



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 05:43 AM EST

PDB ID : 5X5S  
BMRB ID : 36061  
Title : Ligand induced structure of AmyP-SBD  
Authors : Li, X.; Yu, J.; Sun, H.; Zhang, X.  
Deposited on : 2017-02-17

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

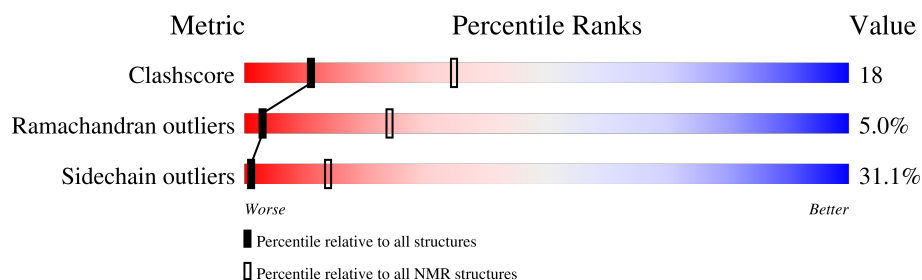
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	157	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:29-A:149 (121)	1.59	2

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 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2201 atoms, of which 1080 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amylase.

Mol	Chain	Residues	Atoms						Trace
1	A	149	Total	C	H	N	O	S	0
			2201	706	1080	186	224	5	

There are 8 discrepancies between the modelled and reference sequences:

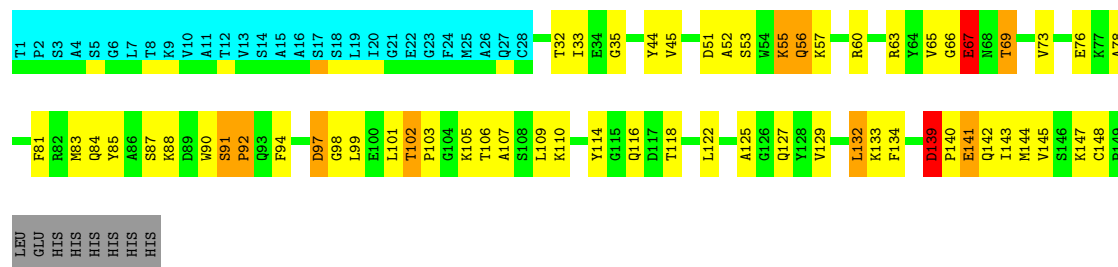
Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LEU	-	expression tag	UNP D9MZ14
A	151	GLU	-	expression tag	UNP D9MZ14
A	152	HIS	-	expression tag	UNP D9MZ14
A	153	HIS	-	expression tag	UNP D9MZ14
A	154	HIS	-	expression tag	UNP D9MZ14
A	155	HIS	-	expression tag	UNP D9MZ14
A	156	HIS	-	expression tag	UNP D9MZ14
A	157	HIS	-	expression tag	UNP D9MZ14



### 4.2.2 Score per residue for model 2 (medoid)

#### • Molecule 1: Amylase

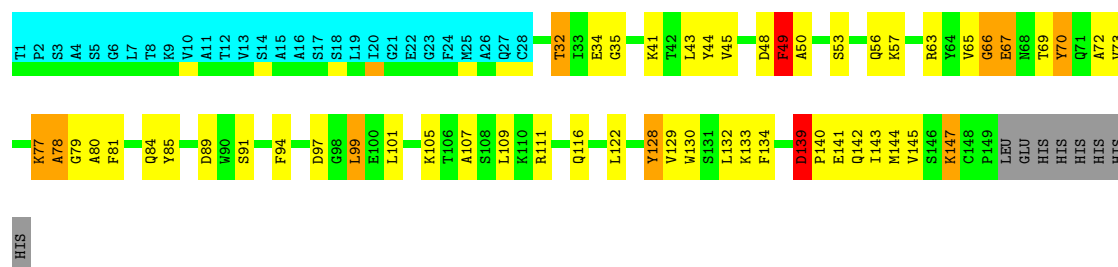
Chain A: 



### 4.2.3 Score per residue for model 3


#### • Molecule 1: Amylase

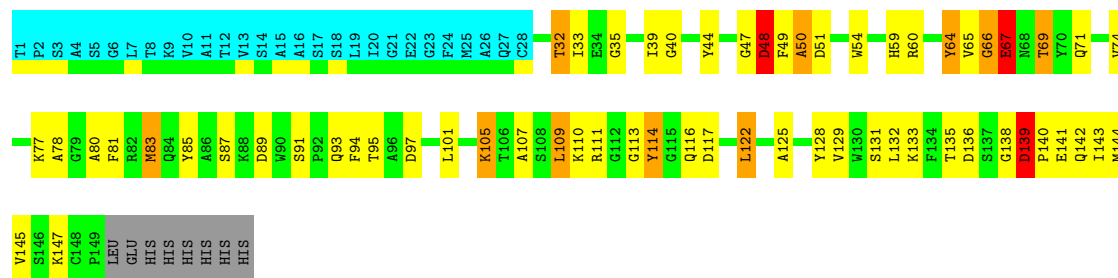
Chain A: 



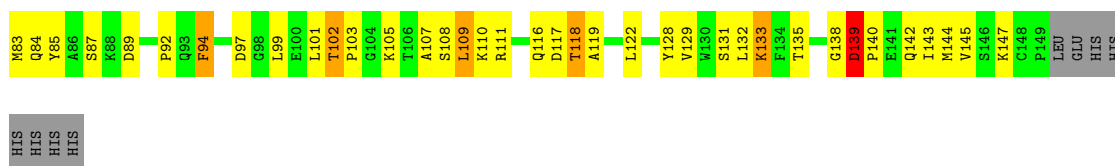
### 4.2.4 Score per residue for model 4

#### • Molecule 1: Amylase

Chain A: 

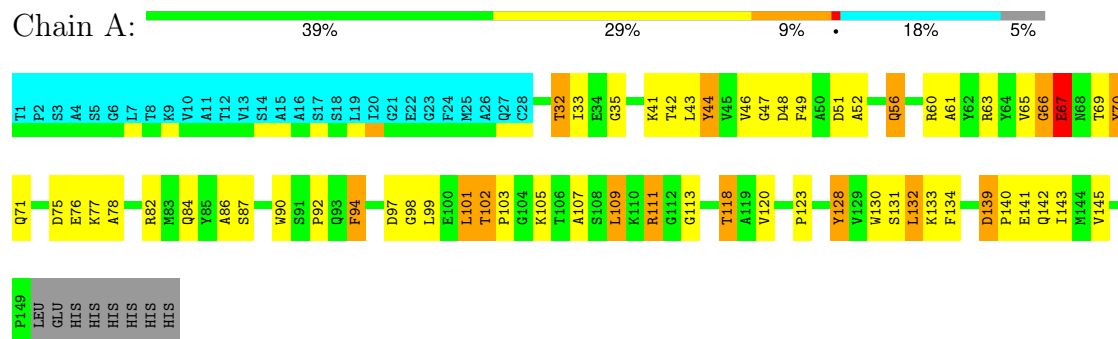






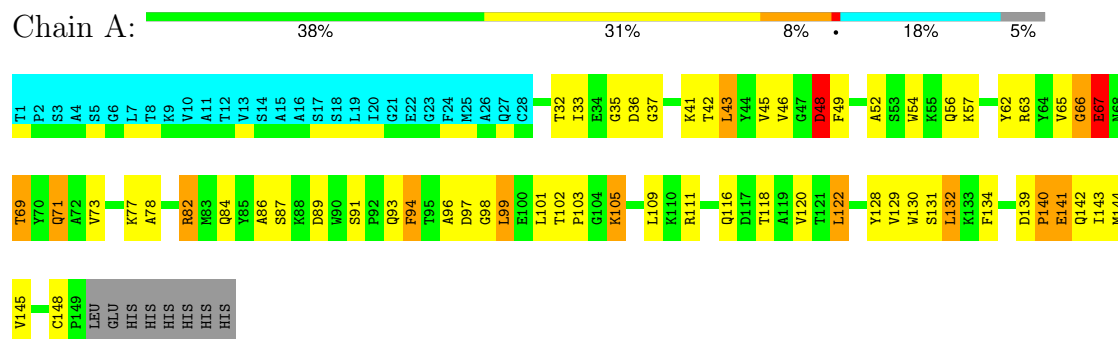
#### 4.2.9 Score per residue for model 9

- Molecule 1: Amylase



#### 4.2.10 Score per residue for model 10

- Molecule 1: Amylase





## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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	
CNS	structure solution	
Sparky	structure solution	

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	1627
Number of shifts mapped to atoms	1627
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	936	891	890	33±5
All	All	9360	8910	8900	328

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:101:LEU:HD21	1:A:145:VAL:HG11	0.86	1.44	9	2
1:A:73:VAL:HG12	1:A:129:VAL:HG12	0.80	1.52	1	2
1:A:42:THR:HG23	1:A:61:ALA:HB1	0.80	1.53	5	1
1:A:39:ILE:HG23	1:A:64:TYR:CE1	0.78	2.12	7	1
1:A:109:LEU:HG	1:A:143:ILE:HD11	0.77	1.57	8	2
1:A:135:THR:HG21	1:A:140:PRO:HD2	0.77	1.56	4	2
1:A:32:THR:HG22	1:A:65:VAL:HA	0.75	1.58	8	5
1:A:109:LEU:HB2	1:A:143:ILE:HD11	0.75	1.58	2	2
1:A:50:ALA:HB1	1:A:77:LYS:HG2	0.74	1.57	7	1
1:A:130:TRP:CE3	1:A:145:VAL:HG21	0.71	2.19	3	1
1:A:132:LEU:HD23	1:A:143:ILE:HD12	0.70	1.64	3	1
1:A:107:ALA:HB3	1:A:143:ILE:HB	0.69	1.64	4	4
1:A:45:VAL:HG12	1:A:85:TYR:CE2	0.69	2.23	8	1
1:A:101:LEU:HD23	1:A:120:VAL:HB	0.69	1.63	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LYS:O	1:A:145:VAL:HG12	0.68	1.88	10	2
1:A:131:SER:O	1:A:132:LEU:HD13	0.68	1.89	9	1
1:A:101:LEU:HD12	1:A:107:ALA:HB2	0.68	1.64	2	3
1:A:99:LEU:HD21	1:A:107:ALA:HB1	0.68	1.66	9	3
1:A:78:ALA:HB1	1:A:122:LEU:O	0.68	1.88	10	1
1:A:82:ARG:HG3	1:A:119:ALA:HB2	0.67	1.66	8	2
1:A:102:THR:HG22	1:A:103:PRO:HD2	0.67	1.66	9	5
1:A:96:ALA:HB1	1:A:99:LEU:HB3	0.67	1.67	1	1
1:A:69:THR:HG22	1:A:133:LYS:HG2	0.65	1.68	5	1
1:A:103:PRO:HG3	1:A:122:LEU:HD23	0.65	1.67	10	1
1:A:69:THR:HG22	1:A:133:LYS:HA	0.65	1.68	2	5
1:A:101:LEU:HD21	1:A:145:VAL:HG12	0.65	1.67	7	1
1:A:99:LEU:HD21	1:A:107:ALA:CB	0.64	2.22	5	3
1:A:48:ASP:HB3	1:A:52:ALA:HB3	0.64	1.68	10	1
1:A:101:LEU:HD11	1:A:145:VAL:HG12	0.63	1.70	1	2
1:A:63:ARG:CZ	1:A:73:VAL:HG13	0.63	2.23	3	1
1:A:101:LEU:HD11	1:A:145:VAL:HG21	0.63	1.71	8	1
1:A:122:LEU:HD11	1:A:147:LYS:CD	0.62	2.25	1	1
1:A:78:ALA:HB2	1:A:125:ALA:HB2	0.62	1.70	4	1
1:A:101:LEU:CD1	1:A:107:ALA:HB2	0.62	2.24	2	2
1:A:132:LEU:N	1:A:132:LEU:HD23	0.62	2.10	1	1
1:A:101:LEU:CG	1:A:145:VAL:HG11	0.62	2.25	4	2
1:A:39:ILE:HD13	1:A:64:TYR:CE2	0.61	2.30	1	1
1:A:82:ARG:CG	1:A:119:ALA:HB2	0.61	2.25	7	1
1:A:35:GLY:HA3	1:A:66:GLY:HA2	0.61	1.71	10	7
1:A:45:VAL:HG11	1:A:74:VAL:HG11	0.61	1.71	1	1
1:A:132:LEU:HD12	1:A:143:ILE:HB	0.61	1.71	9	1
1:A:43:LEU:HD23	1:A:87:SER:HB2	0.60	1.71	10	1
1:A:103:PRO:CG	1:A:122:LEU:HD23	0.60	2.27	10	1
1:A:109:LEU:HD12	1:A:143:ILE:CG1	0.60	2.25	4	1
1:A:132:LEU:HD12	1:A:134:PHE:CZ	0.60	2.31	1	1
1:A:101:LEU:HD11	1:A:145:VAL:CG2	0.59	2.28	8	1
1:A:99:LEU:CD2	1:A:107:ALA:HB1	0.59	2.28	9	2
1:A:101:LEU:HD21	1:A:145:VAL:HG21	0.59	1.75	5	2
1:A:109:LEU:HD23	1:A:141:GLU:HG2	0.59	1.73	2	2
1:A:131:SER:C	1:A:132:LEU:HD13	0.59	2.18	10	2
1:A:139:ASP:CB	1:A:140:PRO:CD	0.58	2.82	4	6
1:A:132:LEU:HD23	1:A:143:ILE:HG12	0.58	1.76	2	1
1:A:78:ALA:HB1	1:A:123:PRO:O	0.58	1.98	5	2
1:A:135:THR:HG21	1:A:140:PRO:CD	0.57	2.29	8	2
1:A:96:ALA:HB3	1:A:118:THR:CG2	0.57	2.29	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LEU:HD13	1:A:132:LEU:N	0.57	2.13	10	1
1:A:50:ALA:HB1	1:A:77:LYS:CG	0.57	2.29	7	1
1:A:132:LEU:HD12	1:A:143:ILE:CB	0.57	2.29	9	1
1:A:122:LEU:HD11	1:A:147:LYS:HD2	0.57	1.77	1	1
1:A:131:SER:C	1:A:132:LEU:HD12	0.57	2.20	8	1
1:A:69:THR:HG23	1:A:133:LYS:HG3	0.57	1.77	4	1
1:A:65:VAL:HG23	1:A:69:THR:O	0.57	1.99	6	2
1:A:60:ARG:HD3	1:A:73:VAL:HG12	0.57	1.75	2	1
1:A:45:VAL:HG11	1:A:74:VAL:CG1	0.56	2.31	1	1
1:A:109:LEU:HD13	1:A:141:GLU:HG2	0.56	1.77	4	1
1:A:101:LEU:HD21	1:A:145:VAL:CG1	0.56	2.30	2	2
1:A:132:LEU:HG	1:A:143:ILE:HG23	0.56	1.77	8	3
1:A:101:LEU:HD11	1:A:145:VAL:CG1	0.56	2.31	1	4
1:A:132:LEU:N	1:A:132:LEU:HD13	0.56	2.16	6	1
1:A:103:PRO:HD3	1:A:120:VAL:HG12	0.55	1.79	7	1
1:A:109:LEU:HD12	1:A:143:ILE:HG12	0.55	1.78	4	1
1:A:99:LEU:C	1:A:99:LEU:HD13	0.55	2.22	2	3
1:A:45:VAL:HG13	1:A:56:GLN:HG3	0.55	1.77	3	1
1:A:139:ASP:CB	1:A:140:PRO:HD3	0.54	2.32	2	5
1:A:103:PRO:CG	1:A:122:LEU:HD13	0.54	2.32	5	1
1:A:129:VAL:O	1:A:145:VAL:HG23	0.53	2.02	3	2
1:A:101:LEU:CD2	1:A:145:VAL:HG11	0.53	2.32	10	1
1:A:109:LEU:HD22	1:A:134:PHE:CE2	0.53	2.38	5	2
1:A:45:VAL:HG12	1:A:56:GLN:OE1	0.53	2.03	10	1
1:A:85:TYR:HB2	1:A:94:PHE:CG	0.53	2.39	8	1
1:A:139:ASP:HB3	1:A:140:PRO:HD2	0.53	1.81	10	1
1:A:135:THR:HG21	1:A:139:ASP:N	0.53	2.18	1	2
1:A:32:THR:CG2	1:A:65:VAL:HG13	0.53	2.34	2	3
1:A:54:TRP:N	1:A:54:TRP:CD1	0.53	2.74	4	1
1:A:101:LEU:HD22	1:A:101:LEU:C	0.53	2.23	7	1
1:A:48:ASP:CB	1:A:52:ALA:HB3	0.53	2.33	10	1
1:A:132:LEU:HD22	1:A:132:LEU:N	0.52	2.19	9	1
1:A:128:TYR:CE1	1:A:145:VAL:HG22	0.52	2.39	3	3
1:A:130:TRP:CZ3	1:A:143:ILE:HG21	0.52	2.39	1	1
1:A:33:ILE:N	1:A:33:ILE:HD13	0.52	2.19	5	1
1:A:69:THR:HG23	1:A:133:LYS:HD3	0.52	1.81	8	1
1:A:42:THR:HG23	1:A:61:ALA:CB	0.52	2.32	5	1
1:A:69:THR:HG21	1:A:133:LYS:HD2	0.52	1.80	7	2
1:A:135:THR:HG23	1:A:138:GLY:H	0.52	1.65	8	2
1:A:101:LEU:HD22	1:A:101:LEU:O	0.52	2.05	7	1
1:A:109:LEU:HD23	1:A:141:GLU:CG	0.51	2.35	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:TRP:CE2	1:A:145:VAL:HG11	0.51	2.41	6	1
1:A:51:ASP:O	1:A:52:ALA:HB3	0.51	2.05	1	1
1:A:107:ALA:HB3	1:A:143:ILE:HG13	0.51	1.82	5	1
1:A:101:LEU:HD11	1:A:145:VAL:CB	0.51	2.36	4	1
1:A:101:LEU:HD11	1:A:145:VAL:HB	0.50	1.82	5	2
1:A:103:PRO:HG3	1:A:122:LEU:HD13	0.49	1.84	1	1
1:A:109:LEU:HD22	1:A:141:GLU:HG2	0.49	1.85	6	2
1:A:69:THR:CG2	1:A:133:LYS:HG2	0.49	2.38	5	1
1:A:43:LEU:HD11	1:A:70:TYR:HD2	0.49	1.68	7	1
1:A:130:TRP:CZ3	1:A:145:VAL:HG21	0.49	2.42	3	1
1:A:122:LEU:HD13	1:A:147:LYS:HD3	0.48	1.84	3	1
1:A:73:VAL:HG22	1:A:129:VAL:HG12	0.48	1.85	10	1
1:A:81:PHE:CE1	1:A:122:LEU:HB2	0.48	2.43	4	1
1:A:109:LEU:HD13	1:A:143:ILE:HG12	0.48	1.84	7	1
1:A:49:PHE:CZ	1:A:83:MET:HB3	0.48	2.43	6	2
1:A:109:LEU:CD1	1:A:143:ILE:HD11	0.48	2.38	1	1
1:A:65:VAL:O	1:A:67:GLU:N	0.48	2.46	10	2
1:A:34:GLU:O	1:A:67:GLU:N	0.48	2.46	6	3
1:A:101:LEU:CD1	1:A:145:VAL:HG11	0.47	2.39	4	1
1:A:86:ALA:CB	1:A:92:PRO:HA	0.47	2.40	9	1
1:A:96:ALA:HB1	1:A:99:LEU:CB	0.47	2.39	1	1
1:A:45:VAL:HG12	1:A:85:TYR:CE1	0.47	2.45	2	1
1:A:101:LEU:HD11	1:A:145:VAL:HG11	0.47	1.86	4	2
1:A:99:LEU:HD23	1:A:118:THR:CG2	0.47	2.38	8	2
1:A:66:GLY:O	1:A:67:GLU:CB	0.47	2.62	10	5
1:A:130:TRP:CD1	1:A:145:VAL:HG21	0.47	2.45	1	1
1:A:101:LEU:HD13	1:A:130:TRP:CH2	0.47	2.44	9	1
1:A:39:ILE:HG12	1:A:64:TYR:CE2	0.47	2.45	6	1
1:A:35:GLY:CA	1:A:66:GLY:HA2	0.46	2.39	2	4
1:A:81:PHE:CE1	1:A:122:LEU:HD22	0.46	2.45	2	1
1:A:109:LEU:HD22	1:A:143:ILE:CG2	0.46	2.40	7	1
1:A:132:LEU:HA	1:A:143:ILE:HG22	0.46	1.86	7	1
1:A:102:THR:HG23	1:A:103:PRO:HD2	0.46	1.88	7	2
1:A:106:THR:HG23	1:A:144:MET:HB3	0.46	1.88	6	1
1:A:109:LEU:HD12	1:A:143:ILE:HD13	0.46	1.87	9	1
1:A:107:ALA:O	1:A:143:ILE:HD12	0.46	2.11	8	1
1:A:132:LEU:HB3	1:A:143:ILE:HG22	0.46	1.87	9	1
1:A:74:VAL:HB	1:A:128:TYR:CE1	0.45	2.45	4	1
1:A:32:THR:O	1:A:65:VAL:HG12	0.45	2.11	7	2
1:A:94:PHE:HA	1:A:109:LEU:HD11	0.45	1.89	6	2
1:A:50:ALA:HB1	1:A:78:ALA:HB3	0.45	1.89	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:TYR:HE1	1:A:145:VAL:HG22	0.45	1.71	5	1
1:A:49:PHE:CB	1:A:81:PHE:HA	0.45	2.40	3	1
1:A:69:THR:HG22	1:A:132:LEU:O	0.45	2.12	10	2
1:A:46:VAL:HG12	1:A:56:GLN:NE2	0.45	2.27	9	1
1:A:78:ALA:HB2	1:A:125:ALA:N	0.45	2.27	2	2
1:A:85:TYR:O	1:A:93:GLN:HB2	0.45	2.12	4	2
1:A:101:LEU:HD11	1:A:105:LYS:O	0.45	2.10	3	1
1:A:49:PHE:CE1	1:A:83:MET:HB3	0.45	2.47	6	1
1:A:45:VAL:HG22	1:A:56:GLN:HG2	0.45	1.88	2	1
1:A:99:LEU:HD12	1:A:101:LEU:HD12	0.45	1.88	7	1
1:A:103:PRO:HD3	1:A:120:VAL:HG23	0.45	1.89	9	1
1:A:81:PHE:CZ	1:A:122:LEU:HD13	0.44	2.47	7	1
1:A:139:ASP:CB	1:A:140:PRO:HD2	0.44	2.42	10	1
1:A:99:LEU:HD23	1:A:118:THR:HG22	0.44	1.88	8	1
1:A:82:ARG:HG2	1:A:119:ALA:HB2	0.44	1.90	7	1
1:A:42:THR:HB	1:A:62:TYR:CD1	0.44	2.47	10	1
1:A:52:ALA:HB1	1:A:55:LYS:HG3	0.44	1.89	2	1
1:A:64:TYR:CD1	1:A:64:TYR:O	0.44	2.70	7	1
1:A:94:PHE:CE1	1:A:143:ILE:HD13	0.44	2.48	10	1
1:A:131:SER:C	1:A:132:LEU:HD23	0.44	2.33	1	1
1:A:70:TYR:CD1	1:A:134:PHE:CE2	0.44	3.05	9	1
1:A:32:THR:HG22	1:A:65:VAL:HG13	0.44	1.90	2	2
1:A:39:ILE:CG1	1:A:64:TYR:CE2	0.44	3.01	6	1
1:A:44:TYR:HB2	1:A:86:ALA:HB3	0.44	1.90	9	1
1:A:132:LEU:HB3	1:A:143:ILE:HG23	0.44	1.88	10	1
1:A:130:TRP:NE1	1:A:145:VAL:HG21	0.43	2.28	1	1
1:A:33:ILE:HG23	1:A:66:GLY:HA3	0.43	1.90	10	1
1:A:60:ARG:CD	1:A:73:VAL:HG12	0.43	2.43	2	1
1:A:79:GLY:N	1:A:122:LEU:O	0.43	2.51	6	3
1:A:97:ASP:O	1:A:99:LEU:N	0.43	2.51	2	1
1:A:109:LEU:HD22	1:A:143:ILE:HD11	0.43	1.89	3	1
1:A:81:PHE:CE2	1:A:120:VAL:CG1	0.43	3.01	6	1
1:A:78:ALA:HB2	1:A:125:ALA:CA	0.43	2.43	1	1
1:A:94:PHE:O	1:A:94:PHE:CD2	0.43	2.71	9	1
1:A:72:ALA:HB3	1:A:85:TYR:OH	0.43	2.12	3	1
1:A:43:LEU:HD12	1:A:70:TYR:CD1	0.43	2.48	3	1
1:A:132:LEU:HD23	1:A:143:ILE:CD1	0.43	2.40	3	1
1:A:39:ILE:CD1	1:A:64:TYR:CE2	0.43	3.02	4	1
1:A:49:PHE:CD1	1:A:49:PHE:N	0.43	2.87	6	1
1:A:122:LEU:HD22	1:A:128:TYR:HE2	0.43	1.74	5	1
1:A:76:GLU:HG3	1:A:128:TYR:CD2	0.43	2.49	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLY:HA3	1:A:52:ALA:HB1	0.42	1.90	9	1
1:A:109:LEU:HD13	1:A:143:ILE:CG2	0.42	2.44	5	1
1:A:96:ALA:HB1	1:A:99:LEU:CD2	0.42	2.43	10	1
1:A:48:ASP:O	1:A:49:PHE:CB	0.42	2.67	3	1
1:A:62:TYR:CE1	1:A:64:TYR:CE1	0.42	3.07	5	1
1:A:35:GLY:O	1:A:37:GLY:N	0.42	2.52	10	1
1:A:82:ARG:HA	1:A:118:THR:O	0.42	2.13	10	1
1:A:69:THR:CG2	1:A:133:LYS:HA	0.42	2.43	2	1
1:A:50:ALA:O	1:A:51:ASP:CB	0.42	2.66	4	1
1:A:101:LEU:HG	1:A:145:VAL:HG11	0.42	1.88	4	1
1:A:33:ILE:O	1:A:66:GLY:CA	0.42	2.68	4	4
1:A:91:SER:CB	1:A:92:PRO:HD2	0.42	2.44	6	2
1:A:79:GLY:O	1:A:80:ALA:HB3	0.42	2.15	3	1
1:A:39:ILE:HG22	1:A:40:GLY:N	0.42	2.30	6	2
1:A:76:GLU:CG	1:A:128:TYR:HB2	0.42	2.45	6	1
1:A:109:LEU:HD11	1:A:132:LEU:HD23	0.42	1.90	8	1
1:A:134:PHE:HB2	1:A:141:GLU:HB3	0.42	1.91	10	1
1:A:101:LEU:O	1:A:120:VAL:HA	0.42	2.15	7	1
1:A:101:LEU:N	1:A:101:LEU:HD13	0.42	2.30	7	1
1:A:47:GLY:O	1:A:48:ASP:CB	0.42	2.67	4	1
1:A:142:GLN:O	1:A:143:ILE:HD13	0.42	2.14	3	1
1:A:122:LEU:HD21	1:A:128:TYR:HE2	0.42	1.75	6	1
1:A:132:LEU:HD22	1:A:132:LEU:O	0.41	2.15	6	1
1:A:102:THR:CG2	1:A:103:PRO:HD2	0.41	2.45	7	1
1:A:131:SER:O	1:A:132:LEU:HD12	0.41	2.14	8	1
1:A:46:VAL:HB	1:A:84:GLN:O	0.41	2.15	8	1
1:A:81:PHE:CZ	1:A:122:LEU:HB2	0.41	2.51	4	1
1:A:101:LEU:N	1:A:101:LEU:CD1	0.41	2.83	7	1
1:A:44:TYR:CB	1:A:86:ALA:HB3	0.41	2.44	9	1
1:A:132:LEU:HB3	1:A:134:PHE:CZ	0.41	2.51	9	1
1:A:132:LEU:N	1:A:132:LEU:CD2	0.41	2.81	1	1
1:A:50:ALA:HB1	1:A:77:LYS:O	0.41	2.15	3	1
1:A:101:LEU:HD22	1:A:120:VAL:CG2	0.41	2.46	10	1
1:A:102:THR:HG22	1:A:103:PRO:CD	0.41	2.42	9	1
1:A:101:LEU:C	1:A:101:LEU:HD23	0.41	2.36	10	1
1:A:65:VAL:CG2	1:A:71:GLN:HB2	0.41	2.45	10	2
1:A:101:LEU:HD13	1:A:101:LEU:H	0.41	1.75	7	1
1:A:132:LEU:N	1:A:132:LEU:CD1	0.41	2.83	10	1
1:A:139:ASP:HB3	1:A:140:PRO:CD	0.41	2.46	10	1
1:A:91:SER:CB	1:A:92:PRO:CD	0.41	2.99	5	1
1:A:47:GLY:O	1:A:54:TRP:CD1	0.41	2.74	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:GLY:O	1:A:67:GLU:CG	0.41	2.69	8	1
1:A:46:VAL:HB	1:A:54:TRP:CG	0.41	2.51	10	1
1:A:48:ASP:O	1:A:49:PHE:HB2	0.40	2.16	8	1
1:A:45:VAL:HG12	1:A:85:TYR:CZ	0.40	2.52	2	1
1:A:94:PHE:CE1	1:A:143:ILE:HD12	0.40	2.51	6	1
1:A:62:TYR:CD2	1:A:62:TYR:N	0.40	2.89	8	1
1:A:62:TYR:HB2	1:A:70:TYR:CE2	0.40	2.52	8	1
1:A:86:ALA:HA	1:A:93:GLN:CB	0.40	2.46	10	1
1:A:94:PHE:CD2	1:A:94:PHE:O	0.40	2.74	8	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	120/157 (76%)	99±2 (82±2%)	15±3 (12±2%)	6±1 (5±1%)	<b>3</b>	<b>24</b>
All	All	1200/1570 (76%)	990 (82%)	150 (12%)	60 (5%)	<b>3</b>	<b>24</b>

All 24 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	66	GLY	7
1	A	67	GLU	7
1	A	139	ASP	6
1	A	49	PHE	4
1	A	98	GLY	4
1	A	111	ARG	4
1	A	48	ASP	3
1	A	80	ALA	2
1	A	114	TYR	2
1	A	53	SER	2
1	A	92	PRO	2
1	A	99	LEU	2
1	A	113	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	36	ASP	2
1	A	140	PRO	2
1	A	97	ASP	1
1	A	78	ALA	1
1	A	50	ALA	1
1	A	62	TYR	1
1	A	51	ASP	1
1	A	112	GLY	1
1	A	38	PRO	1
1	A	100	GLU	1
1	A	61	ALA	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	97/125 (78%)	67±3 (69±4%)	30±3 (31±4%)	1	14
All	All	970/1250 (78%)	668 (69%)	302 (31%)	1	14

All 75 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	94	PHE	10
1	A	32	THR	9
1	A	67	GLU	9
1	A	139	ASP	9
1	A	142	GLN	9
1	A	87	SER	8
1	A	91	SER	8
1	A	97	ASP	8
1	A	105	LYS	8
1	A	44	TYR	7
1	A	77	LYS	7
1	A	116	GLN	7
1	A	128	TYR	7
1	A	144	MET	7

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Mol	Chain	Res	Type	Models (Total)
1	A	84	GLN	7
1	A	56	GLN	6
1	A	89	ASP	6
1	A	147	LYS	6
1	A	110	LYS	6
1	A	63	ARG	5
1	A	69	THR	5
1	A	95	THR	5
1	A	111	ARG	5
1	A	118	THR	5
1	A	132	LEU	5
1	A	83	MET	5
1	A	41	LYS	5
1	A	59	HIS	4
1	A	102	THR	4
1	A	33	ILE	4
1	A	57	LYS	4
1	A	49	PHE	4
1	A	48	ASP	4
1	A	109	LEU	4
1	A	122	LEU	4
1	A	130	TRP	4
1	A	71	GLN	4
1	A	82	ARG	4
1	A	29	ASP	3
1	A	85	TYR	3
1	A	108	SER	3
1	A	141	GLU	3
1	A	51	ASP	3
1	A	76	GLU	3
1	A	114	TYR	3
1	A	70	TYR	3
1	A	60	ARG	3
1	A	117	ASP	3
1	A	65	VAL	3
1	A	43	LEU	3
1	A	36	ASP	2
1	A	88	LYS	2
1	A	100	GLU	2
1	A	127	GLN	2
1	A	55	LYS	2
1	A	90	TRP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	134	PHE	2
1	A	148	CYS	2
1	A	34	GLU	2
1	A	64	TYR	2
1	A	62	TYR	2
1	A	133	LYS	2
1	A	101	LEU	2
1	A	93	GLN	1
1	A	146	SER	1
1	A	106	THR	1
1	A	53	SER	1
1	A	99	LEU	1
1	A	131	SER	1
1	A	136	ASP	1
1	A	30	ASN	1
1	A	143	ILE	1
1	A	137	SER	1
1	A	42	THR	1
1	A	75	ASP	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *AmyP-SBD\_Chemical\_Shifts.txt*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1627
Number of shifts mapped to atoms	1627
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	$-0.09 \pm 0.20$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	128	$-0.27 \pm 0.30$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	135	$0.38 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	137	$0.14 \pm 0.50$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1343 atoms were assigned a chemical shift out of a possible 1560. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	589/602 (98%)	245/247 (99%)	231/242 (95%)	113/113 (100%)
Sidechain	708/811 (87%)	489/524 (93%)	208/257 (81%)	11/30 (37%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	46/147 (31%)	43/70 (61%)	1/72 (1%)	2/5 (40%)
Overall	1343/1560 (86%)	777/841 (92%)	440/571 (77%)	126/148 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1612 atoms were assigned a chemical shift out of a possible 1878. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	717/743 (97%)	298/305 (98%)	282/298 (95%)	137/140 (98%)
Sidechain	847/978 (87%)	586/637 (92%)	249/309 (81%)	12/32 (38%)
Aromatic	48/157 (31%)	45/75 (60%)	1/77 (1%)	2/5 (40%)
Overall	1612/1878 (86%)	929/1017 (91%)	532/684 (78%)	151/177 (85%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

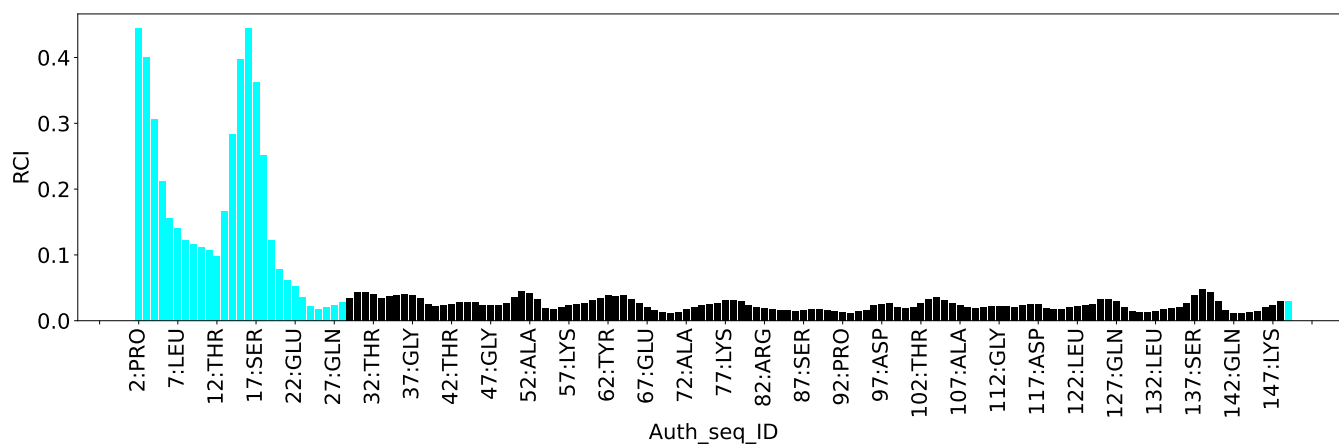
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	54	TRP	CH2	159.24	116.19 – 131.43	23.2
1	A	118	THR	HG1	5.86	0.08 – 2.19	22.4
1	A	32	THR	HG1	5.70	0.08 – 2.19	21.6
1	A	95	THR	HG1	5.67	0.08 – 2.19	21.5
1	A	121	THR	HG1	5.53	0.08 – 2.19	20.8
1	A	106	THR	HG1	5.52	0.08 – 2.19	20.8
1	A	42	THR	HG1	5.20	0.08 – 2.19	19.2
1	A	135	THR	HG1	5.10	0.08 – 2.19	18.8
1	A	145	VAL	HG11	-0.71	-0.48 – 2.12	-5.9
1	A	145	VAL	HG12	-0.71	-0.48 – 2.12	-5.9
1	A	145	VAL	HG13	-0.71	-0.48 – 2.12	-5.9

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2079
Intra-residue ( $ i-j =0$ )	928
Sequential ( $ i-j =1$ )	577
Medium range ( $ i-j >1$ and $ i-j <5$ )	102
Long range ( $ i-j \geq 5$ )	396
Inter-chain	0
Hydrogen bond restraints	76
Disulfide bond restraints	0
Total dihedral-angle restraints	176
Number of unmapped restraints	0
Number of restraints per residue	14.4
Number of long range restraints per residue <sup>1</sup>	3.0

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.2	0.19
0.2-0.5 (Medium)	1.1	0.36
>0.5 (Large)	0.1	0.64



### 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	2.45
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

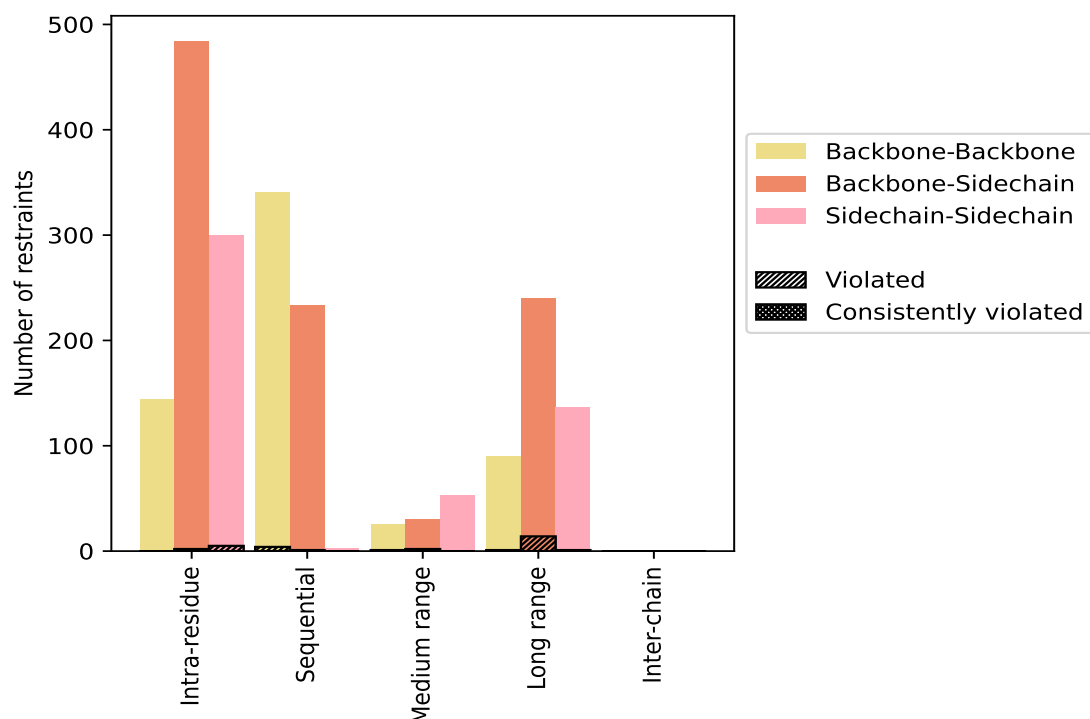
### 9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>928</b>	<b>44.6</b>	<b>7</b>	<b>0.8</b>	<b>0.3</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	144	6.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	484	23.3	2	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	300	14.4	5	1.7	0.2	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>577</b>	<b>27.8</b>	<b>5</b>	<b>0.9</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	341	16.4	4	1.2	0.2	0	0.0	0.0
Backbone-Sidechain	233	11.2	1	0.4	0.0	0	0.0	0.0
Sidechain-Sidechain	3	0.1	0	0.0	0.0	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>102</b>	<b>4.9</b>	<b>2</b>	<b>2.0</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	25	1.2	1	4.0	0.0	0	0.0	0.0
Backbone-Sidechain	24	1.2	1	4.2	0.0	0	0.0	0.0
Sidechain-Sidechain	53	2.5	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>396</b>	<b>19.0</b>	<b>4</b>	<b>1.0</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	90	4.3	1	1.1	0.0	0	0.0	0.0
Backbone-Sidechain	170	8.2	2	1.2	0.1	0	0.0	0.0
Sidechain-Sidechain	136	6.5	1	0.7	0.0	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>76</b>	<b>3.7</b>	<b>13</b>	<b>17.1</b>	<b>0.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>2079</b>	<b>100.0</b>	<b>31</b>	<b>1.5</b>	<b>1.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	600	28.9	6	1.0	0.3	0	0.0	0.0
Backbone-Sidechain	987	47.5	19	1.9	0.9	0	0.0	0.0
Sidechain-Sidechain	492	23.7	6	1.2	0.3	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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

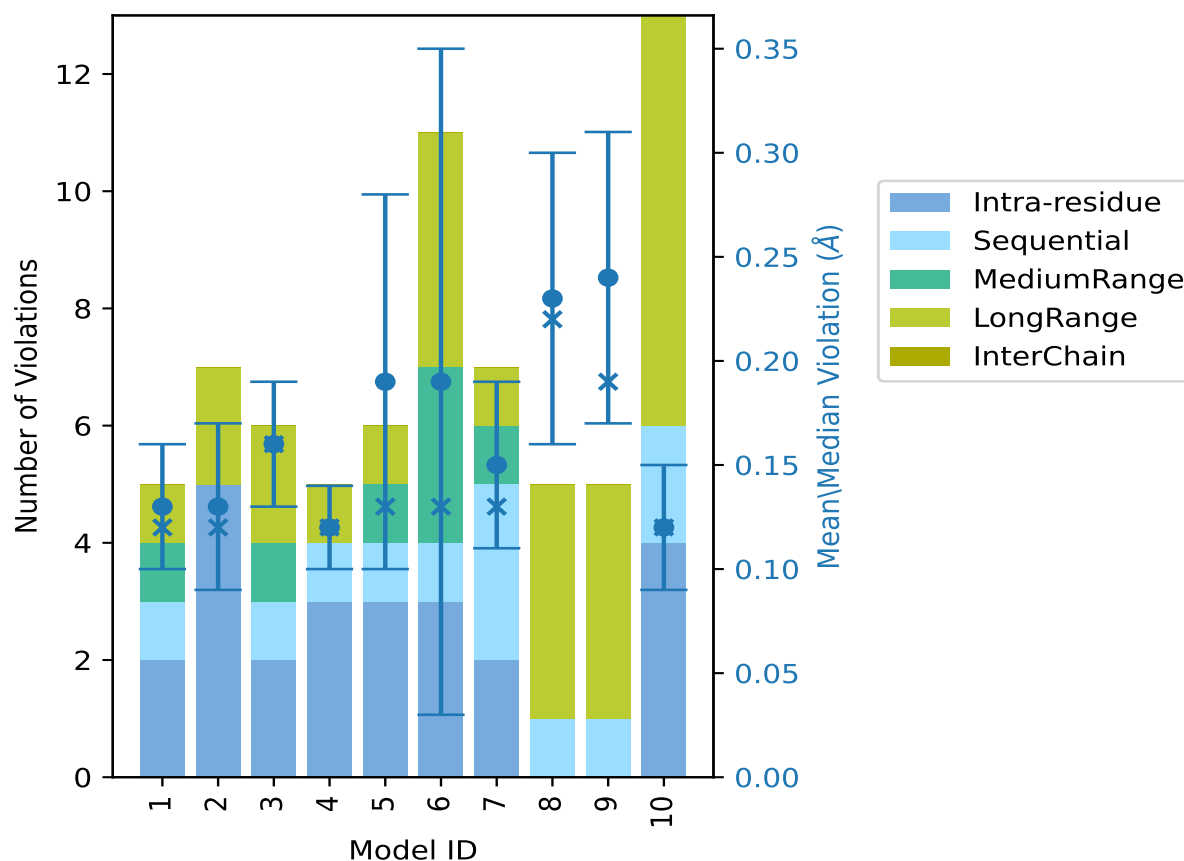
## 9.2 Distance violation statistics for each model [i](#)

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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	2	1	1	1	0	5	0.13	0.18	0.03	0.12
2	5	0	0	2	0	7	0.13	0.24	0.04	0.12
3	2	1	1	2	0	6	0.16	0.22	0.03	0.16
4	3	1	0	1	0	5	0.12	0.17	0.02	0.12
5	3	1	1	1	0	6	0.19	0.32	0.09	0.13
6	3	1	3	4	0	11	0.19	0.64	0.16	0.13
7	2	3	1	1	0	7	0.15	0.23	0.04	0.13
8	0	1	0	4	0	5	0.23	0.34	0.07	0.22
9	0	1	0	4	0	5	0.24	0.36	0.07	0.19
10	4	2	0	7	0	13	0.12	0.19	0.03	0.12

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble ⓘ

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, 1985(IR:921, SQ:572, MR:100, LR:392, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
3	3	1	4	0	11	1	10.0
0	0	0	0	0	0	2	20.0
0	1	1	0	0	2	3	30.0

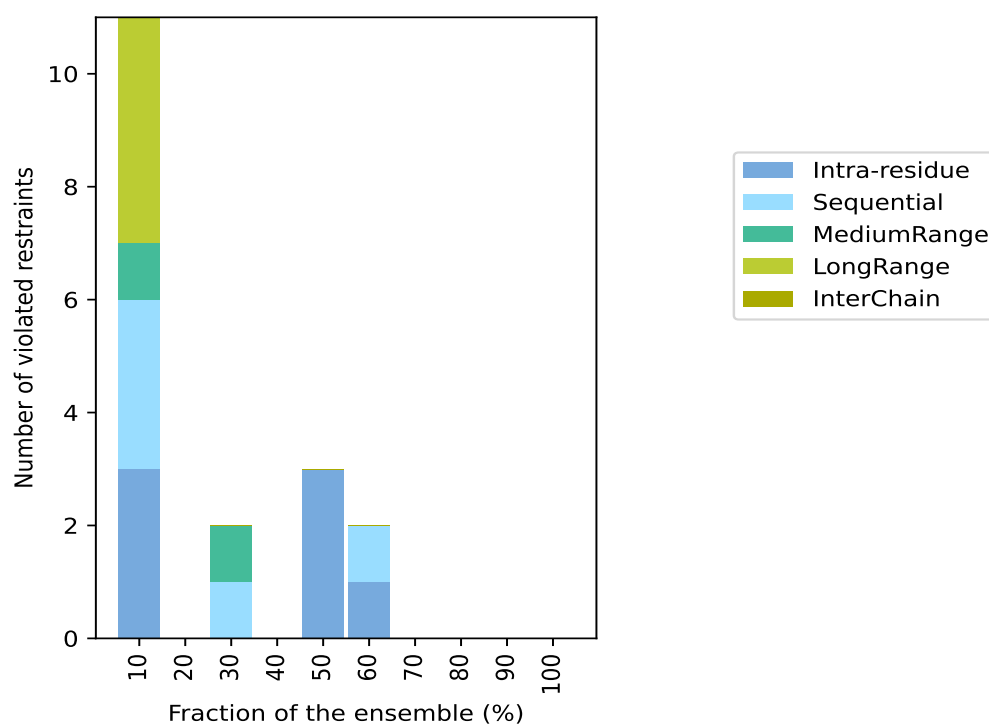
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	4	40.0
3	0	0	0	0	3	5	50.0
1	1	0	0	0	2	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	0	0	0	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

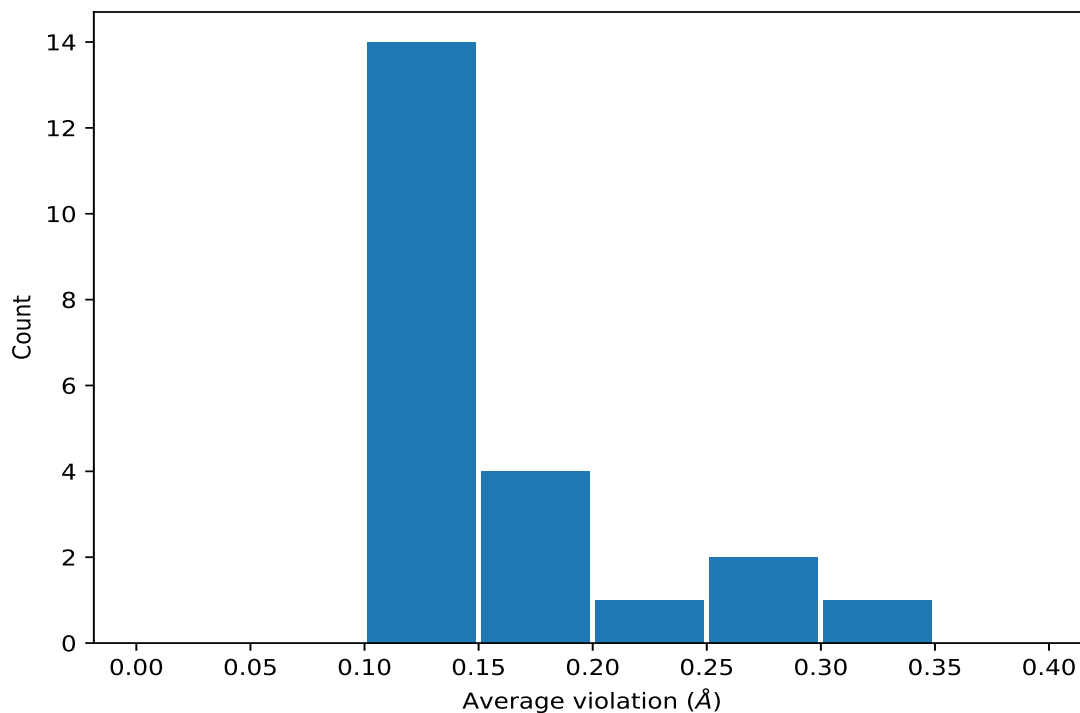


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,980)	1:34:A:GLU:H	1:33:A:ILE:HA	6	0.17	0.01	0.17
(2,742)	1:100:A:GLU:HG2	1:100:A:GLU:HB2	6	0.12	0.01	0.12
(2,742)	1:100:A:GLU:HG3	1:100:A:GLU:HB2	6	0.12	0.01	0.12
(1,59)	1:43:A:LEU:H	1:61:A:ALA:O	5	0.18	0.07	0.14
(2,415)	1:22:A:GLU:HG2	1:22:A:GLU:HB3	5	0.12	0.0	0.12
(2,415)	1:22:A:GLU:HG3	1:22:A:GLU:HB3	5	0.12	0.0	0.12
(2,741)	1:100:A:GLU:HG2	1:100:A:GLU:HB3	5	0.12	0.01	0.12
(2,741)	1:100:A:GLU:HG3	1:100:A:GLU:HB3	5	0.12	0.01	0.12
(2,416)	1:22:A:GLU:HG2	1:22:A:GLU:HB2	5	0.11	0.0	0.11
(2,416)	1:22:A:GLU:HG3	1:22:A:GLU:HB2	5	0.11	0.0	0.11
(1,67)	1:65:A:VAL:H	1:69:A:THR:O	3	0.27	0.08	0.32
(2,1378)	1:32:A:THR:H	1:31:A:PRO:HB3	3	0.15	0.02	0.15
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG21	3	0.12	0.03	0.11
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG22	3	0.12	0.03	0.11
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG23	3	0.12	0.03	0.11

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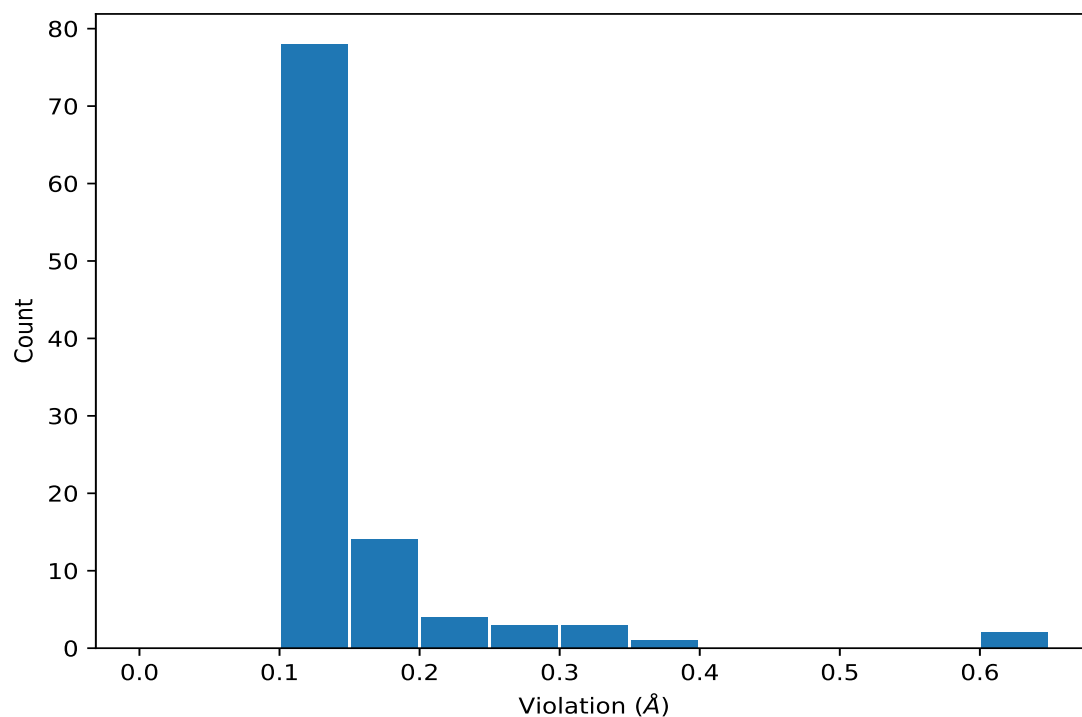
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,71)	1:85:A:TYR:H	1:94:A:PHE:O	2	0.35	0.01	0.35
(1,72)	1:85:A:TYR:N	1:94:A:PHE:O	2	0.28	0.01	0.28
(1,73)	1:94:A:PHE:H	1:85:A:TYR:O	2	0.2	0.02	0.2
(1,53)	1:118:A:THR:H	1:83:A:MET:O	2	0.18	0.01	0.18
(1,7)	1:82:A:ARG:H	1:48:A:ASP:O	2	0.17	0.05	0.17
(1,8)	1:82:A:ARG:N	1:48:A:ASP:O	2	0.13	0.03	0.13
(1,47)	1:105:A:LYS:H	1:145:A:VAL:O	2	0.11	0.0	0.11

<sup>1</sup>Number of violated models, <sup>2</sup>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)
(2,201)	1:63:A:ARG:H	1:63:A:ARG:HH11	6	0.64
(2,201)	1:63:A:ARG:H	1:63:A:ARG:HH12	6	0.64
(1,71)	1:85:A:TYR:H	1:94:A:PHE:O	9	0.36
(1,71)	1:85:A:TYR:H	1:94:A:PHE:O	8	0.34
(1,67)	1:65:A:VAL:H	1:69:A:THR:O	6	0.33
(1,67)	1:65:A:VAL:H	1:69:A:THR:O	5	0.32
(1,59)	1:43:A:LEU:H	1:61:A:ALA:O	5	0.3
(1,72)	1:85:A:TYR:N	1:94:A:PHE:O	9	0.29
(1,72)	1:85:A:TYR:N	1:94:A:PHE:O	8	0.26
(1,59)	1:43:A:LEU:H	1:61:A:ALA:O	2	0.24
(1,63)	1:63:A:ARG:H	1:71:A:GLN:O	7	0.23
(1,73)	1:94:A:PHE:H	1:85:A:TYR:O	8	0.22
(1,7)	1:82:A:ARG:H	1:48:A:ASP:O	3	0.22
(1,53)	1:118:A:THR:H	1:83:A:MET:O	9	0.19
(1,5)	1:48:A:ASP:H	1:82:A:ARG:O	10	0.19
(2,1378)	1:32:A:THR:H	1:31:A:PRO:HB3	7	0.18
(2,980)	1:34:A:GLU:H	1:33:A:ILE:HA	1	0.18
(2,980)	1:34:A:GLU:H	1:33:A:ILE:HA	9	0.18
(1,73)	1:94:A:PHE:H	1:85:A:TYR:O	9	0.18
(1,53)	1:118:A:THR:H	1:83:A:MET:O	8	0.18
(2,980)	1:34:A:GLU:H	1:33:A:ILE:HA	4	0.17
(2,980)	1:34:A:GLU:H	1:33:A:ILE:HA	10	0.17
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG21	3	0.16
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG22	3	0.16
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG23	3	0.16
(2,980)	1:34:A:GLU:H	1:33:A:ILE:HA	3	0.16
(1,8)	1:82:A:ARG:N	1:48:A:ASP:O	3	0.16
(2,1378)	1:32:A:THR:H	1:31:A:PRO:HB3	6	0.15
(2,980)	1:34:A:GLU:H	1:33:A:ILE:HA	8	0.15
(1,67)	1:65:A:VAL:H	1:69:A:THR:O	7	0.15
(1,59)	1:43:A:LEU:H	1:61:A:ALA:O	6	0.14
(2,1393)	1:37:A:GLY:H	1:64:A:TYR:HB2	6	0.13
(2,1378)	1:32:A:THR:H	1:31:A:PRO:HB3	5	0.13
(2,742)	1:100:A:GLU:HG2	1:100:A:GLU:HB2	5	0.13
(2,742)	1:100:A:GLU:HG3	1:100:A:GLU:HB2	5	0.13
(2,741)	1:100:A:GLU:HG2	1:100:A:GLU:HB3	7	0.13
(2,741)	1:100:A:GLU:HG3	1:100:A:GLU:HB3	7	0.13
(1,75)	1:135:A:THR:H	1:140:A:PRO:O	6	0.13
(2,1470)	1:71:A:GLN:H	1:63:A:ARG:HH21	4	0.12
(2,1470)	1:71:A:GLN:H	1:63:A:ARG:HH22	4	0.12
(2,1040)	1:53:A:SER:H	1:52:A:ALA:H	7	0.12
(2,1037)	1:52:A:ALA:H	1:53:A:SER:H	7	0.12
(2,742)	1:100:A:GLU:HG2	1:100:A:GLU:HB2	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,742)	1:100:A:GLU:HG3	1:100:A:GLU:HB2	2	0.12
(2,742)	1:100:A:GLU:HG2	1:100:A:GLU:HB2	3	0.12
(2,742)	1:100:A:GLU:HG3	1:100:A:GLU:HB2	3	0.12
(2,742)	1:100:A:GLU:HG2	1:100:A:GLU:HB2	4	0.12
(2,742)	1:100:A:GLU:HG3	1:100:A:GLU:HB2	4	0.12
(2,742)	1:100:A:GLU:HG2	1:100:A:GLU:HB2	10	0.12
(2,742)	1:100:A:GLU:HG3	1:100:A:GLU:HB2	10	0.12
(2,741)	1:100:A:GLU:HG2	1:100:A:GLU:HB3	3	0.12
(2,741)	1:100:A:GLU:HG3	1:100:A:GLU:HB3	3	0.12
(2,741)	1:100:A:GLU:HG2	1:100:A:GLU:HB3	10	0.12
(2,741)	1:100:A:GLU:HG3	1:100:A:GLU:HB3	10	0.12
(2,416)	1:22:A:GLU:HG2	1:22:A:GLU:HB2	2	0.12
(2,416)	1:22:A:GLU:HG3	1:22:A:GLU:HB2	2	0.12
(2,416)	1:22:A:GLU:HG2	1:22:A:GLU:HB2	5	0.12
(2,416)	1:22:A:GLU:HG3	1:22:A:GLU:HB2	5	0.12
(2,415)	1:22:A:GLU:HG2	1:22:A:GLU:HB3	1	0.12
(2,415)	1:22:A:GLU:HG3	1:22:A:GLU:HB3	1	0.12
(2,415)	1:22:A:GLU:HG2	1:22:A:GLU:HB3	5	0.12
(2,415)	1:22:A:GLU:HG3	1:22:A:GLU:HB3	5	0.12
(2,415)	1:22:A:GLU:HG2	1:22:A:GLU:HB3	6	0.12
(2,415)	1:22:A:GLU:HG3	1:22:A:GLU:HB3	6	0.12
(2,415)	1:22:A:GLU:HG2	1:22:A:GLU:HB3	10	0.12
(2,415)	1:22:A:GLU:HG3	1:22:A:GLU:HB3	10	0.12
(2,398)	1:20:A:ILE:HG12	1:20:A:ILE:HB	2	0.12
(2,398)	1:20:A:ILE:HG13	1:20:A:ILE:HB	2	0.12
(1,59)	1:43:A:LEU:H	1:61:A:ALA:O	1	0.12
(1,59)	1:43:A:LEU:H	1:61:A:ALA:O	10	0.12
(1,37)	1:76:A:GLU:H	1:126:A:GLY:O	2	0.12
(1,7)	1:82:A:ARG:H	1:48:A:ASP:O	10	0.12
(2,1782)	1:67:A:GLU:HG2	1:32:A:THR:HG21	10	0.11
(2,1782)	1:67:A:GLU:HG2	1:32:A:THR:HG22	10	0.11
(2,1782)	1:67:A:GLU:HG2	1:32:A:THR:HG23	10	0.11
(2,1782)	1:67:A:GLU:HG3	1:32:A:THR:HG21	10	0.11
(2,1782)	1:67:A:GLU:HG3	1:32:A:THR:HG22	10	0.11
(2,1782)	1:67:A:GLU:HG3	1:32:A:THR:HG23	10	0.11
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG21	1	0.11
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG22	1	0.11
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG23	1	0.11
(2,992)	1:37:A:GLY:H	1:35:A:GLY:HA2	6	0.11
(2,742)	1:100:A:GLU:HG2	1:100:A:GLU:HB2	7	0.11
(2,742)	1:100:A:GLU:HG3	1:100:A:GLU:HB2	7	0.11
(2,741)	1:100:A:GLU:HG2	1:100:A:GLU:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,741)	1:100:A:GLU:HG3	1:100:A:GLU:HB3	2	0.11
(2,741)	1:100:A:GLU:HG2	1:100:A:GLU:HB3	4	0.11
(2,741)	1:100:A:GLU:HG3	1:100:A:GLU:HB3	4	0.11
(2,416)	1:22:A:GLU:HG2	1:22:A:GLU:HB2	1	0.11
(2,416)	1:22:A:GLU:HG3	1:22:A:GLU:HB2	1	0.11
(2,416)	1:22:A:GLU:HG2	1:22:A:GLU:HB2	6	0.11
(2,416)	1:22:A:GLU:HG3	1:22:A:GLU:HB2	6	0.11
(2,416)	1:22:A:GLU:HG2	1:22:A:GLU:HB2	10	0.11
(2,416)	1:22:A:GLU:HG3	1:22:A:GLU:HB2	10	0.11
(2,415)	1:22:A:GLU:HG2	1:22:A:GLU:HB3	2	0.11
(2,415)	1:22:A:GLU:HG3	1:22:A:GLU:HB3	2	0.11
(1,47)	1:105:A:LYS:H	1:145:A:VAL:O	10	0.11
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG21	6	0.1
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG22	6	0.1
(2,1400)	1:41:A:LYS:H	1:39:A:ILE:HG23	6	0.1
(2,1000)	1:42:A:THR:H	1:41:A:LYS:HA	10	0.1
(2,990)	1:36:A:ASP:H	1:67:A:GLU:HA	10	0.1
(2,288)	1:121:A:THR:H	1:121:A:THR:HB	4	0.1
(1,47)	1:105:A:LYS:H	1:145:A:VAL:O	6	0.1
(1,8)	1:82:A:ARG:N	1:48:A:ASP:O	10	0.1

## 10 Dihedral-angle violation analysis [i](#)

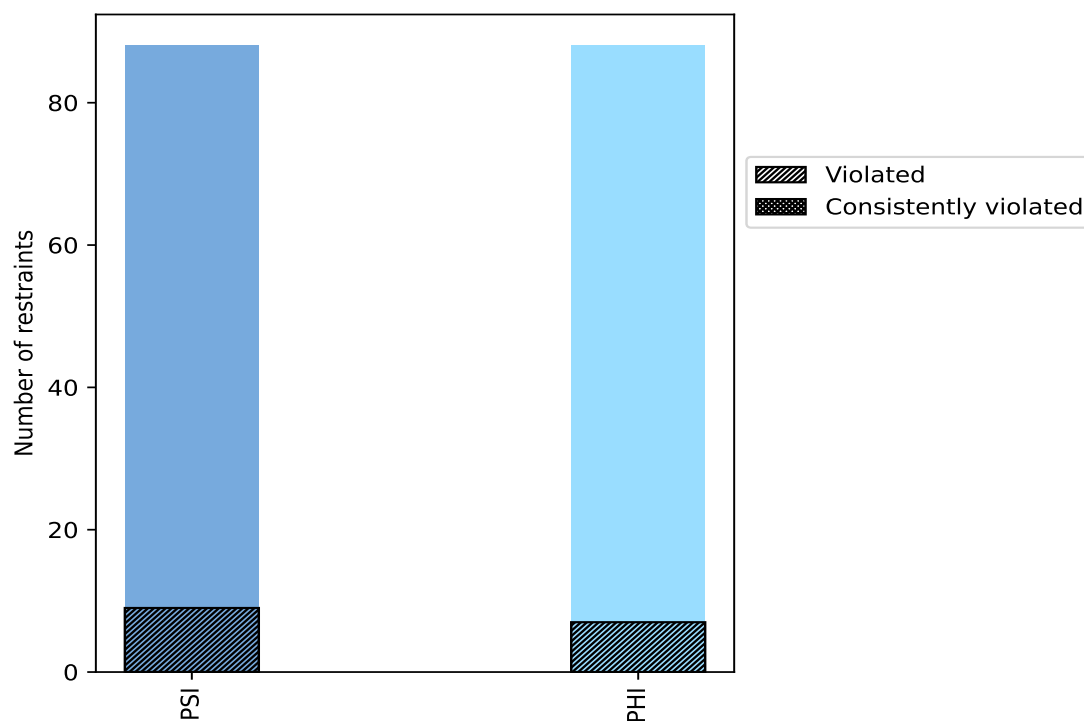
### 10.1 Summary of dihedral-angle violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	88	50.0	9	10.2	5.1	0	0.0	0.0
PHI	88	50.0	7	8.0	4.0	0	0.0	0.0
Total	176	100.0	16	9.1	9.1	0	0.0	0.0

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

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



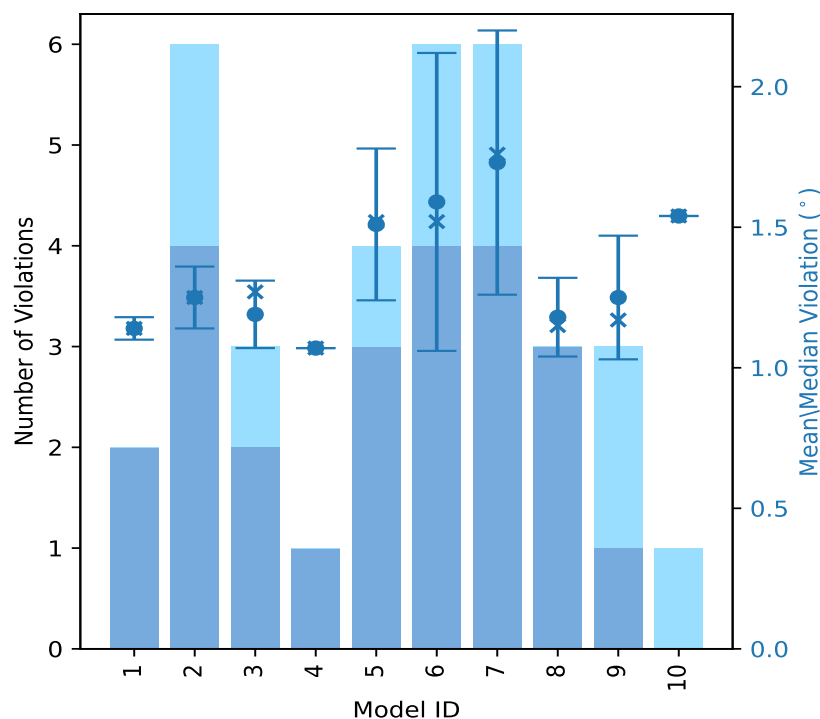
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	2	0	2	1.14	1.19	0.04	1.14
2	4	2	6	1.25	1.37	0.11	1.25
3	2	1	3	1.19	1.28	0.12	1.27
4	1	0	1	1.07	1.07	0.0	1.07
5	3	1	4	1.51	1.82	0.27	1.52
6	4	2	6	1.59	2.45	0.53	1.52
7	4	2	6	1.73	2.23	0.47	1.76
8	3	0	3	1.18	1.36	0.14	1.15
9	1	2	3	1.25	1.54	0.22	1.17
10	0	1	1	1.54	1.54	0.0	1.54

### 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

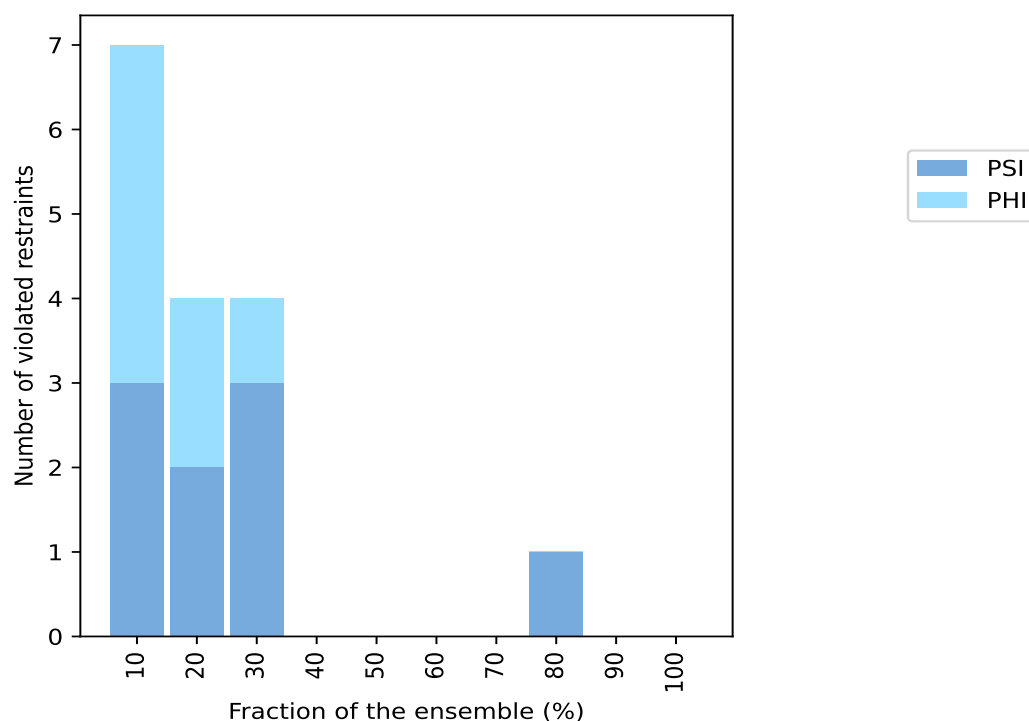
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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 <sup>1</sup>	%
3	4	7	1	10.0
2	2	4	2	20.0
3	1	4	3	30.0
0	0	0	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	7	70.0
1	0	1	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

<sup>1</sup> Number of models with violations

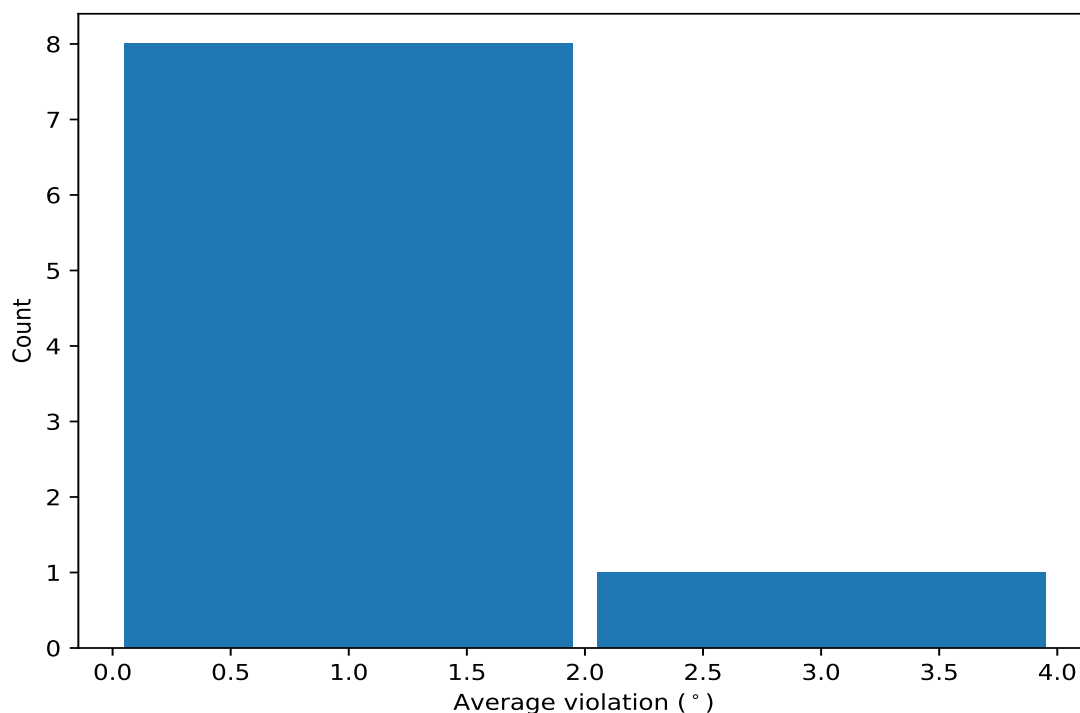
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

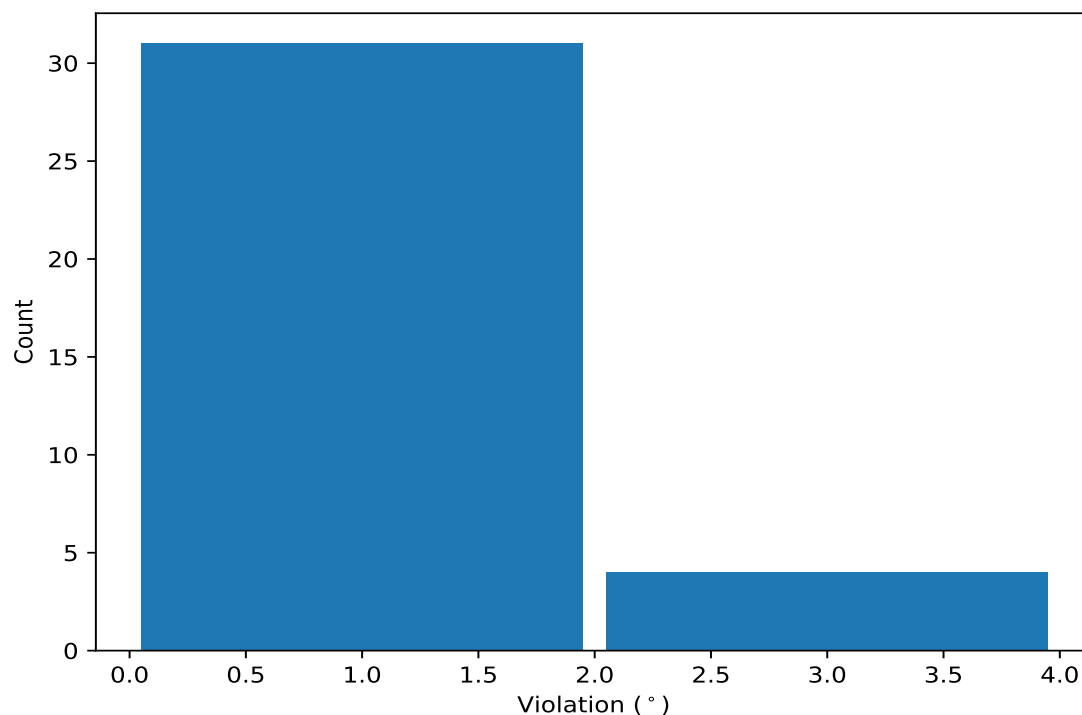
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	8	1.51	0.38	1.33
(1,24)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:GLU:N	3	2.17	0.26	2.23
(1,25)	1:33:A:ILE:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	3	1.76	0.34	1.82
(1,134)	1:123:A:PRO:N	1:123:A:PRO:CA	1:123:A:PRO:C	1:124:A:GLU:N	3	1.17	0.02	1.17
(1,62)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:TYR:N	3	1.07	0.07	1.03
(1,33)	1:41:A:LYS:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	2	1.29	0.08	1.29
(1,59)	1:67:A:GLU:C	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	2	1.2	0.17	1.2
(1,20)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:PRO:N	2	1.15	0.11	1.15
(1,32)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:THR:N	2	1.06	0.03	1.06

<sup>1</sup> Number of violated models, <sup>2</sup>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 (°)
(1,24)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:GLU:N	6	2.45
(1,24)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:GLU:N	7	2.23
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	7	2.2
(1,25)	1:33:A:ILE:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	7	2.15
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	6	1.98
(1,25)	1:33:A:ILE:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	6	1.82
(1,24)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:GLU:N	5	1.82
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	5	1.72
(1,149)	1:131:A:SER:C	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	9	1.54
(1,81)	1:82:A:ARG:C	1:83:A:MET:N	1:83:A:MET:CA	1:83:A:MET:C	10	1.54
(1,21)	1:31:A:PRO:C	1:32:A:THR:N	1:32:A:THR:CA	1:32:A:THR:C	7	1.38
(1,59)	1:67:A:GLU:C	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	2	1.37
(1,33)	1:41:A:LYS:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	2	1.37
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	8	1.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,25)	1:33:A:ILE:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	5	1.32
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	2	1.29
(1,131)	1:121:A:THR:C	1:122:A:LEU:N	1:122:A:LEU:CA	1:122:A:LEU:C	3	1.28
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	3	1.27
(1,20)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:PRO:N	7	1.26
(1,33)	1:41:A:LYS:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	6	1.21
(1,134)	1:123:A:PRO:N	1:123:A:PRO:CA	1:123:A:PRO:C	1:124:A:GLU:N	2	1.2
(1,148)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:LEU:N	1	1.19
(1,134)	1:123:A:PRO:N	1:123:A:PRO:CA	1:123:A:PRO:C	1:124:A:GLU:N	5	1.17
(1,62)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:TYR:N	2	1.17
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	9	1.17
(1,134)	1:123:A:PRO:N	1:123:A:PRO:CA	1:123:A:PRO:C	1:124:A:GLU:N	8	1.15
(1,22)	1:32:A:THR:N	1:32:A:THR:CA	1:32:A:THR:C	1:33:A:ILE:N	7	1.13
(1,26)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:GLY:N	1	1.1
(1,32)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:THR:N	2	1.08
(1,42)	1:46:A:VAL:N	1:46:A:VAL:CA	1:46:A:VAL:C	1:47:A:GLY:N	4	1.07
(1,20)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:PRO:N	6	1.04
(1,62)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:TYR:N	8	1.03
(1,59)	1:67:A:GLU:C	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	9	1.03
(1,32)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:THR:N	6	1.03
(1,62)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:TYR:N	3	1.01