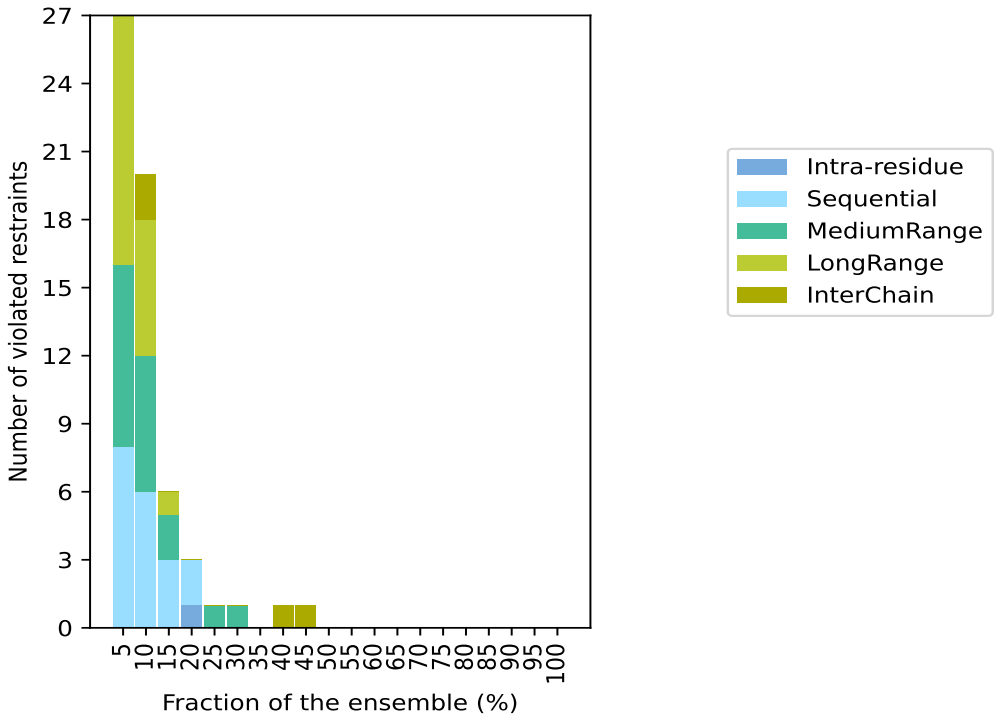
9.3 Distance violation statistics for the ensemble (i)

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, 3962(IR:596, SQ:1038, MR:760, LR:1379, IC:189) 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]	%
0	8	8	11	0	27	1	5.0
0	6	6	6	2	20	2	10.0
0	3	2	1	0	6	3	15.0
1	2	0	0	0	3	4	20.0
0	0	1	0	0	1	5	25.0
0	0	1	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	1	1	8	40.0
0	0	0	0	1	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	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

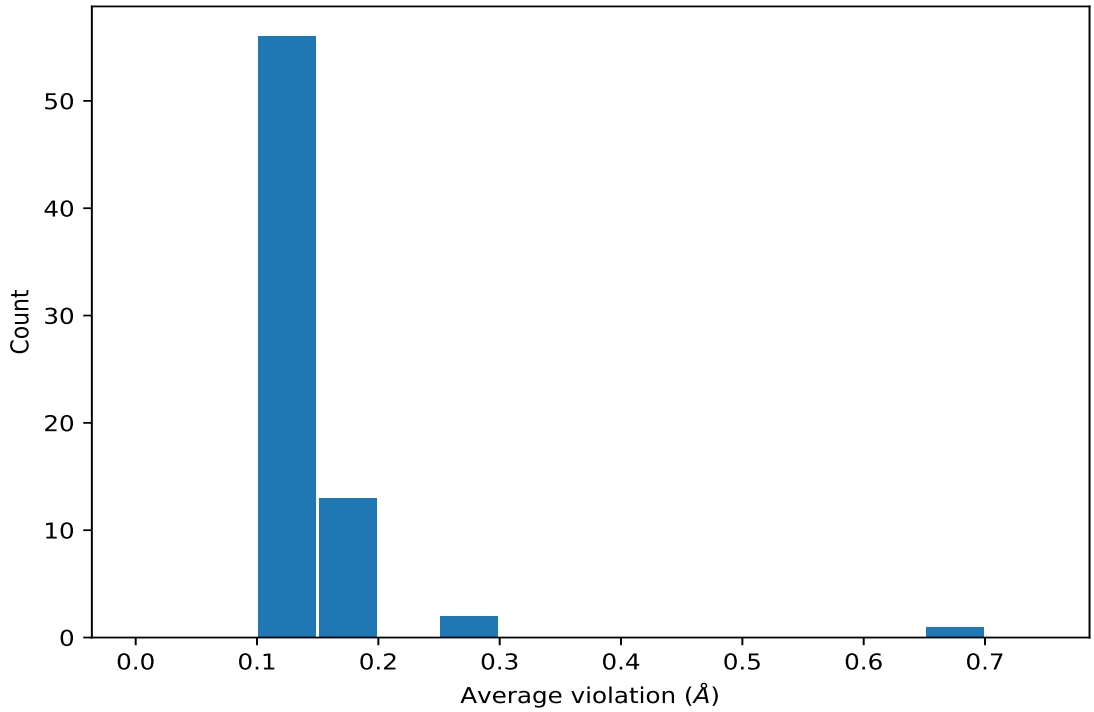
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

The following table provides the mean and the standard deviation of theviolation 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)	Median (Å)
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	9	0.7	0.05	0.72
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG21	8	0.18	0.06	0.16
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG22	8	0.18	0.06	0.16
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG23	8	0.18	0.06	0.16
(3,327)	2:1589:B:GLY:HA2	2:1592:B:ASP:HA	6	0.12	0.01	0.12
(2,1)	1:3:A:THR:HB	1:5:A:LYS:HB3	5	0.12	0.01	0.11
(3,122)	2:1575:B:CYS:HB2	2:1576:B:TYR:HB2	4	0.17	0.03	0.16
(3,122)	2:1575:B:CYS:HB3	2:1576:B:TYR:HB2	4	0.17	0.03	0.16
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD2	4	0.17	0.04	0.18
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD3	4	0.17	0.04	0.18
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE1	4	0.16	0.01	0.16
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE2	4	0.16	0.01	0.16
(1,2526)	1:92:A:SER:HB2	1:93:A:ARG:HB3	3	0.16	0.01	0.16
(1,2526)	1:92:A:SER:HB3	1:93:A:ARG:HB3	3	0.16	0.01	0.16
(1,2712)	1:109:A:THR:HG21	1:110:A:LEU:HG	3	0.13	0.02	0.12
(1,2712)	1:109:A:THR:HG22	1:110:A:LEU:HG	3	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2712)	1:109:A:THR:HG23	1:110:A:LEU:HG	3	0.13	0.02	0.12
(3,695)	2:1610:B:LEU:HD11	2:1611:B:SER:HA	3	0.13	0.01	0.12
(3,695)	2:1610:B:LEU:HD12	2:1611:B:SER:HA	3	0.13	0.01	0.12
(3,695)	2:1610:B:LEU:HD13	2:1611:B:SER:HA	3	0.13	0.01	0.12
(3,695)	2:1610:B:LEU:HD21	2:1611:B:SER:HA	3	0.13	0.01	0.12
(3,695)	2:1610:B:LEU:HD22	2:1611:B:SER:HA	3	0.13	0.01	0.12
(3,695)	2:1610:B:LEU:HD23	2:1611:B:SER:HA	3	0.13	0.01	0.12
(2,120)	1:101:A:TRP:HA	1:105:A:PHE:HA	3	0.12	0.02	0.11
(1,1966)	1:64:A:ILE:H	1:80:A:ASN:HA	3	0.11	0.0	0.11
(4,14)	2:1592:B:ASP:HA	2:1594:B:TRP:HA	3	0.1	0.0	0.1
(3,924)	2:1626:B:GLU:HB2	2:1627:B:ARG:HD2	2	0.3	0.03	0.3
(3,924)	2:1626:B:GLU:HB2	2:1627:B:ARG:HD3	2	0.3	0.03	0.3
(1,2503)	1:88:A:LYS:HA	1:90:A:GLY:H	2	0.18	0.01	0.18
(1,28)	1:4:A:THR:H	1:5:A:LYS:HB3	2	0.17	0.02	0.17
(1,2719)	1:110:A:LEU:HD11	1:111:A:GLU:HB2	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD11	1:111:A:GLU:HB3	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD12	1:111:A:GLU:HB2	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD12	1:111:A:GLU:HB3	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD13	1:111:A:GLU:HB2	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD13	1:111:A:GLU:HB3	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD21	1:111:A:GLU:HB2	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD21	1:111:A:GLU:HB3	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD22	1:111:A:GLU:HB2	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD22	1:111:A:GLU:HB3	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD23	1:111:A:GLU:HB2	2	0.15	0.01	0.15
(1,2719)	1:110:A:LEU:HD23	1:111:A:GLU:HB3	2	0.15	0.01	0.15
(1,2684)	1:104:A:LYS:HA	1:107:A:GLY:HA2	2	0.14	0.02	0.14
(1,2684)	1:104:A:LYS:HA	1:107:A:GLY:HA3	2	0.14	0.02	0.14
(2,75)	1:56:A:LEU:HD11	1:58:A:GLU:HG2	2	0.14	0.0	0.14
(2,75)	1:56:A:LEU:HD11	1:58:A:GLU:HG3	2	0.14	0.0	0.14
(2,75)	1:56:A:LEU:HD12	1:58:A:GLU:HG2	2	0.14	0.0	0.14
(2,75)	1:56:A:LEU:HD12	1:58:A:GLU:HG3	2	0.14	0.0	0.14
(2,75)	1:56:A:LEU:HD13	1:58:A:GLU:HG2	2	0.14	0.0	0.14
(2,75)	1:56:A:LEU:HD13	1:58:A:GLU:HG3	2	0.14	0.0	0.14
(1,2379)	1:78:A:ARG:HD2	1:80:A:ASN:HD21	2	0.13	0.02	0.13
(3,146)	2:1579:B:ASP:HB2	2:1583:B:SER:HB2	2	0.13	0.02	0.13
(3,146)	2:1579:B:ASP:HB2	2:1583:B:SER:HB3	2	0.13	0.02	0.13
(3,146)	2:1579:B:ASP:HB3	2:1583:B:SER:HB2	2	0.13	0.02	0.13
(3,146)	2:1579:B:ASP:HB3	2:1583:B:SER:HB3	2	0.13	0.02	0.13
(1,2440)	1:84:A:PRO:HG2	1:85:A:MET:HG2	2	0.12	0.02	0.12
(1,2440)	1:84:A:PRO:HG2	1:85:A:MET:HG3	2	0.12	0.02	0.12
(3,131)	2:1576:B:TYR:HD1	2:1596:B:HIS:HE1	2	0.12	0.02	0.12

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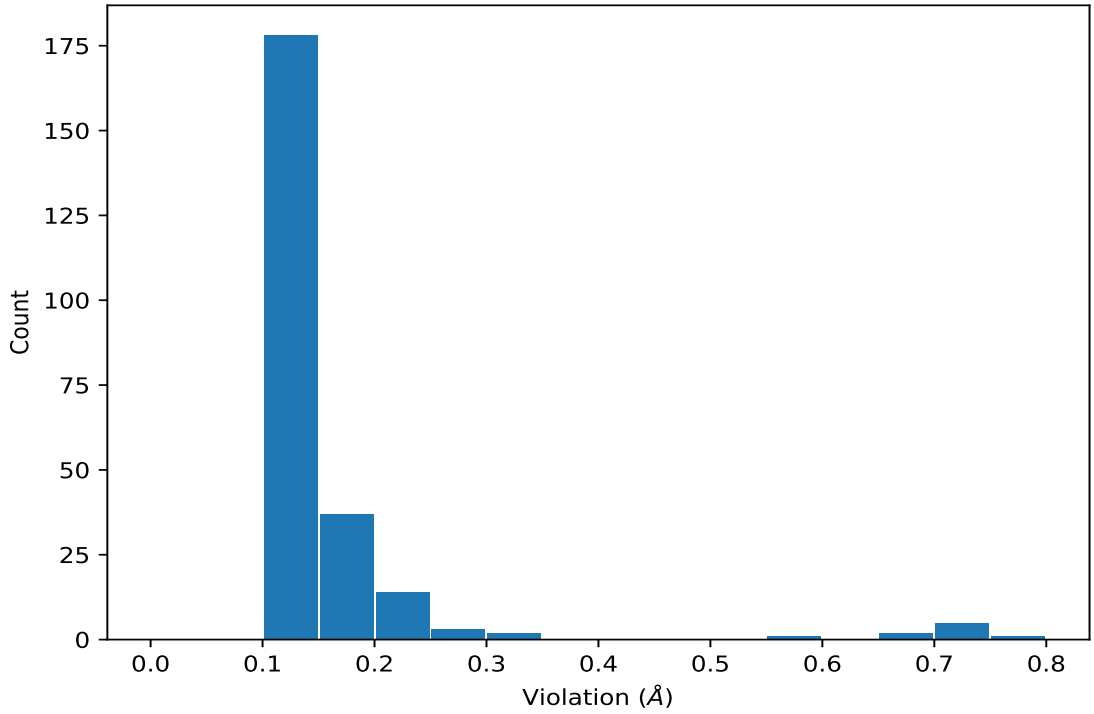
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,131)	2:1576:B:TYR:HD2	2:1596:B:HIS:HE1	2	0.12	0.02	0.12
(2,2)	1:4:A:THR:HB	1:84:A:PRO:HD2	2	0.12	0.0	0.12
(3,36)	2:1566:B:GLY:HA2	2:1593:B:ARG:HD2	2	0.12	0.01	0.12
(3,36)	2:1566:B:GLY:HA2	2:1593:B:ARG:HD3	2	0.12	0.01	0.12
(2,56)	1:40:A:ASP:HA	1:42:A:GLU:HG3	2	0.12	0.02	0.12
(4,11)	2:1588:B:CYS:H	2:1594:B:TRP:HD1	2	0.12	0.0	0.12
(1,1671)	1:51:A:PHE:HE1	1:102:A:LEU:HG	2	0.11	0.0	0.11
(1,1671)	1:51:A:PHE:HE2	1:102:A:LEU:HG	2	0.11	0.0	0.11
(2,22)	1:19:A:ASP:HA	1:20:A:LYS:HE2	2	0.11	0.0	0.11
(2,22)	1:19:A:ASP:HA	1:20:A:LYS:HE3	2	0.11	0.0	0.11
(3,780)	2:1615:B:GLU:H	2:1616:B:SER:HB3	2	0.11	0.01	0.11
(5,35)	1:38:A:PRO:HD3	2:1610:B:LEU:HB3	2	0.11	0.0	0.11
(5,172)	1:103:A:LYS:HA	2:1614:B:PRO:HD3	2	0.11	0.01	0.11
(1,45)	1:5:A:LYS:HB3	1:57:A:ALA:H	2	0.11	0.0	0.11

[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 lists the 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)
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	2	0.76
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	3	0.74
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	4	0.73
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	18	0.73
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	14	0.72
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	1	0.71
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	10	0.69
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	13	0.66
(5,22)	1:36:A:GLN:HG3	2:1627:B:ARG:HB3	11	0.6
(3,924)	2:1626:B:GLU:HB2	2:1627:B:ARG:HD2	7	0.33
(3,924)	2:1626:B:GLU:HB2	2:1627:B:ARG:HD3	7	0.33
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG22	16	0.27
(3,924)	2:1626:B:GLU:HB2	2:1627:B:ARG:HD2	11	0.27
(3,924)	2:1626:B:GLU:HB2	2:1627:B:ARG:HD3	11	0.27
(1,2700)	1:107:A:GLY:HA2	1:108:A:LYS:HG2	12	0.24
(1,2700)	1:107:A:GLY:HA2	1:108:A:LYS:HG3	12	0.24
(1,2700)	1:107:A:GLY:HA3	1:108:A:LYS:HG2	12	0.24
(1,2700)	1:107:A:GLY:HA3	1:108:A:LYS:HG3	12	0.24
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG22	12	0.23
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG22	9	0.22
(3,921)	2:1626:B:GLU:HA	2:1627:B:ARG:HD2	11	0.21
(3,921)	2:1626:B:GLU:HA	2:1627:B:ARG:HD3	11	0.21
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD2	4	0.21
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD3	4	0.21
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD2	7	0.21
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD3	7	0.21
(3,122)	2:1575:B:CYS:HB2	2:1576:B:TYR:HB2	20	0.21
(3,122)	2:1575:B:CYS:HB3	2:1576:B:TYR:HB2	20	0.21
(1,2503)	1:88:A:LYS:HA	1:90:A:GLY:H	1	0.19
(1,28)	1:4:A:THR:H	1:5:A:LYS:HB3	9	0.19
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG21	2	0.18
(1,2526)	1:92:A:SER:HB2	1:93:A:ARG:HB3	13	0.18
(1,2526)	1:92:A:SER:HB3	1:93:A:ARG:HB3	13	0.18
(4,18)	2:1597:B:SER:HB2	2:1608:B:GLU:H	16	0.17
(4,18)	2:1597:B:SER:HB3	2:1608:B:GLU:H	16	0.17
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE1	20	0.17
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE2	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,122)	2:1575:B:CYS:HB2	2:1576:B:TYR:HB2	3	0.17
(3,122)	2:1575:B:CYS:HB3	2:1576:B:TYR:HB2	3	0.17
(1,2503)	1:88:A:LYS:HA	1:90:A:GLY:H	2	0.17
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE1	3	0.16
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE2	3	0.16
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE1	17	0.16
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE2	17	0.16
(3,122)	2:1575:B:CYS:HB2	2:1576:B:TYR:HB2	17	0.16
(3,122)	2:1575:B:CYS:HB3	2:1576:B:TYR:HB2	17	0.16
(1,2719)	1:110:A:LEU:HD11	1:111:A:GLU:HB2	2	0.16
(1,2719)	1:110:A:LEU:HD11	1:111:A:GLU:HB3	2	0.16
(1,2719)	1:110:A:LEU:HD12	1:111:A:GLU:HB2	2	0.16
(1,2719)	1:110:A:LEU:HD12	1:111:A:GLU:HB3	2	0.16
(1,2719)	1:110:A:LEU:HD13	1:111:A:GLU:HB2	2	0.16
(1,2719)	1:110:A:LEU:HD13	1:111:A:GLU:HB3	2	0.16
(1,2719)	1:110:A:LEU:HD21	1:111:A:GLU:HB2	2	0.16
(1,2719)	1:110:A:LEU:HD21	1:111:A:GLU:HB3	2	0.16
(1,2719)	1:110:A:LEU:HD22	1:111:A:GLU:HB2	2	0.16
(1,2719)	1:110:A:LEU:HD22	1:111:A:GLU:HB3	2	0.16
(1,2719)	1:110:A:LEU:HD23	1:111:A:GLU:HB2	2	0.16
(1,2719)	1:110:A:LEU:HD23	1:111:A:GLU:HB3	2	0.16
(1,2712)	1:109:A:THR:HG21	1:110:A:LEU:HG	1	0.16
(1,2712)	1:109:A:THR:HG22	1:110:A:LEU:HG	1	0.16
(1,2712)	1:109:A:THR:HG23	1:110:A:LEU:HG	1	0.16
(1,2684)	1:104:A:LYS:HA	1:107:A:GLY:HA2	19	0.16
(1,2684)	1:104:A:LYS:HA	1:107:A:GLY:HA3	19	0.16
(1,2526)	1:92:A:SER:HB2	1:93:A:ARG:HB3	1	0.16
(1,2526)	1:92:A:SER:HB3	1:93:A:ARG:HB3	1	0.16
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG22	15	0.15
(3,903)	2:1625:B:THR:HB	2:1627:B:ARG:HG2	7	0.15
(3,903)	2:1625:B:THR:HB	2:1627:B:ARG:HG3	7	0.15
(3,695)	2:1610:B:LEU:HD11	2:1611:B:SER:HA	10	0.15
(3,695)	2:1610:B:LEU:HD12	2:1611:B:SER:HA	10	0.15
(3,695)	2:1610:B:LEU:HD13	2:1611:B:SER:HA	10	0.15
(3,695)	2:1610:B:LEU:HD21	2:1611:B:SER:HA	10	0.15
(3,695)	2:1610:B:LEU:HD22	2:1611:B:SER:HA	10	0.15
(3,695)	2:1610:B:LEU:HD23	2:1611:B:SER:HA	10	0.15
(3,146)	2:1579:B:ASP:HB2	2:1583:B:SER:HB2	16	0.15
(3,146)	2:1579:B:ASP:HB2	2:1583:B:SER:HB3	16	0.15
(3,146)	2:1579:B:ASP:HB3	2:1583:B:SER:HB2	16	0.15
(3,146)	2:1579:B:ASP:HB3	2:1583:B:SER:HB3	16	0.15
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE1	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,129)	2:1576:B:TYR:HA	2:1576:B:TYR:HE2	9	0.15
(3,48)	2:1568:B:PHE:HZ	2:1570:B:PRO:HA	17	0.15
(2,120)	1:101:A:TRP:HA	1:105:A:PHE:HA	3	0.15
(1,2718)	1:110:A:LEU:HB2	1:113:A:ASN:H	19	0.15
(1,2718)	1:110:A:LEU:HB3	1:113:A:ASN:H	19	0.15
(1,2526)	1:92:A:SER:HB2	1:93:A:ARG:HB3	10	0.15
(1,2526)	1:92:A:SER:HB3	1:93:A:ARG:HB3	10	0.15
(1,2379)	1:78:A:ARG:HD2	1:80:A:ASN:HD21	14	0.15
(1,28)	1:4:A:THR:H	1:5:A:LYS:HB3	20	0.15
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG22	7	0.14
(4,30)	2:1620:B:THR:HA	2:1625:B:THR:HB	17	0.14
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD2	9	0.14
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD3	9	0.14
(3,131)	2:1576:B:TYR:HD1	2:1596:B:HIS:HE1	8	0.14
(3,131)	2:1576:B:TYR:HD2	2:1596:B:HIS:HE1	8	0.14
(3,122)	2:1575:B:CYS:HB2	2:1576:B:TYR:HB2	9	0.14
(3,122)	2:1575:B:CYS:HB3	2:1576:B:TYR:HB2	9	0.14
(3,65)	2:1569:B:CYS:H	2:1576:B:TYR:HD1	2	0.14
(3,65)	2:1569:B:CYS:H	2:1576:B:TYR:HD2	2	0.14
(2,75)	1:56:A:LEU:HD11	1:58:A:GLU:HG2	4	0.14
(2,75)	1:56:A:LEU:HD11	1:58:A:GLU:HG3	4	0.14
(2,75)	1:56:A:LEU:HD12	1:58:A:GLU:HG2	4	0.14
(2,75)	1:56:A:LEU:HD12	1:58:A:GLU:HG3	4	0.14
(2,75)	1:56:A:LEU:HD13	1:58:A:GLU:HG2	4	0.14
(2,75)	1:56:A:LEU:HD13	1:58:A:GLU:HG3	4	0.14
(2,75)	1:56:A:LEU:HD11	1:58:A:GLU:HG2	12	0.14
(2,75)	1:56:A:LEU:HD11	1:58:A:GLU:HG3	12	0.14
(2,75)	1:56:A:LEU:HD12	1:58:A:GLU:HG2	12	0.14
(2,75)	1:56:A:LEU:HD12	1:58:A:GLU:HG3	12	0.14
(2,75)	1:56:A:LEU:HD13	1:58:A:GLU:HG2	12	0.14
(2,75)	1:56:A:LEU:HD13	1:58:A:GLU:HG3	12	0.14
(2,1)	1:3:A:THR:HB	1:5:A:LYS:HB3	2	0.14
(1,2719)	1:110:A:LEU:HD11	1:111:A:GLU:HB2	16	0.14
(1,2719)	1:110:A:LEU:HD11	1:111:A:GLU:HB3	16	0.14
(1,2719)	1:110:A:LEU:HD12	1:111:A:GLU:HB2	16	0.14
(1,2719)	1:110:A:LEU:HD12	1:111:A:GLU:HB3	16	0.14
(1,2719)	1:110:A:LEU:HD13	1:111:A:GLU:HB2	16	0.14
(1,2719)	1:110:A:LEU:HD13	1:111:A:GLU:HB3	16	0.14
(1,2719)	1:110:A:LEU:HD21	1:111:A:GLU:HB2	16	0.14
(1,2719)	1:110:A:LEU:HD21	1:111:A:GLU:HB3	16	0.14
(1,2719)	1:110:A:LEU:HD22	1:111:A:GLU:HB2	16	0.14
(1,2719)	1:110:A:LEU:HD22	1:111:A:GLU:HB3	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2719)	1:110:A:LEU:HD23	1:111:A:GLU:HB2	16	0.14
(1,2719)	1:110:A:LEU:HD23	1:111:A:GLU:HB3	16	0.14
(1,2440)	1:84:A:PRO:HG2	1:85:A:MET:HG2	16	0.14
(1,2440)	1:84:A:PRO:HG2	1:85:A:MET:HG3	16	0.14
(3,327)	2:1589:B:GLY:HA2	2:1592:B:ASP:HA	1	0.13
(3,327)	2:1589:B:GLY:HA2	2:1592:B:ASP:HA	10	0.13
(3,327)	2:1589:B:GLY:HA2	2:1592:B:ASP:HA	20	0.13
(3,36)	2:1566:B:GLY:HA2	2:1593:B:ARG:HD2	5	0.13
(3,36)	2:1566:B:GLY:HA2	2:1593:B:ARG:HD3	5	0.13
(2,56)	1:40:A:ASP:HA	1:42:A:GLU:HG3	19	0.13
(2,1)	1:3:A:THR:HB	1:5:A:LYS:HB3	10	0.13
(1,2092)	1:68:A:ASN:H	1:69:A:GLU:HG3	15	0.13
(1,3)	1:-1:A:HIS:HB2	1:1:A:MET:HE1	17	0.13
(1,3)	1:-1:A:HIS:HB2	1:1:A:MET:HE2	17	0.13
(1,3)	1:-1:A:HIS:HB2	1:1:A:MET:HE3	17	0.13
(5,172)	1:103:A:LYS:HA	2:1614:B:PRO:HD3	3	0.12
(4,11)	2:1588:B:CYS:H	2:1594:B:TRP:HD1	9	0.12
(3,780)	2:1615:B:GLU:H	2:1616:B:SER:HB3	10	0.12
(3,695)	2:1610:B:LEU:HD11	2:1611:B:SER:HA	11	0.12
(3,695)	2:1610:B:LEU:HD12	2:1611:B:SER:HA	11	0.12
(3,695)	2:1610:B:LEU:HD13	2:1611:B:SER:HA	11	0.12
(3,695)	2:1610:B:LEU:HD21	2:1611:B:SER:HA	11	0.12
(3,695)	2:1610:B:LEU:HD22	2:1611:B:SER:HA	11	0.12
(3,695)	2:1610:B:LEU:HD23	2:1611:B:SER:HA	11	0.12
(3,695)	2:1610:B:LEU:HD11	2:1611:B:SER:HA	18	0.12
(3,695)	2:1610:B:LEU:HD12	2:1611:B:SER:HA	18	0.12
(3,695)	2:1610:B:LEU:HD13	2:1611:B:SER:HA	18	0.12
(3,695)	2:1610:B:LEU:HD21	2:1611:B:SER:HA	18	0.12
(3,695)	2:1610:B:LEU:HD22	2:1611:B:SER:HA	18	0.12
(3,695)	2:1610:B:LEU:HD23	2:1611:B:SER:HA	18	0.12
(3,511)	2:1602:B:LEU:HG	2:1619:B:TYR:HE1	10	0.12
(3,511)	2:1602:B:LEU:HG	2:1619:B:TYR:HE2	10	0.12
(3,453)	2:1597:B:SER:HB2	2:1598:B:LYS:HB2	7	0.12
(3,453)	2:1597:B:SER:HB3	2:1598:B:LYS:HB2	7	0.12
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD2	16	0.12
(3,444)	2:1597:B:SER:HA	2:1598:B:LYS:HD3	16	0.12
(3,425)	2:1595:B:VAL:HB	2:1621:B:CYS:HA	16	0.12
(3,327)	2:1589:B:GLY:HA2	2:1592:B:ASP:HA	17	0.12
(2,2)	1:4:A:THR:HB	1:84:A:PRO:HD2	8	0.12
(2,2)	1:4:A:THR:HB	1:84:A:PRO:HD2	13	0.12
(1,2712)	1:109:A:THR:HG21	1:110:A:LEU:HG	15	0.12
(1,2712)	1:109:A:THR:HG22	1:110:A:LEU:HG	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2712)	1:109:A:THR:HG23	1:110:A:LEU:HG	15	0.12
(1,2684)	1:104:A:LYS:HA	1:107:A:GLY:HA2	4	0.12
(1,2684)	1:104:A:LYS:HA	1:107:A:GLY:HA3	4	0.12
(1,2565)	1:94:A:PRO:HB3	1:96:A:TRP:HZ2	15	0.12
(1,1966)	1:64:A:ILE:H	1:80:A:ASN:HA	7	0.12
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG22	6	0.11
(6,6)	1:51:A:PHE:HB2	2:1609:B:ILE:HG23	17	0.11
(5,35)	1:38:A:PRO:HD3	2:1610:B:LEU:HB3	10	0.11
(5,35)	1:38:A:PRO:HD3	2:1610:B:LEU:HB3	18	0.11
(4,14)	2:1592:B:ASP:HA	2:1594:B:TRP:HA	18	0.11
(4,11)	2:1588:B:CYS:H	2:1594:B:TRP:HD1	16	0.11
(3,493)	2:1601:B:ASN:HB3	2:1602:B:LEU:HD11	19	0.11
(3,493)	2:1601:B:ASN:HB3	2:1602:B:LEU:HD12	19	0.11
(3,493)	2:1601:B:ASN:HB3	2:1602:B:LEU:HD13	19	0.11
(3,493)	2:1601:B:ASN:HB3	2:1602:B:LEU:HD21	19	0.11
(3,493)	2:1601:B:ASN:HB3	2:1602:B:LEU:HD22	19	0.11
(3,493)	2:1601:B:ASN:HB3	2:1602:B:LEU:HD23	19	0.11
(3,328)	2:1589:B:GLY:HA3	2:1590:B:LYS:HE2	19	0.11
(3,328)	2:1589:B:GLY:HA3	2:1590:B:LYS:HE3	19	0.11
(3,327)	2:1589:B:GLY:HA2	2:1592:B:ASP:HA	15	0.11
(3,146)	2:1579:B:ASP:HB2	2:1583:B:SER:HB2	19	0.11
(3,146)	2:1579:B:ASP:HB2	2:1583:B:SER:HB3	19	0.11
(3,146)	2:1579:B:ASP:HB3	2:1583:B:SER:HB2	19	0.11
(3,146)	2:1579:B:ASP:HB3	2:1583:B:SER:HB3	19	0.11
(3,36)	2:1566:B:GLY:HA2	2:1593:B:ARG:HD2	12	0.11
(3,36)	2:1566:B:GLY:HA2	2:1593:B:ARG:HD3	12	0.11
(2,120)	1:101:A:TRP:HA	1:105:A:PHE:HA	16	0.11
(2,27)	1:22:A:LEU:H	1:37:A:ILE:HG12	3	0.11
(2,22)	1:19:A:ASP:HA	1:20:A:LYS:HE2	2	0.11
(2,22)	1:19:A:ASP:HA	1:20:A:LYS:HE3	2	0.11
(2,22)	1:19:A:ASP:HA	1:20:A:LYS:HE2	8	0.11
(2,22)	1:19:A:ASP:HA	1:20:A:LYS:HE3	8	0.11
(2,1)	1:3:A:THR:HB	1:5:A:LYS:HB3	6	0.11
(2,1)	1:3:A:THR:HB	1:5:A:LYS:HB3	14	0.11
(1,2714)	1:110:A:LEU:H	1:113:A:ASN:H	8	0.11
(1,2712)	1:109:A:THR:HG21	1:110:A:LEU:HG	7	0.11
(1,2712)	1:109:A:THR:HG22	1:110:A:LEU:HG	7	0.11
(1,2712)	1:109:A:THR:HG23	1:110:A:LEU:HG	7	0.11
(1,2528)	1:92:A:SER:HB2	1:95:A:VAL:H	5	0.11
(1,2528)	1:92:A:SER:HB3	1:95:A:VAL:H	5	0.11
(1,2379)	1:78:A:ARG:HD2	1:80:A:ASN:HD21	18	0.11
(1,1966)	1:64:A:ILE:H	1:80:A:ASN:HA	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1966)	1:64:A:ILE:H	1:80:A:ASN:HA	19	0.11
(1,1763)	1:55:A:GLU:HB3	1:56:A:LEU:HB3	3	0.11
(1,1671)	1:51:A:PHE:HE1	1:102:A:LEU:HG	2	0.11
(1,1671)	1:51:A:PHE:HE2	1:102:A:LEU:HG	2	0.11
(1,1671)	1:51:A:PHE:HE1	1:102:A:LEU:HG	20	0.11
(1,1671)	1:51:A:PHE:HE2	1:102:A:LEU:HG	20	0.11
(1,1512)	1:42:A:GLU:HB3	1:43:A:THR:HG21	19	0.11
(1,1512)	1:42:A:GLU:HB3	1:43:A:THR:HG22	19	0.11
(1,1512)	1:42:A:GLU:HB3	1:43:A:THR:HG23	19	0.11
(1,611)	1:18:A:ASP:HB2	1:20:A:LYS:HE2	8	0.11
(1,611)	1:18:A:ASP:HB2	1:20:A:LYS:HE3	8	0.11
(1,45)	1:5:A:LYS:HB3	1:57:A:ALA:H	13	0.11
(5,172)	1:103:A:LYS:HA	2:1614:B:PRO:HD3	15	0.1
(4,14)	2:1592:B:ASP:HA	2:1594:B:TRP:HA	11	0.1
(4,14)	2:1592:B:ASP:HA	2:1594:B:TRP:HA	13	0.1
(3,780)	2:1615:B:GLU:H	2:1616:B:SER:HB3	16	0.1
(3,348)	2:1590:B:LYS:HB2	2:1620:B:THR:HG21	12	0.1
(3,348)	2:1590:B:LYS:HB2	2:1620:B:THR:HG22	12	0.1
(3,348)	2:1590:B:LYS:HB2	2:1620:B:THR:HG23	12	0.1
(3,327)	2:1589:B:GLY:HA2	2:1592:B:ASP:HA	14	0.1
(3,131)	2:1576:B:TYR:HD1	2:1596:B:HIS:HE1	1	0.1
(3,131)	2:1576:B:TYR:HD2	2:1596:B:HIS:HE1	1	0.1
(2,120)	1:101:A:TRP:HA	1:105:A:PHE:HA	15	0.1
(2,56)	1:40:A:ASP:HA	1:42:A:GLU:HG3	4	0.1
(2,1)	1:3:A:THR:HB	1:5:A:LYS:HB3	12	0.1
(1,2440)	1:84:A:PRO:HG2	1:85:A:MET:HG2	4	0.1
(1,2440)	1:84:A:PRO:HG2	1:85:A:MET:HG3	4	0.1
(1,1636)	1:49:A:PHE:HD1	1:105:A:PHE:HD1	20	0.1
(1,1636)	1:49:A:PHE:HD1	1:105:A:PHE:HD2	20	0.1
(1,1636)	1:49:A:PHE:HD2	1:105:A:PHE:HD1	20	0.1
(1,1636)	1:49:A:PHE:HD2	1:105:A:PHE:HD2	20	0.1
(1,1201)	1:32:A:ILE:HG21	1:53:A:GLU:HG3	10	0.1
(1,1201)	1:32:A:ILE:HG22	1:53:A:GLU:HG3	10	0.1
(1,1201)	1:32:A:ILE:HG23	1:53:A:GLU:HG3	10	0.1
(1,1099)	1:30:A:GLY:H	1:59:A:ASP:HB3	20	0.1
(1,212)	1:9:A:TYR:HE1	1:80:A:ASN:HB3	13	0.1
(1,212)	1:9:A:TYR:HE2	1:80:A:ASN:HB3	13	0.1
(1,45)	1:5:A:LYS:HB3	1:57:A:ALA:H	8	0.1

10 Dihedral-angle violation analysis

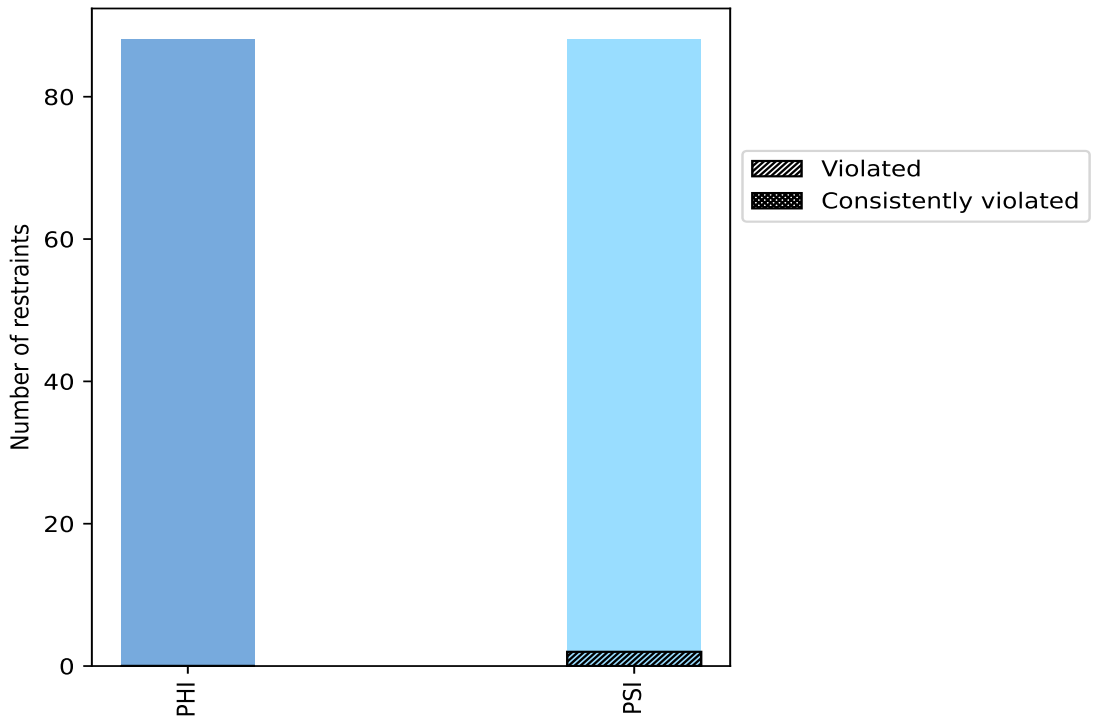
10.1 Summary of dihedral-angle violations

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]
PHI	88	50.0	0	0.0	0.0	0	0.0	0.0
PSI	88	50.0	2	2.3	1.1	0	0.0	0.0
Total	176	100.0	2	1.1	1.1	0	0.0	0.0

[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



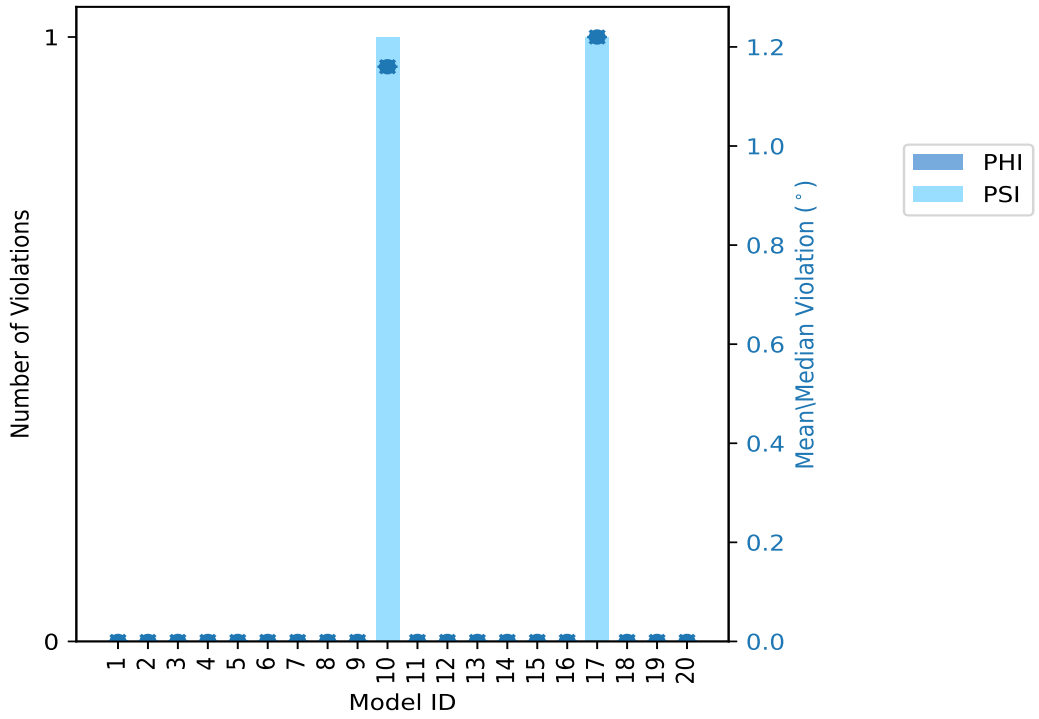
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	1.16	1.16	0.0	1.16
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	1	1	1.22	1.22	0.0	1.22
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

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

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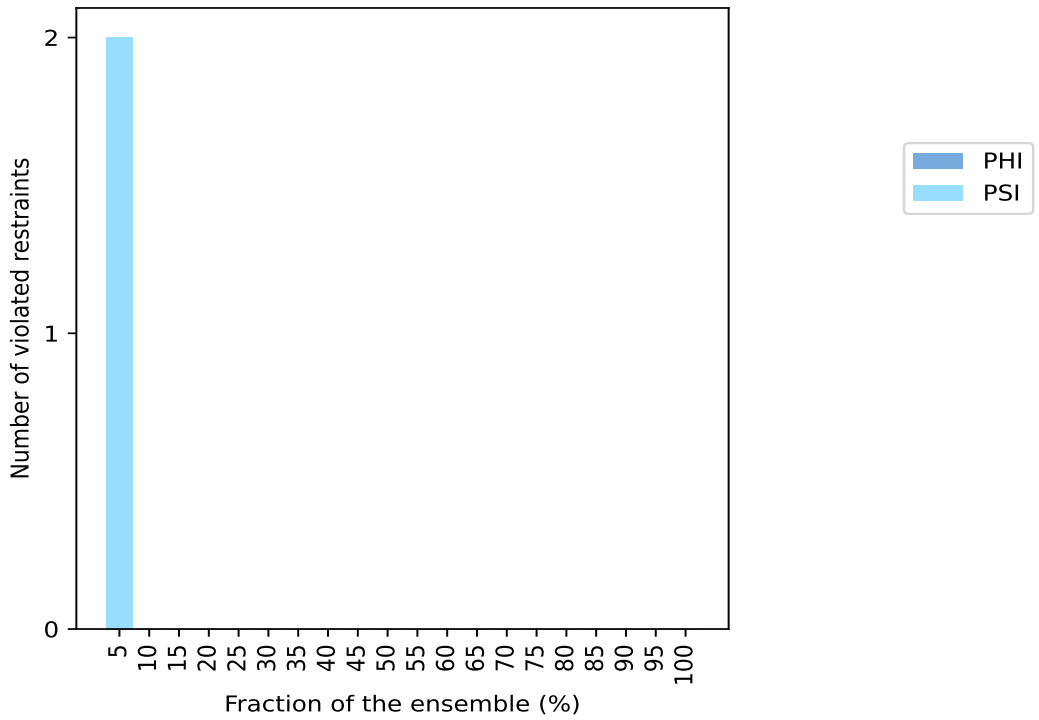
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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



10.4 Most violated dihedral-angle restraints in the ensemble

No violations found

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.
Data insufficient to plot histogram

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

The following table lists the 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,52)	2:1618:B:ALA:N	2:1618:B:ALA:CA	2:1618:B:ALA:C	2:1619:B:TYR:N	17	1.22
(2,14)	2:1584:B:LYS:N	2:1584:B:LYS:CA	2:1584:B:LYS:C	2:1585:B:MET:N	10	1.16