Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 08:59 AM EDT

PDB ID	:	2L89
BMRB ID	:	17398
Title	:	Solution structure of Pdp1 PWWP domain reveals its unique binding sites for methylated H4K20 and DNA
Authors	:	Qiu, Y.; Zhang, J.; Zhang, W.
Deposited on	:	2011-01-07

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:

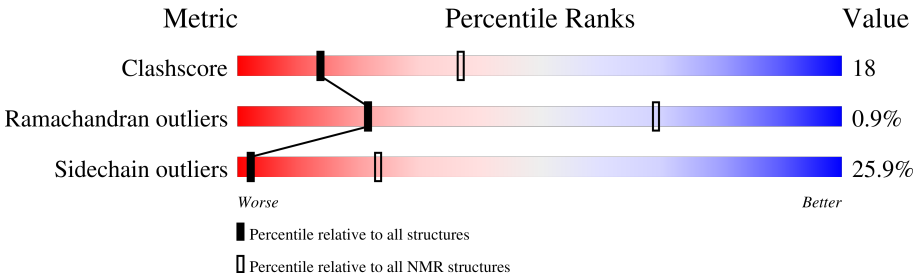
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 75%.

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	108	32% 35% • 31%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 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 averagec.*

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:51-A:76, A:86-A:121, A:127-A:139 (75)	0.58	8

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1766 atoms, of which 885 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PWWP domain-containing protein 1.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	108	1766	568	885	147	166	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LEU	GLU	cloning artifact	UNP O59676

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: PWWP domain-containing protein 1

Chain A: 32% 35% • 31%

S45 A46 D47 D48 R49 L50 R55 I56 L57 V58 K59 W66 P67 A68 L69 L70 L71 R72 R73 K74 K77 D78 S79 L80 N81 T82 N83 S84 S85 L89 Y90 K91 V92 L93 D97 F98 N99 F100 V103 K104 R105 V108 L111 L112 D113 S114 E115 I116 A117 K118 F119 L120

G121 S122 S123 K124 R125 K126 S127 K128 E129 L130 I131 E132 A133 Y134 E135 K138 T139 P140 P141 D142 L143 K144 E145 E146 S147 S148 T149 D150 L151 E152

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: PWWP domain-containing protein 1

Chain A: 36% 31% • 31%

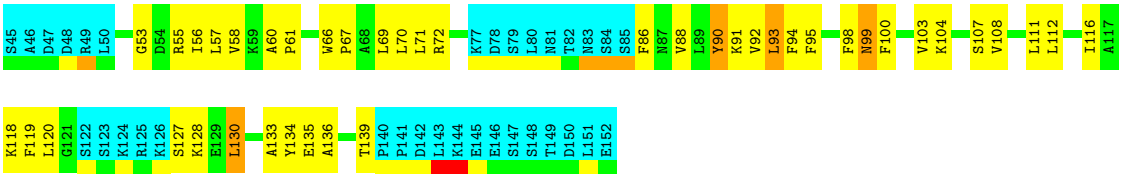
S45 A46 D47 D48 R49 L50 I56 L57 V58 K59 W66 P67 A68 L69 L70 L71 R72 R73 K74 E75 T76 K77 D78 S79 L80 N81 T82 N83 S84 S85 F86 N87 Y90 K91 V92 D97 F98 N99 F100 A101 W102 V103 K104 V108 K109 P110 L111 I116 A117 K118 F119 S122 S123

K124 R125 K126 S127 K128 E132 A133 Y134 E135 A136 S137 K138 T139 P140 P141 D142 L143 K144 E145 E146 S147 S148 T149 D150 L151 E152

4.2.2 Score per residue for model 2

• Molecule 1: PWWP domain-containing protein 1

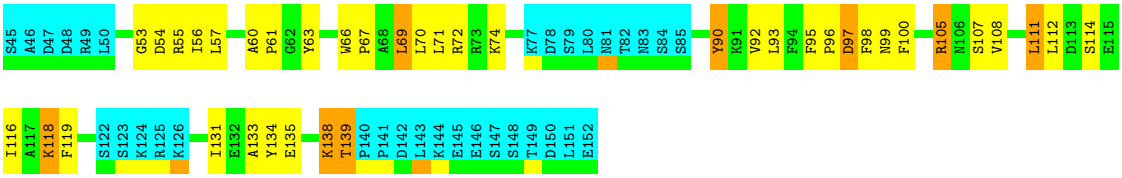
Chain A: 31% 35% • 31%



4.2.3 Score per residue for model 3

- Molecule 1: PWWP domain-containing protein 1

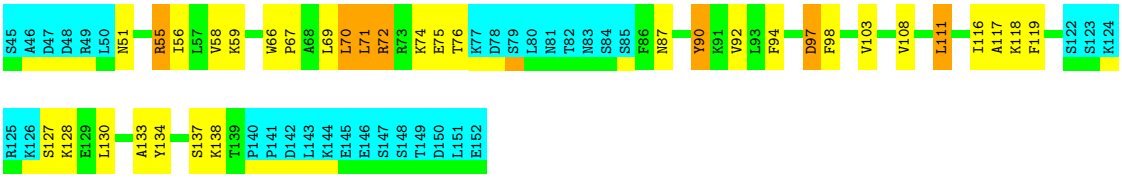
Chain A: 33% 29% 7% 31%



4.2.4 Score per residue for model 4

- Molecule 1: PWWP domain-containing protein 1

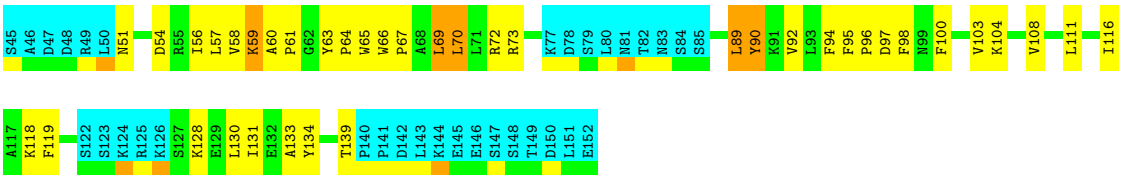
Chain A: 38% 25% 6% 31%



4.2.5 Score per residue for model 5

- Molecule 1: PWWP domain-containing protein 1

Chain A: 33% 31% 5% 31%



4.2.6 Score per residue for model 6

- Molecule 1: PWWP domain-containing protein 1

Chain A: 36% 31% • 31%

S45 A46 D47 D48 R49 L50 R55 I56 L57 V58 K59 A60 P61 G62 Y63 W66 L69 L70 L71 R72 R73 K74 K77 D78 S79 L80 N81 T82 N83 S84 S85 F86 L89 Y90 K91 V92 L93 F94 V103 K104 R105 N106 S107 V108 L111 L112 D113 S114 K118 F119 L120 G121

S122 S123 K124 R125 K126 L130 I131 E132 A133 Y134 E135 T139 P140 P141 D142 L143 K144 E145 E146 S147 S148 T149 D150 L151 E152

4.2.7 Score per residue for model 7

- Molecule 1: PWWP domain-containing protein 1

Chain A: 42% 23% 5% 31%

S45 A46 D47 D48 R49 L50 D54 R55 I56 L57 V58 K59 W66 L69 L70 L71 R72 R73 K74 K77 D78 S79 L80 N81 T82 N83 S84 S85 Y90 K91 V92 L93 D97 F98 N99 F100 V103 V108 L111 L112 D113 S114 E115 I116 A117 K118 F119 S122 S123 K124

R125 K126 I131 E132 A133 Y134 P140 P141 D142 L143 K144 E145 E146 S147 S148 T149 D150 L151 E152

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: PWWP domain-containing protein 1

Chain A: 37% 29% • 31%

S45 A46 D47 D48 R49 L50 D54 R55 I56 L57 V58 K59 W66 L69 L70 L71 R72 R73 K74 K77 D78 S79 L80 N81 T82 N83 S84 S85 F86 N87 V88 L89 Y90 K91 V92 D97 F98 N99 F100 V103 K104 R105 V108 L111 L112 I116 F119 L120 G121 S122

S123 K124 R125 K126 L130 I131 E132 A133 Y134 E135 K138 T139 P140 P141 D142 L143 K144 E145 E146 S147 S148 T149 D150 L151 E152

4.2.9 Score per residue for model 9

- Molecule 1: PWWP domain-containing protein 1

Chain A: 36% 29% 5% 31%

S45 A46 D47 D48 R49 L50 R55 I56 L57 V58 K59 A60 P61 W66 P67 A68 L69 L70 E75 T76 K77 D78 S79 L80 N81 T82 N83 S84 S85 V88 L89 Y90 K91 V92 L93 F98 N99 F100 A101 W102 V103 K104 R105 V108 I116 A117 K118 F119 L120 G121 S122 S123 K124

R125 K126 S127 K128 E129 L130 I131 E132 A133 Y134 E135 K138 T139 P140 P141 D142 L143 K144 E145 E146 S147 S148 T149 D150 L151 E152

4.2.10 Score per residue for model 10

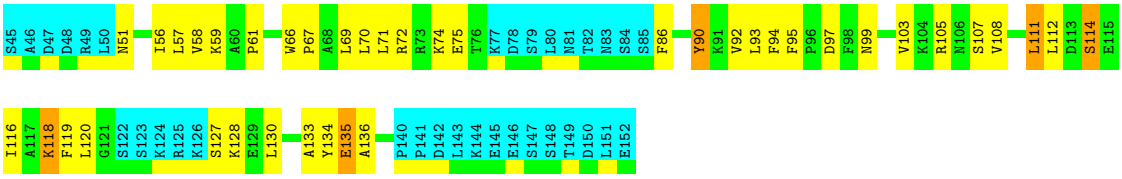
- Molecule 1: PWWP domain-containing protein 1

Chain A: 37% 30% • 31%

4.2.11 Score per residue for model 11

- Molecule 1: PWWP domain-containing protein 1

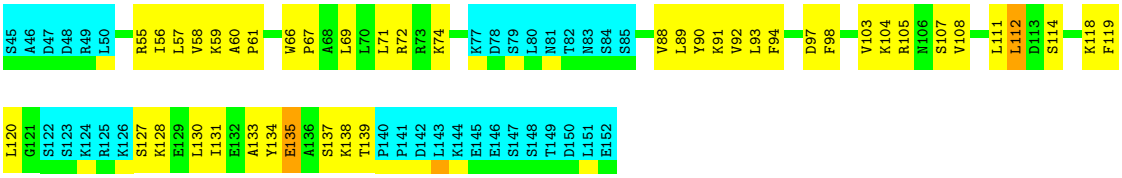
Chain A: 32% 32% 5% 31%



4.2.12 Score per residue for model 12

- Molecule 1: PWWP domain-containing protein 1

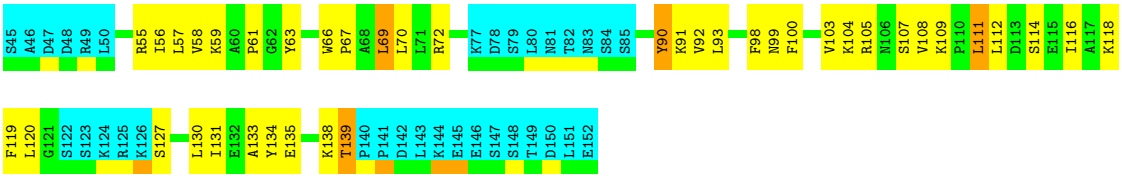
Chain A: 30% 38% • 31%



4.2.13 Score per residue for model 13

- Molecule 1: PWWP domain-containing protein 1

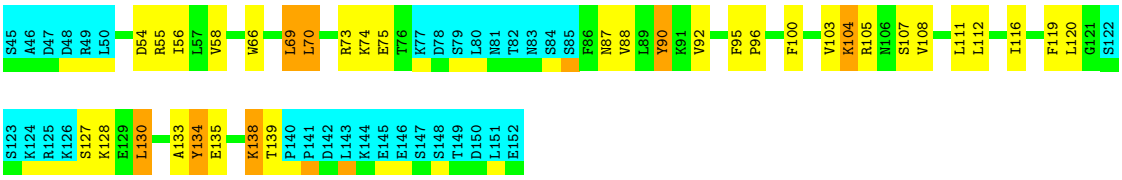
Chain A: 32% 33% • 31%



4.2.14 Score per residue for model 14

- Molecule 1: PWWP domain-containing protein 1

Chain A: 37% 26% 6% 31%



4.2.15 Score per residue for model 15

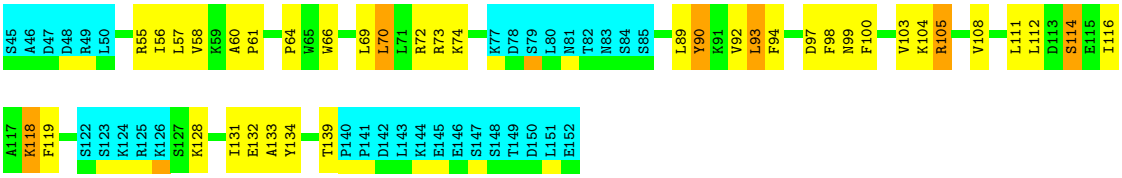
- Molecule 1: PWWP domain-containing protein 1

Chain A: 31% 32% 6% 31%

4.2.16 Score per residue for model 16

- Molecule 1: PWWP domain-containing protein 1

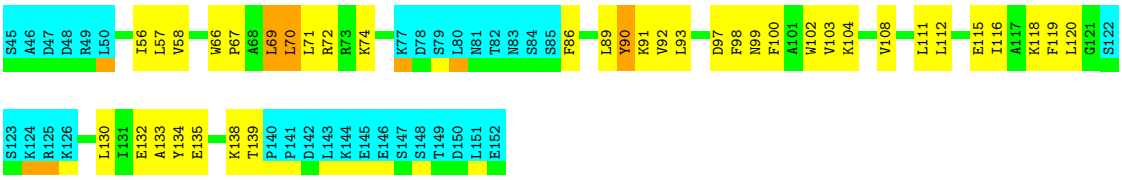
Chain A: 34% 30% 6% 31%



4.2.17 Score per residue for model 17

- Molecule 1: PWWP domain-containing protein 1

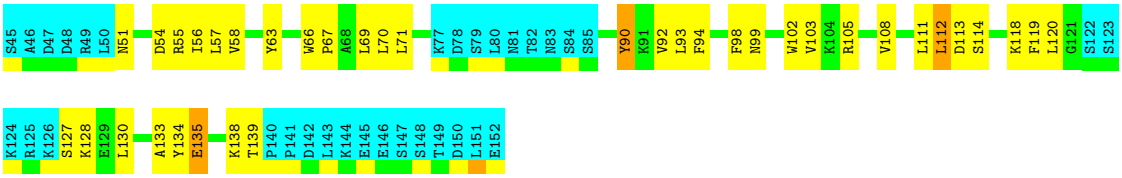
Chain A: 34% 32% • 31%



4.2.18 Score per residue for model 18

- Molecule 1: PWWP domain-containing protein 1

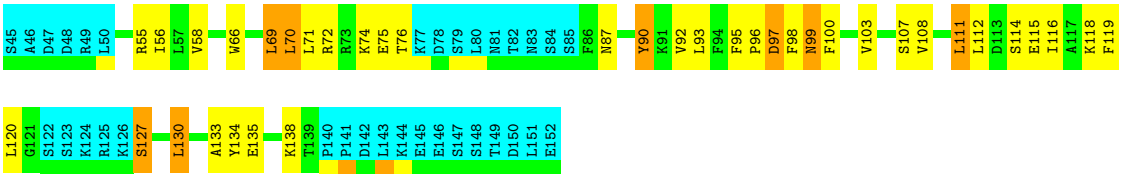
Chain A: 35% 31% • 31%



4.2.19 Score per residue for model 19

- Molecule 1: PWWP domain-containing protein 1

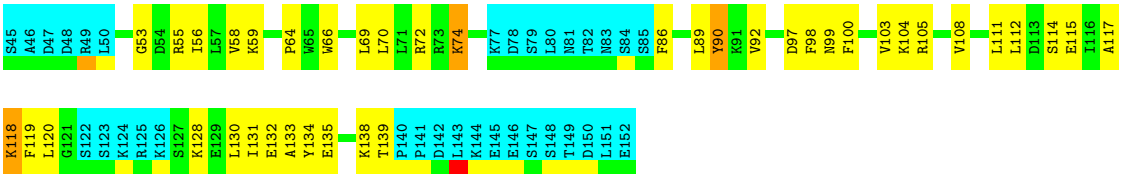
Chain A: 34% 28% 7% 31%



4.2.20 Score per residue for model 20

- Molecule 1: PWWP domain-containing protein 1

Chain A: 32% 34% • 31%



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
CNS	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	1148
Number of shifts mapped to atoms	1148
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

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	626	638	638	22±3
All	All	12520	12760	12760	449

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 18.

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:VAL:HG21	1:A:103:VAL:HG21	1.03	1.30	16	8
1:A:56:ILE:HD12	1:A:108:VAL:HG11	0.96	1.34	16	13
1:A:56:ILE:HD11	1:A:92:VAL:HG11	0.91	1.39	10	15
1:A:58:VAL:HG13	1:A:103:VAL:HG21	0.83	1.51	15	3
1:A:58:VAL:CG2	1:A:103:VAL:HG21	0.82	2.05	10	11
1:A:56:ILE:HD13	1:A:70:LEU:HD12	0.81	1.53	16	11
1:A:58:VAL:HG21	1:A:103:VAL:HG11	0.79	1.53	14	2
1:A:57:LEU:HD13	1:A:111:LEU:HD13	0.78	1.55	6	4
1:A:66:TRP:CZ2	1:A:133:ALA:HB2	0.74	2.18	15	20
1:A:58:VAL:HG11	1:A:103:VAL:HG21	0.73	1.59	8	2
1:A:56:ILE:HD13	1:A:108:VAL:HG13	0.73	1.58	19	3
1:A:57:LEU:HD13	1:A:111:LEU:CD1	0.72	2.15	17	4
1:A:58:VAL:HG21	1:A:92:VAL:HG21	0.71	1.62	13	3
1:A:58:VAL:CG2	1:A:103:VAL:HG11	0.71	2.15	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD11	1:A:90:TYR:CE1	0.69	2.22	18	13
1:A:105:ARG:O	1:A:108:VAL:HG12	0.69	1.88	3	2
1:A:56:ILE:HD12	1:A:108:VAL:CG1	0.68	2.17	1	13
1:A:56:ILE:CD1	1:A:92:VAL:HG11	0.68	2.18	19	5
1:A:70:LEU:HA	1:A:92:VAL:HG12	0.68	1.66	17	8
1:A:58:VAL:HG12	1:A:108:VAL:HG22	0.68	1.63	17	1
1:A:57:LEU:HB2	1:A:111:LEU:HD23	0.68	1.64	11	1
1:A:69:LEU:HD13	1:A:95:PHE:CZ	0.67	2.24	5	1
1:A:111:LEU:HD22	1:A:116:ILE:HG13	0.66	1.68	7	4
1:A:120:LEU:HD21	1:A:135:GLU:N	0.65	2.06	8	12
1:A:89:LEU:HD23	1:A:104:LYS:HG2	0.65	1.68	17	6
1:A:58:VAL:CG1	1:A:103:VAL:HG21	0.65	2.21	8	5
1:A:57:LEU:HD11	1:A:134:TYR:OH	0.65	1.91	6	4
1:A:71:LEU:HD11	1:A:93:LEU:HG	0.64	1.69	7	5
1:A:58:VAL:HG21	1:A:103:VAL:CG2	0.64	2.22	2	3
1:A:104:LYS:O	1:A:108:VAL:HG23	0.63	1.94	17	4
1:A:56:ILE:HD12	1:A:108:VAL:CG2	0.63	2.24	3	2
1:A:70:LEU:HD21	1:A:90:TYR:CD1	0.63	2.28	17	10
1:A:56:ILE:HD13	1:A:108:VAL:CG1	0.62	2.24	19	4
1:A:116:ILE:HG23	1:A:134:TYR:CD2	0.61	2.31	7	10
1:A:57:LEU:HD13	1:A:111:LEU:HD22	0.60	1.73	16	5
1:A:56:ILE:HD11	1:A:92:VAL:CG1	0.60	2.26	2	18
1:A:70:LEU:HD11	1:A:90:TYR:CD1	0.60	2.32	18	12
1:A:76:THR:HG22	1:A:87:ASN:O	0.59	1.97	19	4
1:A:71:LEU:HD21	1:A:93:LEU:HD12	0.59	1.74	11	4
1:A:74:LYS:HE2	1:A:89:LEU:HD12	0.59	1.73	20	1
1:A:95:PHE:HB3	1:A:136:ALA:HB3	0.58	1.74	11	2
1:A:71:LEU:HD21	1:A:93:LEU:CD1	0.58	2.28	7	2
1:A:56:ILE:CD1	1:A:70:LEU:HD12	0.58	2.29	9	2
1:A:103:VAL:HG11	1:A:108:VAL:HG23	0.56	1.76	16	2
1:A:56:ILE:HD12	1:A:108:VAL:HG21	0.55	1.77	8	2
1:A:55:ARG:HG2	1:A:69:LEU:HD11	0.55	1.78	4	1
1:A:70:LEU:HD21	1:A:90:TYR:CE1	0.55	2.37	6	2
1:A:89:LEU:HD23	1:A:104:LYS:HG3	0.55	1.78	8	2
1:A:56:ILE:HD11	1:A:92:VAL:HG12	0.54	1.79	9	3
1:A:111:LEU:HD11	1:A:134:TYR:OH	0.54	2.01	13	1
1:A:57:LEU:CD1	1:A:111:LEU:HD22	0.53	2.33	8	1
1:A:66:TRP:CZ3	1:A:130:LEU:HD12	0.53	2.38	15	3
1:A:103:VAL:CG1	1:A:108:VAL:HG23	0.53	2.34	15	2
1:A:89:LEU:HD13	1:A:102:TRP:HB2	0.53	1.80	15	1
1:A:117:ALA:HB2	1:A:138:LYS:HE2	0.52	1.81	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:PHE:CD1	1:A:134:TYR:CG	0.52	2.97	9	20
1:A:71:LEU:HD21	1:A:93:LEU:HG	0.51	1.81	3	1
1:A:71:LEU:HD11	1:A:93:LEU:HD13	0.51	1.83	19	1
1:A:112:LEU:HD12	1:A:114:SER:OG	0.51	2.05	18	1
1:A:57:LEU:HD12	1:A:67:PRO:HA	0.51	1.82	2	2
1:A:58:VAL:HB	1:A:103:VAL:HG21	0.51	1.82	17	1
1:A:58:VAL:HG22	1:A:108:VAL:HG22	0.51	1.82	18	1
1:A:119:PHE:HZ	1:A:130:LEU:HD12	0.51	1.64	5	2
1:A:111:LEU:HD21	1:A:116:ILE:HG12	0.50	1.82	5	6
1:A:60:ALA:HB1	1:A:61:PRO:HD2	0.50	1.84	15	7
1:A:127:SER:CB	1:A:130:LEU:HD12	0.50	2.36	19	1
1:A:119:PHE:CZ	1:A:130:LEU:HD22	0.49	2.42	9	2
1:A:69:LEU:HD12	1:A:95:PHE:CE2	0.49	2.43	14	1
1:A:88:VAL:O	1:A:89:LEU:HD23	0.48	2.08	9	2
1:A:93:LEU:HD23	1:A:99:ASN:O	0.48	2.09	9	1
1:A:66:TRP:CZ2	1:A:133:ALA:CB	0.48	2.94	2	11
1:A:58:VAL:HG23	1:A:103:VAL:HG21	0.48	1.81	10	3
1:A:71:LEU:HD21	1:A:93:LEU:CG	0.48	2.38	3	1
1:A:119:PHE:CE1	1:A:134:TYR:CD1	0.48	3.00	2	8
1:A:71:LEU:HD11	1:A:93:LEU:HB2	0.47	1.85	15	1
1:A:93:LEU:HA	1:A:100:PHE:HA	0.47	1.86	16	1
1:A:130:LEU:O	1:A:133:ALA:HB3	0.47	2.10	17	2
1:A:66:TRP:CZ3	1:A:130:LEU:HD13	0.47	2.44	12	4
1:A:139:THR:O	1:A:139:THR:HG23	0.47	2.10	20	1
1:A:97:ASP:O	1:A:99:ASN:N	0.47	2.47	20	4
1:A:60:ALA:HB3	1:A:63:TYR:HB2	0.47	1.87	5	1
1:A:66:TRP:CG	1:A:67:PRO:HD2	0.46	2.45	11	11
1:A:93:LEU:HD21	1:A:98:PHE:CD2	0.46	2.46	13	1
1:A:67:PRO:HG3	1:A:134:TYR:CD1	0.46	2.45	11	6
1:A:120:LEU:HD22	1:A:135:GLU:HG2	0.46	1.87	10	1
1:A:93:LEU:HD22	1:A:99:ASN:O	0.45	2.12	2	1
1:A:57:LEU:HD13	1:A:111:LEU:HD12	0.45	1.88	3	1
1:A:71:LEU:HD11	1:A:93:LEU:HD12	0.45	1.88	15	1
1:A:55:ARG:CG	1:A:69:LEU:HD11	0.45	2.41	4	1
1:A:97:ASP:O	1:A:98:PHE:HB2	0.45	2.12	8	4
1:A:58:VAL:HG11	1:A:103:VAL:CG2	0.45	2.39	8	1
1:A:114:SER:O	1:A:118:LYS:HB2	0.44	2.12	11	4
1:A:89:LEU:HD13	1:A:102:TRP:HB3	0.44	1.89	17	1
1:A:111:LEU:HD12	1:A:116:ILE:HG13	0.44	1.88	11	1
1:A:95:PHE:HB3	1:A:96:PRO:HA	0.44	1.90	19	4
1:A:57:LEU:HB2	1:A:111:LEU:HD13	0.44	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LYS:CE	1:A:89:LEU:HD12	0.44	2.43	20	1
1:A:57:LEU:HD11	1:A:134:TYR:CZ	0.44	2.47	6	1
1:A:70:LEU:HD11	1:A:90:TYR:CZ	0.44	2.48	6	1
1:A:94:PHE:O	1:A:98:PHE:HA	0.44	2.13	4	3
1:A:90:TYR:CE2	1:A:105:ARG:HG2	0.43	2.49	16	2
1:A:117:ALA:HB2	1:A:138:LYS:HE3	0.43	1.90	20	1
1:A:116:ILE:HG22	1:A:138:LYS:HG2	0.43	1.91	3	1
1:A:116:ILE:HG23	1:A:134:TYR:HD2	0.43	1.72	10	1
1:A:71:LEU:HD11	1:A:93:LEU:CG	0.43	2.42	12	1
1:A:70:LEU:HD23	1:A:71:LEU:N	0.43	2.29	3	3
1:A:94:PHE:HB2	1:A:99:ASN:O	0.43	2.14	18	2
1:A:59:LYS:HB3	1:A:65:TRP:CD2	0.43	2.49	5	1
1:A:111:LEU:HD23	1:A:116:ILE:HD11	0.42	1.91	17	1
1:A:116:ILE:HA	1:A:134:TYR:CD2	0.42	2.50	10	2
1:A:89:LEU:HD23	1:A:104:LYS:CG	0.42	2.44	10	1
1:A:112:LEU:N	1:A:112:LEU:HD23	0.42	2.29	12	1
1:A:119:PHE:CZ	1:A:134:TYR:CD1	0.42	3.08	12	1
1:A:127:SER:HB3	1:A:130:LEU:HD12	0.42	1.92	14	1
1:A:93:LEU:HD13	1:A:94:PHE:N	0.41	2.30	2	1
1:A:119:PHE:HZ	1:A:130:LEU:HD22	0.41	1.74	9	1
1:A:119:PHE:CD1	1:A:119:PHE:C	0.41	2.93	14	2
1:A:120:LEU:HD23	1:A:131:ILE:HG23	0.41	1.91	12	1
1:A:111:LEU:CD2	1:A:116:ILE:HG13	0.41	2.46	19	1
1:A:111:LEU:HD22	1:A:116:ILE:CG1	0.41	2.45	10	1
1:A:58:VAL:HG11	1:A:94:PHE:CZ	0.41	2.51	6	1
1:A:58:VAL:HG13	1:A:94:PHE:CZ	0.41	2.51	16	1
1:A:55:ARG:CZ	1:A:69:LEU:HD12	0.41	2.46	3	1
1:A:119:PHE:CD1	1:A:134:TYR:CD1	0.40	3.09	4	1
1:A:71:LEU:HG	1:A:72:ARG:N	0.40	2.31	4	1
1:A:56:ILE:HD12	1:A:58:VAL:HG13	0.40	1.93	17	1
1:A:73:ARG:HB3	1:A:90:TYR:CE1	0.40	2.51	7	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	75/108 (69%)	67±2 (89±2%)	8±2 (10±3%)	1±1 (1±1%)	21 69
All	All	1500/2160 (69%)	1336 (89%)	150 (10%)	14 (1%)	21 69

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	98	PHE	7
1	A	61	PRO	3
1	A	64	PRO	3
1	A	86	PHE	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	66/98 (67%)	49±2 (74±3%)	17±2 (26±3%)	2 23
All	All	1320/1960 (67%)	978 (74%)	342 (26%)	2 23

All 44 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	90	TYR	20
1	A	69	LEU	19
1	A	118	LYS	18
1	A	72	ARG	17
1	A	74	LYS	15
1	A	100	PHE	14
1	A	70	LEU	13
1	A	139	THR	13
1	A	55	ARG	13
1	A	59	LYS	12
1	A	105	ARG	12
1	A	128	LYS	11
1	A	112	LEU	11
1	A	107	SER	10

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Mol	Chain	Res	Type	Models (Total)
1	A	127	SER	10
1	A	138	LYS	9
1	A	97	ASP	9
1	A	135	GLU	8
1	A	54	ASP	8
1	A	111	LEU	8
1	A	114	SER	8
1	A	75	GLU	7
1	A	132	GLU	6
1	A	99	ASN	6
1	A	91	LYS	5
1	A	93	LEU	5
1	A	87	ASN	4
1	A	98	PHE	4
1	A	130	LEU	4
1	A	63	TYR	4
1	A	51	ASN	4
1	A	73	ARG	4
1	A	113	ASP	4
1	A	102	TRP	3
1	A	104	LYS	3
1	A	109	LYS	3
1	A	137	SER	3
1	A	88	VAL	3
1	A	86	PHE	3
1	A	115	GLU	3
1	A	71	LEU	2
1	A	89	LEU	2
1	A	134	TYR	1
1	A	129	GLU	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 75% for the well-defined parts and 76% 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	1148
Number of shifts mapped to atoms	1148
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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	105	-0.14 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	102	0.03 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	93	0.10 ± 0.15	None needed (< 0.5 ppm)
^{15}N	96	0.13 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 832 atoms were assigned a chemical shift out of a possible 1103. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	354/368 (96%)	146/148 (99%)	140/150 (93%)	68/70 (97%)
Sidechain	416/602 (69%)	285/392 (73%)	127/186 (68%)	4/24 (17%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	62/133 (47%)	59/65 (91%)	0/65 (0%)	3/3 (100%)
Overall	832/1103 (75%)	490/605 (81%)	267/401 (67%)	75/97 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1147 atoms were assigned a chemical shift out of a possible 1517. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	498/529 (94%)	204/212 (96%)	198/216 (92%)	96/101 (95%)
Sidechain	587/855 (69%)	400/551 (73%)	181/268 (68%)	6/36 (17%)
Aromatic	62/133 (47%)	59/65 (91%)	0/65 (0%)	3/3 (100%)
Overall	1147/1517 (76%)	663/828 (80%)	379/549 (69%)	105/140 (75%)

7.1.4 Statistically unusual chemical shifts (i)

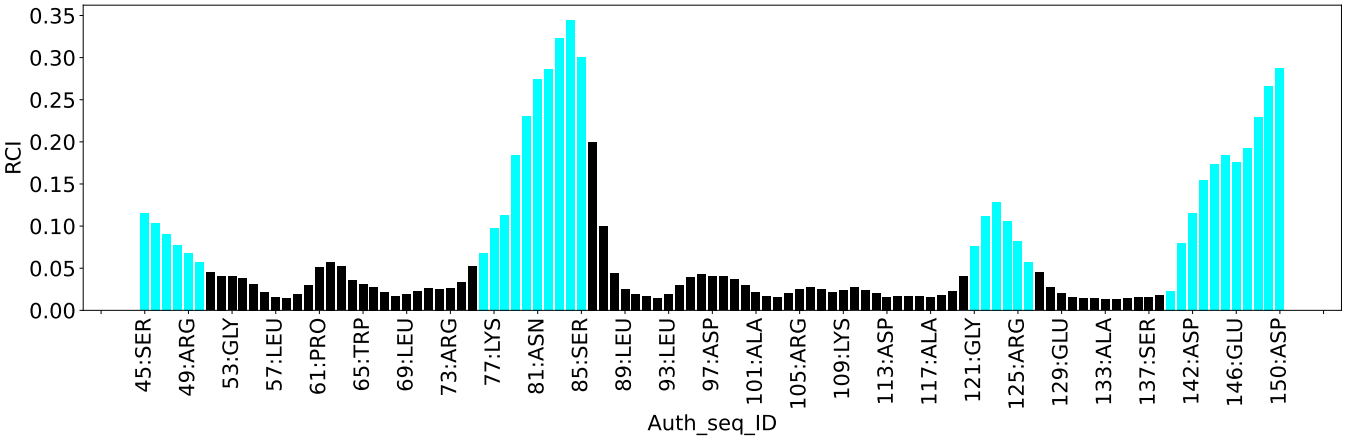
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	137	SER	HB2	2.47	2.61 – 5.13	-5.6
1	A	137	SER	HB3	2.47	2.49 – 5.20	-5.1

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:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
45:SER
49:ARG
53:GLY
57:LEU
61:PRO
65:TRP
69:LEU
73:ARG
77:LYS
81:ASN
85:SER
89:LEU
93:LEU
97:ASP
101:ALA
105:ARG
109:LYS
113:ASP
117:ALA
121:GLY
125:ARG
129:GLU
133:ALA
137:SER
142:ASP
146:GLU
150:ASP
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	1630
Intra-residue (|i-j|=0)	521
Sequential (|i-j|=1)	443
Medium range (|i-j|>1 and |i-j|<5)	204
Long range (|i-j|≥5)	430
Inter-chain	0
Hydrogen bond restraints	32
Disulfide bond restraints	0
Total dihedral-angle restraints	113
Number of unmapped restraints	0
Number of restraints per residue	16.1
Number of long range restraints per residue[1]	4.3

[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)	3.0	0.2
0.2-0.5 (Medium)	0.1	0.25
>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)	2.0	2.4
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

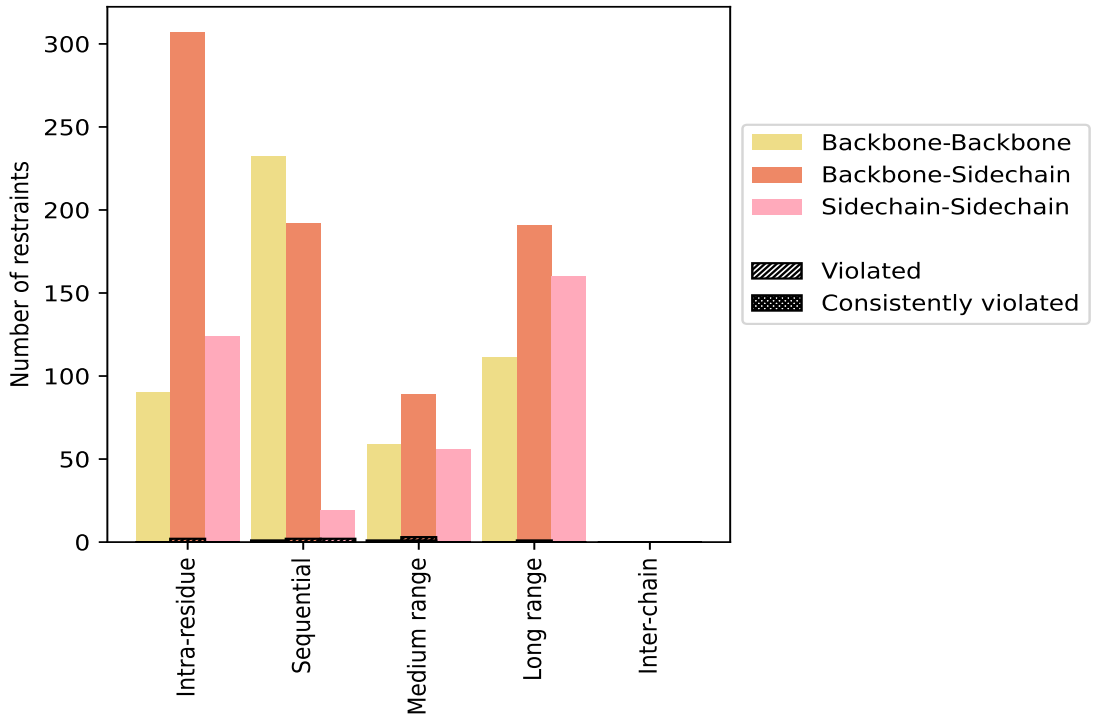
9.1 Summary of distance violations (i)

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)	521	32.0	2	0.4	0.1	0	0.0	0.0
Backbone-Backbone	90	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	307	18.8	2	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	124	7.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	443	27.2	5	1.1	0.3	0	0.0	0.0
Backbone-Backbone	232	14.2	1	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	192	11.8	2	1.0	0.1	0	0.0	0.0
Sidechain-Sidechain	19	1.2	2	10.5	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	204	12.5	4	2.0	0.2	1	0.5	0.1
Backbone-Backbone	59	3.6	1	1.7	0.1	0	0.0	0.0
Backbone-Sidechain	89	5.5	3	3.4	0.2	1	1.1	0.1
Sidechain-Sidechain	56	3.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	430	26.4	1	0.2	0.1	0	0.0	0.0
Backbone-Backbone	79	4.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	191	11.7	1	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	160	9.8	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	32	2.0	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	1630	100.0	12	0.7	0.7	1	0.1	0.1
Backbone-Backbone	492	30.2	2	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	779	47.8	8	1.0	0.5	1	0.1	0.1
Sidechain-Sidechain	359	22.0	2	0.6	0.1	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	0	0	3	0	0	3	0.14	0.2	0.04	0.12
2	0	0	2	0	0	2	0.14	0.15	0.02	0.14
3	0	0	2	0	0	2	0.16	0.19	0.03	0.16
4	0	1	3	1	0	5	0.12	0.17	0.02	0.11
5	1	0	1	0	0	2	0.13	0.14	0.01	0.13
6	0	3	1	0	0	4	0.14	0.15	0.01	0.15
7	1	2	1	0	0	4	0.15	0.17	0.02	0.15
8	0	0	2	0	0	2	0.15	0.15	0.0	0.15
9	0	0	2	0	0	2	0.13	0.15	0.02	0.13
10	0	2	1	0	0	3	0.14	0.15	0.01	0.15
11	0	0	3	1	0	4	0.12	0.14	0.02	0.12

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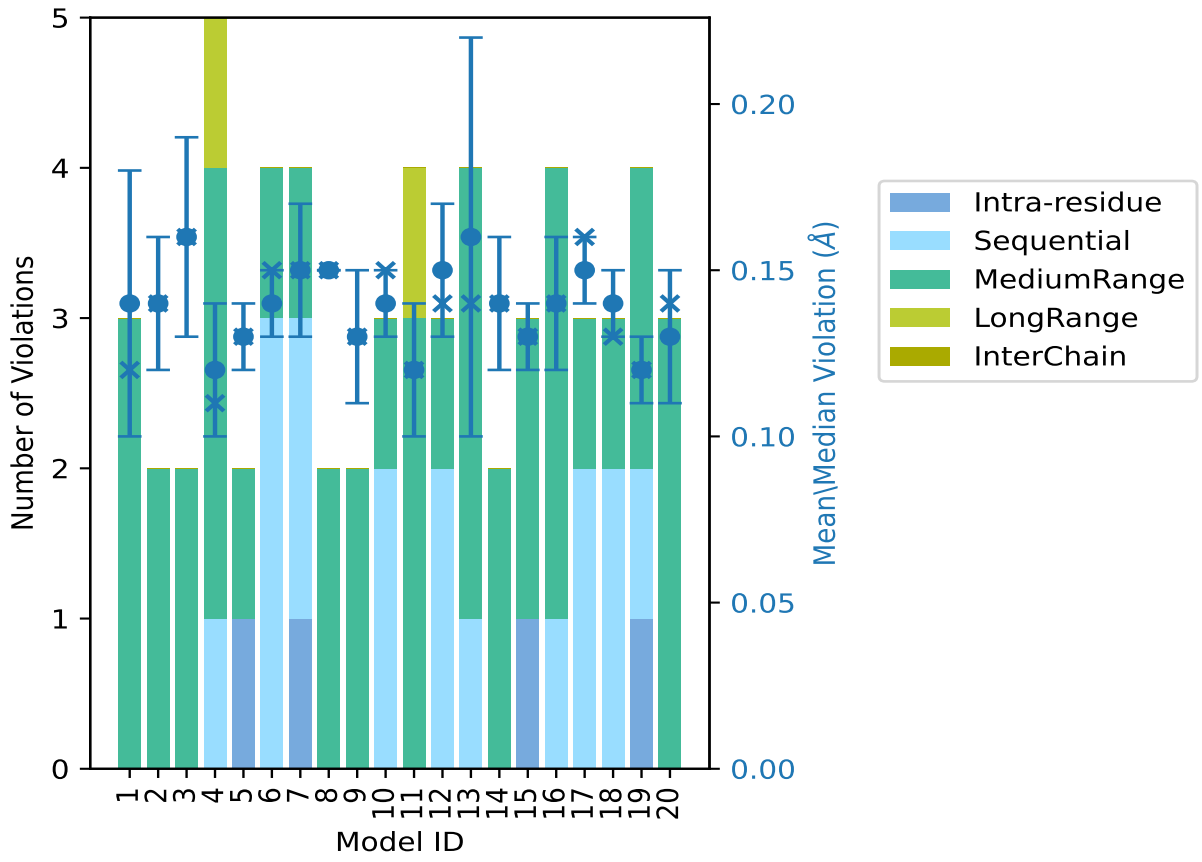
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	1	0	0	3	0.15	0.17	0.02	0.14
13	0	1	3	0	0	4	0.16	0.25	0.06	0.14
14	0	0	2	0	0	2	0.14	0.15	0.02	0.14
15	1	0	2	0	0	3	0.13	0.14	0.01	0.13
16	0	1	3	0	0	4	0.14	0.15	0.02	0.14
17	0	2	1	0	0	3	0.15	0.16	0.01	0.16
18	0	2	1	0	0	3	0.14	0.16	0.01	0.13
19	1	1	2	0	0	4	0.12	0.14	0.01	0.12
20	0	0	3	0	0	3	0.13	0.15	0.02	0.14

[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

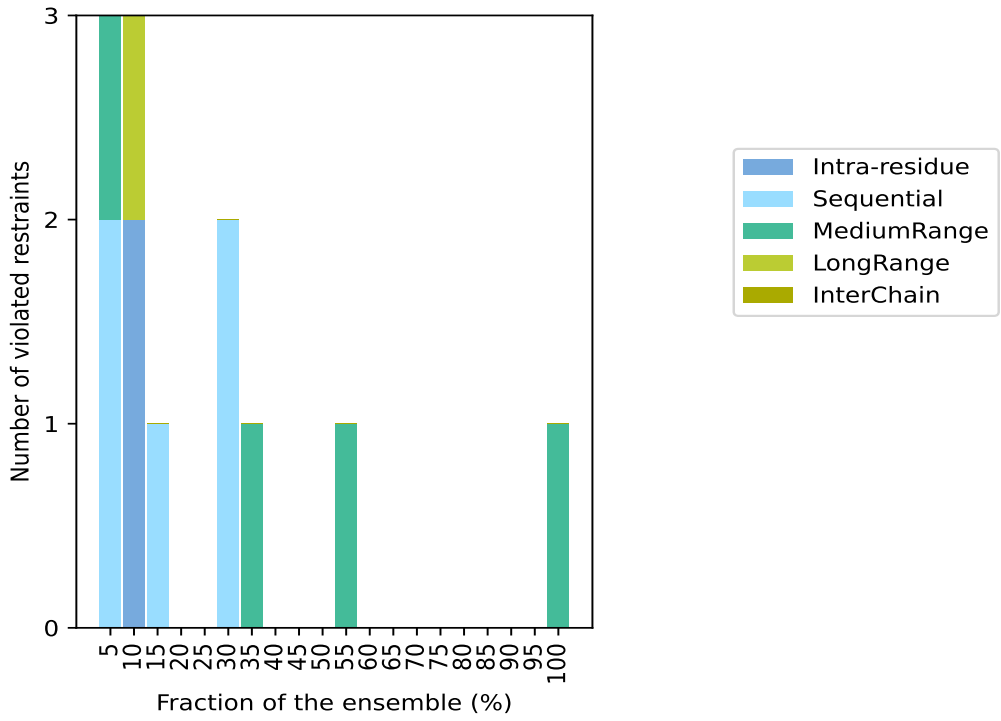
9.3 Distance violation statistics for the ensemble (i)

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, 1586(IR:519, SQ:438, MR:200, LR:429, 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	2	1	0	0	3	1	5.0
2	0	0	1	0	3	2	10.0
0	1	0	0	0	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	2	0	0	0	2	6	30.0
0	0	1	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	1	0	0	1	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	1	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

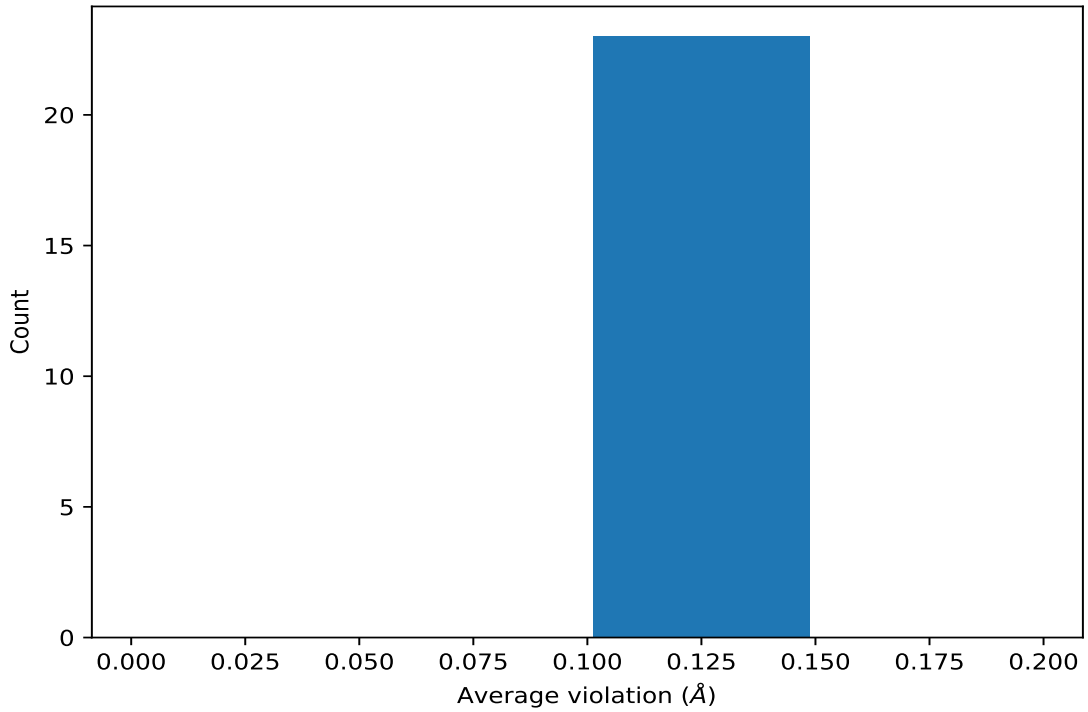
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	20	0.15	0.02	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	20	0.15	0.02	0.15
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	11	0.13	0.01	0.13
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	11	0.13	0.01	0.13
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	7	0.11	0.0	0.11
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB2	6	0.15	0.01	0.15
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB3	6	0.15	0.01	0.15
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD2	6	0.14	0.01	0.14
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD3	6	0.14	0.01	0.14
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD2	6	0.14	0.01	0.14
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD3	6	0.14	0.01	0.14
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD2	6	0.14	0.01	0.14
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD3	6	0.14	0.01	0.14
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB2	3	0.14	0.02	0.15
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB3	3	0.14	0.02	0.15
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB2	3	0.14	0.02	0.15

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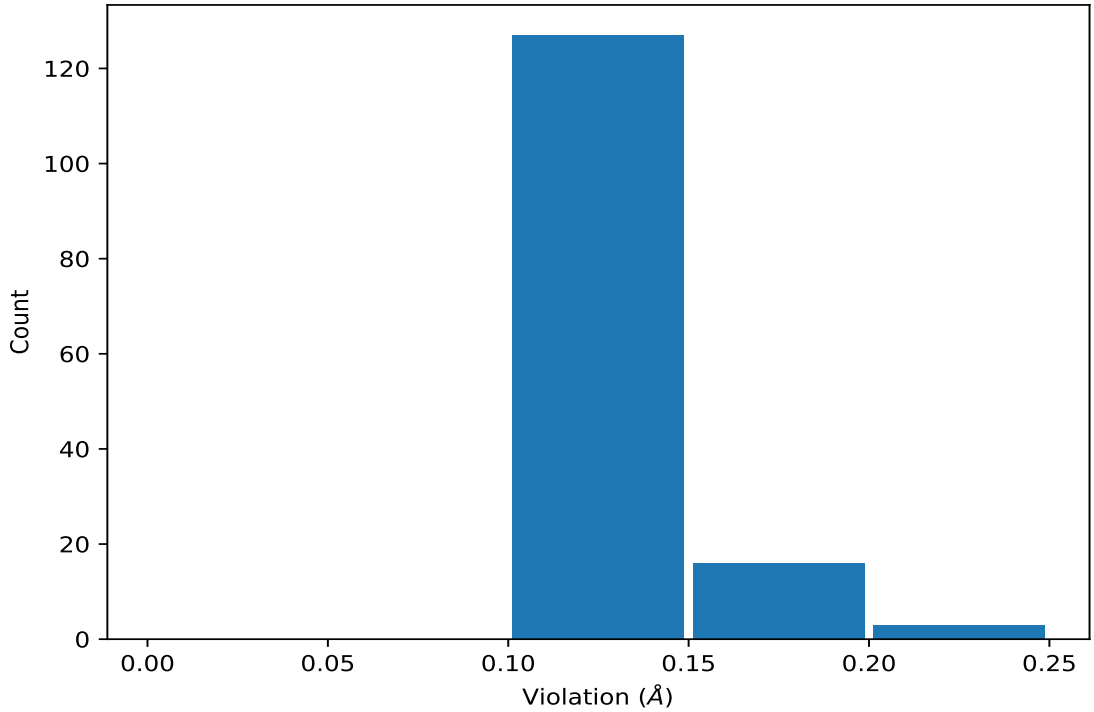
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB3	3	0.14	0.02	0.15
(1,881)	1:A:100:PHE:H	1:A:100:PHE:HE1	2	0.12	0.0	0.12
(1,881)	1:A:100:PHE:H	1:A:100:PHE:HE2	2	0.12	0.0	0.12
(1,1544)	1:A:142:ASP:H	1:A:142:ASP:HB2	2	0.12	0.0	0.12
(1,1544)	1:A:142:ASP:H	1:A:142:ASP:HB3	2	0.12	0.0	0.12
(1,799)	1:A:94:PHE:H	1:A:100:PHE:HD1	2	0.11	0.0	0.11
(1,799)	1:A:94:PHE:H	1:A:100:PHE:HD2	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)
(1,557)	1:A:78:ASP:HA	1:A:79:SER:HA	13	0.25
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	1	0.2
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	1	0.2
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	3	0.19
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	3	0.19
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	4	0.17
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	4	0.17
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	12	0.17
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	12	0.17
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB2	7	0.17
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB3	7	0.17
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	13	0.16
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	13	0.16
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	17	0.16
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	17	0.16
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	18	0.16
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	18	0.16
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB2	17	0.16
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB3	17	0.16
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB2	6	0.15
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB3	6	0.15
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB2	6	0.15
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB3	6	0.15
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB2	16	0.15
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB3	16	0.15
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB2	16	0.15
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB3	16	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	2	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	2	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	9	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	9	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	14	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	14	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	16	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	16	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	20	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	20	0.15
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	8	0.15
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	8	0.15
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB2	6	0.15
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB3	6	0.15
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB2	10	0.15
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB3	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD2	7	0.15
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD3	7	0.15
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD2	7	0.15
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD3	7	0.15
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD2	7	0.15
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD3	7	0.15
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD2	10	0.15
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD3	10	0.15
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD2	10	0.15
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD3	10	0.15
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD2	10	0.15
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD3	10	0.15
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	5	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	5	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	6	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	6	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	7	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	7	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	8	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	8	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	11	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	11	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	19	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	19	0.14
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	11	0.14
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	11	0.14
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	15	0.14
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	15	0.14
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	20	0.14
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	20	0.14
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD2	12	0.14
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD3	12	0.14
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD2	12	0.14
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD3	12	0.14
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD2	12	0.14
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD3	12	0.14
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	10	0.13
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	10	0.13
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG2	15	0.13
(1,1310)	1:A:126:LYS:H	1:A:124:LYS:HG3	15	0.13
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	3	0.13
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	16	0.13
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	16	0.13
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB2	12	0.13
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB3	12	0.13
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB2	18	0.13
(1,1226)	1:A:119:PHE:H	1:A:118:LYS:HB3	18	0.13
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD2	6	0.13
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD3	6	0.13
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD2	6	0.13
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD3	6	0.13
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD2	6	0.13
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD3	6	0.13
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD2	17	0.13
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD3	17	0.13
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD2	17	0.13
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD3	17	0.13
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD2	17	0.13
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD3	17	0.13
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD2	18	0.13
(1,1207)	1:A:117:ALA:HB1	1:A:118:LYS:HD3	18	0.13
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD2	18	0.13
(1,1207)	1:A:117:ALA:HB2	1:A:118:LYS:HD3	18	0.13
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD2	18	0.13
(1,1207)	1:A:117:ALA:HB3	1:A:118:LYS:HD3	18	0.13
(1,881)	1:A:100:PHE:H	1:A:100:PHE:HE1	5	0.12
(1,881)	1:A:100:PHE:H	1:A:100:PHE:HE2	5	0.12
(1,881)	1:A:100:PHE:H	1:A:100:PHE:HE1	15	0.12
(1,881)	1:A:100:PHE:H	1:A:100:PHE:HE2	15	0.12
(1,1544)	1:A:142:ASP:H	1:A:142:ASP:HB2	7	0.12
(1,1544)	1:A:142:ASP:H	1:A:142:ASP:HB3	7	0.12
(1,1544)	1:A:142:ASP:H	1:A:142:ASP:HB2	19	0.12
(1,1544)	1:A:142:ASP:H	1:A:142:ASP:HB3	19	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	1	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	1	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	4	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	4	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	13	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	13	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	14	0.12
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	14	0.12
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	2	0.12
(1,1227)	1:A:119:PHE:H	1:A:118:LYS:HG2	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1227)	1:A:119:PHE:H	1:A:118:LYS:HG3	19	0.12
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB2	4	0.11
(1,887)	1:A:100:PHE:HD1	1:A:99:ASN:HB3	4	0.11
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB2	4	0.11
(1,887)	1:A:100:PHE:HD2	1:A:99:ASN:HB3	4	0.11
(1,799)	1:A:94:PHE:H	1:A:100:PHE:HD1	4	0.11
(1,799)	1:A:94:PHE:H	1:A:100:PHE:HD2	4	0.11
(1,799)	1:A:94:PHE:H	1:A:100:PHE:HD1	11	0.11
(1,799)	1:A:94:PHE:H	1:A:100:PHE:HD2	11	0.11
(1,1525)	1:A:139:THR:HA	1:A:141:PRO:HB2	13	0.11
(1,1525)	1:A:139:THR:HA	1:A:141:PRO:HB3	13	0.11
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG2	19	0.11
(1,1257)	1:A:121:GLY:H	1:A:118:LYS:HG3	19	0.11
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	1	0.11
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	4	0.11
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	9	0.11
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	11	0.11
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	16	0.11
(1,1235)	1:A:119:PHE:H	1:A:116:ILE:H	20	0.11

10 Dihedral-angle violation analysis (i)

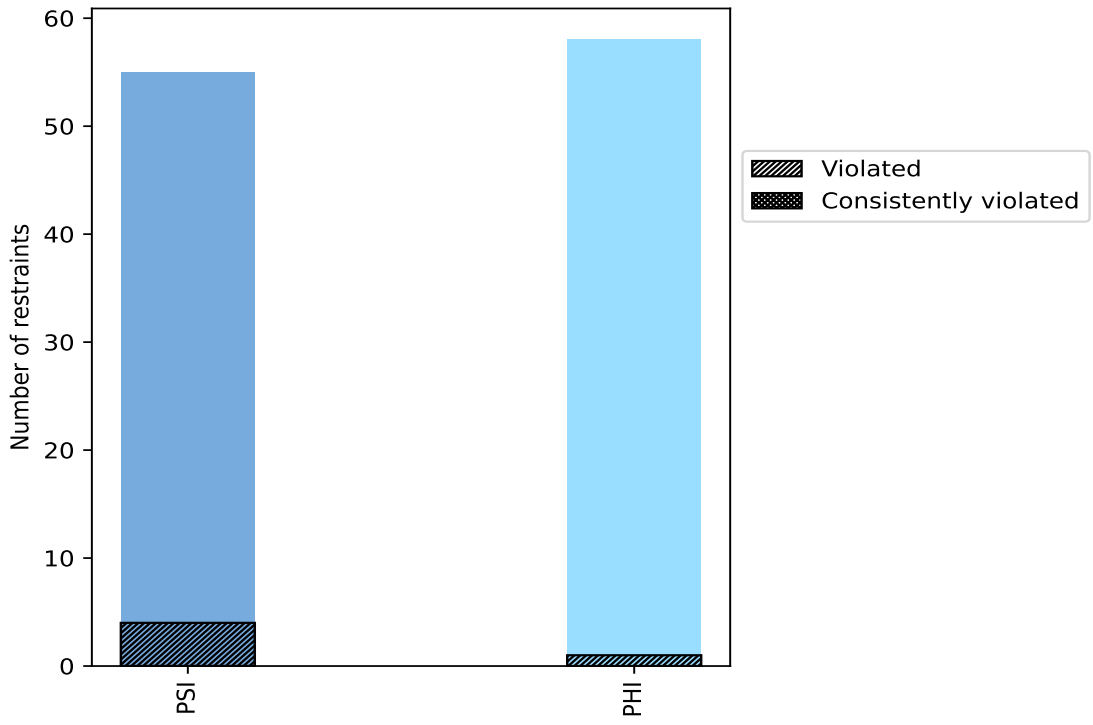
10.1 Summary of dihedral-angle violations (i)

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]
PSI	55	48.7	4	7.3	3.5	0	0.0	0.0
PHI	58	51.3	1	1.7	0.9	0	0.0	0.0
Total	113	100.0	5	4.4	4.4	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)



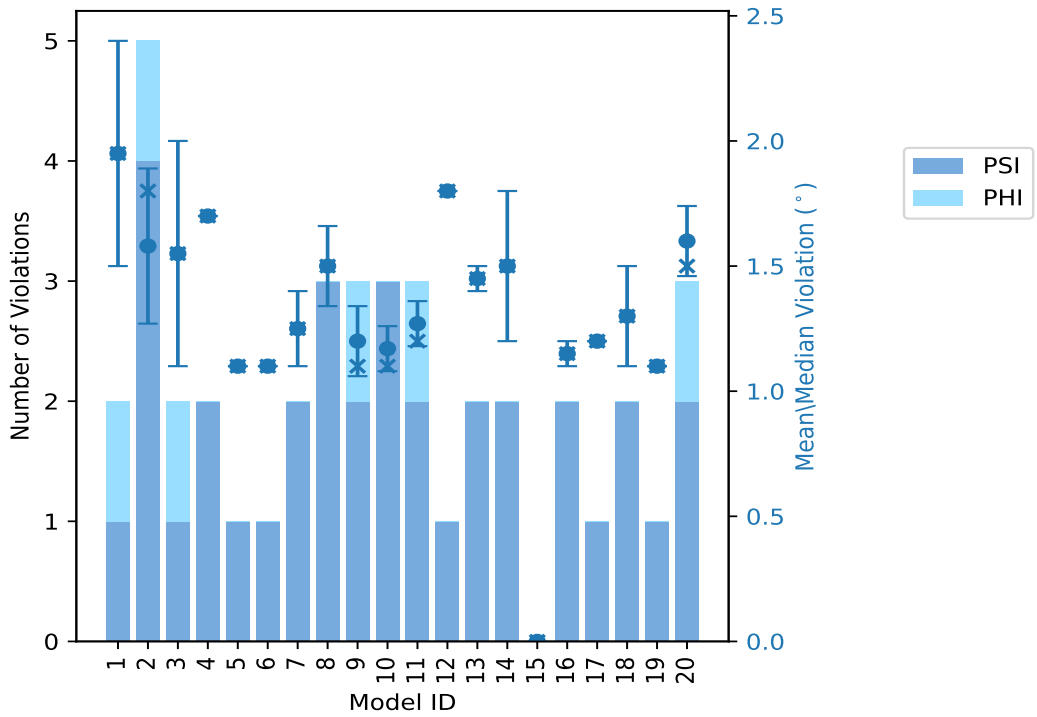
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	1	2	1.95	2.4	0.45	1.95
2	4	1	5	1.58	1.9	0.31	1.8
3	1	1	2	1.55	2.0	0.45	1.55
4	2	0	2	1.7	1.7	0.0	1.7
5	1	0	1	1.1	1.1	0.0	1.1
6	1	0	1	1.1	1.1	0.0	1.1
7	2	0	2	1.25	1.4	0.15	1.25
8	3	0	3	1.5	1.7	0.16	1.5
9	2	1	3	1.2	1.4	0.14	1.1
10	3	0	3	1.17	1.3	0.09	1.1
11	2	1	3	1.27	1.4	0.09	1.2
12	1	0	1	1.8	1.8	0.0	1.8
13	2	0	2	1.45	1.5	0.05	1.45
14	2	0	2	1.5	1.8	0.3	1.5
15	0	0	0	0.0	0.0	0.0	0.0
16	2	0	2	1.15	1.2	0.05	1.15
17	1	0	1	1.2	1.2	0.0	1.2
18	2	0	2	1.3	1.5	0.2	1.3
19	1	0	1	1.1	1.1	0.0	1.1
20	2	1	3	1.6	1.8	0.14	1.5

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]	%
0	0	0	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	1	1	6	30.0
0	0	0	7	35.0
2	0	2	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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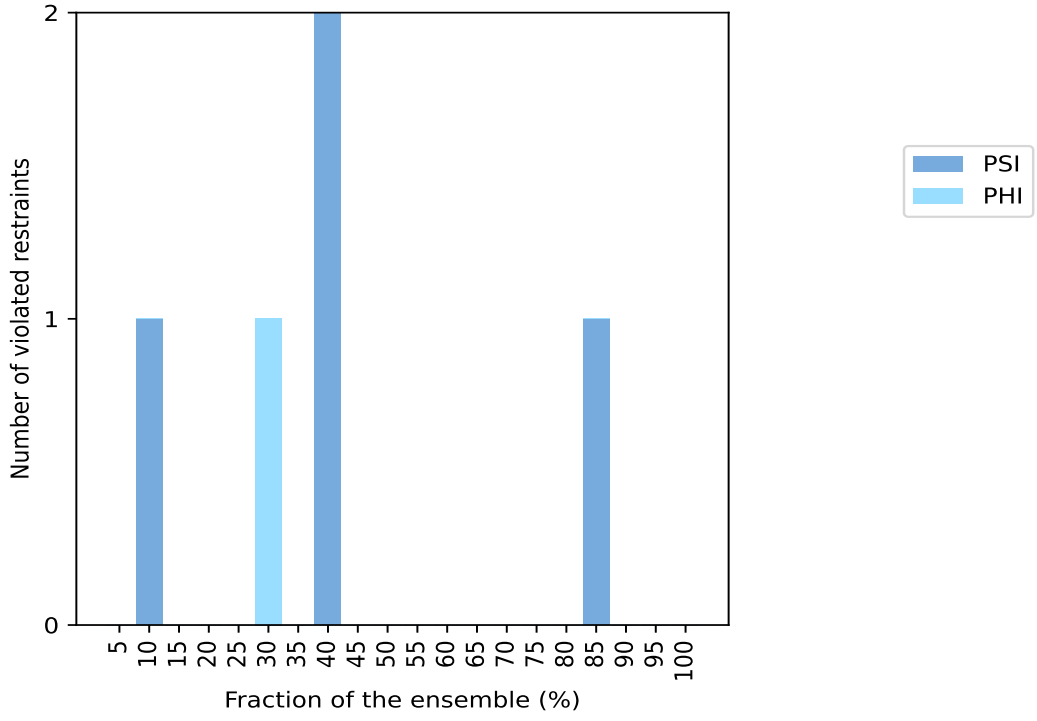
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

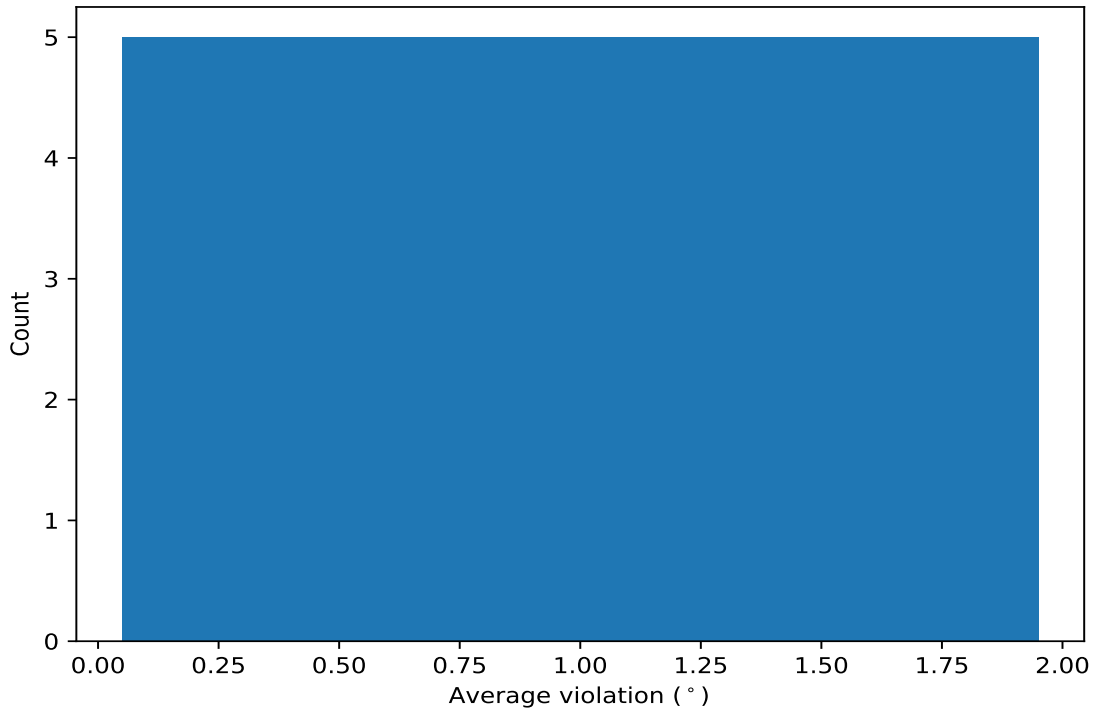


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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.

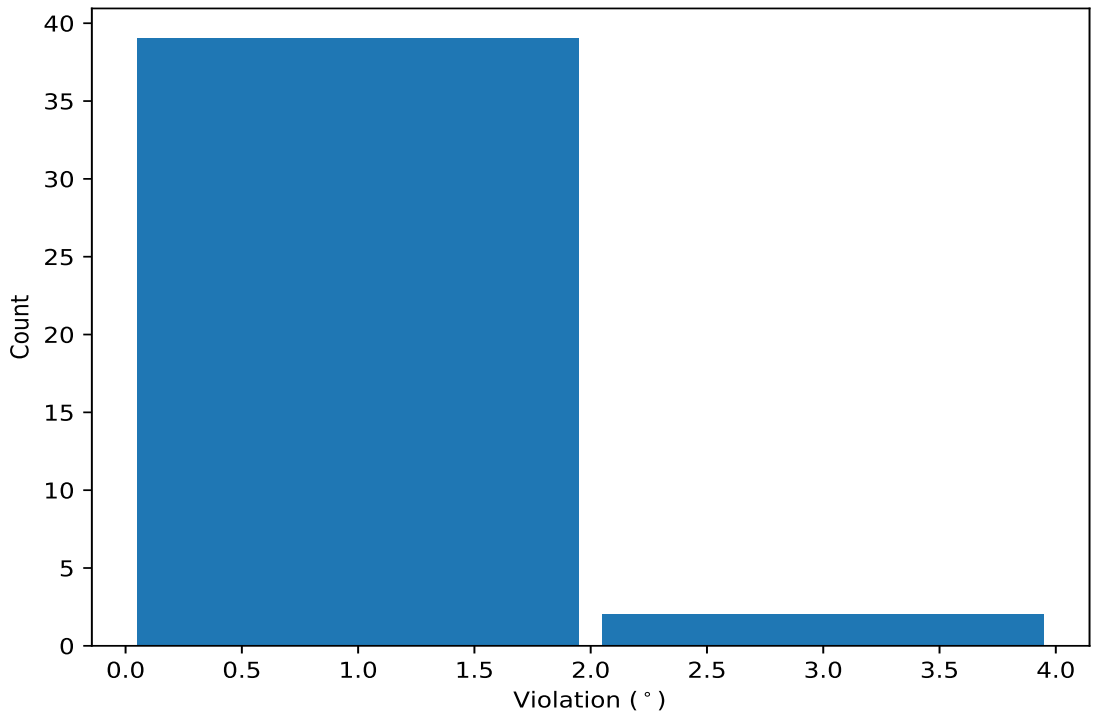
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	17	1.54	0.35	1.5
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	8	1.39	0.33	1.2
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	8	1.24	0.16	1.2
(1,87)	1:A:124:LYS:C	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	6	1.3	0.17	1.3
(1,50)	1:A:93:LEU:N	1:A:93:LEU:CA	1:A:93:LEU:C	1:A:94:PHE:N	2	1.6	0.2	1.6

[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 (°)
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	1	2.4
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	3	2.0
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	2	1.9
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	2	1.8
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	12	1.8
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	20	1.8
(1,50)	1:A:93:LEU:N	1:A:93:LEU:CA	1:A:93:LEU:C	1:A:94:PHE:N	2	1.8
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	14	1.8
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	4	1.7
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	8	1.7
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	4	1.7
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	13	1.5
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	18	1.5
(1,87)	1:A:124:LYS:C	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1	1.5
(1,87)	1:A:124:LYS:C	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	20	1.5
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	8	1.5
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	20	1.5
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	7	1.4
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	9	1.4
(1,87)	1:A:124:LYS:C	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	11	1.4
(1,50)	1:A:93:LEU:N	1:A:93:LEU:CA	1:A:93:LEU:C	1:A:94:PHE:N	13	1.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	10	1.3
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	8	1.3
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	11	1.2
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	16	1.2
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	17	1.2
(1,87)	1:A:124:LYS:C	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	2	1.2
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	2	1.2
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	11	1.2
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	14	1.2
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	5	1.1
(1,88)	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	1:A:126:LYS:N	19	1.1
(1,87)	1:A:124:LYS:C	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	3	1.1
(1,87)	1:A:124:LYS:C	1:A:125:ARG:N	1:A:125:ARG:CA	1:A:125:ARG:C	9	1.1
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	7	1.1
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	9	1.1
(1,86)	1:A:124:LYS:N	1:A:124:LYS:CA	1:A:124:LYS:C	1:A:125:ARG:N	10	1.1
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	6	1.1
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	10	1.1
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	16	1.1
(1,38)	1:A:87:ASN:N	1:A:87:ASN:CA	1:A:87:ASN:C	1:A:88:VAL:N	18	1.1