Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 05:26 PM EDT

PDB ID	:	2LAS
BMRB ID	:	17536
Title	:	Molecular Determinants of Paralogue-Specific SUMO-SIM Recognition
Authors	:	Namanja, A.; Li, Y.; Su, Y.; Wong, S.; Lu, J.; Colson, L.; Wu, C.; Li, S.; Chen, Y.
Deposited on	:	2011-03-20

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:

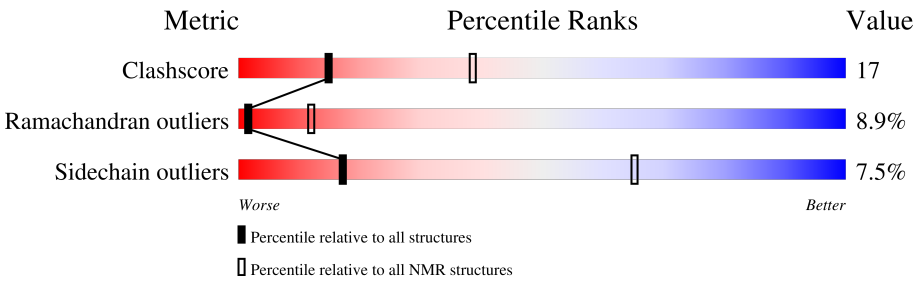
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 28%.

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	101	29% 13% • 32% 23%
2	B	13	100%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:52-A:97 (46)	0.04	4

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 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 8, 9
2	5, 6
Single-model clusters	7; 10

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1500 atoms, of which 750 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Small ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	78	1269	400	633	109	123	4	0

- Molecule 2 is a protein called M-IR2_peptide.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	13	231	74	117	17	23	0

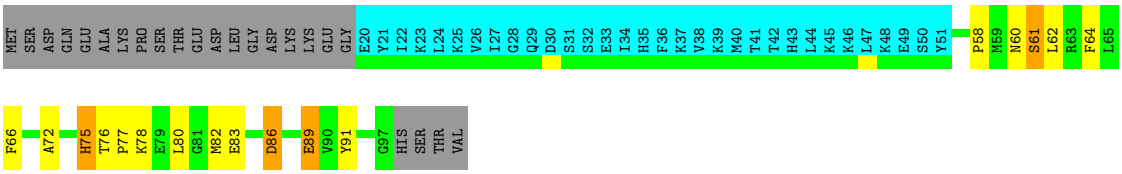
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

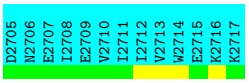
• Molecule 1: Small ubiquitin-related modifier 1

Chain A: 29% 13% • 32% 23%



• Molecule 2: M-IR2_peptide

Chain B: 100%



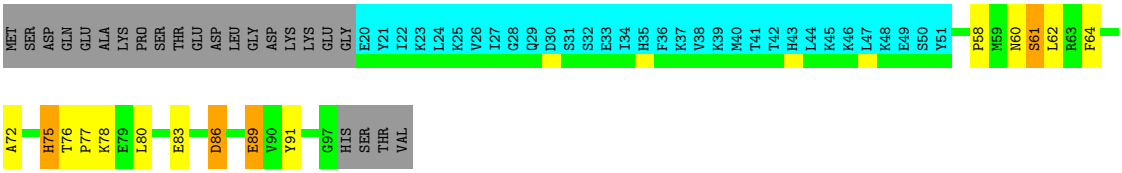
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Small ubiquitin-related modifier 1

Chain A: 31% 11% • 32% 23%



• Molecule 2: M-IR2_peptide

Chain B: 100%

D2705 N2706 E2707 I2708 E2709 V2710 I2711 I2712 V2713 W2714 E2715 K2716 K2717

4.2.2 Score per residue for model 2

- Molecule 1: Small ubiquitin-related modifier 1

Chain A: 28% 14% • 32% 23%

MET SER ASP GLN GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY E20 Y21 I22 K23 L24 K25 V26 I27 G28 Q29 D30 S31 S32 E33 I34 H35 F36 K37 V38 K39 M40 T41 T42 H43 L44 K45 K46 L47 K48 E49 S50 Y51 C52 P58 M59 N60 S61 L62 R63 F64

A72 H75 T76 P77 K78 E79 L80 E83 E84 E85 D86 E89 V90 Y91 G97 HIS SER THR VAL

- Molecule 2: M-IR2_peptide

Chain B: 100%

D2705 N2706 E2707 I2708 E2709 V2710 I2711 I2712 V2713 W2714 E2715 K2716 K2717

4.2.3 Score per residue for model 3

- Molecule 1: Small ubiquitin-related modifier 1

Chain A: 29% 13% • 32% 23%

MET SER ASP GLN GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY E20 Y21 I22 K23 L24 K25 V26 I27 G28 Q29 D30 S31 S32 E33 I34 H35 F36 K37 V38 K39 M40 T41 T42 H43 L44 K45 K46 L47 K48 E49 S50 Y51 P58 M59 N60 S61 L62 R63 F64 L65

F66 A72 H75 T76 P77 K78 E79 L80 G81 M82 E83 D86 E89 V90 Y91 G97 HIS SER THR VAL

- Molecule 2: M-IR2_peptide

Chain B: 100%

D2705 N2706 E2707 I2708 E2709 V2710 I2711 I2712 V2713 W2714 E2715 K2716 K2717

4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Small ubiquitin-related modifier 1

Chain A: 31% 11% • 32% 23%

MET SER ASP GLN GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY E20 Y21 I22 K23 L24 K25 V26 I27 G28 Q29 D30 S31 S32 E33 I34 H35 F36 K37 V38 K39 M40 T41 T42 H43 L44 K45 K46 L47 K48 E49 S50 Y51 P58 M59 N60 S61 L62 R63 F64

A72 H75 T76 P77 K78 E79 L80 E83 D86 E89 V90 Y91 G97 HIS SER THR VAL

• Molecule 2: M-IR2_peptide

Chain B: 100%

D2705 N2706 E2707 I2708 E2709 V2710 I2711 I2712 V2713 W2714 E2715 K2716 K2717

4.2.5 Score per residue for model 5

• Molecule 1: Small ubiquitin-related modifier 1

Chain A: 27% 15% • 32% 23%

MET SER ASP GLN GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY E20 Y21 I22 K23 L24 K25 V26 I27 G28 Q29 D30 S31 S32 E33 I34 H35 F36 K37 V38 K39 M40 T41 T42 H43 L44 K45 K46 L47 K48 E49 S50 Y51 C52 P58 M59 N60 S61 L62 R63 F64

L65 F66 A72 H75 T76 P77 K78 E79 L80 G81 M82 E83 D86 E89 V90 Y91 G97 HIS SER THR VAL

• Molecule 2: M-IR2_peptide

Chain B: 100%

D2705 N2706 E2707 I2708 E2709 V2710 I2711 I2712 V2713 W2714 E2715 K2716 K2717

4.2.6 Score per residue for model 6

• Molecule 1: Small ubiquitin-related modifier 1

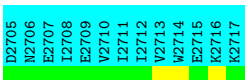
Chain A: 29% 13% • 32% 23%

MET SER ASP GLN GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY E20 Y21 I22 K23 L24 K25 V26 I27 G28 Q29 D30 S31 S32 E33 I34 H35 F36 K37 V38 K39 M40 T41 T42 H43 L44 K45 K46 L47 K48 E49 S50 Y51 P58 M59 N60 S61 L62 R63 F64 L65

F66 A72 H75 T76 P77 K78 E79 L80 G81 M82 E83 D86 E89 V90 Y91 G97 HIS SER THR VAL

• Molecule 2: M-IR2_peptide

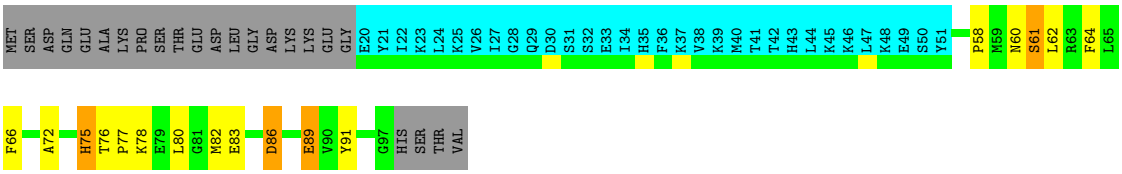
Chain B: 100%



4.2.7 Score per residue for model 7

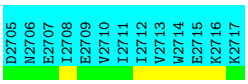
- Molecule 1: Small ubiquitin-related modifier 1

Chain A: 29% 13% • 32% 23%



- Molecule 2: M-IR2_peptide

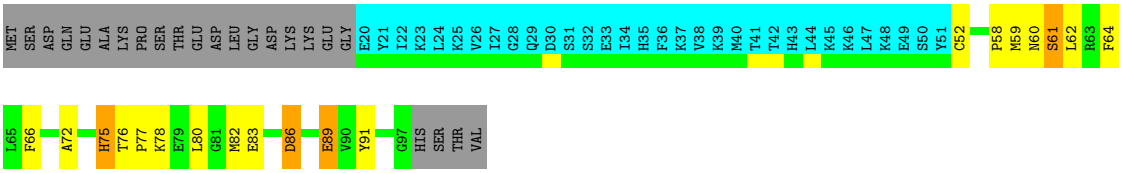
Chain B: 100%



4.2.8 Score per residue for model 8

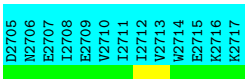
- Molecule 1: Small ubiquitin-related modifier 1

Chain A: 27% 15% • 32% 23%



- Molecule 2: M-IR2_peptide

Chain B: 100%



4.2.9 Score per residue for model 9

- Molecule 1: Small ubiquitin-related modifier 1

Chain A: 29% 13% • 32% 23%

MET SER ASP GLN GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY E20 Y21 I22 K23 L24 K25 V26 I27 G28 Q29 D30 S31 S32 E33 I34 H35 F36 K37 V38 K39 M40 T41 T42 H43 L44 K45 K46 L47 K48 E49 S50 Y51 C52 P58 M59 N60 S61 L62 R63 F64

A72 H75 T76 P77 K78 E79 L80 E83 D86 E89 V90 Y91 G97 HIS SER THR VAL

• Molecule 2: M-IR2_peptide

Chain B: 100%

D2705 N2706 E2707 I2708 E2709 V2710 I2711 I2712 V2713 W2714 E2715 K2716 K2717

4.2.10 Score per residue for model 10

• Molecule 1: Small ubiquitin-related modifier 1

Chain A: 29% 13% • 32% 23%

MET SER ASP GLN GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY E20 Y21 I22 K23 L24 K25 V26 I27 G28 Q29 D30 S31 S32 E33 I34 H35 F36 K37 V38 K39 M40 T41 T42 H43 L44 K45 K46 L47 K48 E49 S50 Y51 P58 M59 N60 S61 L62 R63 F64 L65

F66 A72 H75 T76 P77 K78 E79 L80 G81 M82 E83 D86 E89 V90 Y91 G97 HIS SER THR VAL

• Molecule 2: M-IR2_peptide

Chain B: 100%

D2705 N2706 E2707 I2708 E2709 V2710 I2711 I2712 V2713 W2714 E2715 K2716 K2717

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *all calculated structures submitted*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	structure solution	2.0
CNS	refinement	
HADDOCK	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	515
Number of shifts mapped to atoms	447
Number of unparsed shifts	0
Number of shifts with mapping errors	68
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	28%

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	368	346	346	12±1
2	B	0	0	0	0±0
All	All	3680	3460	3460	121

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:PRO:HG2	1:A:61:SER:HB2	0.74	1.59	9	10
1:A:60:ASN:O	1:A:62:LEU:N	0.52	2.42	3	10
1:A:76:THR:O	1:A:78:LYS:N	0.52	2.43	2	10
1:A:75:HIS:CE1	1:A:80:LEU:HG	0.51	2.41	2	10
1:A:76:THR:C	1:A:78:LYS:N	0.51	2.64	6	10
1:A:72:ALA:H	1:A:75:HIS:HD2	0.48	1.52	8	10
1:A:89:GLU:HB3	1:A:91:TYR:CE1	0.47	2.45	5	10
1:A:64:PHE:CD1	1:A:64:PHE:N	0.46	2.83	5	10
1:A:76:THR:C	1:A:78:LYS:H	0.46	2.14	10	10
1:A:75:HIS:O	1:A:76:THR:OG1	0.42	2.38	1	1
1:A:52:CYS:SG	1:A:59:MET:HA	0.42	2.55	5	4
1:A:58:PRO:HB2	1:A:60:ASN:OD1	0.41	2.15	2	9
1:A:60:ASN:O	1:A:61:SER:C	0.41	2.59	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:PHE:CZ	1:A:82:MET:HG2	0.41	2.52	3	6
1:A:85:GLU:HG3	1:A:85:GLU:O	0.40	2.17	2	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	45/101 (45%)	34±0 (76±0%)	7±0 (16±0%)	4±0 (9±0%)	1 12
2	B	0	-	-	-	-
All	All	450/1140 (39%)	340 (76%)	70 (16%)	40 (9%)	1 12

All 4 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	61	SER	10
1	A	77	PRO	10
1	A	83	GLU	10
1	A	86	ASP	10

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	40/91 (44%)	37±0 (92±0%)	3±0 (8±0%)	17 65
2	B	0	-	-	-
All	All	400/1040 (38%)	370 (92%)	30 (8%)	17 65

All 3 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	HIS	10
1	A	86	ASP	10
1	A	89	GLU	10

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 28% for the well-defined parts and 35% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	515
Number of shifts mapped to atoms	447
Number of unparsed shifts	0
Number of shifts with mapping errors	68
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 68 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	CA	55.302	0.010	1
1	A	1	MET	CB	31.712	0.186	1
1	A	2	SER	CA	58.021	0.043	1
1	A	2	SER	CB	63.127	0.053	1
1	A	2	SER	H	8.403	0.003	1
1	A	2	SER	N	116.863	0.038	1
1	A	3	ASP	CA	54.245	0.192	1
1	A	3	ASP	CB	40.137	0.104	1
1	A	3	ASP	H	8.416	0.004	1
1	A	3	ASP	N	122.15	0.141	1
1	A	4	GLN	CA	55.591	0.012	1
1	A	4	GLN	CB	28.501	0.150	1
1	A	4	GLN	H	8.24	0.003	1
1	A	4	GLN	N	119.654	0.023	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	GLU	CA	55.905	0.150	1
1	A	5	GLU	CB	29.285	0.167	1
1	A	5	GLU	H	8.246	0.002	1
1	A	5	GLU	N	121.372	0.033	1
1	A	6	ALA	CA	51.816	0.103	1
1	A	6	ALA	CB	18.095	0.174	1
1	A	6	ALA	H	8.221	0.003	1
1	A	6	ALA	N	125.157	0.031	1
1	A	7	LYS	CA	53.627	0.000	1
1	A	7	LYS	CB	31.407	0.000	1
1	A	7	LYS	H	8.261	0.003	1
1	A	7	LYS	N	122.199	0.045	1
1	A	8	PRO	CA	62.971	0.169	1
1	A	8	PRO	CB	31.002	0.168	1
1	A	9	SER	CA	57.685	0.120	1
1	A	9	SER	CB	63.075	0.073	1
1	A	9	SER	H	8.546	0.003	1
1	A	9	SER	N	116.665	0.017	1
1	A	10	THR	CA	61.51	0.065	1
1	A	10	THR	CB	68.933	0.058	1
1	A	10	THR	H	8.207	0.001	1
1	A	10	THR	N	115.608	0.021	1
1	A	11	GLU	CA	56.094	0.145	1
1	A	11	GLU	CB	29.355	0.184	1
1	A	11	GLU	H	8.359	0.002	1
1	A	11	GLU	N	122.691	0.033	1
1	A	12	ASP	CA	53.789	0.026	1
1	A	12	ASP	CB	40.455	0.070	1
1	A	12	ASP	H	8.364	0.003	1
1	A	12	ASP	N	121.8	0.030	1
1	A	13	LEU	CA	54.928	0.114	1
1	A	13	LEU	CB	40.93	0.136	1
1	A	13	LEU	H	8.314	0.005	1
1	A	13	LEU	N	123.492	0.015	1
1	A	14	GLY	CA	44.972	0.137	1
1	A	14	GLY	H	8.409	0.003	1
1	A	14	GLY	N	108.9	0.016	1
1	A	15	ASP	CA	53.859	0.000	1
1	A	15	ASP	CB	40.53	0.000	1
1	A	15	ASP	H	8.242	0.000	1
1	A	15	ASP	N	120.554	0.023	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	LYS	CA	55.654	0.062	1
1	A	16	LYS	CB	31.097	0.000	1
1	A	17	LYS	CA	55.959	0.108	1
1	A	17	LYS	CB	31.51	0.155	1
1	A	17	LYS	H	8.387	0.003	1
1	A	17	LYS	N	122.439	0.034	1
1	A	18	GLU	CA	56.379	0.098	1
1	A	18	GLU	CB	29.168	0.182	1
1	A	18	GLU	H	8.479	0.002	1
1	A	18	GLU	N	121.817	0.026	1
1	A	19	GLY	CA	44.752	0.186	1
1	A	19	GLY	H	8.448	0.002	1
1	A	19	GLY	N	109.532	0.019	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	102	0.26 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	96	0.78 ± 0.13	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	92	0.73 ± 0.39	None needed (imprecise)

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 28%, i.e. 175 atoms were assigned a chemical shift out of a possible 622. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	134/231 (58%)	44/95 (46%)	46/92 (50%)	44/44 (100%)
Sidechain	41/355 (12%)	0/226 (0%)	41/112 (37%)	0/17 (0%)
Aromatic	0/36 (0%)	0/18 (0%)	0/17 (0%)	0/1 (0%)
Overall	175/622 (28%)	44/339 (13%)	87/221 (39%)	44/62 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 447 atoms were assigned a chemical shift out of a possible 1292. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	260/457 (57%)	101/186 (54%)	83/182 (46%)	76/89 (85%)
Sidechain	176/745 (24%)	75/478 (16%)	101/239 (42%)	0/28 (0%)
Aromatic	11/90 (12%)	6/45 (13%)	5/41 (12%)	0/4 (0%)
Overall	447/1292 (35%)	182/709 (26%)	189/462 (41%)	76/121 (63%)

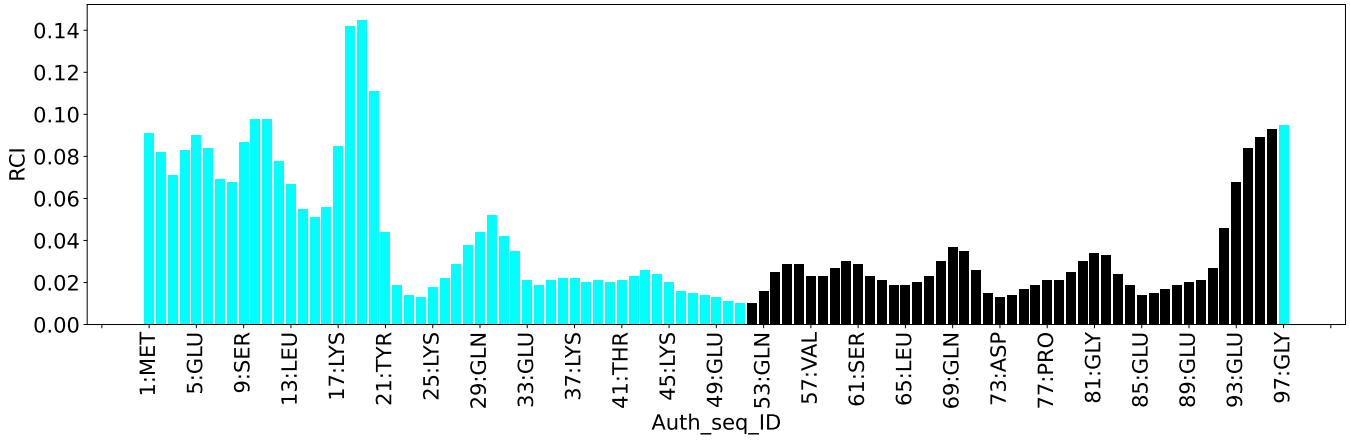
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

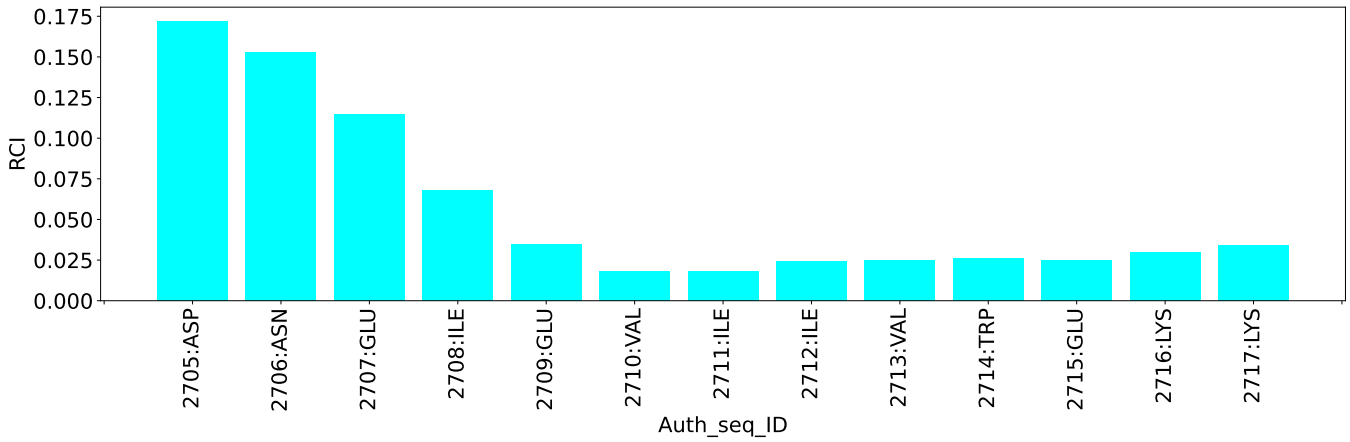
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:


0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
RCI
2705:ASP
2706:ASN
2707:GLU
2708:ILE
2709:GLU
2710:VAL
2711:ILE
2712:ILE
2713:VAL
2714:TRP
2715:GLU
2716:LYS
2717:LYS
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	84
Intra-residue (|i-j|=0)	41
Sequential (|i-j|=1)	3
Medium range (|i-j|>1 and |i-j|<5)	7
Long range (|i-j|≥5)	0
Inter-chain	33
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	64
Number of unmapped restraints	0
Number of restraints per residue	1.3
Number of long range restraints per residue[1]	0.0

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.0	0.2
0.2-0.5 (Medium)	0.1	0.22
>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)	3.5	3.7
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

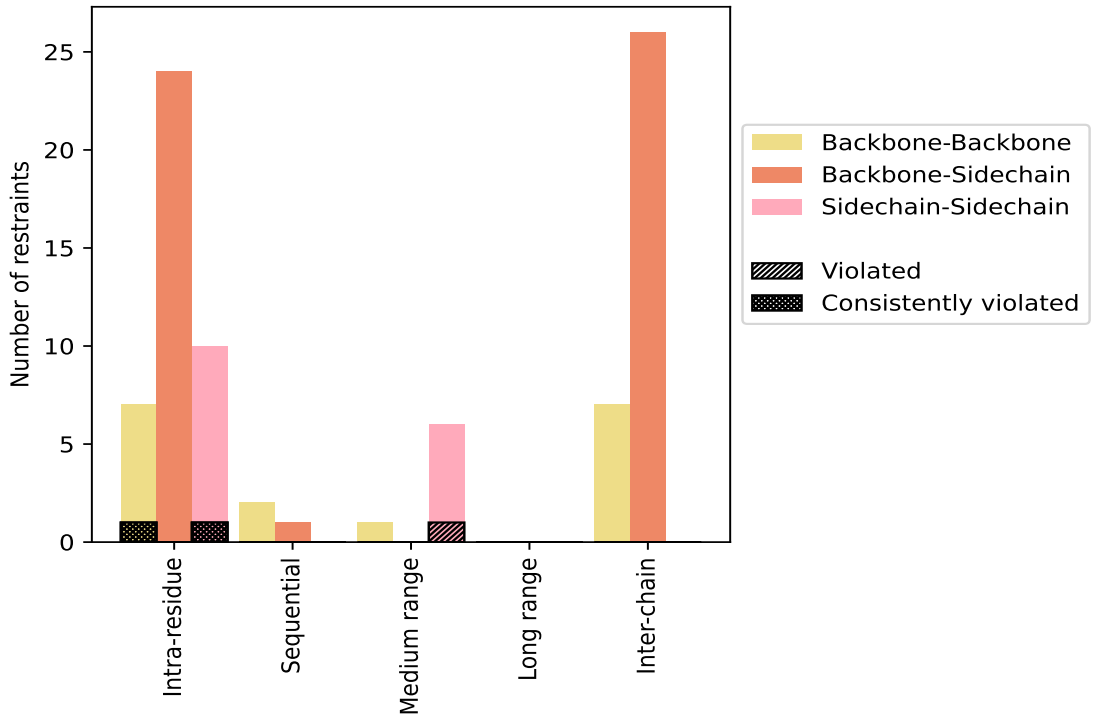
9.1 Summary of distance violations (i)

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)	41	48.8	2	4.9	2.4	2	4.9	2.4
Backbone-Backbone	7	8.3	1	14.3	1.2	1	14.3	1.2
Backbone-Sidechain	24	28.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	10	11.9	1	10.0	1.2	1	10.0	1.2
Sequential (|i-j|=1)	3	3.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	1.2	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
Medium range (|i-j|>1 & |i-j|<5)	7	8.3	1	14.3	1.2	0	0.0	0.0
Backbone-Backbone	1	1.2	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	6	7.1	1	16.7	1.2	0	0.0	0.0
Long range (|i-j|≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	33	39.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	7	8.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	26	31.0	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	84	100.0	3	3.6	3.6	2	2.4	2.4
Backbone-Backbone	17	20.2	1	5.9	1.2	1	5.9	1.2
Backbone-Sidechain	51	60.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	16	19.0	2	12.5	2.4	1	6.2	1.2

[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)

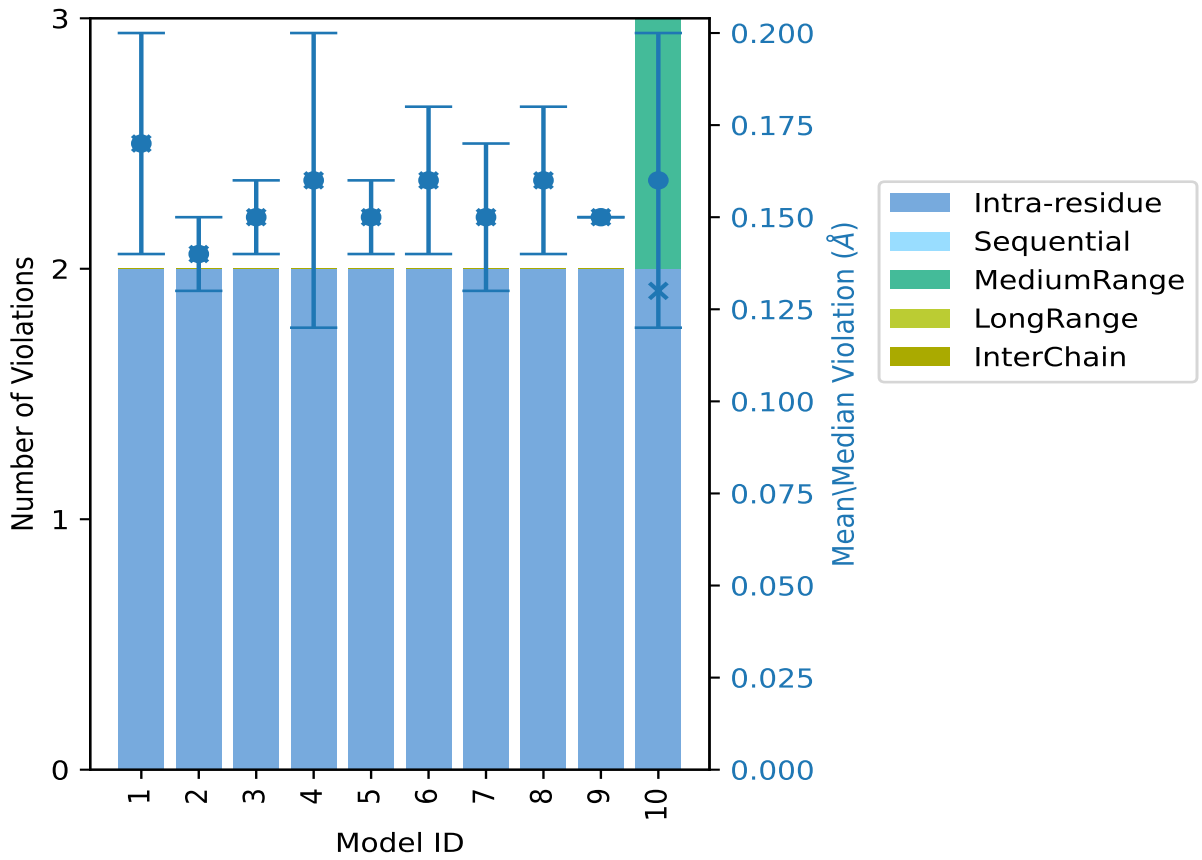
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	0	0	0	0	2	0.17	0.2	0.03	0.17
2	2	0	0	0	0	2	0.14	0.15	0.01	0.14
3	2	0	0	0	0	2	0.15	0.16	0.01	0.15
4	2	0	0	0	0	2	0.16	0.2	0.04	0.16
5	2	0	0	0	0	2	0.15	0.16	0.01	0.15
6	2	0	0	0	0	2	0.16	0.17	0.02	0.16
7	2	0	0	0	0	2	0.15	0.17	0.02	0.15
8	2	0	0	0	0	2	0.16	0.17	0.02	0.16
9	2	0	0	0	0	2	0.15	0.15	0.0	0.15
10	2	0	1	0	0	3	0.16	0.22	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 (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, 81(IR:39, SQ:3, MR:6, LR:0, IC:33) 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	0	1	0	0	1	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0
0	0	0	0	0	0	4	40.0

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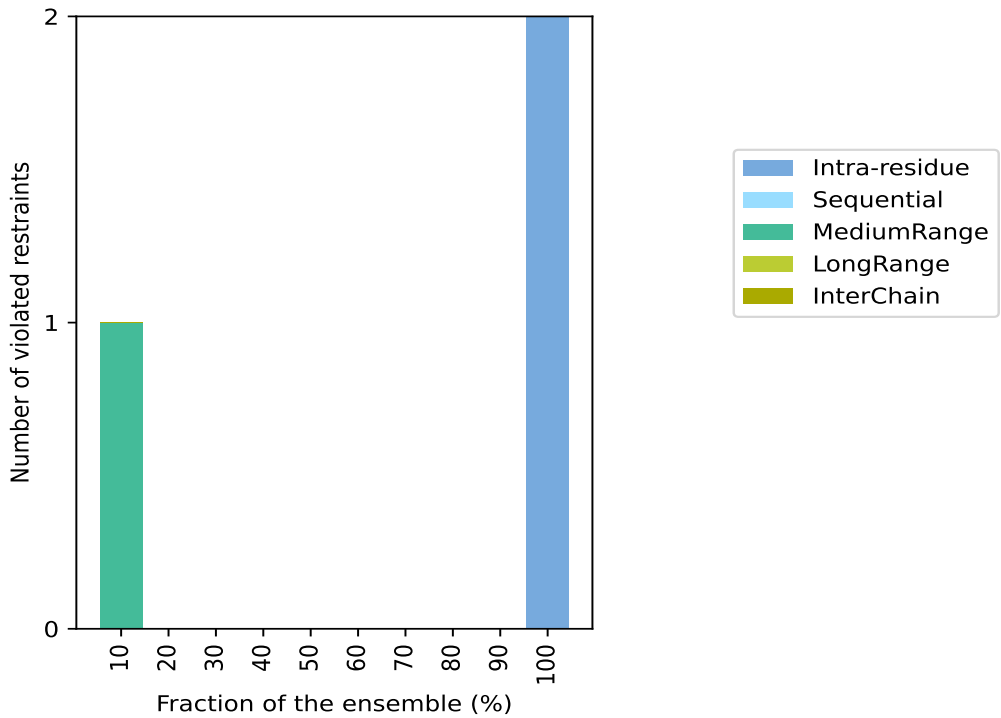
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
2	0	0	0	0	2	10	100.0

[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

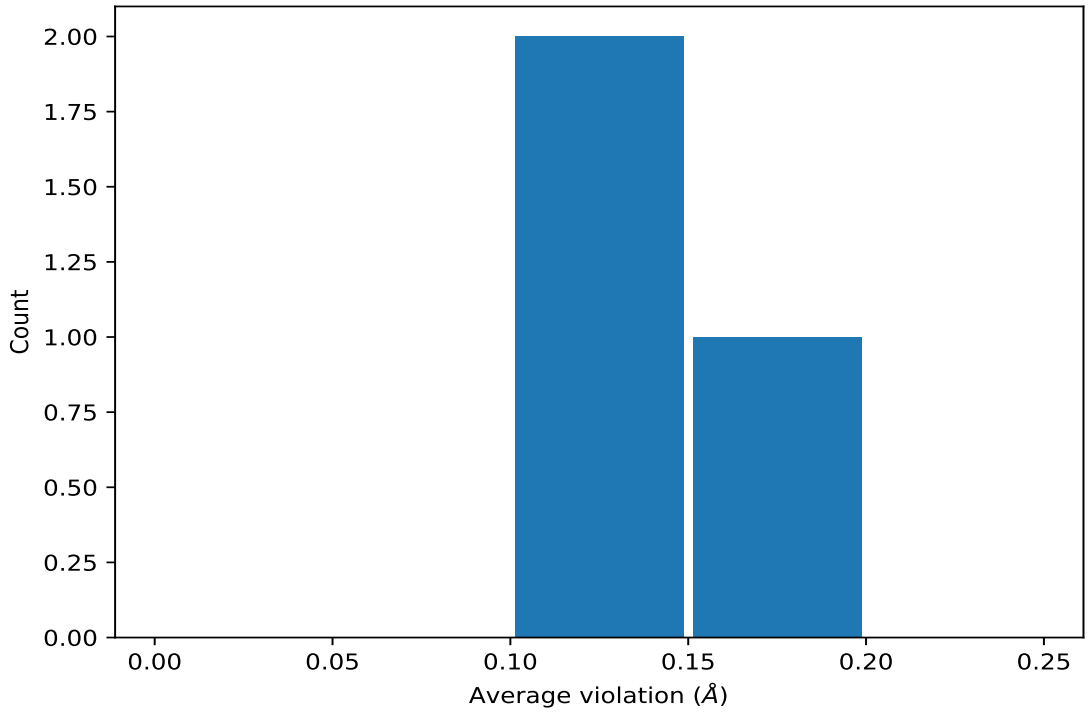
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

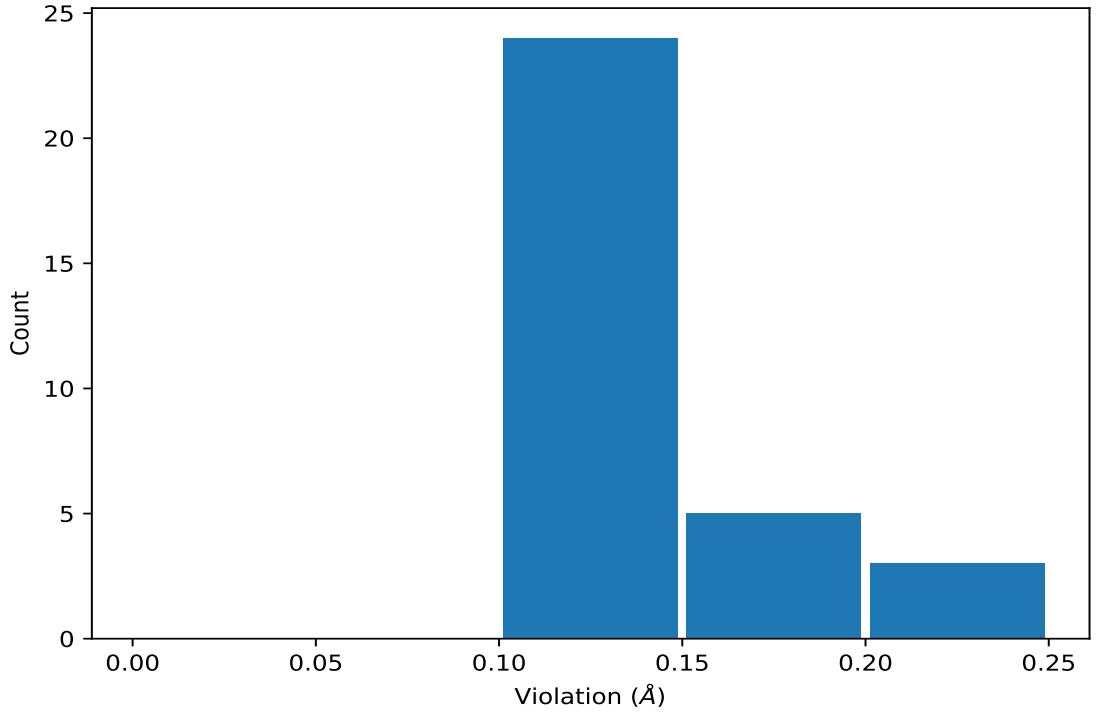
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	10	0.18	0.02	0.17
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	10	0.14	0.0	0.14
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	10	0.14	0.0	0.14

[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)
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	10	0.22
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	1	0.2
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	4	0.2
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	6	0.17
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	7	0.17
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	8	0.17
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	3	0.16
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	5	0.16
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	2	0.15
(1,35)	2:B:2713:VAL:HA	2:B:2713:VAL:H	9	0.15
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	1	0.14
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	1	0.14
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	3	0.14
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	3	0.14
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	5	0.14
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	6	0.14
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	6	0.14
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	8	0.14
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	8	0.14
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	9	0.14
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	9	0.14
(1,77)	2:B:2717:LYS:HB2	2:B:2714:TRP:HH2	10	0.13
(1,77)	2:B:2717:LYS:HB3	2:B:2714:TRP:HH2	10	0.13
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	2	0.13
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	2	0.13
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	4	0.13
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	4	0.13
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	7	0.13
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	7	0.13
(1,47)	2:B:2714:TRP:HB2	2:B:2714:TRP:HB3	10	0.13
(1,47)	2:B:2714:TRP:HB3	2:B:2714:TRP:HB2	10	0.13

10 Dihedral-angle violation analysis (i)

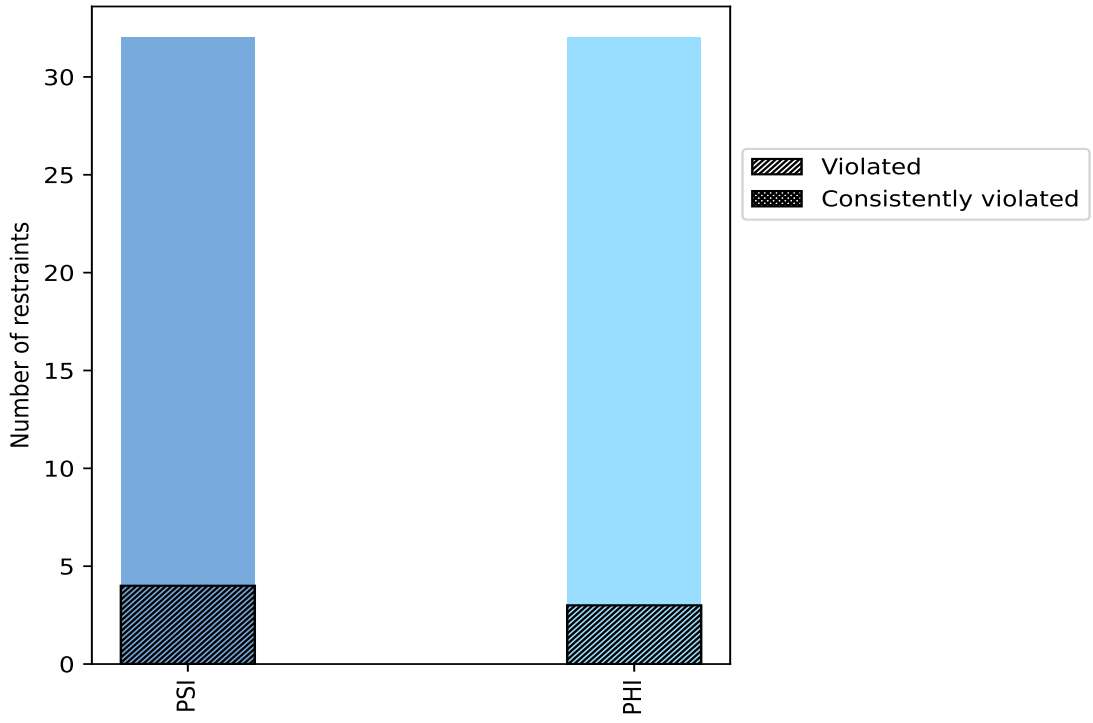
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	32	50.0	4	12.5	6.2	0	0.0	0.0
PHI	32	50.0	3	9.4	4.7	0	0.0	0.0
Total	64	100.0	7	10.9	10.9	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)



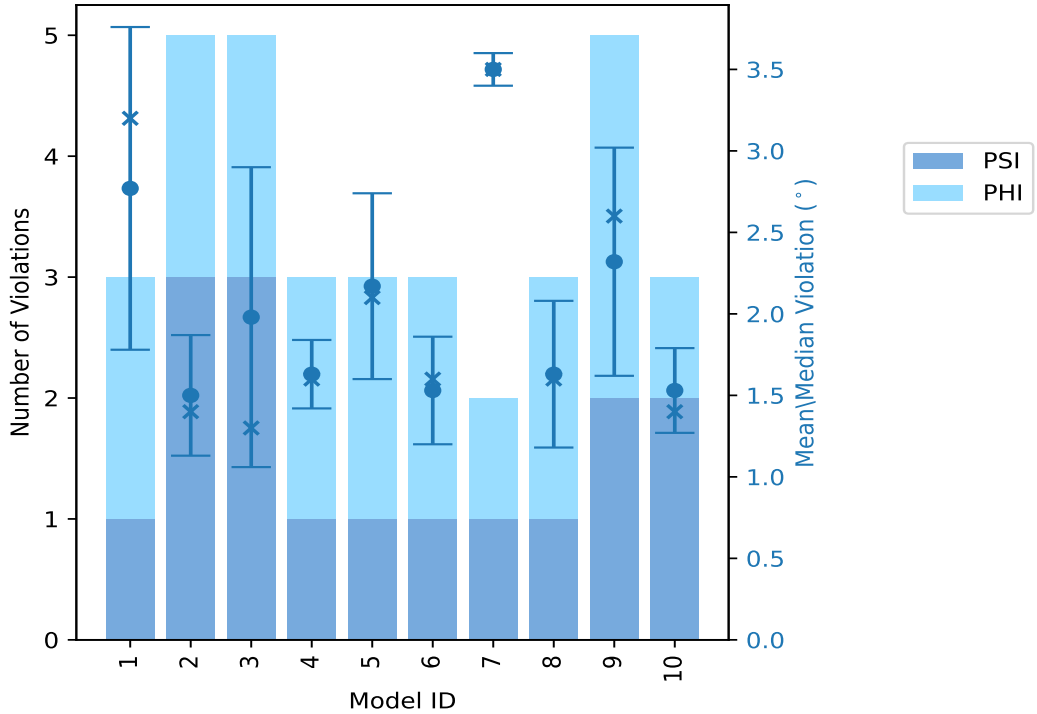
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	1	2	3	2.77	3.7	0.99	3.2
2	3	2	5	1.5	2.2	0.37	1.4
3	3	2	5	1.98	3.2	0.92	1.3
4	1	2	3	1.63	1.9	0.21	1.6
5	1	2	3	2.17	2.9	0.57	2.1
6	1	2	3	1.53	1.9	0.33	1.6
7	1	1	2	3.5	3.6	0.1	3.5
8	1	2	3	1.63	2.2	0.45	1.6
9	2	3	5	2.32	3.2	0.7	2.6
10	2	1	3	1.53	1.9	0.26	1.4

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

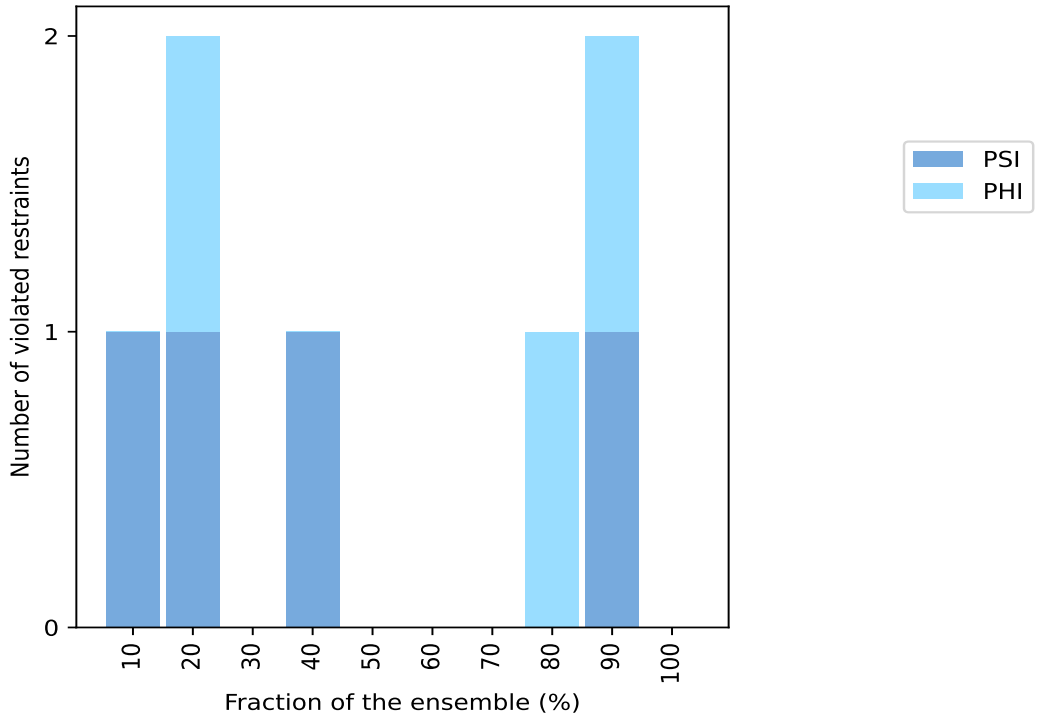
10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	0	1	1	10.0
1	1	2	2	20.0
0	0	0	3	30.0
1	0	1	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	7	70.0
0	1	1	8	80.0
1	1	2	9	90.0
0	0	0	10	100.0

[1] Number of models with violations

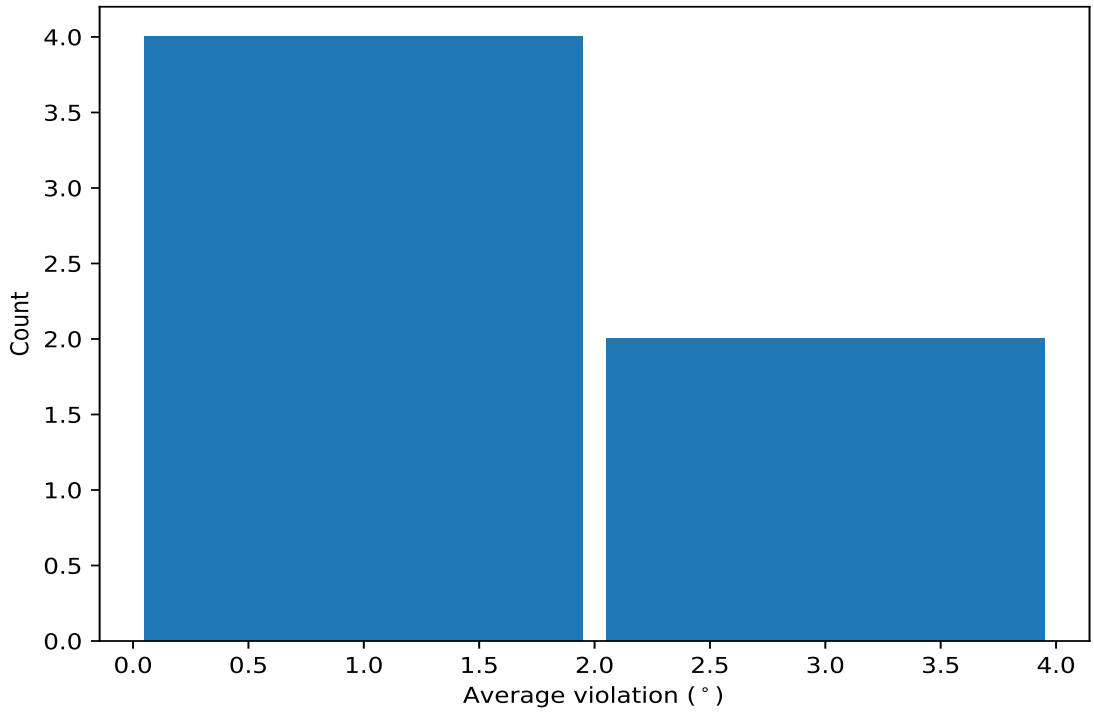
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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.

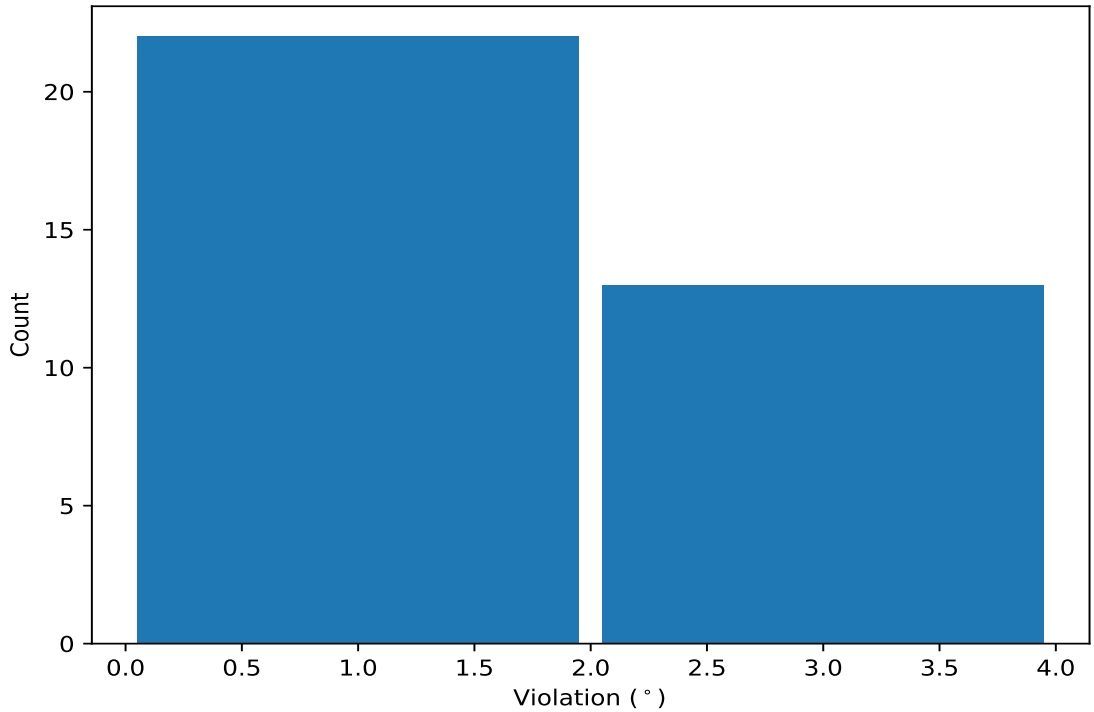
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	9	2.6	0.62	2.8
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	9	2.4	0.8	2.1
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	8	1.34	0.15	1.4
(1,8)	2:B:2709:GLU:N	2:B:2709:GLU:CA	2:B:2709:GLU:C	2:B:2710:VAL:N	4	1.93	0.78	1.6
(1,9)	2:B:2709:GLU:C	2:B:2710:VAL:N	2:B:2710:VAL:CA	2:B:2710:VAL:C	2	1.4	0.1	1.4
(1,20)	2:B:2715:GLU:N	2:B:2715:GLU:CA	2:B:2715:GLU:C	2:B:2716:LYS:N	2	1.1	0.0	1.1

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

The following table 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 (°)
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	1	3.7
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	7	3.6
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	7	3.4
(1,8)	2:B:2709:GLU:N	2:B:2709:GLU:CA	2:B:2709:GLU:C	2:B:2710:VAL:N	9	3.2
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	3	3.2
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	1	3.2
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	3	3.0
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	5	2.9
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	9	2.8
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	9	2.6
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	2	2.2
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	8	2.2
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	5	2.1
(1,8)	2:B:2709:GLU:N	2:B:2709:GLU:CA	2:B:2709:GLU:C	2:B:2710:VAL:N	10	1.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	6	1.9
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	4	1.9
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	4	1.6
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	8	1.6
(1,16)	2:B:2713:VAL:N	2:B:2713:VAL:CA	2:B:2713:VAL:C	2:B:2714:TRP:N	6	1.6
(1,9)	2:B:2709:GLU:C	2:B:2710:VAL:N	2:B:2710:VAL:CA	2:B:2710:VAL:C	9	1.5
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	5	1.5
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	9	1.5
(1,17)	2:B:2713:VAL:C	2:B:2714:TRP:N	2:B:2714:TRP:CA	2:B:2714:TRP:C	2	1.5
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	1	1.4
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	2	1.4
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	4	1.4
(1,34)	1:A:33:GLU:N	1:A:33:GLU:CA	1:A:33:GLU:C	1:A:34:ILE:N	10	1.4
(1,9)	2:B:2709:GLU:C	2:B:2710:VAL:N	2:B:2710:VAL:CA	2:B:2710:VAL:C	10	1.3
(1,8)	2:B:2709:GLU:N	2:B:2709:GLU:CA	2:B:2709:GLU:C	2:B:2710:VAL:N	2	1.3
(1,8)	2:B:2709:GLU:N	2:B:2709:GLU:CA	2:B:2709:GLU:C	2:B:2710:VAL:N	3	1.3
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	3	1.3
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	6	1.1
(1,37)	1:A:34:ILE:C	1:A:35:HIS:N	1:A:35:HIS:CA	1:A:35:HIS:C	8	1.1
(1,20)	2:B:2715:GLU:N	2:B:2715:GLU:CA	2:B:2715:GLU:C	2:B:2716:LYS:N	2	1.1
(1,20)	2:B:2715:GLU:N	2:B:2715:GLU:CA	2:B:2715:GLU:C	2:B:2716:LYS:N	3	1.1