Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 01:14 PM JST

PDB ID	:	6L8R
BMRB ID	:	36293
Title	:	membrane-bound PD-L1-CD
Authors	:	Maorong, W.; Cao, Y.; Bin, W.; Bo, O.
Deposited on	:	2019-11-07

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 (1)) were used in the production of this report:

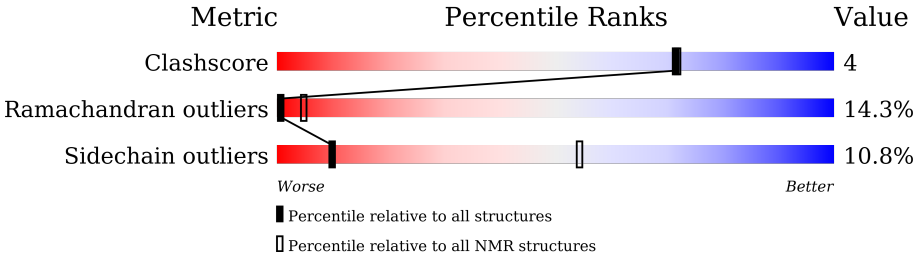
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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	33	61% 18% • 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:259-A:285 (27)	1.75	3

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 533 atoms, of which 271 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	33	533	155	271	52	52	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	GLY	-	expression tag	UNP Q9NZQ7
A	259	PRO	-	expression tag	UNP Q9NZQ7

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: Programmed cell death 1 ligand 1

Chain A:

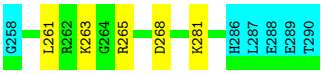
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Programmed cell death 1 ligand 1

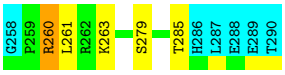
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Programmed cell death 1 ligand 1

Chain A:



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Programmed cell death 1 ligand 1

Chain A: 58% 18% 6% 18%

G258 P259 R260 L261 R262 K263 D268 S279 D284 T285 H286 L287 E288 E289 T290

4.2.4 Score per residue for model 4

- Molecule 1: Programmed cell death 1 ligand 1

Chain A: 67% 9% 6% 18%

G258 P259 R260 L261 R262 K263 M266 H286 L287 E288 E289 T290

4.2.5 Score per residue for model 5

- Molecule 1: Programmed cell death 1 ligand 1

Chain A: 48% 21% 12% 18%

G258 P259 R260 L261 R262 K263 D268 C272 S279 Q282 S283 D284 T285 H286 L287 E288 E289 T290

4.2.6 Score per residue for model 6

- Molecule 1: Programmed cell death 1 ligand 1

Chain A: 61% 18% • 18%

G258 P259 R260 L261 R262 K263 G264 R265 I274 K280 K281 Q282 H286 L287 E288 E289 T290

4.2.7 Score per residue for model 7

- Molecule 1: Programmed cell death 1 ligand 1

Chain A: 61% 15% 6% 18%

G258 P259 R260 L261 R262 K263 C272 S279 D284 T285 H286 L287 E288 E289 T290

4.2.8 Score per residue for model 8

- Molecule 1: Programmed cell death 1 ligand 1

Chain A:

4.2.9 Score per residue for model 9

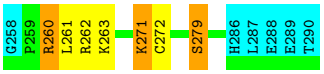
- Molecule 1: Programmed cell death 1 ligand 1

Chain A:

4.2.10 Score per residue for model 10

- Molecule 1: Programmed cell death 1 ligand 1

Chain A:



4.2.11 Score per residue for model 11

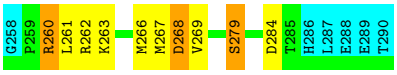
- Molecule 1: Programmed cell death 1 ligand 1

Chain A:

4.2.12 Score per residue for model 12

- Molecule 1: Programmed cell death 1 ligand 1

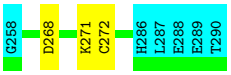
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Programmed cell death 1 ligand 1

Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Programmed cell death 1 ligand 1

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: Programmed cell death 1 ligand 1

Chain A:

4.2.16 Score per residue for model 16

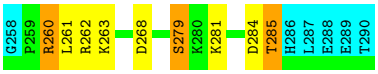
• Molecule 1: Programmed cell death 1 ligand 1

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: Programmed cell death 1 ligand 1

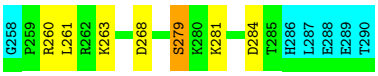
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Programmed cell death 1 ligand 1

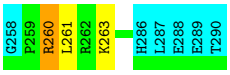
Chain A: 61% 18% • 18%



4.2.19 Score per residue for model 19

- Molecule 1: Programmed cell death 1 ligand 1

Chain A: 73% 6% • 18%



4.2.20 Score per residue for model 20

- Molecule 1: Programmed cell death 1 ligand 1

Chain A: 70% 9% • 18%

5 Refinement protocol and experimental data overview (i)

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

Of the 200 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	structure calculation	
X-PLOR NIH	refinement	

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	394
Number of shifts mapped to atoms	394
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	214	229	229	2±1
All	All	4280	4580	4580	31

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:284:ASP:O	1:A:285:THR:O	0.53	2.27	14	2
1:A:267:MET:O	1:A:269:VAL:HG13	0.51	2.04	15	2
1:A:267:MET:O	1:A:268:ASP:C	0.51	2.49	15	2
1:A:261:LEU:HD22	1:A:261:LEU:C	0.50	2.27	4	1
1:A:261:LEU:HD12	1:A:261:LEU:C	0.48	2.29	16	17
1:A:284:ASP:O	1:A:285:THR:C	0.47	2.53	17	4
1:A:261:LEU:CD1	1:A:261:LEU:N	0.43	2.82	4	1
1:A:261:LEU:N	1:A:261:LEU:HD13	0.40	2.32	4	1
1:A:261:LEU:C	1:A:261:LEU:HD12	0.40	2.37	8	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	27/33 (82%)	17±2 (62±6%)	6±2 (24±7%)	4±2 (14±6%)	1 5
All	All	540/660 (82%)	335 (62%)	128 (24%)	77 (14%)	1 5

All 11 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	263	LYS	17
1	A	260	ARG	15
1	A	268	ASP	13
1	A	279	SER	13
1	A	284	ASP	6
1	A	285	THR	6
1	A	259	PRO	2
1	A	266	MET	2
1	A	274	ILE	1
1	A	271	LYS	1
1	A	265	ARG	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	25/30 (83%)	22±1 (89±5%)	3±1 (11±5%)	10 54
All	All	500/600 (83%)	446 (89%)	54 (11%)	10 54

All 14 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	260	ARG	17
1	A	279	SER	7
1	A	262	ARG	6
1	A	272	CYS	5
1	A	265	ARG	3
1	A	281	LYS	3
1	A	285	THR	2
1	A	259	PRO	2
1	A	261	LEU	2
1	A	282	GLN	2
1	A	271	LYS	2
1	A	263	LYS	1
1	A	266	MET	1
1	A	280	LYS	1

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 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	394
Number of shifts mapped to atoms	394
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	31	-0.41 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	29	0.15 ± 0.05	None needed (< 0.5 ppm)
$^{13}C'$	31	-0.20 ± 0.08	None needed (< 0.5 ppm)
^{15}N	31	-1.09 ± 0.18	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 88%, i.e. 335 atoms were assigned a chemical shift out of a possible 379. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	132/135 (98%)	54/55 (98%)	52/54 (96%)	26/26 (100%)
Sidechain	203/244 (83%)	136/154 (88%)	61/73 (84%)	6/17 (35%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Overall	335/379 (88%)	190/209 (91%)	113/127 (89%)	32/43 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 394 atoms were assigned a chemical shift out of a possible 453. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	157/166 (95%)	64/68 (94%)	62/66 (94%)	31/32 (97%)
Sidechain	237/280 (85%)	159/177 (90%)	72/86 (84%)	6/17 (35%)
Aromatic	0/7 (0%)	0/4 (0%)	0/2 (0%)	0/1 (0%)
Overall	394/453 (87%)	223/249 (90%)	134/154 (87%)	37/50 (74%)

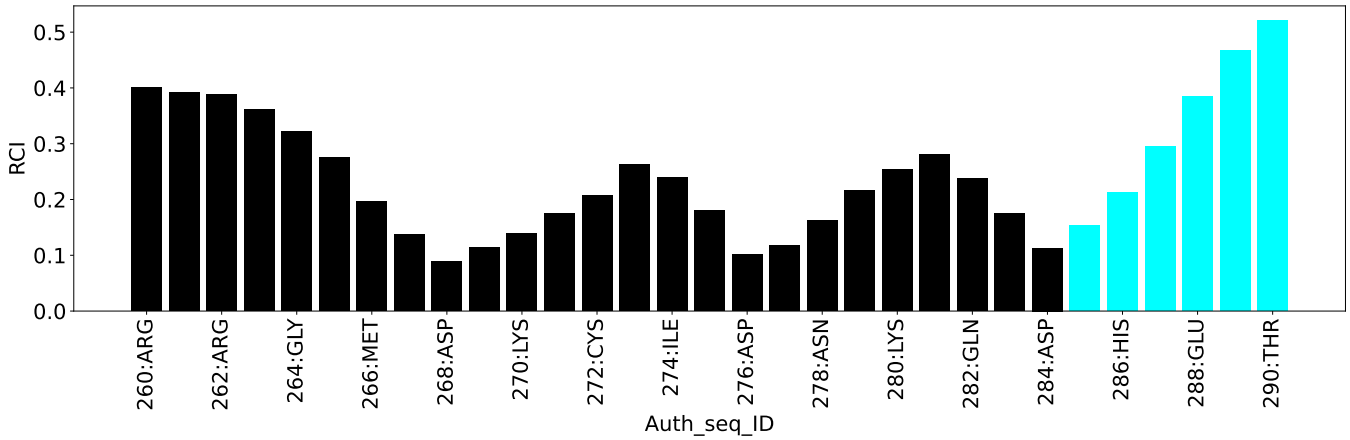
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis (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	397
Intra-residue (|i-j|=0)	189
Sequential (|i-j|=1)	153
Medium range (|i-j|>1 and |i-j|<5)	49
Long range (|i-j|≥5)	6
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	48
Number of unmapped restraints	0
Number of restraints per residue	13.5
Number of long range restraints per residue[1]	0.2

[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)	3.9	0.2
0.2-0.5 (Medium)	0.9	0.47
>0.5 (Large)	None	None

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	2.2
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

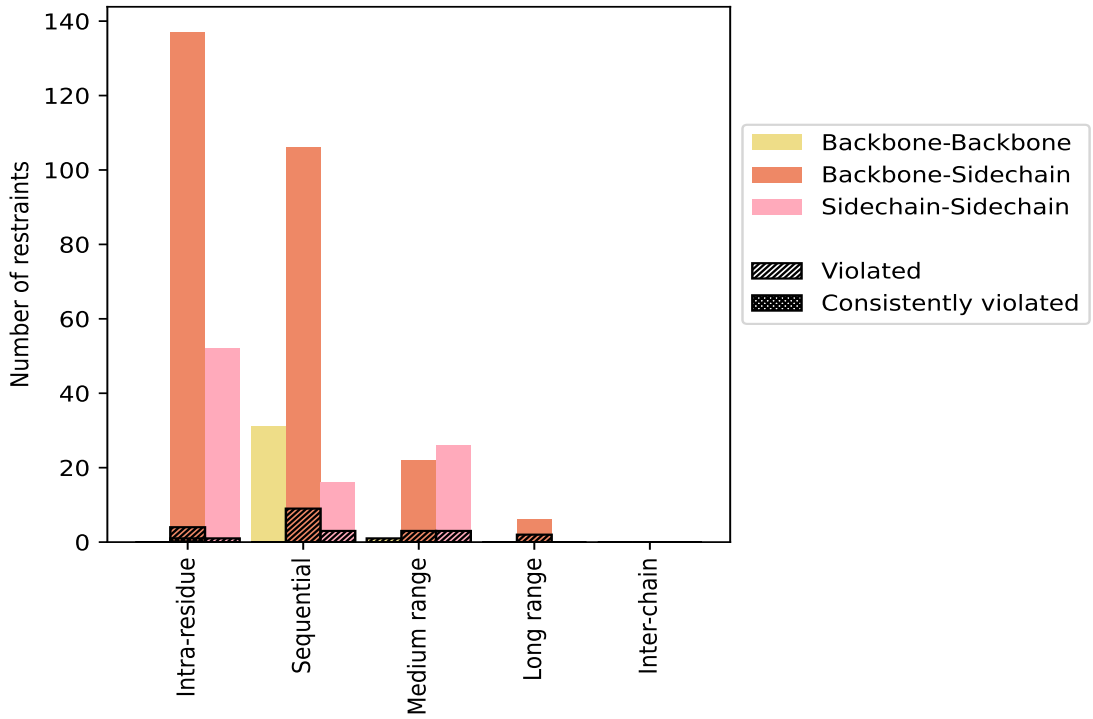
9.1 Summary of distance violations (i)

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)	189	47.6	5	2.6	1.3	1	0.5	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	137	34.5	4	2.9	1.0	1	0.7	0.3
Sidechain-Sidechain	52	13.1	1	1.9	0.3	0	0.0	0.0
Sequential (|i-j|=1)	153	38.5	12	7.8	3.0	0	0.0	0.0
Backbone-Backbone	31	7.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	106	26.7	9	8.5	2.3	0	0.0	0.0
Sidechain-Sidechain	16	4.0	3	18.8	0.8	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	49	12.3	7	14.3	1.8	0	0.0	0.0
Backbone-Backbone	1	0.3	1	100.0	0.3	0	0.0	0.0
Backbone-Sidechain	22	5.5	3	13.6	0.8	0	0.0	0.0
Sidechain-Sidechain	26	6.5	3	11.5	0.8	0	0.0	0.0
Long range (|i-j|≥5)	6	1.5	2	33.3	0.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	1.5	2	33.3	0.5	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	397	100.0	26	6.5	6.5	1	0.3	0.3
Backbone-Backbone	32	8.1	1	3.1	0.3	0	0.0	0.0
Backbone-Sidechain	271	68.3	18	6.6	4.5	1	0.4	0.3
Sidechain-Sidechain	94	23.7	7	7.4	1.8	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 (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	2	1	2	0	0	5	0.13	0.16	0.02	0.12
2	2	2	1	0	0	5	0.21	0.46	0.13	0.18
3	1	1	1	1	0	4	0.12	0.15	0.02	0.12
4	2	2	2	0	0	6	0.18	0.3	0.08	0.14
5	2	1	1	1	0	5	0.17	0.3	0.07	0.14
6	3	1	3	1	0	8	0.17	0.35	0.09	0.13
7	2	0	1	0	0	3	0.19	0.3	0.08	0.14
8	2	2	1	1	0	6	0.22	0.47	0.13	0.15
9	2	2	3	1	0	8	0.15	0.3	0.06	0.12
10	4	1	2	1	0	8	0.22	0.38	0.09	0.19
11	1	1	2	0	0	4	0.13	0.17	0.02	0.12

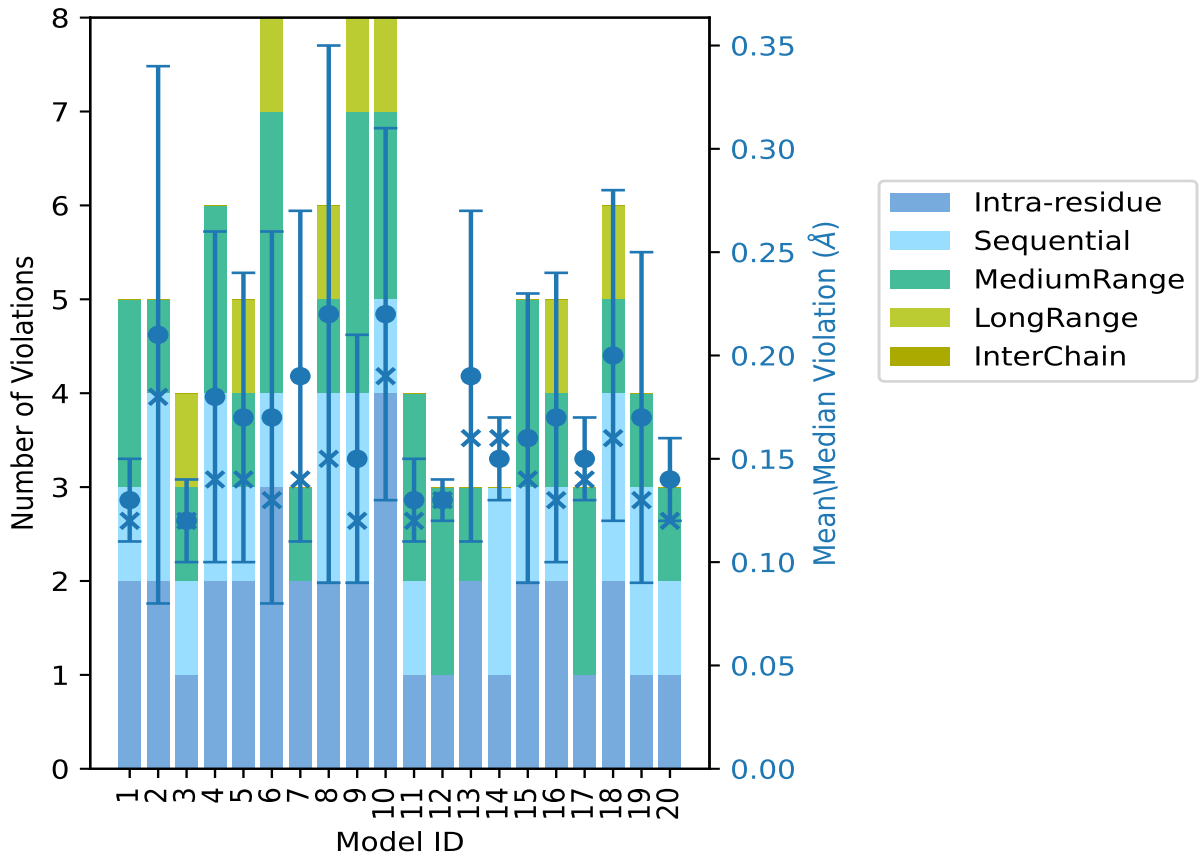
Continued on next page...

Continued from previous page...

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	1	0	2	0	0	3	0.13	0.14	0.01	0.13
13	2	0	1	0	0	3	0.19	0.3	0.08	0.16
14	1	2	0	0	0	3	0.15	0.18	0.02	0.16
15	2	1	2	0	0	5	0.16	0.3	0.07	0.14
16	2	1	1	1	0	5	0.17	0.3	0.07	0.13
17	1	0	2	0	0	3	0.15	0.18	0.02	0.14
18	2	2	1	1	0	6	0.2	0.32	0.08	0.16
19	1	2	1	0	0	4	0.17	0.3	0.08	0.13
20	1	1	1	0	0	3	0.14	0.17	0.02	0.12

[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

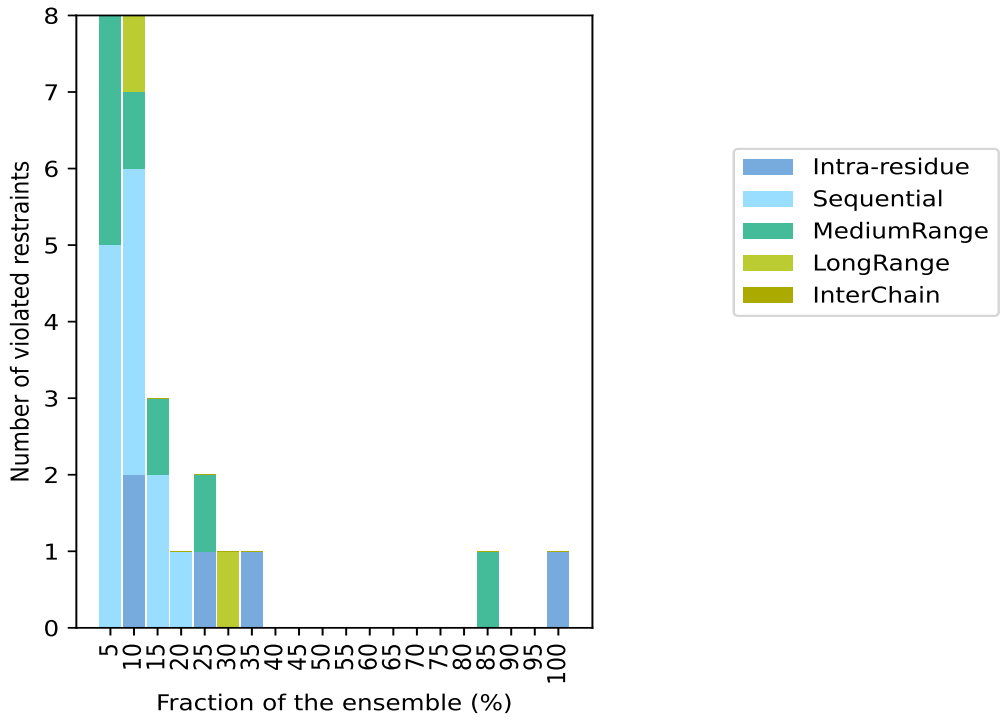
9.3 Distance violation statistics for the ensemble (i)

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, 371(IR:184, SQ:141, MR:42, LR:4, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	5	3	0	0	8	1	5.0
2	4	1	1	0	8	2	10.0
0	2	1	0	0	3	3	15.0
0	1	0	0	0	1	4	20.0
1	0	1	0	0	2	5	25.0
0	0	0	1	0	1	6	30.0
1	0	0	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	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	1	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
1	0	0	0	0	1	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

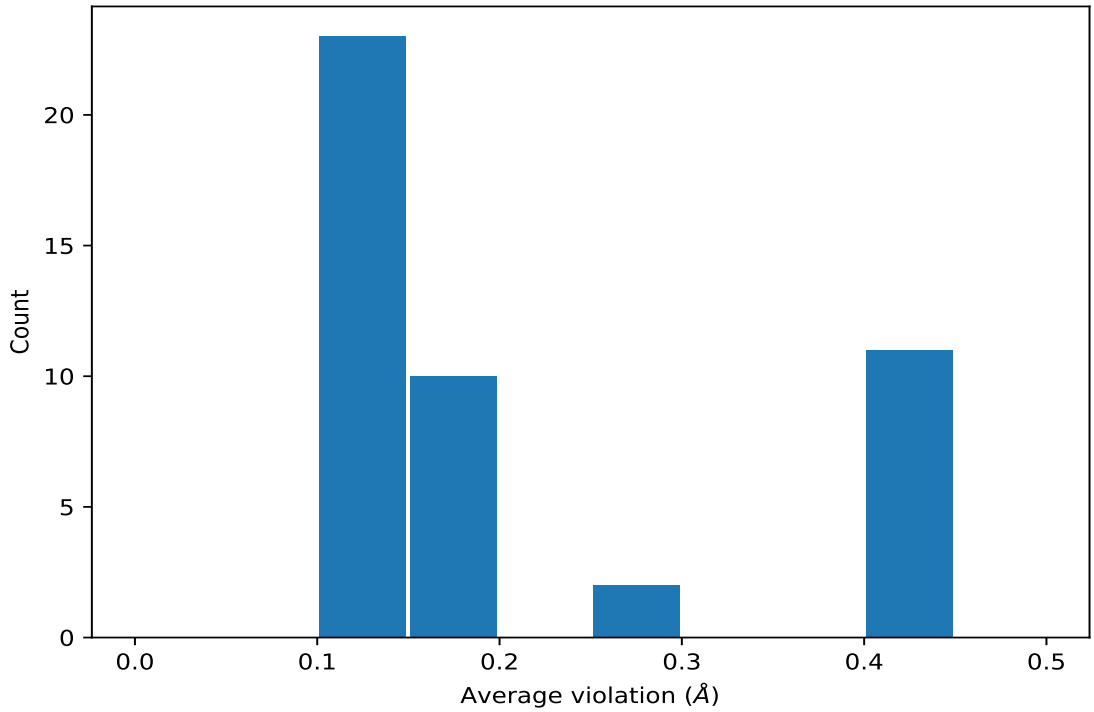
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	20	0.12	0.01	0.12
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	17	0.15	0.02	0.15
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	17	0.15	0.02	0.15
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	17	0.15	0.02	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	17	0.15	0.02	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	17	0.15	0.02	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	17	0.15	0.02	0.15
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	7	0.3	0.0	0.3
(1,183)	1:A:268:ASP:HB3	1:A:273:GLY:HA3	6	0.14	0.02	0.15
(1,396)	1:A:290:THR:HA	1:A:290:THR:HB	5	0.3	0.0	0.3
(1,133)	1:A:266:MET:HB2	1:A:270:LYS:HG3	5	0.12	0.01	0.12
(1,133)	1:A:266:MET:HB3	1:A:270:LYS:HG3	5	0.12	0.01	0.12
(1,41)	1:A:261:LEU:HD11	1:A:262:ARG:HE	4	0.16	0.06	0.12
(1,41)	1:A:261:LEU:HD12	1:A:262:ARG:HE	4	0.16	0.06	0.12
(1,41)	1:A:261:LEU:HD13	1:A:262:ARG:HE	4	0.16	0.06	0.12
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD11	3	0.19	0.09	0.14

Continued on next page...

Continued from previous page...

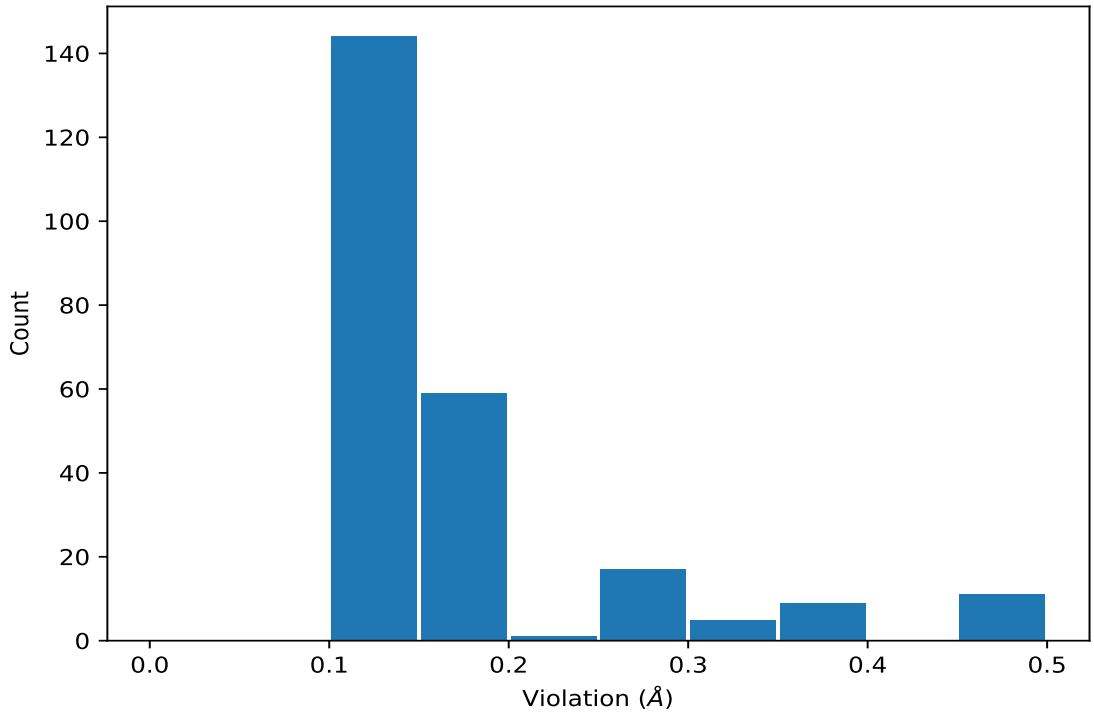
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD12	3	0.19	0.09	0.14
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD13	3	0.19	0.09	0.14
(1,243)	1:A:271:LYS:HE2	1:A:272:CYS:H	3	0.19	0.08	0.14
(1,243)	1:A:271:LYS:HE3	1:A:272:CYS:H	3	0.19	0.08	0.14
(1,86)	1:A:263:LYS:H	1:A:265:ARG:H	3	0.12	0.0	0.12
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD11	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD12	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD13	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD11	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD12	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD13	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD11	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD12	2	0.42	0.04	0.42
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD13	2	0.42	0.04	0.42
(1,303)	1:A:275:GLN:HB2	1:A:276:ASP:H	2	0.41	0.06	0.41
(1,303)	1:A:275:GLN:HB3	1:A:276:ASP:H	2	0.41	0.06	0.41
(1,264)	1:A:273:GLY:HA3	1:A:274:ILE:HG12	2	0.18	0.0	0.18
(1,185)	1:A:268:ASP:HB2	1:A:273:GLY:HA3	2	0.16	0.04	0.16
(1,288)	1:A:274:ILE:HD11	1:A:275:GLN:H	2	0.15	0.03	0.15
(1,288)	1:A:274:ILE:HD12	1:A:275:GLN:H	2	0.15	0.03	0.15
(1,288)	1:A:274:ILE:HD13	1:A:275:GLN:H	2	0.15	0.03	0.15
(1,100)	1:A:265:ARG:H	1:A:265:ARG:HG2	2	0.15	0.02	0.15
(1,100)	1:A:265:ARG:H	1:A:265:ARG:HG3	2	0.15	0.02	0.15
(1,106)	1:A:265:ARG:HE	1:A:266:MET:H	2	0.12	0.02	0.12
(1,44)	1:A:261:LEU:HD11	1:A:263:LYS:HE2	2	0.12	0.0	0.12
(1,44)	1:A:261:LEU:HD11	1:A:263:LYS:HE3	2	0.12	0.0	0.12
(1,44)	1:A:261:LEU:HD12	1:A:263:LYS:HE2	2	0.12	0.0	0.12
(1,44)	1:A:261:LEU:HD12	1:A:263:LYS:HE3	2	0.12	0.0	0.12
(1,44)	1:A:261:LEU:HD13	1:A:263:LYS:HE2	2	0.12	0.0	0.12
(1,44)	1:A:261:LEU:HD13	1:A:263:LYS:HE3	2	0.12	0.0	0.12

[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)
(1,303)	1:A:275:GLN:HB2	1:A:276:ASP:H	8	0.47
(1,303)	1:A:275:GLN:HB3	1:A:276:ASP:H	8	0.47
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD11	2	0.46
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD12	2	0.46
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD13	2	0.46
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD11	2	0.46
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD12	2	0.46
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD13	2	0.46
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD11	2	0.46
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD12	2	0.46
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD13	2	0.46
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD11	10	0.38
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD12	10	0.38
(1,281)	1:A:274:ILE:HG21	1:A:274:ILE:HD13	10	0.38
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD11	10	0.38
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD12	10	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:A:274:ILE:HG22	1:A:274:ILE:HD13	10	0.38
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD11	10	0.38
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD12	10	0.38
(1,281)	1:A:274:ILE:HG23	1:A:274:ILE:HD13	10	0.38
(1,303)	1:A:275:GLN:HB2	1:A:276:ASP:H	6	0.35
(1,303)	1:A:275:GLN:HB3	1:A:276:ASP:H	6	0.35
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD11	18	0.32
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD12	18	0.32
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD13	18	0.32
(1,396)	1:A:290:THR:HA	1:A:290:THR:HB	10	0.3
(1,396)	1:A:290:THR:HA	1:A:290:THR:HB	15	0.3
(1,396)	1:A:290:THR:HA	1:A:290:THR:HB	16	0.3
(1,396)	1:A:290:THR:HA	1:A:290:THR:HB	18	0.3
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	4	0.3
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	5	0.3
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	7	0.3
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	8	0.3
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	9	0.3
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	10	0.3
(1,311)	1:A:277:THR:HA	1:A:277:THR:HB	13	0.3
(1,243)	1:A:271:LYS:HE2	1:A:272:CYS:H	19	0.3
(1,243)	1:A:271:LYS:HE3	1:A:272:CYS:H	19	0.3
(1,396)	1:A:290:THR:HA	1:A:290:THR:HB	6	0.29
(1,41)	1:A:261:LEU:HD11	1:A:262:ARG:HE	4	0.27
(1,41)	1:A:261:LEU:HD12	1:A:262:ARG:HE	4	0.27
(1,41)	1:A:261:LEU:HD13	1:A:262:ARG:HE	4	0.27
(1,185)	1:A:268:ASP:HB2	1:A:273:GLY:HA3	10	0.2
(1,288)	1:A:274:ILE:HD11	1:A:275:GLN:H	14	0.18
(1,288)	1:A:274:ILE:HD12	1:A:275:GLN:H	14	0.18
(1,288)	1:A:274:ILE:HD13	1:A:275:GLN:H	14	0.18
(1,264)	1:A:273:GLY:HA3	1:A:274:ILE:HG12	2	0.18
(1,264)	1:A:273:GLY:HA3	1:A:274:ILE:HG12	10	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	2	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	2	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	2	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	2	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	2	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	2	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	16	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	16	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	16	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	16	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	16	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	16	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	17	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	17	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	17	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	17	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	17	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	17	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	18	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	18	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	18	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	18	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	18	0.18
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	18	0.18
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	11	0.17
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	11	0.17
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	11	0.17
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	11	0.17
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	11	0.17
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	11	0.17
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	20	0.17
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	20	0.17
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	20	0.17
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	20	0.17
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	20	0.17
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	20	0.17
(1,272)	1:A:273:GLY:HA2	1:A:274:ILE:HG12	14	0.16
(1,272)	1:A:273:GLY:HA3	1:A:274:ILE:HG12	14	0.16
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	5	0.16
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	5	0.16
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	5	0.16
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	5	0.16
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	5	0.16
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	5	0.16
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	13	0.16
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	13	0.16
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	13	0.16
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	13	0.16
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	13	0.16
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	13	0.16
(1,183)	1:A:268:ASP:HB3	1:A:273:GLY:HA3	8	0.16
(1,183)	1:A:268:ASP:HB3	1:A:273:GLY:HA3	9	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:A:265:ARG:H	1:A:265:ARG:HG2	1	0.16
(1,100)	1:A:265:ARG:H	1:A:265:ARG:HG3	1	0.16
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	4	0.15
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	4	0.15
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	4	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	4	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	4	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	4	0.15
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	15	0.15
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	15	0.15
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	15	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	15	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	15	0.15
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	15	0.15
(1,183)	1:A:268:ASP:HB3	1:A:273:GLY:HA3	3	0.15
(1,42)	1:A:261:LEU:HA	1:A:262:ARG:HE	15	0.14
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	7	0.14
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	7	0.14
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	7	0.14
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	7	0.14
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	7	0.14
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	7	0.14
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	12	0.14
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	12	0.14
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	12	0.14
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	12	0.14
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	12	0.14
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	12	0.14
(1,243)	1:A:271:LYS:HE2	1:A:272:CYS:H	5	0.14
(1,243)	1:A:271:LYS:HE3	1:A:272:CYS:H	5	0.14
(1,199)	1:A:269:VAL:HG11	1:A:270:LYS:HE2	19	0.14
(1,199)	1:A:269:VAL:HG11	1:A:270:LYS:HE3	19	0.14
(1,199)	1:A:269:VAL:HG12	1:A:270:LYS:HE2	19	0.14
(1,199)	1:A:269:VAL:HG12	1:A:270:LYS:HE3	19	0.14
(1,199)	1:A:269:VAL:HG13	1:A:270:LYS:HE2	19	0.14
(1,199)	1:A:269:VAL:HG13	1:A:270:LYS:HE3	19	0.14
(1,183)	1:A:268:ASP:HB3	1:A:273:GLY:HA3	18	0.14
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD11	9	0.14
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD12	9	0.14
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD13	9	0.14
(1,171)	1:A:268:ASP:HB2	1:A:270:LYS:H	17	0.14
(1,106)	1:A:265:ARG:HE	1:A:266:MET:H	18	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	8	0.13
(1,41)	1:A:261:LEU:HD11	1:A:262:ARG:HE	16	0.13
(1,41)	1:A:261:LEU:HD12	1:A:262:ARG:HE	16	0.13
(1,41)	1:A:261:LEU:HD13	1:A:262:ARG:HE	16	0.13
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	1	0.13
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	1	0.13
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	1	0.13
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	1	0.13
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	1	0.13
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	1	0.13
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	10	0.13
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	10	0.13
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	10	0.13
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	10	0.13
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	10	0.13
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	10	0.13
(1,247)	1:A:271:LYS:HE2	1:A:273:GLY:HA3	6	0.13
(1,247)	1:A:271:LYS:HE3	1:A:273:GLY:HA3	6	0.13
(1,243)	1:A:271:LYS:HE2	1:A:272:CYS:H	8	0.13
(1,243)	1:A:271:LYS:HE3	1:A:272:CYS:H	8	0.13
(1,185)	1:A:268:ASP:HB2	1:A:273:GLY:HA3	6	0.13
(1,133)	1:A:266:MET:HB2	1:A:270:LYS:HG3	12	0.13
(1,133)	1:A:266:MET:HB3	1:A:270:LYS:HG3	12	0.13
(1,122)	1:A:266:MET:HG3	1:A:267:MET:H	4	0.13
(1,100)	1:A:265:ARG:H	1:A:265:ARG:HG2	6	0.13
(1,100)	1:A:265:ARG:H	1:A:265:ARG:HG3	6	0.13
(1,86)	1:A:263:LYS:H	1:A:265:ARG:H	1	0.12
(1,86)	1:A:263:LYS:H	1:A:265:ARG:H	9	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	1	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	2	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	3	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	4	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	6	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	7	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	9	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	10	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	14	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	15	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	16	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	17	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	19	0.12
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	20	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:A:261:LEU:HD11	1:A:263:LYS:HE2	9	0.12
(1,44)	1:A:261:LEU:HD11	1:A:263:LYS:HE3	9	0.12
(1,44)	1:A:261:LEU:HD12	1:A:263:LYS:HE2	9	0.12
(1,44)	1:A:261:LEU:HD12	1:A:263:LYS:HE3	9	0.12
(1,44)	1:A:261:LEU:HD13	1:A:263:LYS:HE2	9	0.12
(1,44)	1:A:261:LEU:HD13	1:A:263:LYS:HE3	9	0.12
(1,41)	1:A:261:LEU:HD11	1:A:262:ARG:HE	1	0.12
(1,41)	1:A:261:LEU:HD12	1:A:262:ARG:HE	1	0.12
(1,41)	1:A:261:LEU:HD13	1:A:262:ARG:HE	1	0.12
(1,41)	1:A:261:LEU:HD11	1:A:262:ARG:HE	20	0.12
(1,41)	1:A:261:LEU:HD12	1:A:262:ARG:HE	20	0.12
(1,41)	1:A:261:LEU:HD13	1:A:262:ARG:HE	20	0.12
(1,288)	1:A:274:ILE:HD11	1:A:275:GLN:H	2	0.12
(1,288)	1:A:274:ILE:HD12	1:A:275:GLN:H	2	0.12
(1,288)	1:A:274:ILE:HD13	1:A:275:GLN:H	2	0.12
(1,183)	1:A:268:ASP:HB3	1:A:273:GLY:HA3	5	0.12
(1,172)	1:A:268:ASP:HB3	1:A:270:LYS:H	11	0.12
(1,133)	1:A:266:MET:HB2	1:A:270:LYS:HG3	6	0.12
(1,133)	1:A:266:MET:HB3	1:A:270:LYS:HG3	6	0.12
(1,133)	1:A:266:MET:HB2	1:A:270:LYS:HG3	10	0.12
(1,133)	1:A:266:MET:HB3	1:A:270:LYS:HG3	10	0.12
(1,86)	1:A:263:LYS:H	1:A:265:ARG:H	6	0.11
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	5	0.11
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	11	0.11
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	12	0.11
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	13	0.11
(1,70)	1:A:263:LYS:H	1:A:263:LYS:HB2	18	0.11
(1,44)	1:A:261:LEU:HD11	1:A:263:LYS:HE2	4	0.11
(1,44)	1:A:261:LEU:HD11	1:A:263:LYS:HE3	4	0.11
(1,44)	1:A:261:LEU:HD12	1:A:263:LYS:HE2	4	0.11
(1,44)	1:A:261:LEU:HD12	1:A:263:LYS:HE3	4	0.11
(1,44)	1:A:261:LEU:HD13	1:A:263:LYS:HE2	4	0.11
(1,44)	1:A:261:LEU:HD13	1:A:263:LYS:HE3	4	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	3	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	3	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	3	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	3	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	3	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	3	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	8	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	8	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	8	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	8	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	8	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG21	19	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG22	19	0.11
(1,256)	1:A:272:CYS:HB2	1:A:274:ILE:HG23	19	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG21	19	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG22	19	0.11
(1,256)	1:A:272:CYS:HB3	1:A:274:ILE:HG23	19	0.11
(1,183)	1:A:268:ASP:HB3	1:A:273:GLY:HA3	16	0.11
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD11	11	0.11
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD12	11	0.11
(1,18)	1:A:260:ARG:HE	1:A:261:LEU:HD13	11	0.11
(1,133)	1:A:266:MET:HB2	1:A:270:LYS:HG3	9	0.11
(1,133)	1:A:266:MET:HB3	1:A:270:LYS:HG3	9	0.11
(1,133)	1:A:266:MET:HB2	1:A:270:LYS:HG3	15	0.11
(1,133)	1:A:266:MET:HB3	1:A:270:LYS:HG3	15	0.11
(1,106)	1:A:265:ARG:HE	1:A:266:MET:H	3	0.11
(1,105)	1:A:265:ARG:HD2	1:A:266:MET:H	9	0.11
(1,105)	1:A:265:ARG:HD3	1:A:266:MET:H	9	0.11

10 Dihedral-angle violation analysis (i)

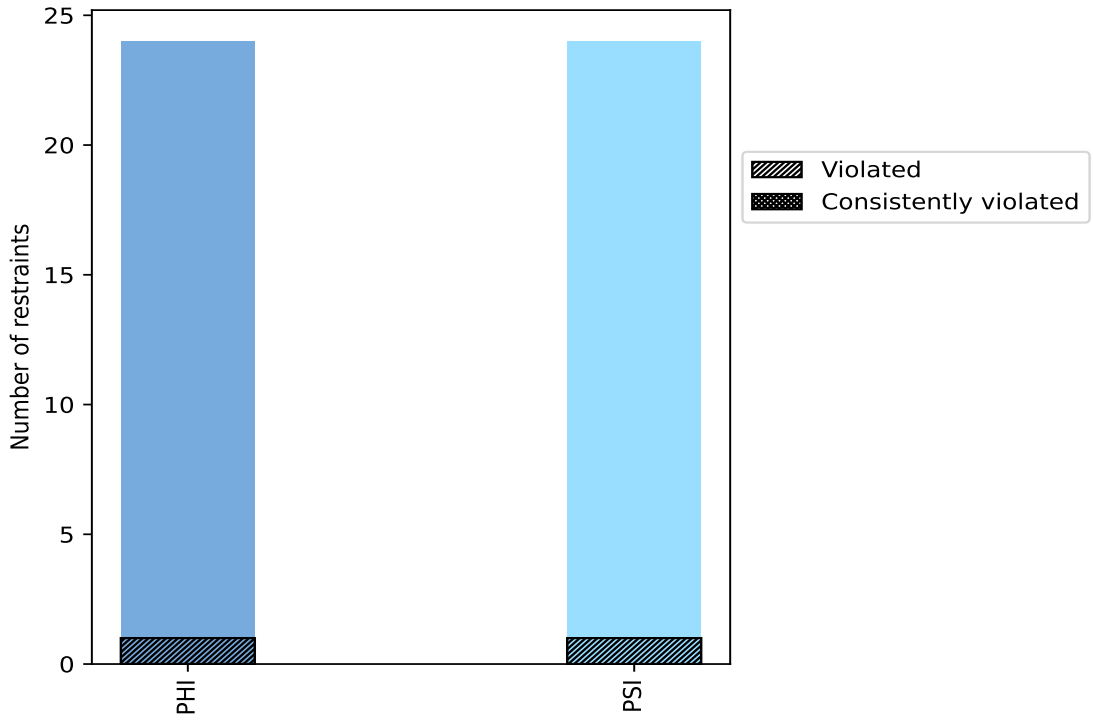
10.1 Summary of dihedral-angle violations (i)

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]
PHI	24	50.0	1	4.2	2.1	0	0.0	0.0
PSI	24	50.0	1	4.2	2.1	0	0.0	0.0
Total	48	100.0	2	4.2	4.2	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 (i)



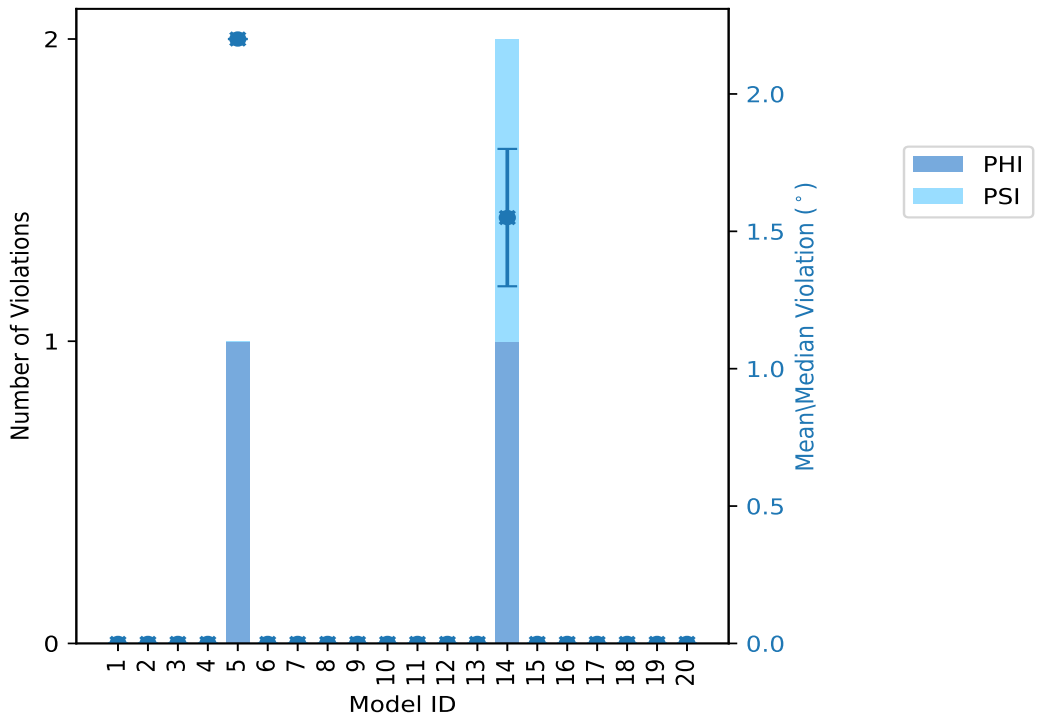
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	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	1	0	1	2.2	2.2	0.0	2.2
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	0	0	0.0	0.0	0.0	0.0
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	1	1	2	1.55	1.8	0.25	1.55
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	0	0	0.0	0.0	0.0	0.0
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 (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	
PHI	PSI	Total	Count[1]	%
0	1	1	1	5.0
1	0	1	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

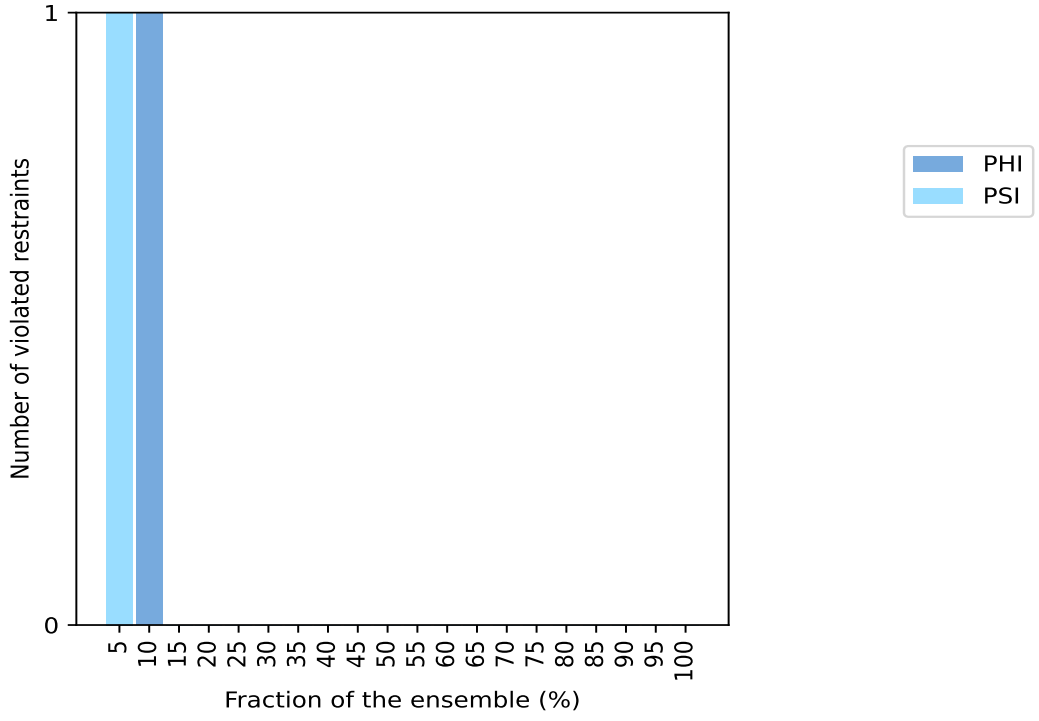
Continued on next page...

Continued from previous page...

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 (i)

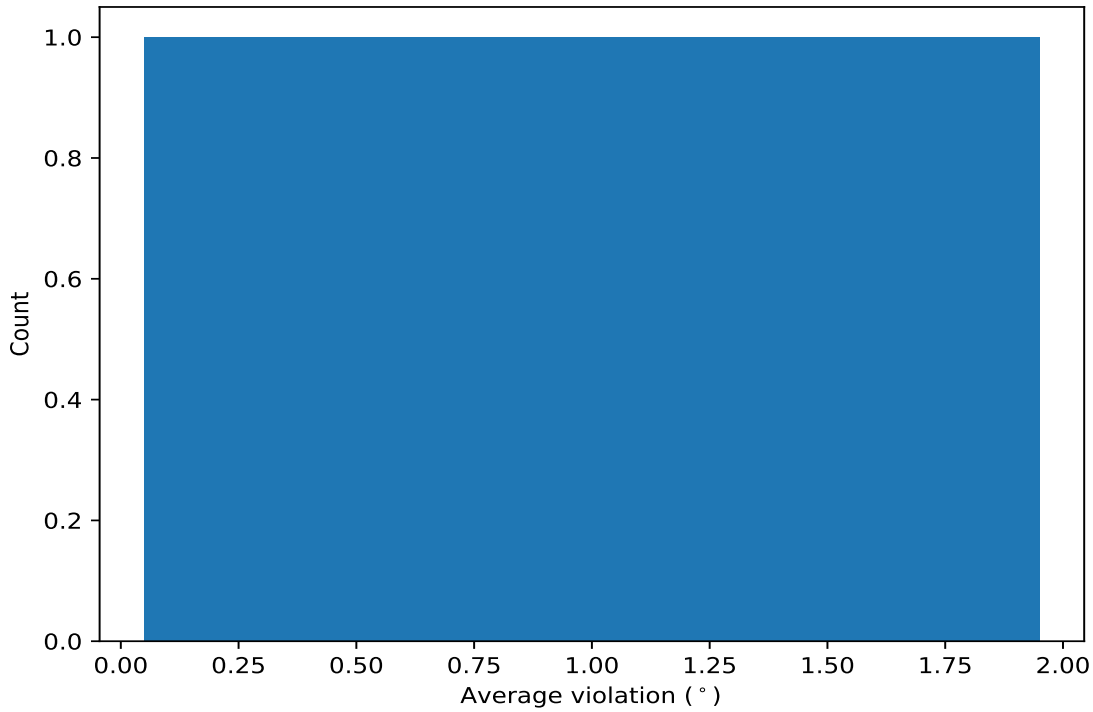


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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 violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,39)	1:A:284:ASP:C	1:A:285:THR:N	1:A:285:THR:CA	1:A:285:THR:C	2	2.0	0.2	2.0

[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.
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 (°)
(1,39)	1:A:284:ASP:C	1:A:285:THR:N	1:A:285:THR:CA	1:A:285:THR:C	5	2.2
(1,39)	1:A:284:ASP:C	1:A:285:THR:N	1:A:285:THR:CA	1:A:285:THR:C	14	1.8
(1,40)	1:A:285:THR:N	1:A:285:THR:CA	1:A:285:THR:C	1:A:286:HIS:N	14	1.3