Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 05:08 PM EDT

PDB ID	:	2MPH
BMRB ID	:	19551
Title	:	Solution Structure of human FK506 binding Protein 25
Authors	:	Shin, J.; Prakash, A.; Yoon, H.
Deposited on	:	2014-05-18

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

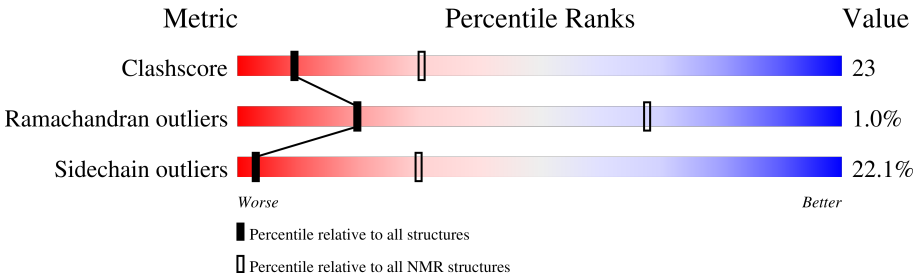
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	224	42% 33% . 22%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:5-A:73, A:110-A:149, A:159-A:224 (175)	0.50	4

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3600 atoms, of which 1825 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	224	3600	1129	1825	306	337	3	0

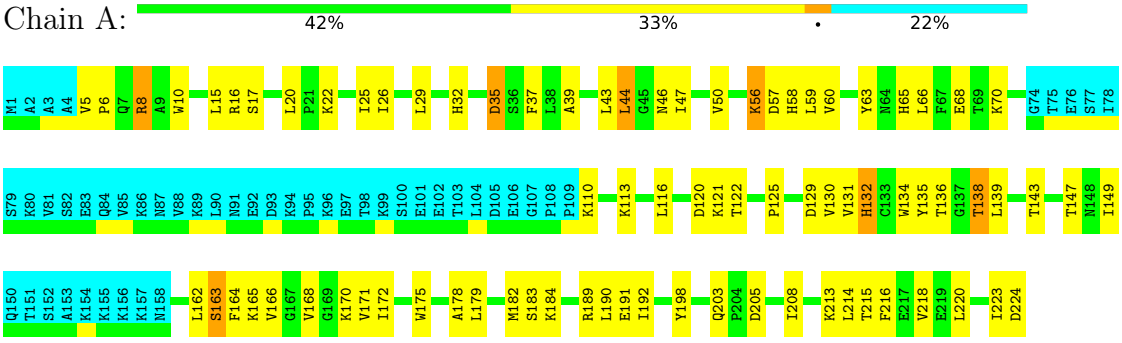
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

Chain A:



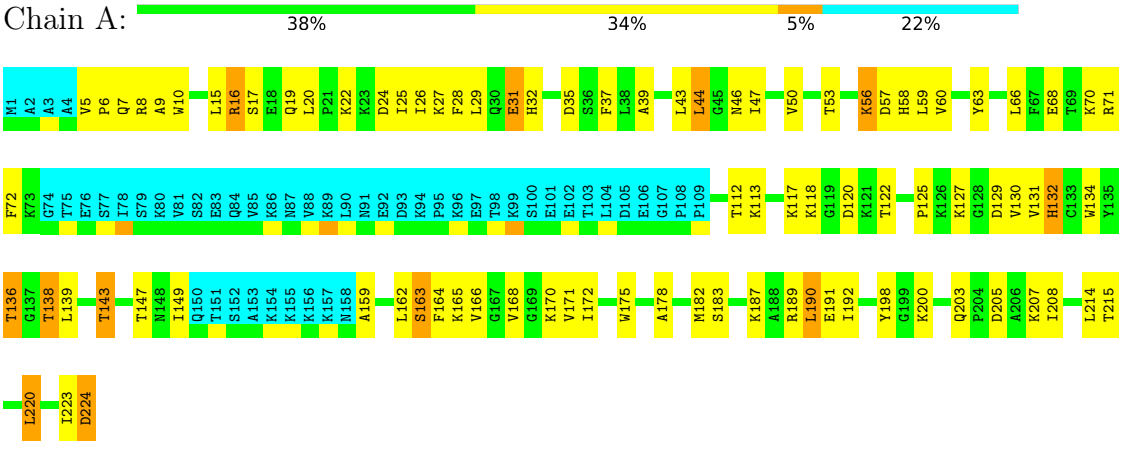
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

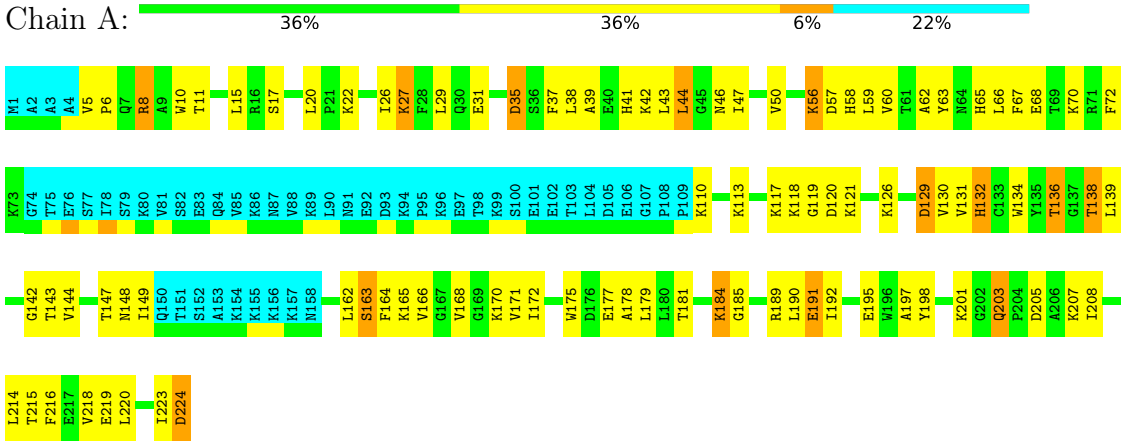
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

Chain A:



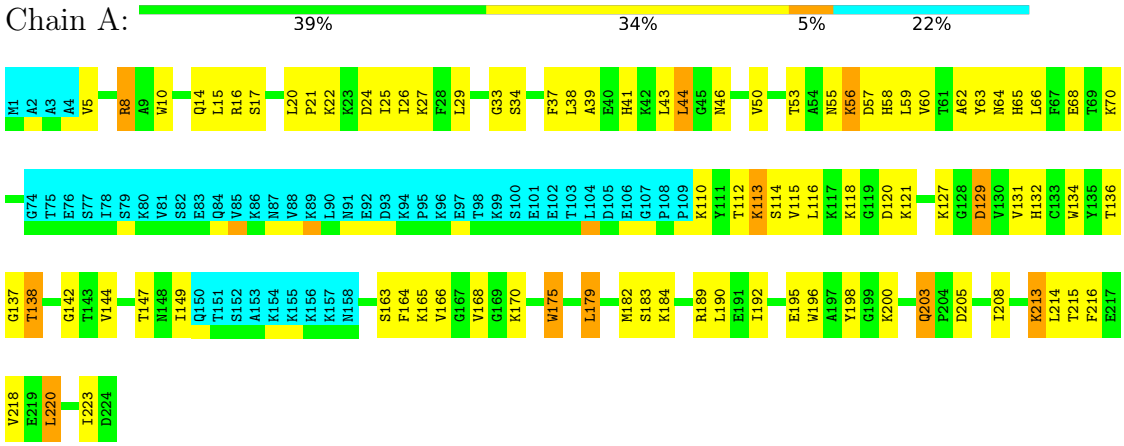
4.2.2 Score per residue for model 2

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



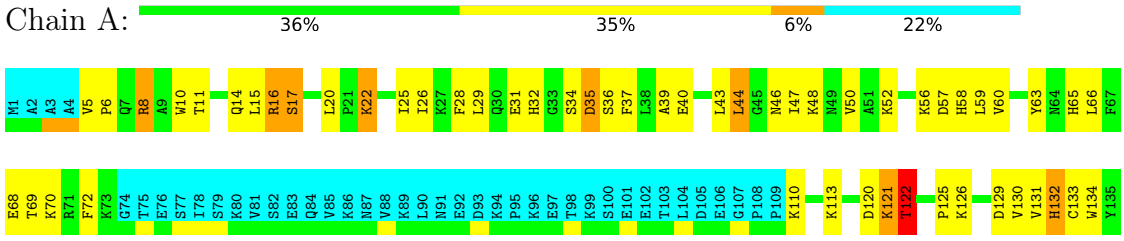
4.2.3 Score per residue for model 3

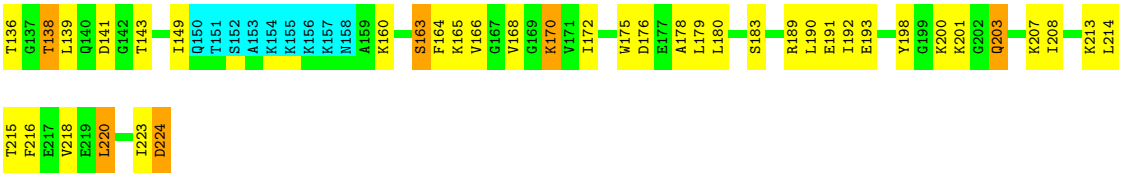
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



4.2.4 Score per residue for model 4 (medoid)

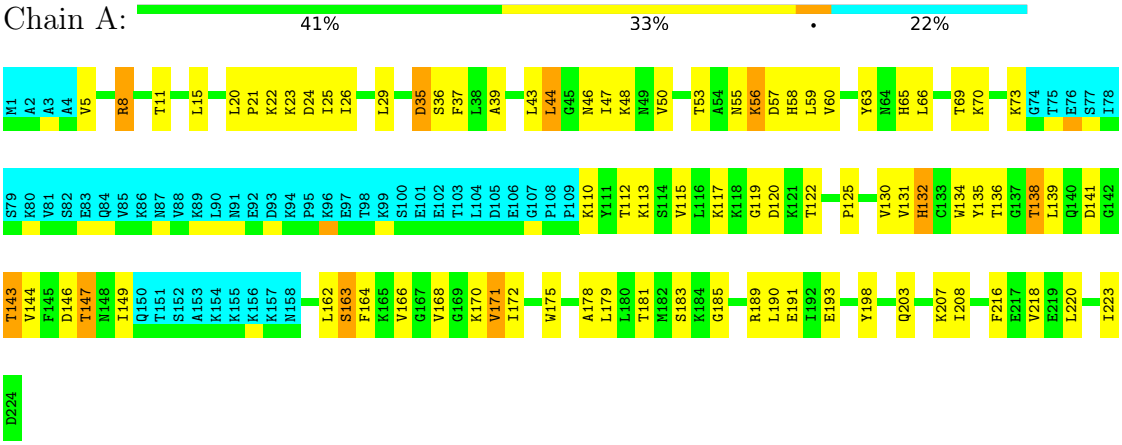
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3





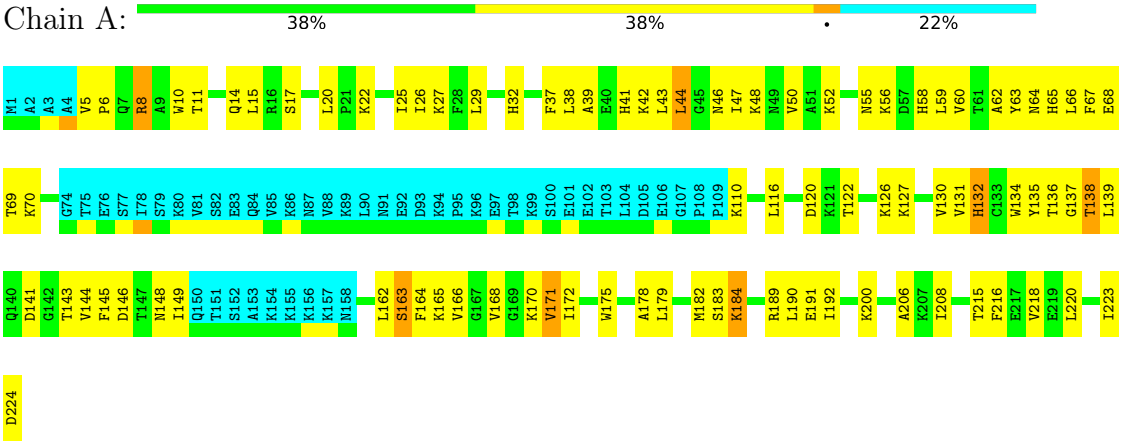
4.2.5 Score per residue for model 5

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



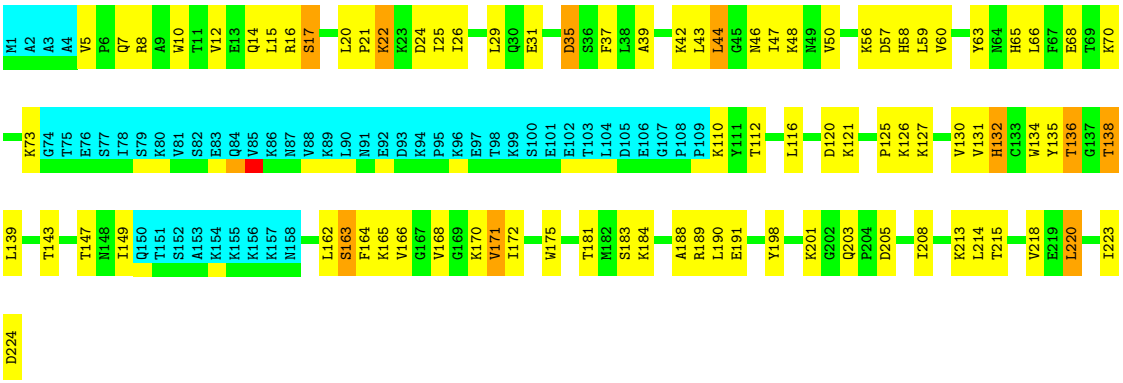
4.2.6 Score per residue for model 6

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



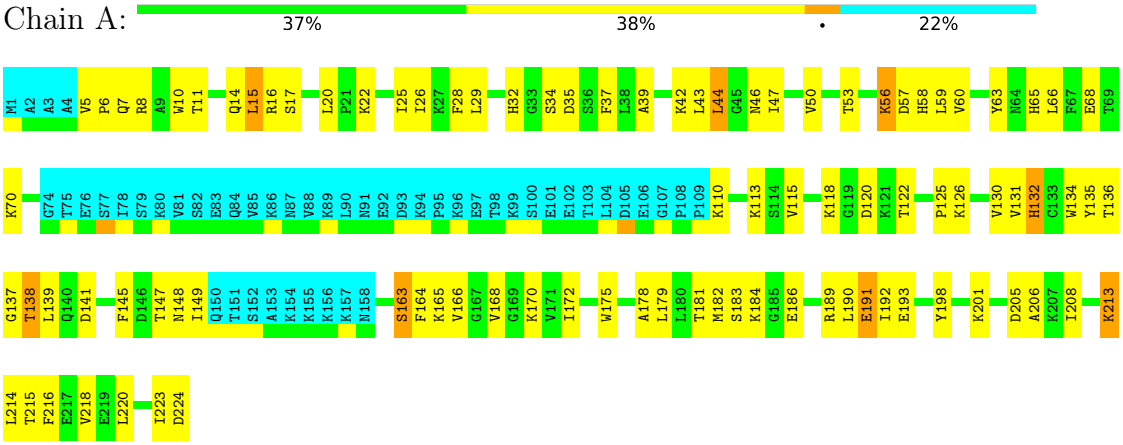
4.2.7 Score per residue for model 7

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



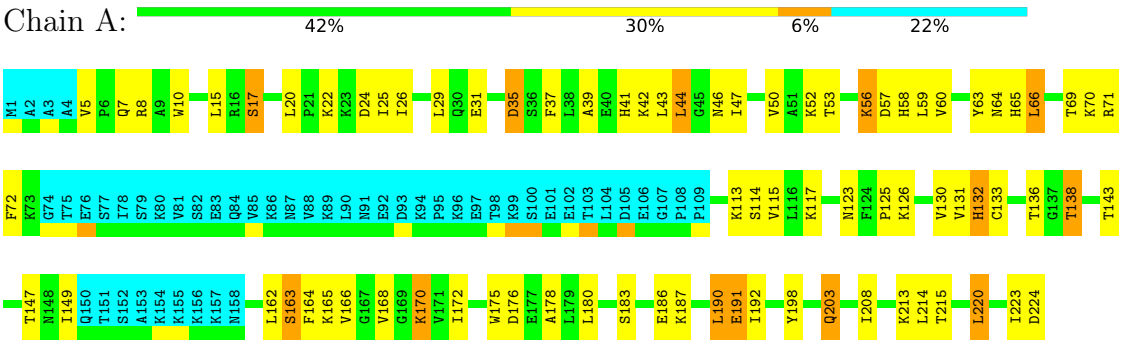
4.2.8 Score per residue for model 8

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



4.2.9 Score per residue for model 9

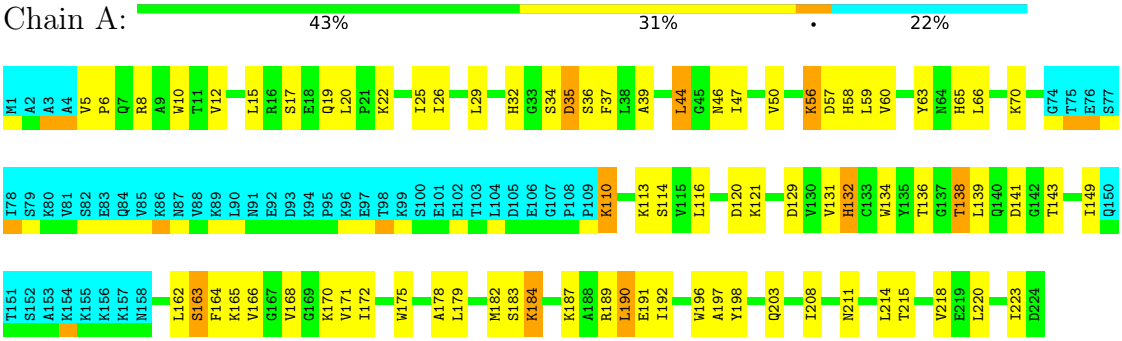
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



4.2.10 Score per residue for model 10

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

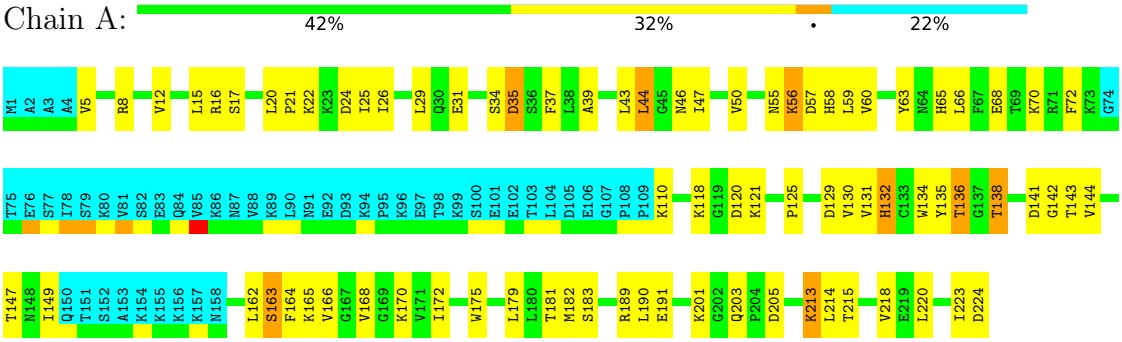
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

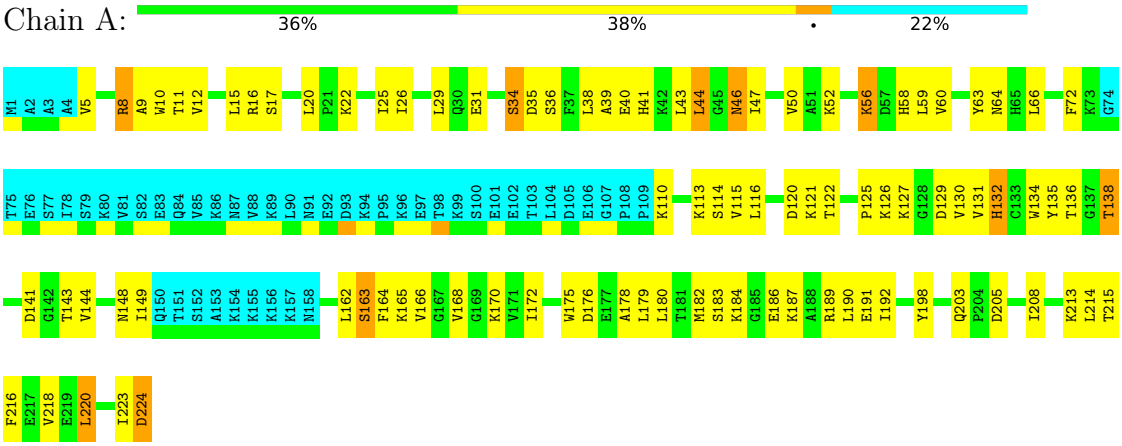
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

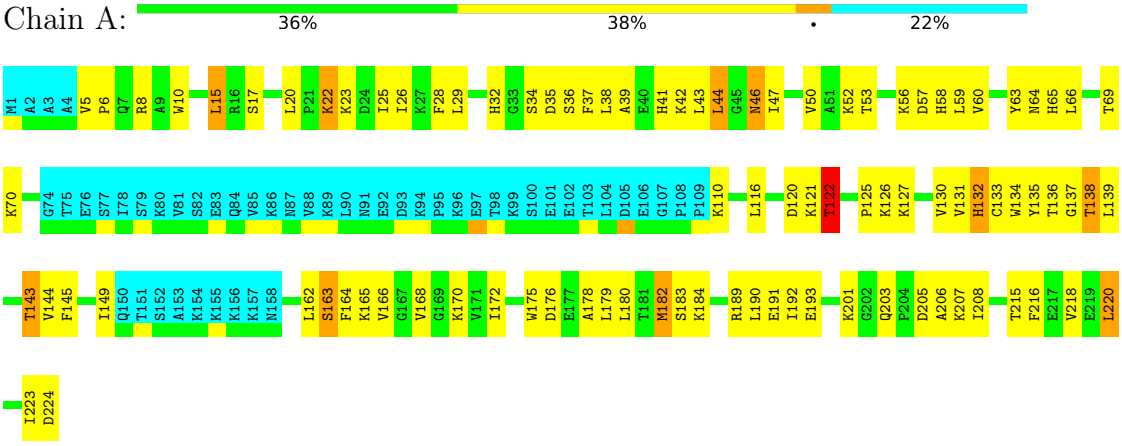
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

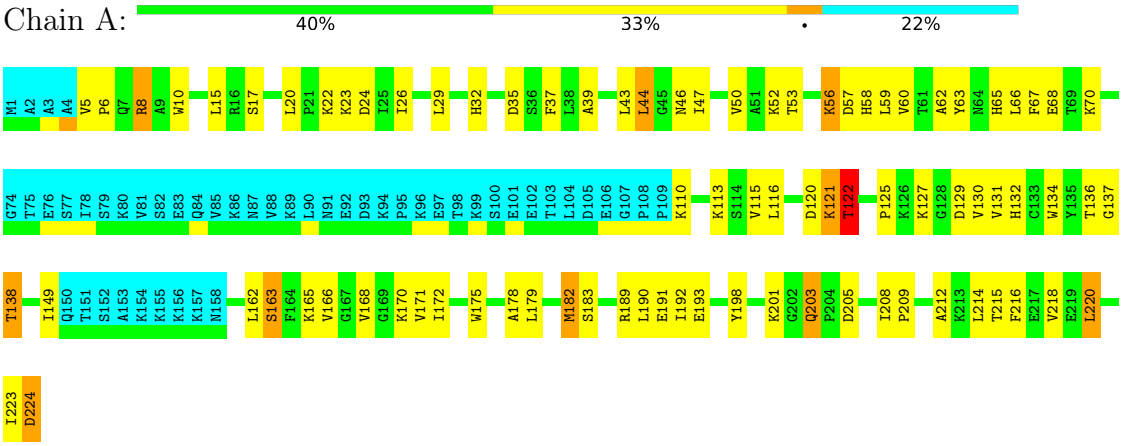
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

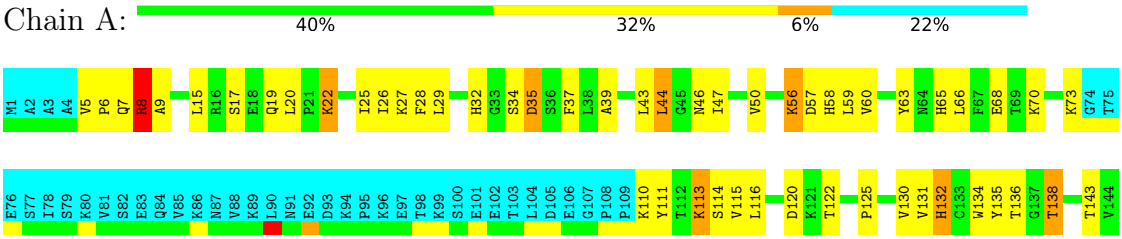
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

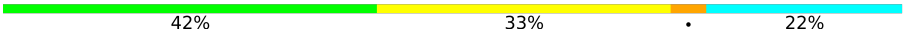
Chain A:

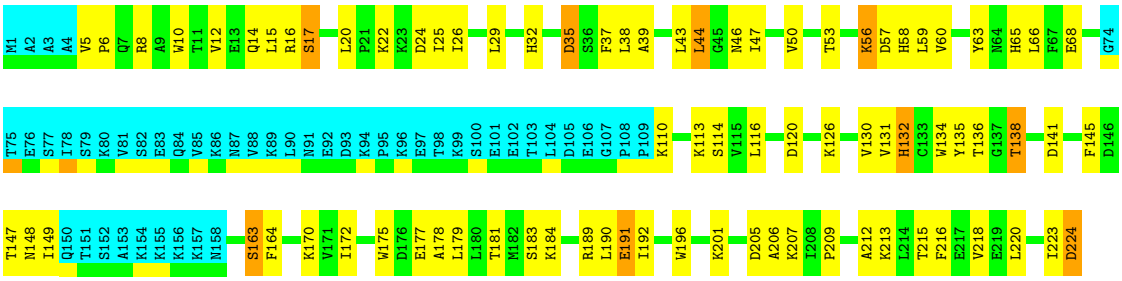


4.2.16 Score per residue for model 16

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

Chain A:

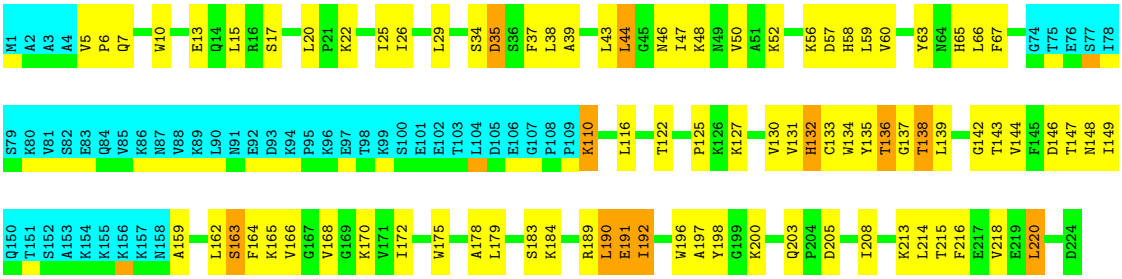




4.2.17 Score per residue for model 17

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

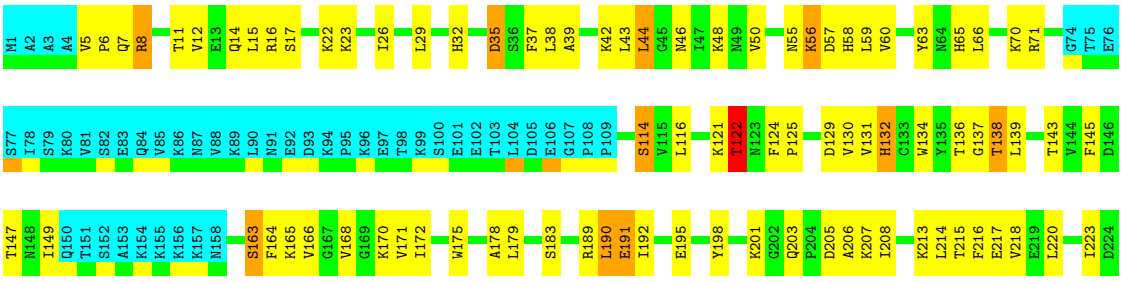
Chain A:



4.2.18 Score per residue for model 18

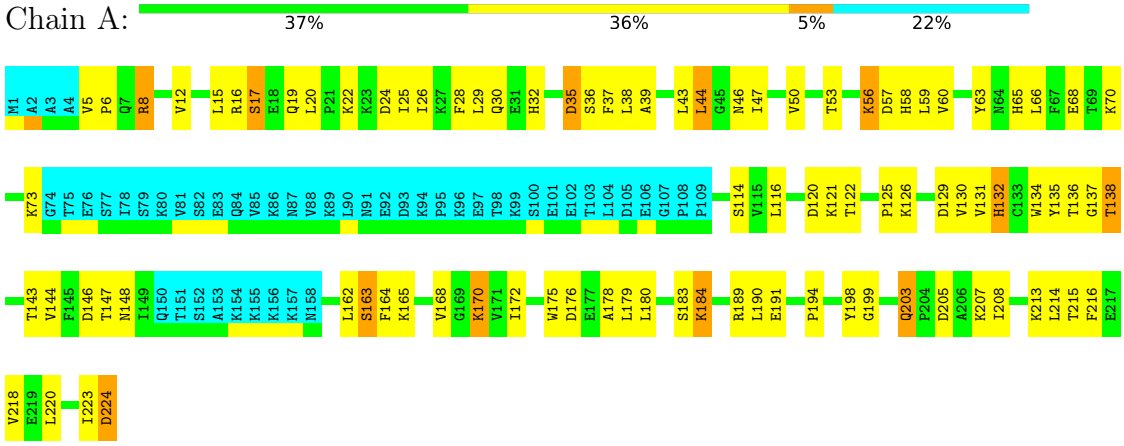
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3

Chain A:



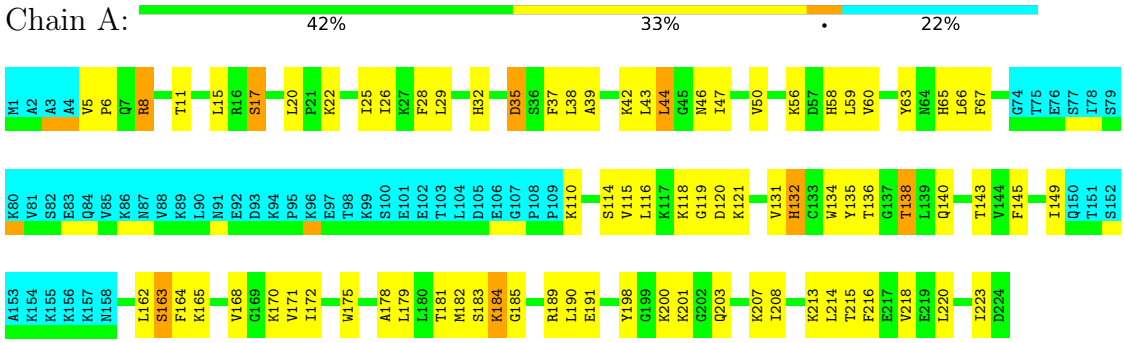
4.2.19 Score per residue for model 19

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



4.2.20 Score per residue for model 20

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP3



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, 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	2804
Number of shifts mapped to atoms	2804
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	1404	1440	1435	64±6
All	All	28080	28800	28700	1278

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:VAL:HG11	1:A:136:THR:HG21	0.97	1.34	3	19
1:A:20:LEU:HD12	1:A:25:ILE:HD11	0.94	1.39	7	4
1:A:29:LEU:HD23	1:A:66:LEU:HD12	0.82	1.50	18	13
1:A:139:LEU:HD21	1:A:208:ILE:HD12	0.82	1.49	7	5
1:A:190:LEU:HD21	1:A:216:PHE:CE2	0.81	2.10	19	1
1:A:37:PHE:CZ	1:A:66:LEU:HD12	0.80	2.10	1	3
1:A:131:VAL:HG22	1:A:164:PHE:O	0.79	1.78	13	15
1:A:198:TYR:CE2	1:A:208:ILE:HD13	0.79	2.12	19	12
1:A:46:ASN:O	1:A:50:VAL:HG23	0.78	1.78	10	20
1:A:213:LYS:O	1:A:214:LEU:HD23	0.78	1.78	19	6
1:A:5:VAL:HG23	1:A:138:THR:OG1	0.77	1.78	7	20
1:A:5:VAL:HG11	1:A:136:THR:CG2	0.77	2.09	7	18
1:A:39:ALA:HB2	1:A:44:LEU:HD11	0.76	1.56	3	5
1:A:20:LEU:HD22	1:A:25:ILE:HD11	0.75	1.56	17	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:THR:HG23	1:A:147:THR:HG23	0.74	1.56	1	6
1:A:136:THR:HG23	1:A:147:THR:OG1	0.74	1.83	17	5
1:A:190:LEU:O	1:A:215:THR:HG23	0.74	1.81	3	1
1:A:29:LEU:HD13	1:A:43:LEU:HD13	0.73	1.60	16	11
1:A:35:ASP:HA	1:A:38:LEU:HD12	0.73	1.61	2	2
1:A:131:VAL:HG12	1:A:223:ILE:HG23	0.73	1.60	16	19
1:A:198:TYR:CE2	1:A:214:LEU:HD11	0.71	2.21	10	10
1:A:16:ARG:HD2	1:A:60:VAL:HG11	0.71	1.62	4	2
1:A:176:ASP:O	1:A:180:LEU:HD13	0.71	1.86	12	6
1:A:39:ALA:HB2	1:A:44:LEU:HD21	0.70	1.62	16	15
1:A:182:MET:SD	1:A:220:LEU:HD23	0.70	2.27	13	2
1:A:134:TRP:HB3	1:A:149:ILE:HD11	0.70	1.63	16	9
1:A:220:LEU:HD13	1:A:223:ILE:HD11	0.70	1.63	12	2
1:A:203:GLN:CB	1:A:208:ILE:HD12	0.70	2.17	14	8
1:A:220:LEU:HD21	1:A:223:ILE:HG13	0.69	1.64	19	11
1:A:7:GLN:OE1	1:A:149:ILE:HD11	0.69	1.87	7	4
1:A:191:GLU:HG2	1:A:215:THR:HG23	0.68	1.65	7	4
1:A:198:TYR:CD2	1:A:208:ILE:HG21	0.67	2.24	7	1
1:A:177:GLU:O	1:A:181:THR:HG23	0.67	1.90	16	2
1:A:191:GLU:HG3	1:A:215:THR:HG23	0.66	1.68	10	6
1:A:203:GLN:HB3	1:A:208:ILE:HD12	0.66	1.65	19	6
1:A:22:LYS:HA	1:A:25:ILE:HD12	0.66	1.68	13	3
1:A:164:PHE:CZ	1:A:179:LEU:HD12	0.66	2.25	3	7
1:A:56:LYS:O	1:A:60:VAL:HG23	0.66	1.90	19	19
1:A:116:LEU:HD12	1:A:188:ALA:HA	0.66	1.67	7	1
1:A:136:THR:HG23	1:A:147:THR:HG22	0.66	1.66	5	1
1:A:7:GLN:CD	1:A:149:ILE:HD11	0.65	2.12	1	2
1:A:26:ILE:HB	1:A:47:ILE:HG23	0.65	1.68	20	15
1:A:29:LEU:HD21	1:A:63:TYR:HA	0.65	1.67	18	20
1:A:178:ALA:O	1:A:181:THR:HG22	0.65	1.92	8	1
1:A:35:ASP:O	1:A:44:LEU:HD23	0.64	1.92	9	15
1:A:220:LEU:HD11	1:A:223:ILE:HD11	0.64	1.70	6	8
1:A:15:LEU:HB3	1:A:60:VAL:HG22	0.64	1.69	5	19
1:A:190:LEU:HD12	1:A:192:ILE:HD11	0.64	1.70	15	4
1:A:149:ILE:HD12	1:A:149:ILE:N	0.64	2.07	10	6
1:A:139:LEU:HD11	1:A:208:ILE:HG12	0.64	1.69	10	2
1:A:175:TRP:NE1	1:A:179:LEU:HD21	0.63	2.08	14	6
1:A:191:GLU:HB3	1:A:215:THR:HG23	0.63	1.70	15	7
1:A:134:TRP:HB3	1:A:149:ILE:HD13	0.63	1.69	1	4
1:A:66:LEU:HD23	1:A:66:LEU:O	0.63	1.93	16	19
1:A:190:LEU:HD21	1:A:216:PHE:CE1	0.63	2.29	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:O	1:A:29:LEU:HD12	0.63	1.94	12	7
1:A:168:VAL:HG22	1:A:168:VAL:O	0.62	1.94	8	1
1:A:178:ALA:CB	1:A:190:LEU:HD13	0.62	2.24	1	17
1:A:139:LEU:HD21	1:A:208:ILE:HG23	0.62	1.71	17	2
1:A:203:GLN:HB2	1:A:208:ILE:HD12	0.62	1.72	14	2
1:A:209:PRO:HG2	1:A:212:ALA:HB2	0.62	1.72	16	1
1:A:38:LEU:HD23	1:A:43:LEU:CB	0.62	2.25	20	2
1:A:20:LEU:HD12	1:A:25:ILE:CD1	0.62	2.22	7	4
1:A:41:HIS:ND1	1:A:62:ALA:HB2	0.61	2.11	2	3
1:A:220:LEU:HD21	1:A:223:ILE:CG1	0.61	2.26	5	12
1:A:10:TRP:CD1	1:A:20:LEU:HD11	0.60	2.30	13	12
1:A:145:PHE:HB2	1:A:206:ALA:HB1	0.60	1.71	13	5
1:A:125:PRO:HB2	1:A:166:VAL:HG21	0.60	1.73	1	10
1:A:175:TRP:CD1	1:A:190:LEU:HD11	0.60	2.32	16	9
1:A:190:LEU:N	1:A:190:LEU:HD23	0.60	2.11	13	11
1:A:168:VAL:HG23	1:A:170:LYS:HG2	0.60	1.72	1	8
1:A:29:LEU:O	1:A:38:LEU:HD21	0.59	1.97	19	5
1:A:131:VAL:O	1:A:163:SER:HA	0.59	1.98	11	20
1:A:148:ASN:C	1:A:149:ILE:HD12	0.59	2.18	12	2
1:A:38:LEU:HD22	1:A:43:LEU:HB3	0.59	1.74	3	3
1:A:38:LEU:HD23	1:A:43:LEU:HB2	0.59	1.74	20	1
1:A:138:THR:HG23	1:A:144:VAL:CG1	0.59	2.27	2	5
1:A:129:ASP:O	1:A:166:VAL:HG22	0.59	1.98	10	4
1:A:130:VAL:HG12	1:A:224:ASP:O	0.58	1.97	4	4
1:A:220:LEU:CD1	1:A:223:ILE:HD11	0.58	2.28	19	9
1:A:138:THR:HG23	1:A:144:VAL:HG13	0.58	1.75	2	3
1:A:5:VAL:CG1	1:A:136:THR:HG21	0.58	2.26	9	5
1:A:139:LEU:HD21	1:A:208:ILE:CD1	0.58	2.28	18	4
1:A:66:LEU:HD21	1:A:72:PHE:CD2	0.58	2.34	1	1
1:A:192:ILE:HD12	1:A:192:ILE:N	0.57	2.14	1	2
1:A:179:LEU:HD21	1:A:218:VAL:HG21	0.57	1.76	18	1
1:A:134:TRP:O	1:A:218:VAL:HG13	0.57	1.99	19	15
1:A:26:ILE:HG12	1:A:59:LEU:HD21	0.57	1.77	8	18
1:A:168:VAL:HG23	1:A:170:LYS:HG3	0.57	1.76	17	2
1:A:135:TYR:CE1	1:A:162:LEU:HD13	0.57	2.35	17	1
1:A:175:TRP:CE2	1:A:179:LEU:HD11	0.56	2.36	14	4
1:A:26:ILE:HD12	1:A:47:ILE:HG23	0.56	1.77	17	3
1:A:165:LYS:O	1:A:168:VAL:HG22	0.55	2.00	3	10
1:A:165:LYS:O	1:A:168:VAL:HG12	0.55	2.01	8	1
1:A:175:TRP:HE1	1:A:218:VAL:HG21	0.55	1.61	19	16
1:A:125:PRO:HB3	1:A:166:VAL:HG11	0.55	1.77	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:VAL:HG23	1:A:165:LYS:HG3	0.55	1.77	17	1
1:A:139:LEU:HD11	1:A:208:ILE:HD13	0.55	1.78	8	4
1:A:198:TYR:CD2	1:A:214:LEU:HD11	0.55	2.37	7	7
1:A:115:VAL:O	1:A:115:VAL:HG13	0.54	2.03	9	6
1:A:10:TRP:NE1	1:A:20:LEU:HD11	0.54	2.16	17	8
1:A:121:LYS:O	1:A:122:THR:HG23	0.54	2.01	4	3
1:A:130:VAL:HG12	1:A:165:LYS:HG3	0.54	1.80	18	6
1:A:133:CYS:HB3	1:A:220:LEU:HD22	0.54	1.78	4	4
1:A:20:LEU:HD23	1:A:21:PRO:N	0.54	2.18	5	2
1:A:44:LEU:HD12	1:A:44:LEU:O	0.53	2.04	8	10
1:A:130:VAL:HG23	1:A:165:LYS:CG	0.53	2.33	17	1
1:A:165:LYS:CB	1:A:168:VAL:HG21	0.53	2.32	2	5
1:A:39:ALA:HB2	1:A:44:LEU:CD1	0.53	2.31	3	3
1:A:43:LEU:HD21	1:A:59:LEU:HD23	0.53	1.80	7	7
1:A:137:GLY:HA2	1:A:216:PHE:HB3	0.53	1.80	3	8
1:A:15:LEU:HD23	1:A:25:ILE:HG12	0.53	1.81	13	3
1:A:70:LYS:HD3	1:A:144:VAL:HG21	0.52	1.82	3	2
1:A:168:VAL:HG23	1:A:170:LYS:CG	0.52	2.34	12	4
1:A:184:LYS:HA	1:A:220:LEU:HD22	0.52	1.81	20	7
1:A:10:TRP:CE2	1:A:20:LEU:HD11	0.52	2.40	14	3
1:A:15:LEU:HD13	1:A:60:VAL:HG13	0.52	1.82	20	3
1:A:37:PHE:CZ	1:A:65:HIS:CE1	0.52	2.98	15	9
1:A:125:PRO:CB	1:A:166:VAL:HG11	0.52	2.35	8	3
1:A:139:LEU:HD12	1:A:143:THR:HB	0.52	1.82	1	4
1:A:114:SER:O	1:A:116:LEU:HD12	0.51	2.05	16	2
1:A:190:LEU:HD21	1:A:216:PHE:CD2	0.51	2.40	19	1
1:A:26:ILE:CB	1:A:47:ILE:HG23	0.51	2.36	11	9
1:A:27:LYS:HG3	1:A:47:ILE:HD11	0.51	1.81	2	1
1:A:190:LEU:H	1:A:190:LEU:HD23	0.51	1.65	5	3
1:A:29:LEU:HD13	1:A:43:LEU:CD1	0.51	2.35	16	5
1:A:116:LEU:N	1:A:116:LEU:HD22	0.51	2.20	3	9
1:A:37:PHE:CE1	1:A:65:HIS:CE1	0.51	2.99	5	11
1:A:175:TRP:CD1	1:A:190:LEU:CD1	0.51	2.94	3	1
1:A:66:LEU:HD22	1:A:72:PHE:CE2	0.51	2.41	11	4
1:A:113:LYS:HD2	1:A:178:ALA:HB1	0.51	1.82	4	2
1:A:220:LEU:HD12	1:A:223:ILE:HD11	0.51	1.83	13	2
1:A:60:VAL:HG12	1:A:64:ASN:ND2	0.50	2.21	12	5
1:A:164:PHE:HZ	1:A:179:LEU:HD12	0.50	1.67	20	12
1:A:171:VAL:HG11	1:A:175:TRP:CE3	0.50	2.41	7	1
1:A:28:PHE:CZ	1:A:32:HIS:CE1	0.50	3.00	4	5
1:A:131:VAL:HG23	1:A:164:PHE:CE1	0.50	2.41	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:THR:HG23	1:A:147:THR:CG2	0.50	2.37	8	1
1:A:20:LEU:CD2	1:A:25:ILE:HD11	0.50	2.33	17	1
1:A:192:ILE:HG21	1:A:196:TRP:O	0.49	2.05	16	2
1:A:132:HIS:CD2	1:A:132:HIS:N	0.49	2.80	7	10
1:A:37:PHE:CE2	1:A:65:HIS:CE1	0.49	3.00	2	3
1:A:126:LYS:O	1:A:166:VAL:HG23	0.49	2.07	6	1
1:A:213:LYS:C	1:A:214:LEU:HD23	0.49	2.27	19	1
1:A:130:VAL:HG22	1:A:131:VAL:N	0.49	2.23	7	8
1:A:191:GLU:CG	1:A:215:THR:HG23	0.49	2.37	4	2
1:A:66:LEU:C	1:A:66:LEU:HD23	0.49	2.28	1	1
1:A:20:LEU:HD22	1:A:25:ILE:CD1	0.49	2.38	3	2
1:A:172:ILE:CD1	1:A:192:ILE:HD13	0.48	2.38	8	1
1:A:130:VAL:HG22	1:A:224:ASP:O	0.48	2.08	1	4
1:A:138:THR:HG22	1:A:142:GLY:C	0.48	2.29	17	3
1:A:162:LEU:HD23	1:A:164:PHE:CD1	0.48	2.44	7	1
1:A:172:ILE:CG1	1:A:175:TRP:HB2	0.48	2.38	18	19
1:A:192:ILE:CD1	1:A:216:PHE:CZ	0.48	2.96	16	8
1:A:132:HIS:N	1:A:132:HIS:CD2	0.48	2.81	11	8
1:A:190:LEU:HD23	1:A:190:LEU:N	0.48	2.23	5	2
1:A:138:THR:HG23	1:A:144:VAL:HG12	0.48	1.86	6	1
1:A:66:LEU:HD22	1:A:72:PHE:CZ	0.48	2.44	9	1
1:A:209:PRO:O	1:A:212:ALA:HB2	0.48	2.08	14	1
1:A:12:VAL:O	1:A:16:ARG:CG	0.48	2.62	16	3
1:A:162:LEU:C	1:A:162:LEU:HD23	0.48	2.29	17	3
1:A:37:PHE:CE2	1:A:66:LEU:HD12	0.48	2.44	4	3
1:A:7:GLN:NE2	1:A:149:ILE:HD11	0.48	2.23	9	2
1:A:165:LYS:HB3	1:A:168:VAL:HG21	0.48	1.85	2	5
1:A:70:LYS:HE2	1:A:136:THR:HG21	0.48	1.86	4	1
1:A:130:VAL:HG12	1:A:224:ASP:C	0.48	2.29	7	6
1:A:116:LEU:HD12	1:A:188:ALA:CA	0.48	2.39	7	1
1:A:162:LEU:O	1:A:162:LEU:HD23	0.48	2.09	12	1
1:A:15:LEU:HD23	1:A:25:ILE:CD1	0.48	2.38	1	1
1:A:149:ILE:N	1:A:149:ILE:CD1	0.48	2.77	10	6
1:A:125:PRO:HA	1:A:223:ILE:HG21	0.48	1.86	19	3
1:A:162:LEU:HD23	1:A:162:LEU:C	0.47	2.30	12	1
1:A:192:ILE:HD11	1:A:216:PHE:CZ	0.47	2.44	2	4
1:A:26:ILE:CG2	1:A:47:ILE:HG23	0.47	2.39	11	4
1:A:37:PHE:CE1	1:A:43:LEU:HD12	0.47	2.44	20	1
1:A:66:LEU:HD22	1:A:72:PHE:CE1	0.47	2.45	2	1
1:A:16:ARG:CG	1:A:60:VAL:HG21	0.47	2.40	8	1
1:A:110:LYS:CG	1:A:196:TRP:CD1	0.47	2.97	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TRP:CD1	1:A:20:LEU:CD1	0.47	2.97	17	11
1:A:165:LYS:NZ	1:A:168:VAL:HG11	0.47	2.25	10	1
1:A:37:PHE:CD1	1:A:71:ARG:HB2	0.47	2.44	18	1
1:A:135:TYR:H	1:A:149:ILE:HD11	0.47	1.69	12	2
1:A:172:ILE:HD11	1:A:192:ILE:HD13	0.47	1.86	8	1
1:A:26:ILE:CD1	1:A:47:ILE:HG23	0.46	2.40	2	2
1:A:175:TRP:HE1	1:A:179:LEU:HD21	0.46	1.71	13	2
1:A:198:TYR:HD2	1:A:208:ILE:HG21	0.46	1.66	7	1
1:A:20:LEU:C	1:A:20:LEU:HD23	0.46	2.30	2	4
1:A:130:VAL:HG22	1:A:224:ASP:C	0.46	2.30	11	2
1:A:135:TYR:CE1	1:A:148:ASN:CB	0.46	2.99	6	2
1:A:192:ILE:HD13	1:A:192:ILE:N	0.46	2.26	17	1
1:A:20:LEU:HD22	1:A:21:PRO:HD2	0.46	1.88	11	2
1:A:198:TYR:CE2	1:A:214:LEU:CD1	0.46	2.99	3	12
1:A:28:PHE:CZ	1:A:32:HIS:ND1	0.46	2.84	4	4
1:A:37:PHE:CD1	1:A:71:ARG:CB	0.46	2.98	9	2
1:A:6:PRO:CB	1:A:32:HIS:CE1	0.45	3.00	4	11
1:A:28:PHE:CE1	1:A:32:HIS:ND1	0.45	2.84	1	4
1:A:8:ARG:NE	1:A:149:ILE:HD13	0.45	2.26	3	1
1:A:162:LEU:CD2	1:A:164:PHE:CD1	0.45	2.99	7	2
1:A:29:LEU:HD21	1:A:63:TYR:CA	0.45	2.41	3	7
1:A:114:SER:O	1:A:116:LEU:HD22	0.45	2.11	18	1
1:A:29:LEU:HD22	1:A:37:PHE:HZ	0.45	1.71	20	1
1:A:66:LEU:CD2	1:A:72:PHE:CD2	0.45	2.99	4	2
1:A:50:VAL:HA	1:A:53:THR:HG22	0.45	1.88	5	2
1:A:182:MET:HE1	1:A:218:VAL:O	0.45	2.11	15	1
1:A:9:ALA:HB2	1:A:187:LYS:NZ	0.45	2.26	12	2
1:A:139:LEU:HD12	1:A:143:THR:CB	0.45	2.42	5	2
1:A:192:ILE:CD1	1:A:216:PHE:CE2	0.45	3.00	2	5
1:A:135:TYR:CE2	1:A:148:ASN:ND2	0.45	2.85	16	1
1:A:43:LEU:HD11	1:A:62:ALA:HB1	0.45	1.89	2	1
1:A:66:LEU:HD23	1:A:66:LEU:C	0.45	2.32	20	9
1:A:12:VAL:O	1:A:16:ARG:HG2	0.45	2.12	16	3
1:A:12:VAL:HG22	1:A:64:ASN:OD1	0.45	2.12	12	1
1:A:37:PHE:CE1	1:A:66:LEU:HD12	0.45	2.46	1	1
1:A:41:HIS:O	1:A:42:LYS:CG	0.45	2.65	9	1
1:A:65:HIS:O	1:A:69:THR:N	0.44	2.50	5	2
1:A:39:ALA:HB2	1:A:44:LEU:CD2	0.44	2.38	16	2
1:A:29:LEU:HD22	1:A:37:PHE:CZ	0.44	2.47	20	1
1:A:131:VAL:CG2	1:A:164:PHE:CE1	0.44	3.00	9	4
1:A:115:VAL:HG13	1:A:186:GLU:CD	0.44	2.33	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ASP:O	1:A:44:LEU:HD21	0.44	2.12	17	1
1:A:125:PRO:CB	1:A:166:VAL:HG21	0.44	2.42	18	1
1:A:198:TYR:CE2	1:A:208:ILE:CD1	0.44	3.00	14	6
1:A:190:LEU:CD2	1:A:216:PHE:CE1	0.44	2.99	4	5
1:A:184:LYS:HA	1:A:223:ILE:HD11	0.44	1.88	3	1
1:A:137:GLY:O	1:A:144:VAL:HG23	0.44	2.13	19	1
1:A:110:LYS:CB	1:A:196:TRP:CD2	0.44	3.00	10	2
1:A:113:LYS:CE	1:A:115:VAL:HG22	0.44	2.43	15	1
1:A:66:LEU:CD2	1:A:72:PHE:CE2	0.44	3.00	1	1
1:A:20:LEU:HD23	1:A:20:LEU:C	0.44	2.32	5	2
1:A:130:VAL:HG13	1:A:131:VAL:N	0.44	2.27	17	1
1:A:145:PHE:CD1	1:A:146:ASP:N	0.44	2.85	15	1
1:A:113:LYS:CG	1:A:190:LEU:HD22	0.43	2.43	3	1
1:A:135:TYR:CD1	1:A:135:TYR:N	0.43	2.86	13	2
1:A:175:TRP:HD1	1:A:190:LEU:HD23	0.43	1.73	7	1
1:A:115:VAL:HG23	1:A:186:GLU:CD	0.43	2.33	8	1
1:A:192:ILE:HD12	1:A:216:PHE:CE2	0.43	2.48	14	2
1:A:26:ILE:HG12	1:A:59:LEU:HD22	0.43	1.88	18	1
1:A:164:PHE:CE1	1:A:179:LEU:HD12	0.43	2.48	3	1
1:A:26:ILE:CG1	1:A:59:LEU:HD22	0.43	2.43	18	1
1:A:41:HIS:NE2	1:A:65:HIS:CE1	0.43	2.86	2	2
1:A:162:LEU:HD23	1:A:162:LEU:O	0.43	2.14	13	3
1:A:138:THR:N	1:A:145:PHE:CE2	0.43	2.86	20	1
1:A:116:LEU:HD12	1:A:116:LEU:H	0.43	1.74	7	1
1:A:16:ARG:HG3	1:A:60:VAL:HG11	0.43	1.91	3	1
1:A:220:LEU:HD11	1:A:223:ILE:CD1	0.43	2.43	19	2
1:A:135:TYR:OH	1:A:162:LEU:HD13	0.43	2.13	11	2
1:A:14:GLN:OE1	1:A:20:LEU:HD23	0.43	2.14	7	1
1:A:29:LEU:CD2	1:A:66:LEU:HD12	0.43	2.43	9	1
1:A:12:VAL:HG12	1:A:16:ARG:HD2	0.43	1.91	11	3
1:A:135:TYR:N	1:A:149:ILE:HD11	0.43	2.29	20	1
1:A:175:TRP:CD1	1:A:179:LEU:HG	0.43	2.49	12	5
1:A:111:TYR:CE2	1:A:178:ALA:HB2	0.43	2.49	15	1
1:A:110:LYS:HG3	1:A:196:TRP:CD1	0.42	2.49	16	1
1:A:168:VAL:O	1:A:168:VAL:CG2	0.42	2.65	8	1
1:A:20:LEU:HD22	1:A:25:ILE:CG1	0.42	2.45	10	2
1:A:182:MET:O	1:A:220:LEU:HD13	0.42	2.15	6	1
1:A:12:VAL:HA	1:A:15:LEU:HD12	0.42	1.90	7	1
1:A:139:LEU:CD2	1:A:208:ILE:HG23	0.42	2.43	17	1
1:A:190:LEU:HD23	1:A:190:LEU:H	0.42	1.75	17	1
1:A:6:PRO:O	1:A:67:PHE:CE2	0.42	2.73	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:HIS:CD2	1:A:41:HIS:N	0.42	2.87	12	1
1:A:190:LEU:CG	1:A:216:PHE:CE1	0.42	3.02	13	1
1:A:6:PRO:HB3	1:A:32:HIS:CE1	0.42	2.50	20	1
1:A:135:TYR:CE1	1:A:148:ASN:HB2	0.42	2.50	6	1
1:A:190:LEU:N	1:A:190:LEU:CD2	0.42	2.82	13	1
1:A:6:PRO:HB2	1:A:32:HIS:CE1	0.42	2.50	1	1
1:A:15:LEU:CB	1:A:60:VAL:HG22	0.42	2.45	10	4
1:A:38:LEU:CD2	1:A:43:LEU:CB	0.41	2.98	2	1
1:A:175:TRP:CD1	1:A:190:LEU:HD23	0.41	2.50	7	1
1:A:8:ARG:NH1	1:A:149:ILE:HD12	0.41	2.29	15	1
1:A:194:PRO:O	1:A:199:GLY:N	0.41	2.53	19	1
1:A:63:TYR:CD1	1:A:63:TYR:O	0.41	2.74	6	3
1:A:184:LYS:HB2	1:A:223:ILE:HD13	0.41	1.92	3	1
1:A:130:VAL:CG2	1:A:131:VAL:N	0.41	2.82	5	5
1:A:165:LYS:HB3	1:A:168:VAL:HG11	0.41	1.93	3	1
1:A:113:LYS:CG	1:A:190:LEU:CD2	0.41	2.99	3	1
1:A:164:PHE:CE2	1:A:171:VAL:HG22	0.41	2.50	5	2
1:A:22:LYS:O	1:A:26:ILE:HD12	0.41	2.16	15	1
1:A:30:GLN:HA	1:A:38:LEU:HD11	0.41	1.92	19	1
1:A:216:PHE:O	1:A:216:PHE:CD1	0.41	2.73	3	1
1:A:190:LEU:HD21	1:A:216:PHE:HE1	0.41	1.74	14	1
1:A:134:TRP:CB	1:A:149:ILE:HD11	0.41	2.45	13	1
1:A:20:LEU:CD2	1:A:25:ILE:CG1	0.41	2.99	6	1
1:A:135:TYR:CD1	1:A:148:ASN:OD1	0.41	2.74	12	2
1:A:38:LEU:O	1:A:42:LYS:N	0.41	2.54	20	2
1:A:119:GLY:CA	1:A:185:GLY:O	0.41	2.69	2	3
1:A:37:PHE:CZ	1:A:66:LEU:HG	0.41	2.51	13	4
1:A:110:LYS:HB3	1:A:196:TRP:CD2	0.41	2.51	10	1
1:A:135:TYR:CZ	1:A:148:ASN:HB2	0.41	2.51	15	2
1:A:178:ALA:HB1	1:A:190:LEU:HD13	0.41	1.93	15	1
1:A:192:ILE:N	1:A:192:ILE:CD1	0.41	2.84	1	1
1:A:29:LEU:HD13	1:A:43:LEU:CD2	0.40	2.45	2	1
1:A:130:VAL:HG23	1:A:224:ASP:HB2	0.40	1.93	2	1
1:A:41:HIS:CD2	1:A:65:HIS:CE1	0.40	3.09	6	1
1:A:172:ILE:HG13	1:A:175:TRP:HB2	0.40	1.93	9	2
1:A:192:ILE:N	1:A:192:ILE:HD13	0.40	2.31	4	1
1:A:46:ASN:C	1:A:50:VAL:HG23	0.40	2.36	6	1
1:A:10:TRP:NE1	1:A:20:LEU:HD21	0.40	2.31	7	1
1:A:136:THR:O	1:A:216:PHE:CB	0.40	2.69	8	2
1:A:110:LYS:HB2	1:A:196:TRP:CD2	0.40	2.52	17	1
1:A:114:SER:O	1:A:116:LEU:CD2	0.40	2.69	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:VAL:O	1:A:144:VAL:HG13	0.40	2.16	5	1
1:A:116:LEU:N	1:A:116:LEU:CD2	0.40	2.85	6	1
1:A:148:ASN:O	1:A:149:ILE:HD13	0.40	2.17	6	1
1:A:7:GLN:NE2	1:A:149:ILE:CD1	0.40	2.84	9	1
1:A:43:LEU:HD11	1:A:62:ALA:CB	0.40	2.47	14	1
1:A:7:GLN:O	1:A:9:ALA:N	0.40	2.55	15	1
1:A:31:GLU:OE2	1:A:32:HIS:CD2	0.40	2.75	1	1
1:A:29:LEU:O	1:A:33:GLY:N	0.40	2.54	3	1
1:A:6:PRO:CB	1:A:32:HIS:ND1	0.40	2.84	4	2
1:A:43:LEU:HD21	1:A:59:LEU:CD2	0.40	2.46	15	1
1:A:35:ASP:CA	1:A:44:LEU:HD21	0.40	2.45	17	1
1:A:63:TYR:O	1:A:63:TYR:CD1	0.40	2.75	17	1
1:A:122:THR:O	1:A:124:PHE:CD1	0.40	2.75	18	1
1:A:165:LYS:HB2	1:A:168:VAL:HG21	0.40	1.94	18	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	174/224 (78%)	157±2 (90±1%)	15±2 (9±1%)	2±1 (1±1%)	20	68
All	All	3480/4480 (78%)	3144 (90%)	300 (9%)	36 (1%)	20	68

All 7 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	8	ARG	10
1	A	122	THR	8
1	A	17	SER	7
1	A	44	LEU	5
1	A	197	ALA	3
1	A	34	SER	2
1	A	211	ASN	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	152/195 (78%)	118±4 (78±2%)	34±4 (22±2%)	3 30
All	All	3040/3900 (78%)	2367 (78%)	673 (22%)	3 30

All 87 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	22	LYS	20
1	A	58	HIS	20
1	A	132	HIS	20
1	A	138	THR	20
1	A	8	ARG	19
1	A	163	SER	19
1	A	189	ARG	19
1	A	17	SER	18
1	A	183	SER	18
1	A	57	ASP	17
1	A	120	ASP	17
1	A	44	LEU	15
1	A	56	LYS	15
1	A	143	THR	15
1	A	110	LYS	15
1	A	203	GLN	15
1	A	70	LYS	13
1	A	205	ASP	13
1	A	35	ASP	13
1	A	170	LYS	13
1	A	68	GLU	12
1	A	121	LYS	11
1	A	113	LYS	10
1	A	182	MET	10
1	A	184	LYS	10
1	A	201	LYS	10
1	A	24	ASP	9
1	A	171	VAL	9
1	A	207	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	220	LEU	9
1	A	224	ASP	9
1	A	126	LYS	9
1	A	213	LYS	9
1	A	122	THR	8
1	A	127	LYS	8
1	A	129	ASP	8
1	A	11	THR	8
1	A	191	GLU	8
1	A	34	SER	8
1	A	141	ASP	8
1	A	31	GLU	7
1	A	53	THR	7
1	A	200	LYS	7
1	A	162	LEU	7
1	A	52	LYS	7
1	A	118	LYS	6
1	A	190	LEU	6
1	A	14	GLN	6
1	A	114	SER	6
1	A	36	SER	6
1	A	48	LYS	6
1	A	193	GLU	6
1	A	27	LYS	5
1	A	136	THR	5
1	A	55	ASN	5
1	A	42	LYS	5
1	A	19	GLN	4
1	A	112	THR	4
1	A	117	LYS	4
1	A	23	LYS	4
1	A	146	ASP	4
1	A	181	THR	4
1	A	195	GLU	3
1	A	69	THR	3
1	A	73	LYS	3
1	A	16	ARG	2
1	A	40	GLU	2
1	A	15	LEU	2
1	A	187	LYS	2
1	A	46	ASN	2
1	A	71	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	219	GLU	1
1	A	175	TRP	1
1	A	179	LEU	1
1	A	160	LYS	1
1	A	147	THR	1
1	A	168	VAL	1
1	A	66	LEU	1
1	A	123	ASN	1
1	A	186	GLU	1
1	A	180	LEU	1
1	A	215	THR	1
1	A	13	GLU	1
1	A	192	ILE	1
1	A	7	GLN	1
1	A	217	GLU	1
1	A	65	HIS	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 monosaccharides 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 (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% 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

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	2804
Number of shifts mapped to atoms	2804
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	223	0.02 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	209	0.09 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	213	0.20 ± 0.10	None needed (< 0.5 ppm)
^{15}N	206	-0.22 ± 0.22	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 91%, i.e. 2234 atoms were assigned a chemical shift out of a possible 2451. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	863/871 (99%)	352/354 (99%)	347/350 (99%)	164/167 (98%)
Sidechain	1245/1376 (90%)	861/888 (97%)	369/435 (85%)	15/53 (28%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	126/204 (62%)	89/100 (89%)	33/90 (37%)	4/14 (29%)
Overall	2234/2451 (91%)	1302/1342 (97%)	749/875 (86%)	183/234 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 2802 atoms were assigned a chemical shift out of a possible 3081. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1086/1112 (98%)	444/451 (98%)	436/448 (97%)	206/213 (97%)
Sidechain	1590/1765 (90%)	1095/1135 (96%)	476/562 (85%)	19/68 (28%)
Aromatic	126/204 (62%)	89/100 (89%)	33/90 (37%)	4/14 (29%)
Overall	2802/3081 (91%)	1628/1686 (97%)	945/1100 (86%)	229/295 (78%)

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.

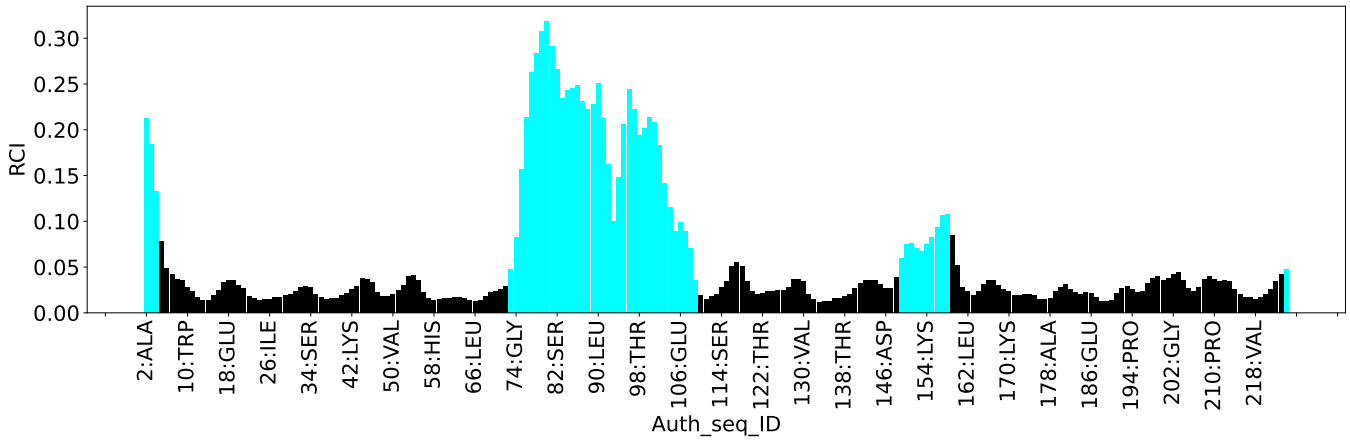
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	147	THR	HG1	5.37	0.08 – 2.19	20.1
1	A	110	LYS	HB3	-0.20	0.46 – 3.04	-7.6
1	A	171	VAL	HG11	-1.09	-0.48 – 2.12	-7.4
1	A	171	VAL	HG12	-1.09	-0.48 – 2.12	-7.4
1	A	171	VAL	HG13	-1.09	-0.48 – 2.12	-7.4
1	A	173	ARG	HD3	1.66	1.81 – 4.39	-5.6
1	A	183	SER	HB3	2.40	2.49 – 5.20	-5.3
1	A	8	ARG	HB3	0.35	0.43 – 3.11	-5.3
1	A	137	GLY	HA3	2.03	2.08 – 5.71	-5.1
1	A	175	TRP	HE1	6.82	6.88 – 13.28	-5.1
1	A	66	LEU	HD21	-0.66	-0.65 – 2.13	-5.0
1	A	66	LEU	HD22	-0.66	-0.65 – 2.13	-5.0
1	A	66	LEU	HD23	-0.66	-0.65 – 2.13	-5.0
1	A	175	TRP	NE1	118.50	118.53 – 139.98	-5.0

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

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	5972
Intra-residue (|i-j|=0)	1008
Sequential (|i-j|=1)	1568
Medium range (|i-j|>1 and |i-j|<5)	1011
Long range (|i-j|≥5)	2249
Inter-chain	0
Hydrogen bond restraints	136
Disulfide bond restraints	0
Total dihedral-angle restraints	281
Number of unmapped restraints	0
Number of restraints per residue	27.9
Number of long range restraints per residue[1]	10.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.6	0.12
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.5	1.4
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

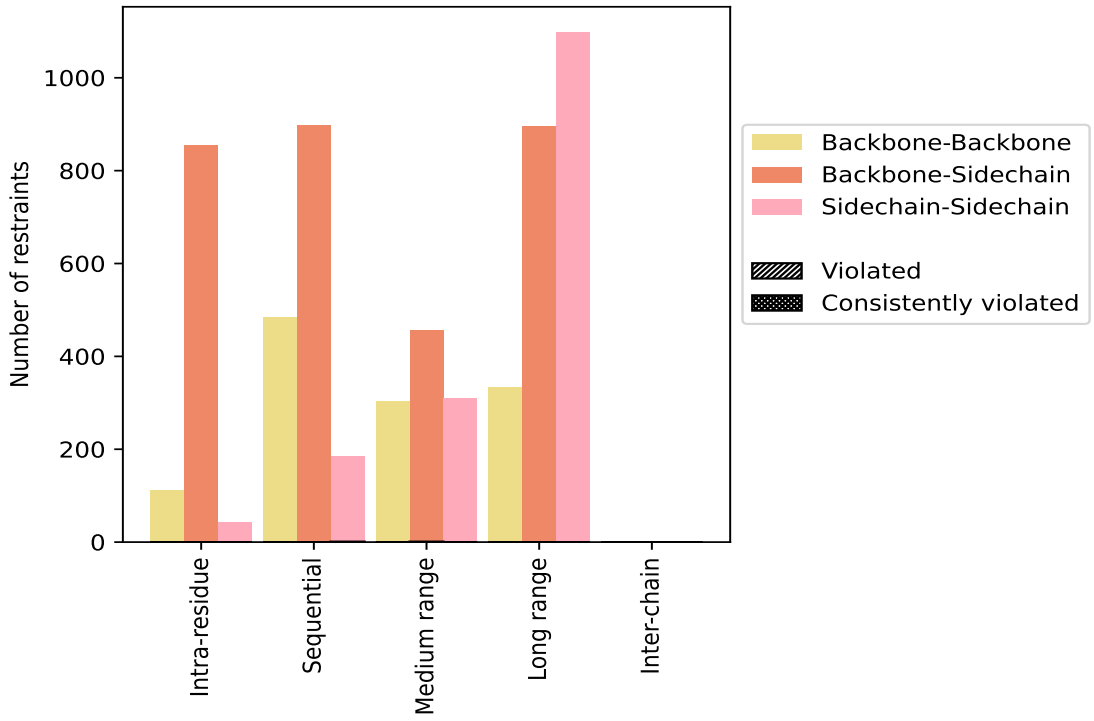
9.1 Summary of distance violations (i)

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)	1008	16.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	112	1.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	854	14.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	42	0.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1568	26.3	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	485	8.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	898	15.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	185	3.1	1	0.5	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1011	16.9	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	244	4.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	457	7.7	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	310	5.2	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	2249	37.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	255	4.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	896	15.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1098	18.4	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	136	2.3	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	5972	100.0	2	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1232	20.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3105	52.0	1	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1635	27.4	1	0.1	0.0	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	1	0	0	1	0.11	0.11	0.0	0.11
4	0	0	1	0	0	1	0.11	0.11	0.0	0.11
5	0	0	1	0	0	1	0.11	0.11	0.0	0.11
6	0	0	1	0	0	1	0.11	0.11	0.0	0.11
7	0	0	1	0	0	1	0.11	0.11	0.0	0.11
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	1	0	0	1	0.11	0.11	0.0	0.11
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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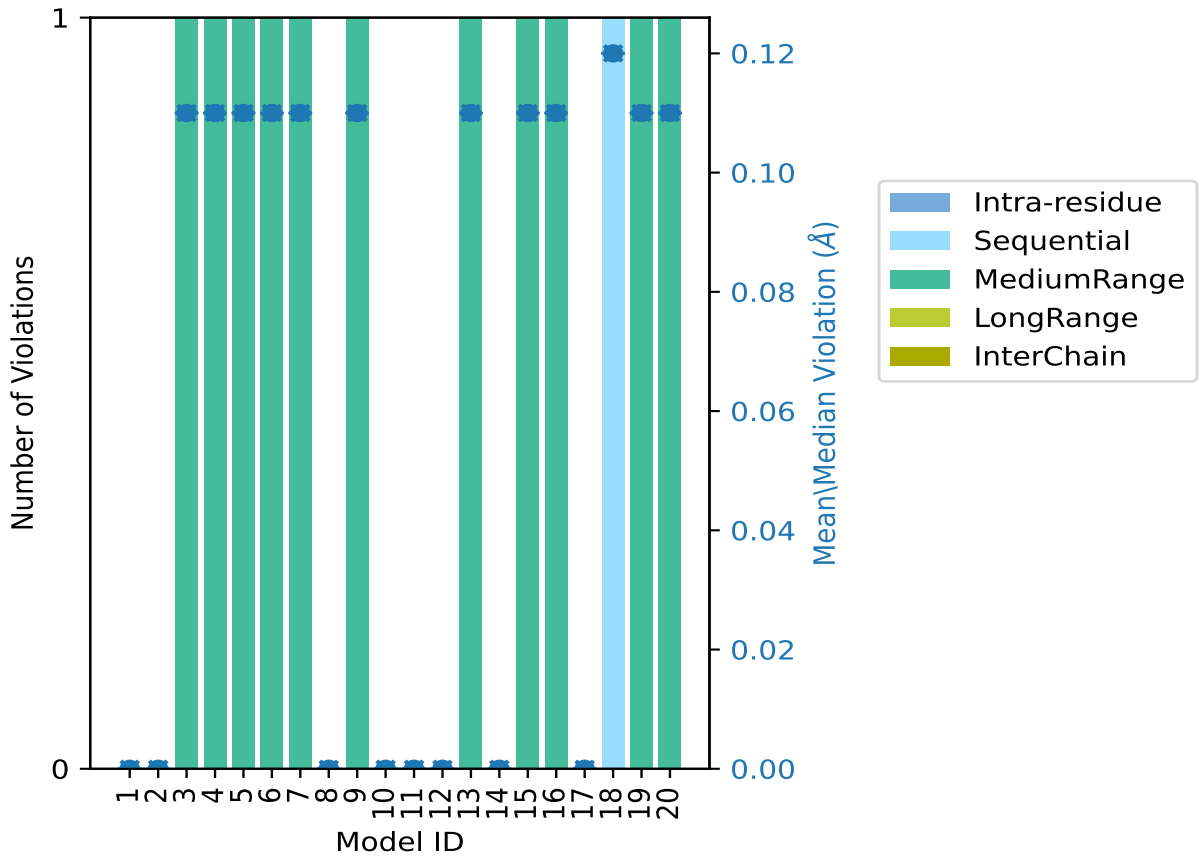
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	1	0	0	1	0.11	0.11	0.0	0.11
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	1	0	0	1	0.11	0.11	0.0	0.11
16	0	0	1	0	0	1	0.11	0.11	0.0	0.11
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	1	0	0	0	1	0.12	0.12	0.0	0.12
19	0	0	1	0	0	1	0.11	0.11	0.0	0.11
20	0	0	1	0	0	1	0.11	0.11	0.0	0.11

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



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

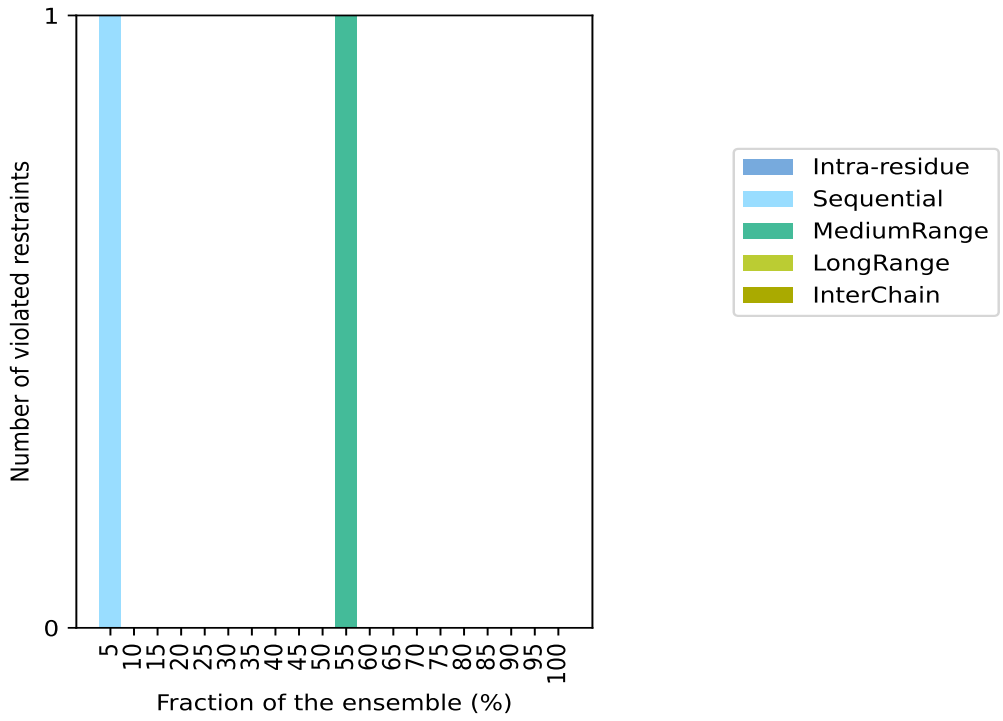
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5834(IR:1008, SQ:1567, MR:1010, LR:2249, 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	1	0	0	0	1	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	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	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

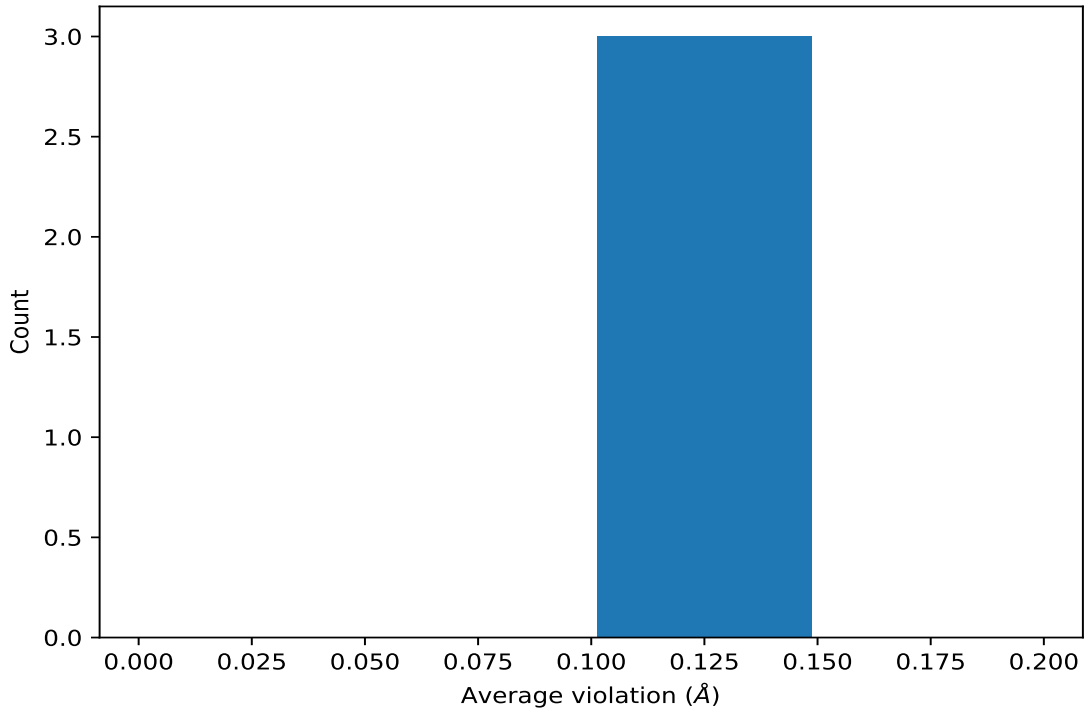
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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.

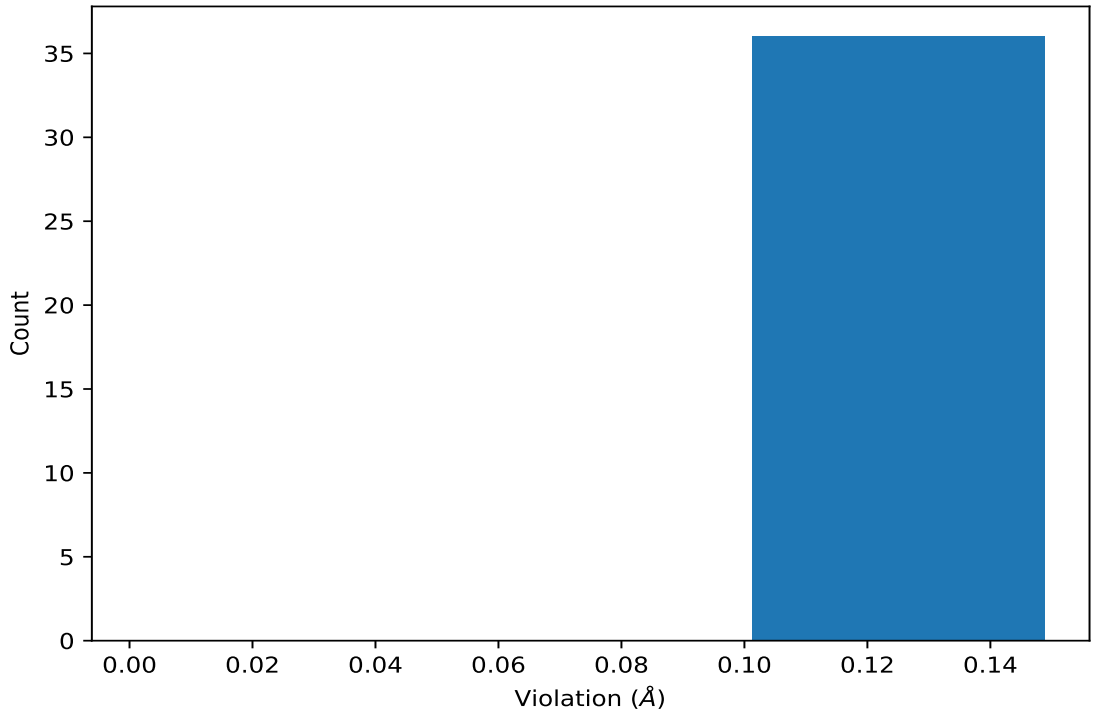
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	11	0.11	0.0	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	11	0.11	0.0	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	11	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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)
(1,5726)	1:A:217:GLU:HG2	1:A:218:VAL:HG21	18	0.12
(1,5726)	1:A:217:GLU:HG2	1:A:218:VAL:HG22	18	0.12
(1,5726)	1:A:217:GLU:HG2	1:A:218:VAL:HG23	18	0.12
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	3	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	3	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	3	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	4	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	4	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	4	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	5	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	5	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	5	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	6	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	6	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	6	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	7	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	7	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	9	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	9	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	9	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	13	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	13	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	13	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	15	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	15	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	15	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	16	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	16	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	16	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	19	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	19	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	19	0.11
(1,4639)	1:A:172:ILE:HG21	1:A:175:TRP:HA	20	0.11
(1,4639)	1:A:172:ILE:HG22	1:A:175:TRP:HA	20	0.11
(1,4639)	1:A:172:ILE:HG23	1:A:175:TRP:HA	20	0.11

10 Dihedral-angle violation analysis

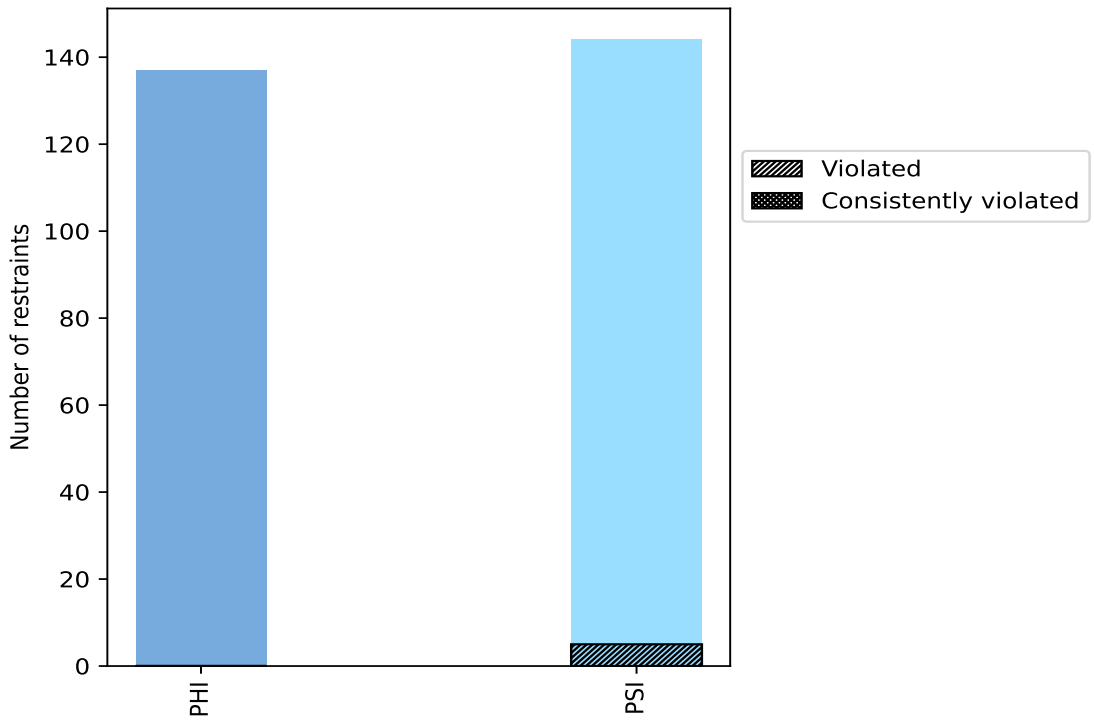
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	137	48.8	0	0.0	0.0	0	0.0	0.0
PSI	144	51.2	5	3.5	1.8	0	0.0	0.0
Total	281	100.0	5	1.8	1.8	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



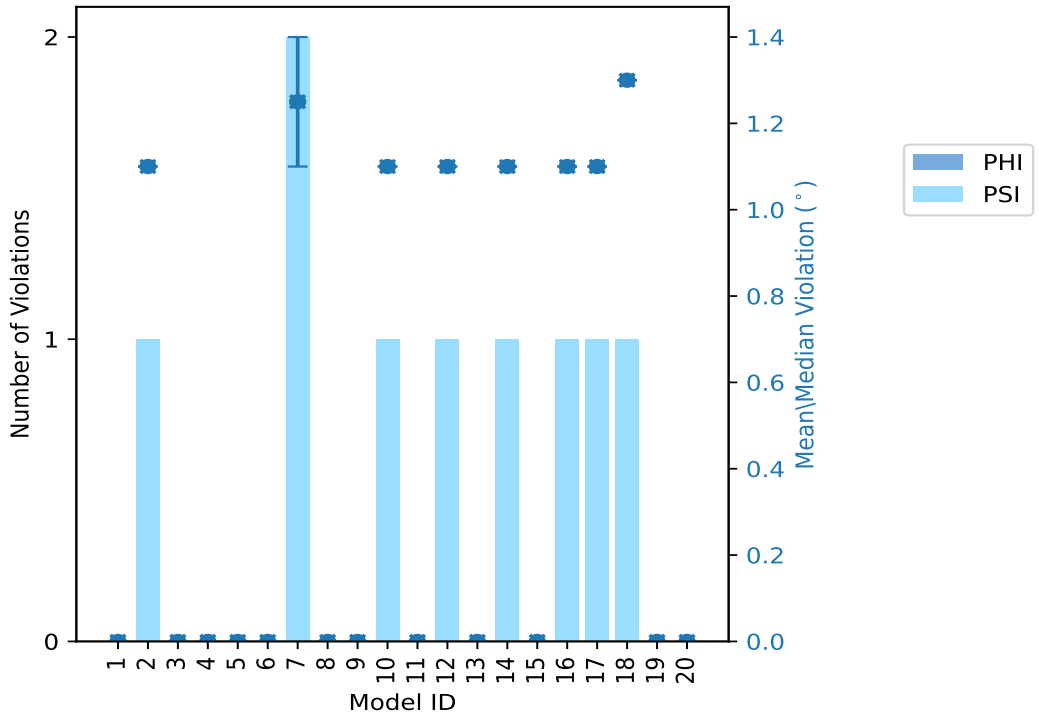
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	1	1	1.1	1.1	0.0	1.1
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	2	2	1.25	1.4	0.15	1.25
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	1.1	1.1	0.0	1.1
11	0	0	0	0.0	0.0	0.0	0.0
12	0	1	1	1.1	1.1	0.0	1.1
13	0	0	0	0.0	0.0	0.0	0.0
14	0	1	1	1.1	1.1	0.0	1.1
15	0	0	0	0.0	0.0	0.0	0.0
16	0	1	1	1.1	1.1	0.0	1.1
17	0	1	1	1.1	1.1	0.0	1.1
18	0	1	1	1.3	1.3	0.0	1.3
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

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

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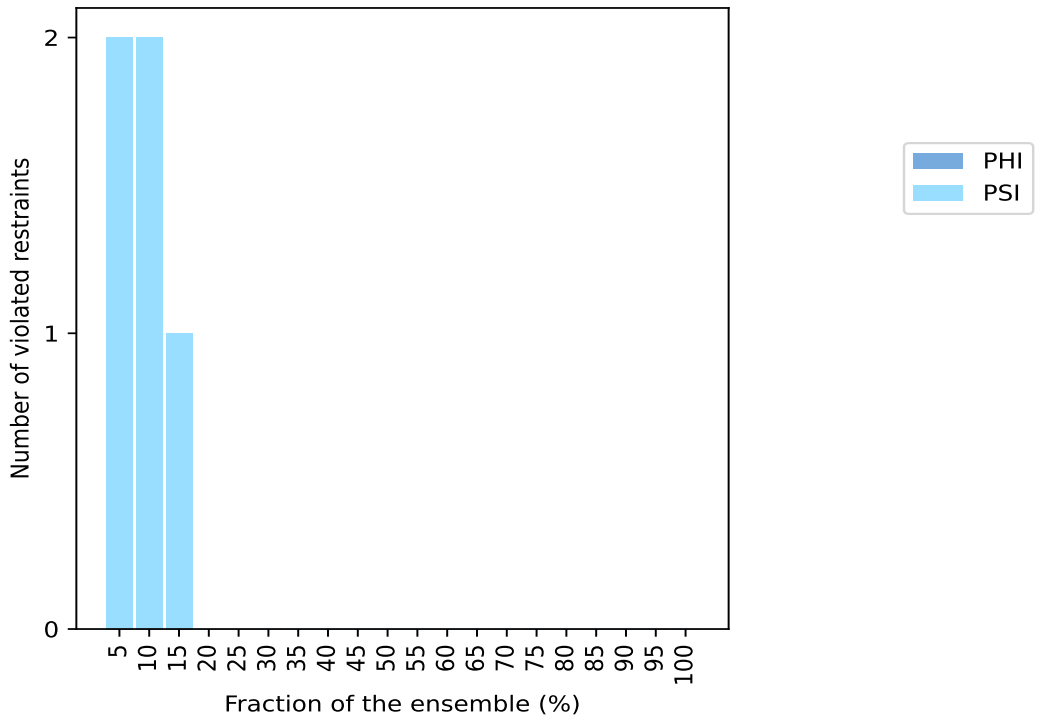
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

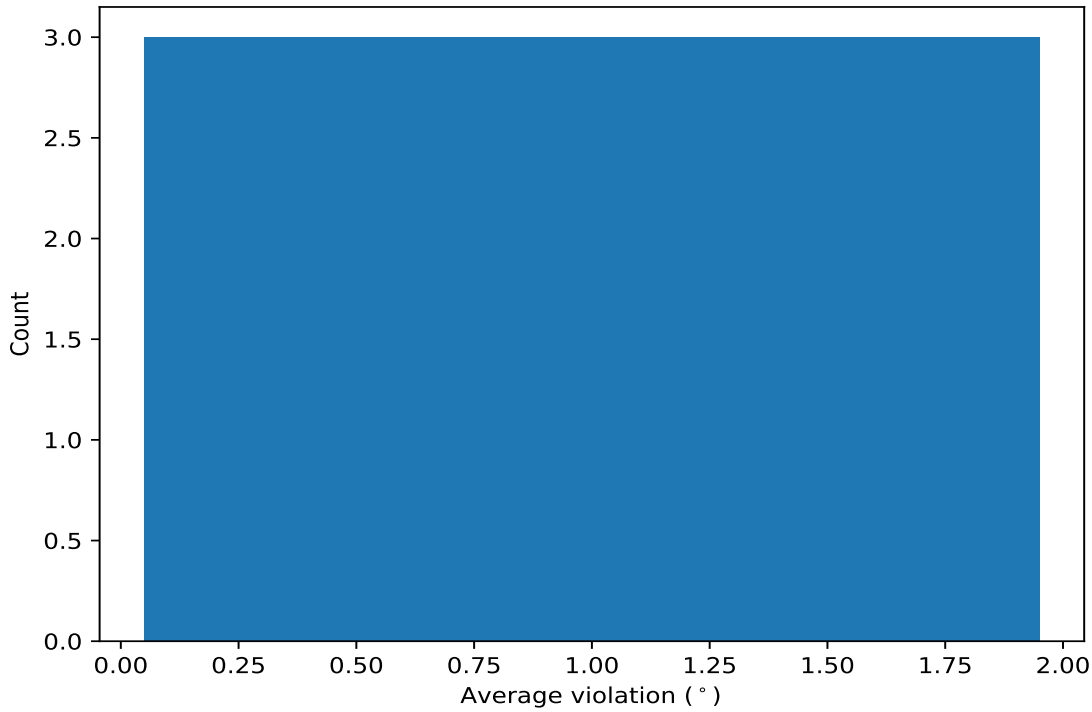


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints

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.

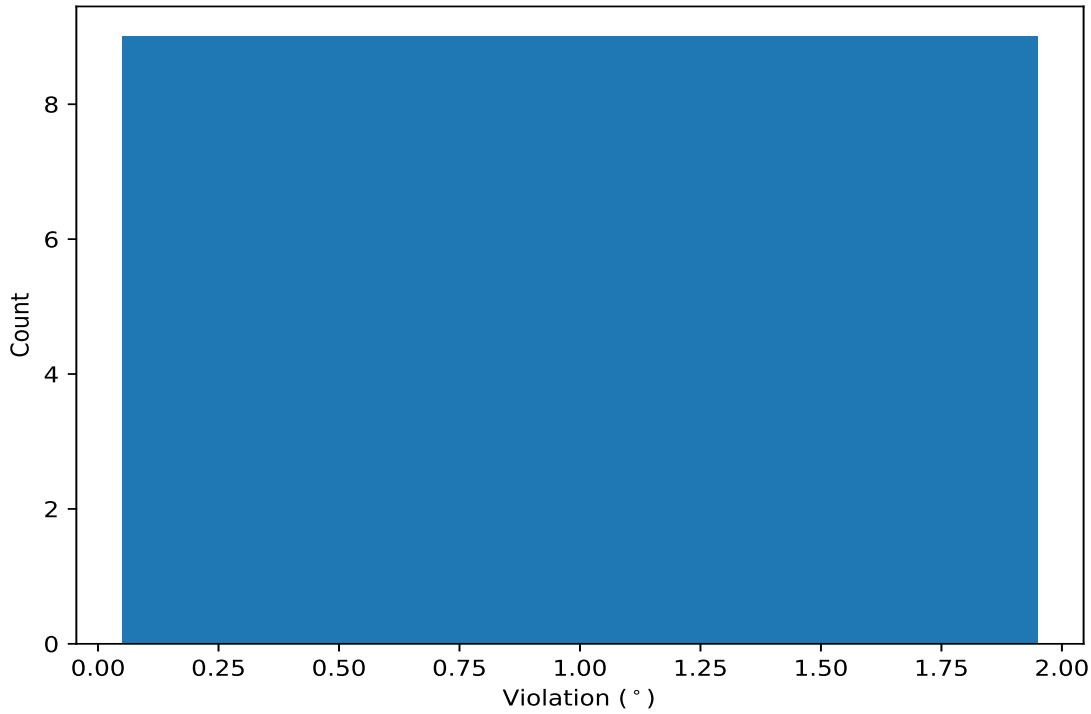
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,148)	1:A:132:HIS:N	1:A:132:HIS:CA	1:A:132:HIS:C	1:A:133:CYS:N	3	1.1	0.0	1.1
(1,197)	1:A:166:VAL:N	1:A:166:VAL:CA	1:A:166:VAL:C	1:A:167:GLY:N	2	1.25	0.15	1.25
(1,17)	1:A:15:LEU:N	1:A:15:LEU:CA	1:A:15:LEU:C	1:A:16:ARG:N	2	1.1	0.0	1.1

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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

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 (°)
(1,197)	1:A:166:VAL:N	1:A:166:VAL:CA	1:A:166:VAL:C	1:A:167:GLY:N	7	1.4
(1,21)	1:A:18:GLU:N	1:A:18:GLU:CA	1:A:18:GLU:C	1:A:19:GLN:N	18	1.3
(1,267)	1:A:214:LEU:N	1:A:214:LEU:CA	1:A:214:LEU:C	1:A:215:THR:N	17	1.1
(1,197)	1:A:166:VAL:N	1:A:166:VAL:CA	1:A:166:VAL:C	1:A:167:GLY:N	12	1.1
(1,17)	1:A:15:LEU:N	1:A:15:LEU:CA	1:A:15:LEU:C	1:A:16:ARG:N	7	1.1
(1,17)	1:A:15:LEU:N	1:A:15:LEU:CA	1:A:15:LEU:C	1:A:16:ARG:N	16	1.1
(1,148)	1:A:132:HIS:N	1:A:132:HIS:CA	1:A:132:HIS:C	1:A:133:CYS:N	2	1.1
(1,148)	1:A:132:HIS:N	1:A:132:HIS:CA	1:A:132:HIS:C	1:A:133:CYS:N	10	1.1
(1,148)	1:A:132:HIS:N	1:A:132:HIS:CA	1:A:132:HIS:C	1:A:133:CYS:N	14	1.1