



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 11:49 AM UTC

PDB ID : 6POJ / pdb_00006poj
BMRB ID : 30624
Title : STRUCTURAL REFINEMENT OF AQUAPORIN 1 VIA SSNMR
Authors : Dingwell, D.A.; Brown, L.S.; Ladizhansky, V.
Deposited on : 2019-07-04

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

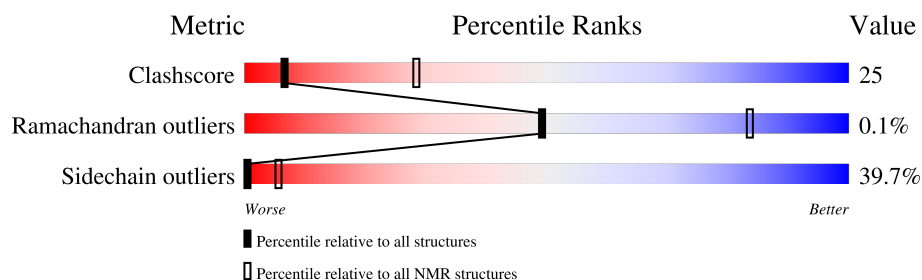
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 37%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	292	

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 9 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:12-A:32, A:48-A:84, A:93-A:116, A:125-A:156, A:168-A:201, A:211-A:227 (165)	0.26	9

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 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4417 atoms, of which 2216 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Aquaporin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	292	Total	C	H	N	O	S	0
			4417	1406	2216	381	407	7	

There are 23 discrepancies between the modelled and reference sequences:

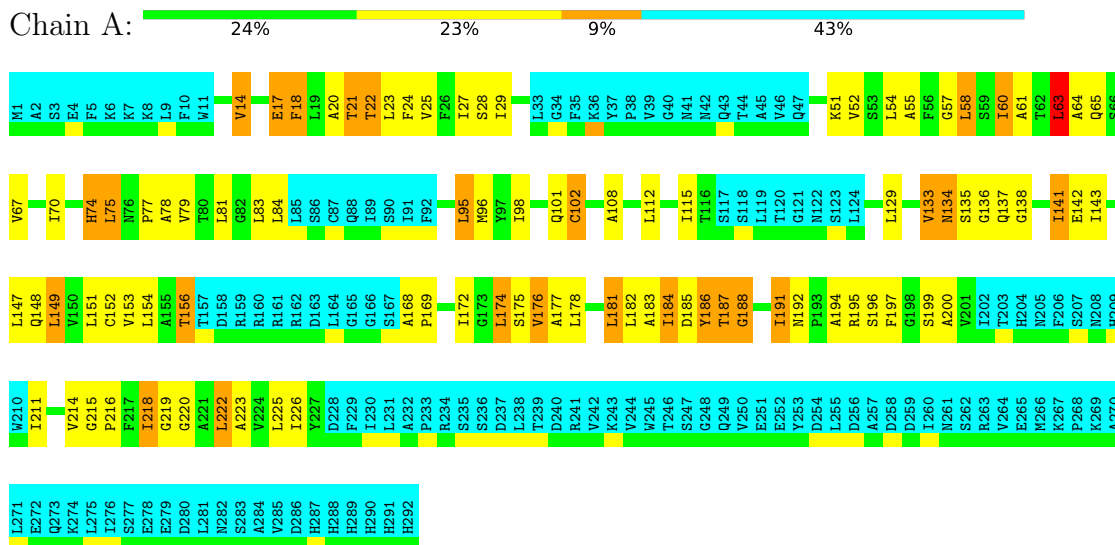
Chain	Residue	Modelled	Actual	Comment	Reference
A	270	ALA	-	expression tag	UNP P29972
A	271	LEU	-	expression tag	UNP P29972
A	272	GLU	-	expression tag	UNP P29972
A	273	GLN	-	expression tag	UNP P29972
A	274	LYS	-	expression tag	UNP P29972
A	275	LEU	-	expression tag	UNP P29972
A	276	ILE	-	expression tag	UNP P29972
A	277	SER	-	expression tag	UNP P29972
A	278	GLU	-	expression tag	UNP P29972
A	279	GLU	-	expression tag	UNP P29972
A	280	ASP	-	expression tag	UNP P29972
A	281	LEU	-	expression tag	UNP P29972
A	282	ASN	-	expression tag	UNP P29972
A	283	SER	-	expression tag	UNP P29972
A	284	ALA	-	expression tag	UNP P29972
A	285	VAL	-	expression tag	UNP P29972
A	286	ASP	-	expression tag	UNP P29972
A	287	HIS	-	expression tag	UNP P29972
A	288	HIS	-	expression tag	UNP P29972
A	289	HIS	-	expression tag	UNP P29972
A	290	HIS	-	expression tag	UNP P29972
A	291	HIS	-	expression tag	UNP P29972
A	292	HIS	-	expression tag	UNP P29972

4 Residue-property plots

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: Aquaporin-1

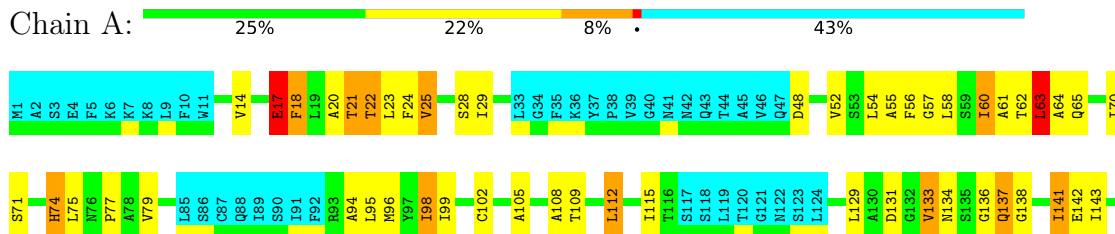


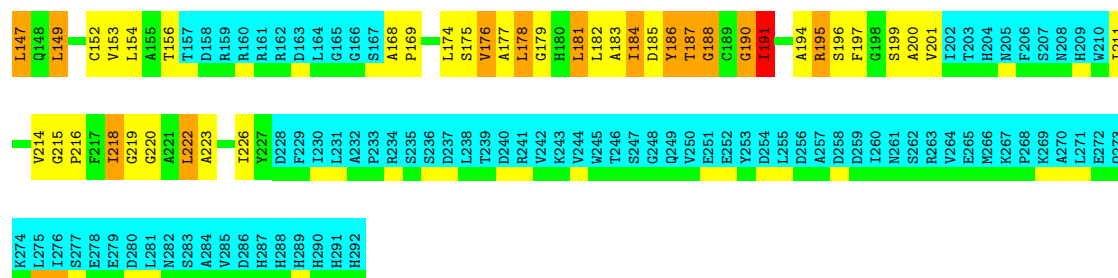
4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

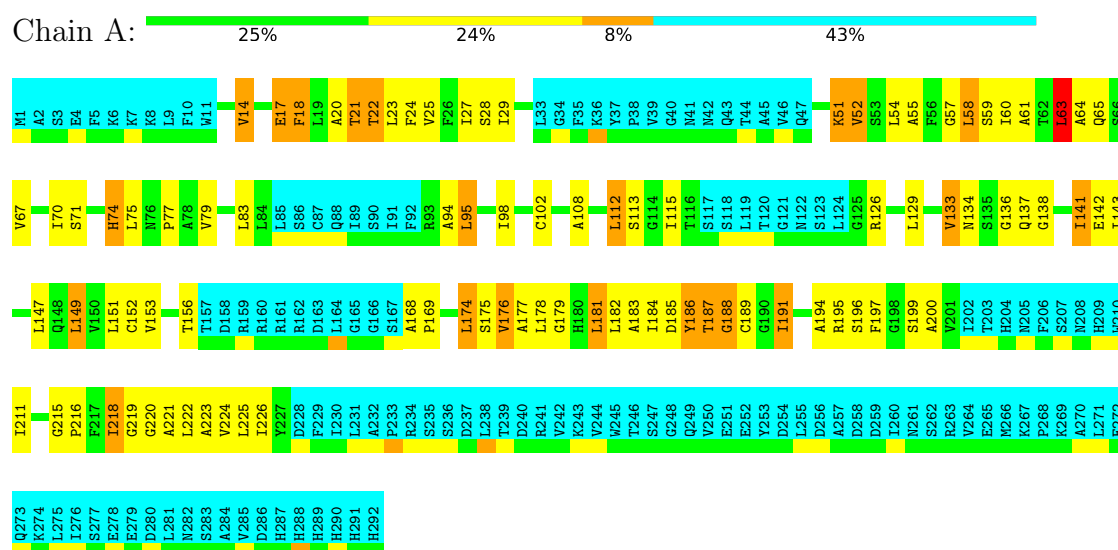
- Molecule 1: Aquaporin-1





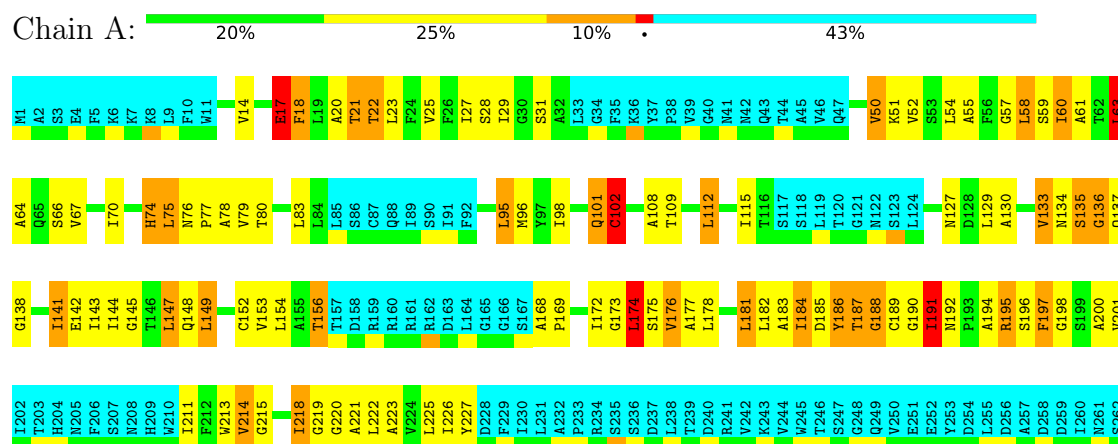
4.2.2 Score per residue for model 2

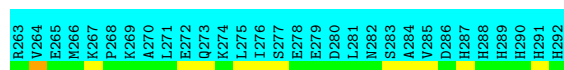
- Molecule 1: Aquaporin-1



4.2.3 Score per residue for model 3

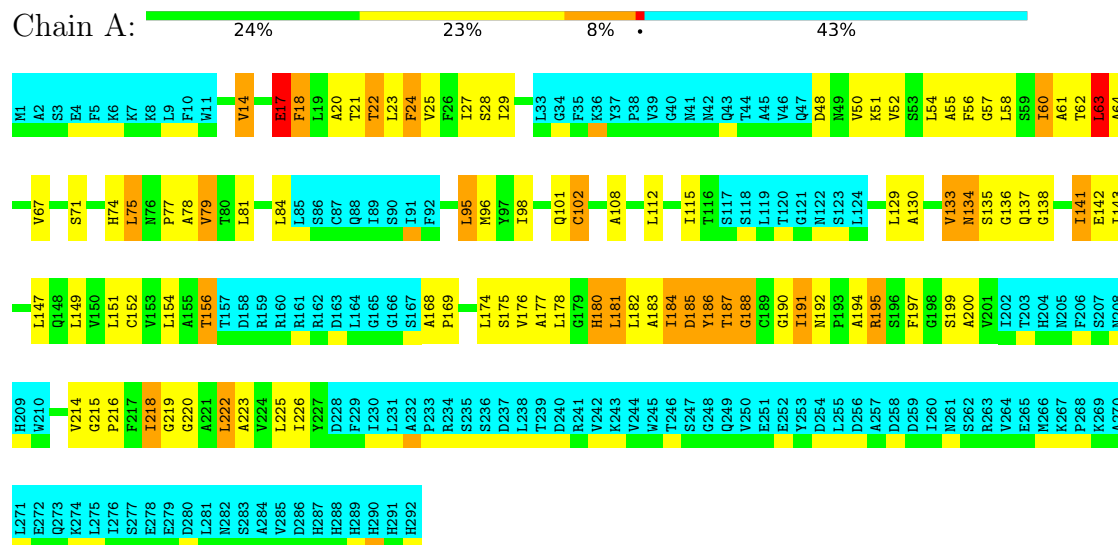
- Molecule 1: Aquaporin-1





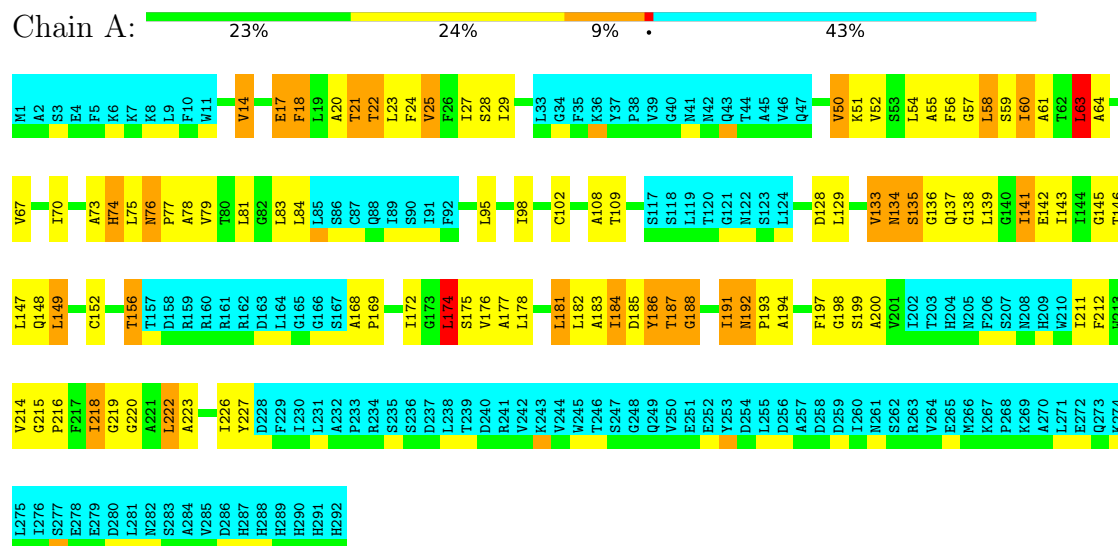
4.2.4 Score per residue for model 4

- Molecule 1: Aquaporin-1



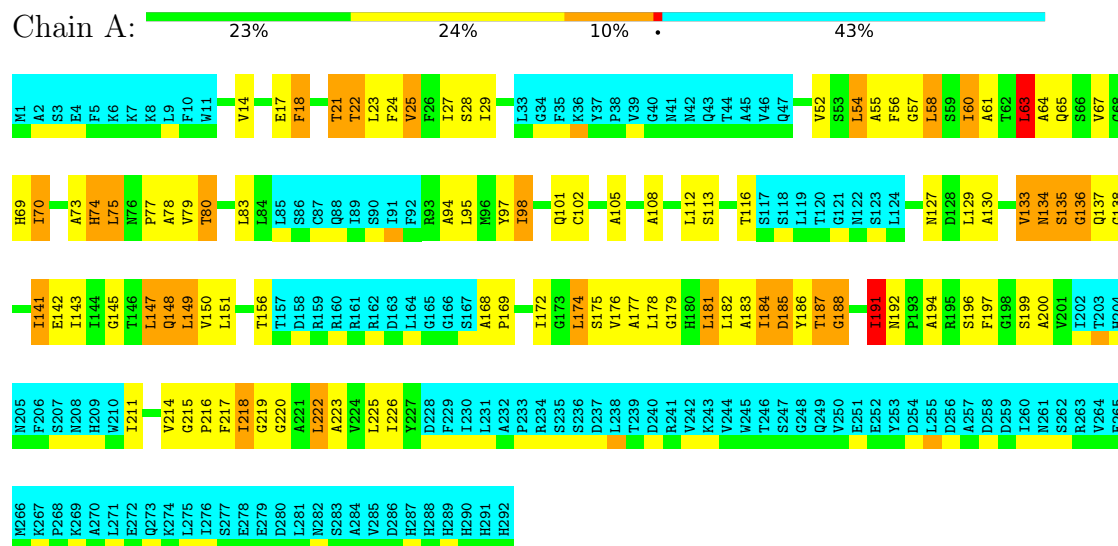
4.2.5 Score per residue for model 5

- Molecule 1: Aquaporin-1



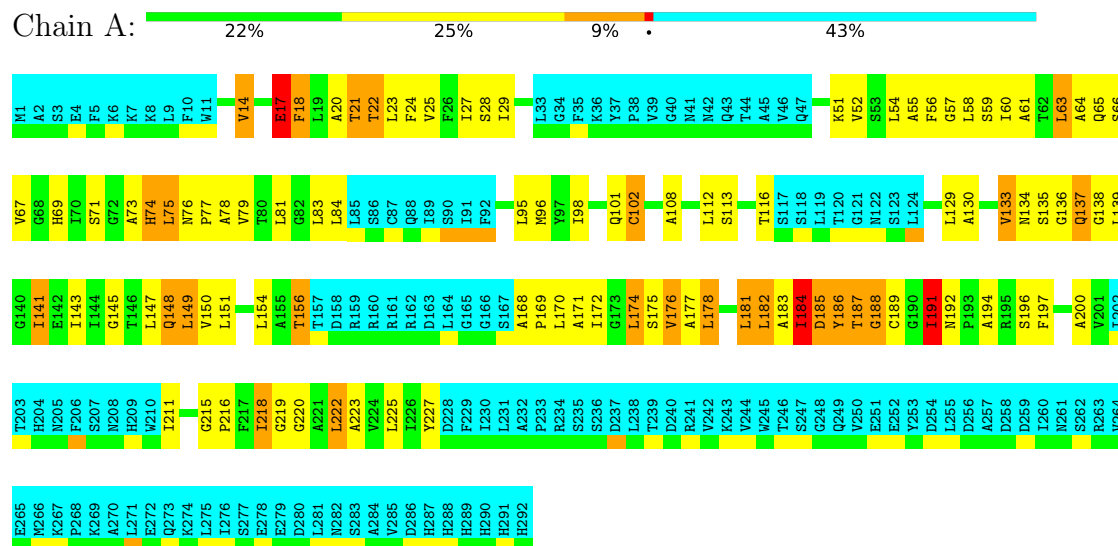
4.2.6 Score per residue for model 6

• Molecule 1: Aquaporin-1



4.2.7 Score per residue for model 7

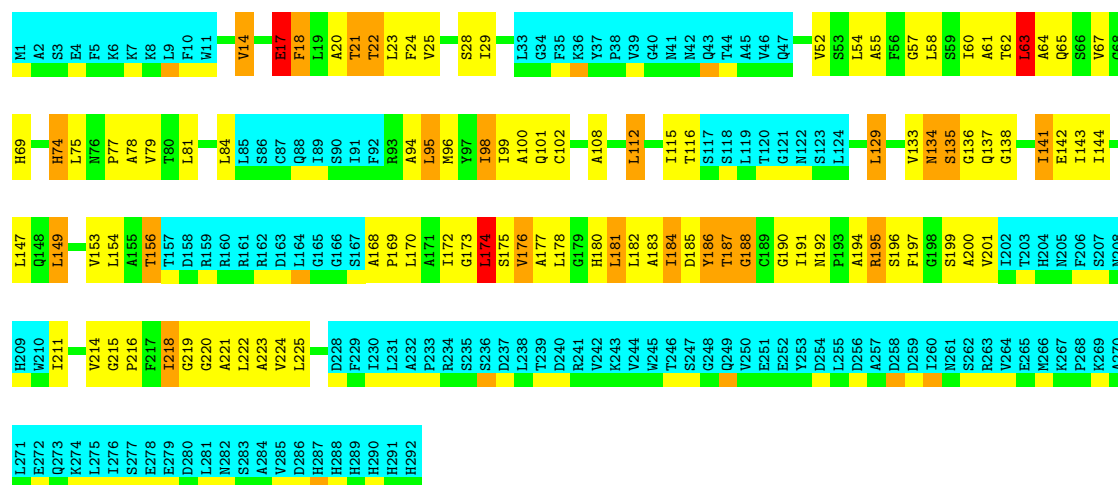
• Molecule 1: Aquaporin-1



4.2.8 Score per residue for model 8

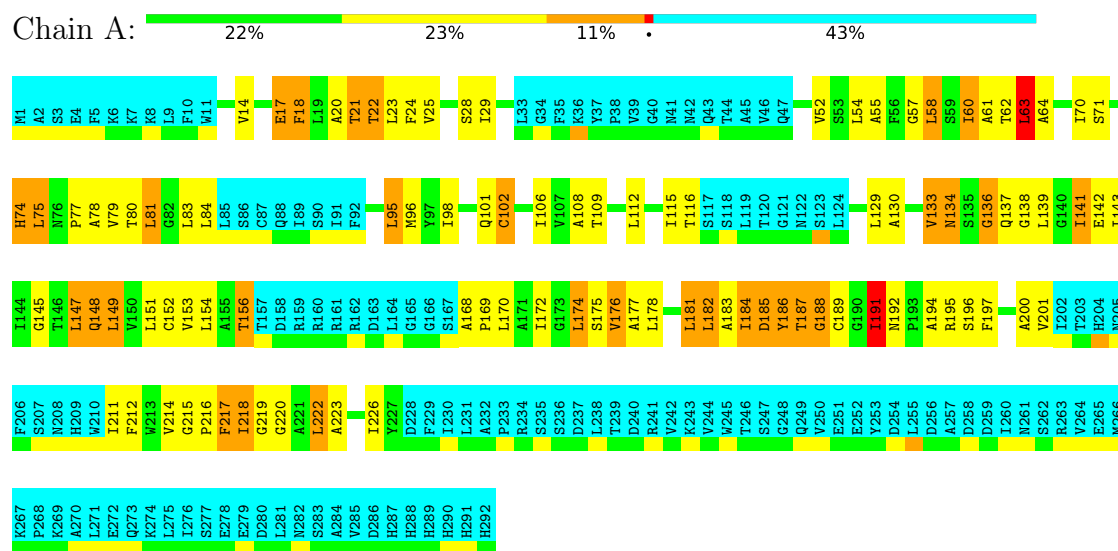
• Molecule 1: Aquaporin-1





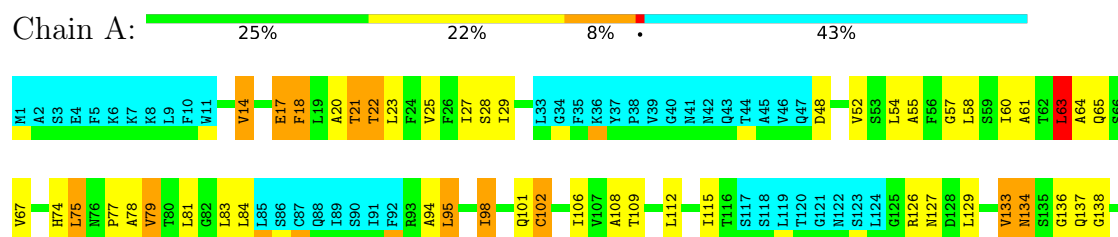
4.2.9 Score per residue for model 9 (medoid)

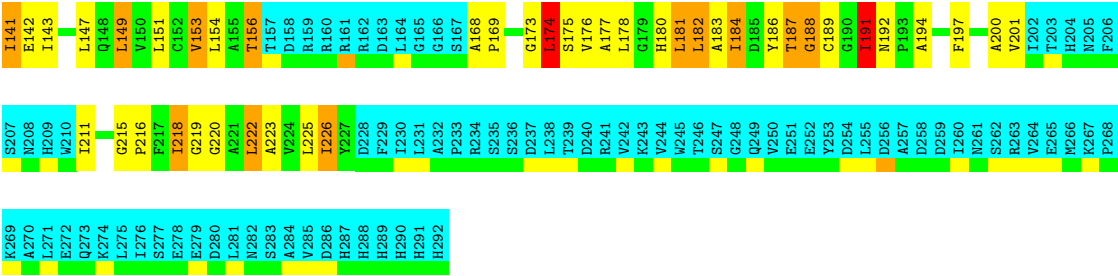
- Molecule 1: Aquaporin-1



4.2.10 Score per residue for model 10

- Molecule 1: Aquaporin-1





5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	refinement	2.48
X-PLOR NIH	structure calculation	2.48

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	951
Number of shifts mapped to atoms	951
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	37%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.09±0.01	2±1/1190 (0.2± 0.1%)	1.44±0.01	14±1/1627 (0.8± 0.1%)
All	All	1.09	24/11900 (0.2%)	1.44	135/16270 (0.8%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	136	GLY	C-N	-6.51	1.25	1.33	3	10
1	A	218	ILE	C-O	-6.02	1.17	1.24	2	3
1	A	184	ILE	C-O	-5.79	1.17	1.24	6	9
1	A	189	CYS	CA-C	-5.51	1.46	1.52	3	2

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	VAL	N-CA-C	-7.75	102.89	110.72	8	10
1	A	18	PHE	N-CA-C	-7.21	103.46	111.82	8	10
1	A	188	GLY	N-CA-C	-7.10	105.98	115.21	6	10
1	A	74	HIS	N-CA-C	-6.79	104.25	112.54	3	10
1	A	218	ILE	O-C-N	6.59	128.76	121.90	1	10
1	A	102	CYS	N-CA-C	-6.54	104.15	111.28	8	10
1	A	63	LEU	N-CA-C	-6.50	104.20	111.28	1	10
1	A	191	ILE	N-CA-C	-6.36	104.30	110.72	6	6
1	A	17	GLU	N-CA-C	6.24	117.88	111.14	8	10
1	A	176	VAL	N-CA-C	5.95	116.12	110.53	1	6
1	A	218	ILE	CA-C-N	5.69	126.14	119.94	1	8
1	A	218	ILE	C-N-CA	5.69	126.14	119.94	1	8
1	A	174	LEU	N-CA-C	-5.68	105.09	111.28	9	10
1	A	95	LEU	N-CA-C	-5.59	104.57	111.33	9	10
1	A	179	GLY	N-CA-C	-5.12	106.58	112.73	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	214	VAL	N-CA-C	5.12	115.34	110.53	3	1
1	A	178	LEU	N-CA-CB	-5.11	102.66	110.07	7	1
1	A	198	GLY	N-CA-C	-5.10	106.61	112.73	3	1
1	A	224	VAL	N-CA-CB	-5.09	104.60	110.55	8	2
1	A	197	PHE	CA-CB-CG	-5.01	108.79	113.80	3	1

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	1171	1233	1235	60±5
All	All	11710	12330	12350	600

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:ALA:HB3	1:A:191:ILE:HG22	0.90	1.41	8	3
1:A:149:LEU:HD11	1:A:176:VAL:HG22	0.84	1.50	3	10
1:A:63:LEU:HD13	1:A:75:LEU:HD12	0.84	1.49	6	1
1:A:21:THR:HG23	1:A:75:LEU:O	0.71	1.85	3	7
1:A:109:THR:HG21	1:A:198:GLY:O	0.69	1.88	5	1
1:A:133:VAL:HG21	1:A:141:ILE:CD1	0.69	2.18	6	2
1:A:94:ALA:O	1:A:98:ILE:HG23	0.69	1.88	2	5
1:A:133:VAL:HG21	1:A:141:ILE:HG13	0.67	1.66	7	1
1:A:133:VAL:HG21	1:A:141:ILE:HD13	0.67	1.65	2	9
1:A:61:ALA:O	1:A:64:ALA:HB3	0.66	1.91	6	10
1:A:222:LEU:O	1:A:226:ILE:HG23	0.66	1.89	10	1
1:A:29:ILE:HG21	1:A:112:LEU:HD22	0.66	1.66	4	9
1:A:147:LEU:HD12	1:A:219:GLY:O	0.66	1.91	3	1
1:A:182:LEU:HD13	1:A:182:LEU:N	0.66	2.05	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:VAL:HG22	1:A:137:GLN:HB3	0.65	1.66	3	10
1:A:197:PHE:HA	1:A:200:ALA:HB3	0.65	1.67	5	10
1:A:170:LEU:HD12	1:A:171:ALA:N	0.65	2.07	7	1
1:A:63:LEU:HG	1:A:75:LEU:HD22	0.64	1.68	3	3
1:A:52:VAL:O	1:A:55:ALA:HB3	0.64	1.92	3	10
1:A:133:VAL:HG13	1:A:137:GLN:HB2	0.63	1.70	3	10
1:A:54:LEU:HA	1:A:177:ALA:HB1	0.63	1.71	5	10
1:A:17:GLU:O	1:A:20:ALA:HB3	0.62	1.95	8	9
1:A:183:ALA:HB3	1:A:191:ILE:HG23	0.61	1.71	3	2
1:A:80:THR:HG21	1:A:97:TYR:CD2	0.61	2.31	6	1
1:A:143:ILE:HG23	1:A:219:GLY:CA	0.60	2.25	4	10
1:A:156:THR:OG1	1:A:172:ILE:HD11	0.60	1.96	5	4
1:A:133:VAL:HG21	1:A:141:ILE:CG1	0.60	2.26	7	1
1:A:57:GLY:HA3	1:A:177:ALA:HB2	0.60	1.73	2	10
1:A:50:VAL:HG22	1:A:181:LEU:HD21	0.60	1.73	4	1
1:A:21:THR:CG2	1:A:105:ALA:HB2	0.60	2.26	6	2
1:A:143:ILE:HG23	1:A:219:GLY:HA2	0.59	1.72	2	5
1:A:149:LEU:HD13	1:A:191:ILE:HD11	0.59	1.74	8	3
1:A:95:LEU:O	1:A:98:ILE:HG13	0.59	1.98	2	1
1:A:75:LEU:O	1:A:75:LEU:HD12	0.59	1.98	1	4
1:A:58:LEU:O	1:A:61:ALA:HB3	0.58	1.98	9	10
1:A:138:GLY:O	1:A:142:GLU:N	0.58	2.35	6	8
1:A:22:THR:HG23	1:A:108:ALA:HB2	0.58	1.75	6	10
1:A:75:LEU:HD22	1:A:75:LEU:O	0.58	1.99	7	1
1:A:218:ILE:O	1:A:222:LEU:HG	0.57	2.00	2	10
1:A:156:THR:OG1	1:A:168:ALA:HB1	0.57	1.99	3	5
1:A:133:VAL:HG13	1:A:137:GLN:CB	0.57	2.29	7	10
1:A:63:LEU:HD13	1:A:75:LEU:CD1	0.57	2.25	6	1
1:A:149:LEU:CD1	1:A:176:VAL:HG22	0.56	2.28	7	8
1:A:78:ALA:HB2	1:A:192:ASN:HA	0.56	1.77	6	8
1:A:24:PHE:CD2	1:A:75:LEU:HD13	0.56	2.35	1	4
1:A:22:THR:HA	1:A:108:ALA:HB2	0.56	1.77	7	10
1:A:139:LEU:HD13	1:A:211:ILE:HD11	0.55	1.76	7	1
1:A:147:LEU:HD12	1:A:147:LEU:O	0.55	2.01	6	3
1:A:147:LEU:CD1	1:A:223:ALA:HB2	0.55	2.31	5	7
1:A:21:THR:HG21	1:A:105:ALA:HB2	0.55	1.77	6	1
1:A:178:LEU:O	1:A:182:LEU:HD22	0.55	2.01	7	2
1:A:156:THR:CB	1:A:172:ILE:HD11	0.54	2.32	9	1
1:A:183:ALA:HB3	1:A:191:ILE:HG12	0.54	1.80	9	1
1:A:183:ALA:HB3	1:A:191:ILE:HG13	0.54	1.79	7	2
1:A:20:ALA:HB1	1:A:75:LEU:HB3	0.54	1.78	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PHE:CD2	1:A:75:LEU:HD23	0.54	2.37	7	1
1:A:183:ALA:CB	1:A:191:ILE:HG22	0.53	2.26	8	1
1:A:17:GLU:OE1	1:A:100:ALA:HB3	0.53	2.04	8	1
1:A:63:LEU:HG	1:A:75:LEU:HD23	0.53	1.81	9	3
1:A:156:THR:HB	1:A:168:ALA:HB1	0.53	1.81	6	3
1:A:81:LEU:HD22	1:A:217:PHE:HA	0.53	1.82	9	1
1:A:21:THR:O	1:A:25:VAL:HG13	0.52	2.04	5	1
1:A:215:GLY:N	1:A:216:PRO:CD	0.52	2.72	2	9
1:A:136:GLY:HA2	1:A:211:ILE:HG21	0.52	1.81	3	3
1:A:183:ALA:CB	1:A:191:ILE:HG23	0.52	2.35	3	2
1:A:75:LEU:HD22	1:A:75:LEU:C	0.51	2.30	7	1
1:A:184:ILE:O	1:A:188:GLY:N	0.51	2.42	4	10
1:A:63:LEU:CD1	1:A:75:LEU:HD12	0.51	2.27	6	1
1:A:106:ILE:HG23	1:A:201:VAL:HG11	0.51	1.80	10	1
1:A:77:PRO:CD	1:A:194:ALA:HB2	0.51	2.36	5	8
1:A:60:ILE:HD13	1:A:75:LEU:HD21	0.51	1.83	3	1
1:A:184:ILE:O	1:A:188:GLY:HA2	0.51	2.05	3	5
1:A:178:LEU:O	1:A:181:LEU:HB2	0.50	2.06	7	10
1:A:218:ILE:O	1:A:221:ALA:HB3	0.50	2.06	8	3
1:A:184:ILE:O	1:A:188:GLY:CA	0.50	2.59	3	10
1:A:63:LEU:CG	1:A:75:LEU:HD22	0.50	2.36	3	1
1:A:141:ILE:N	1:A:141:ILE:HD13	0.50	2.20	7	1
1:A:156:THR:CG2	1:A:168:ALA:HB1	0.50	2.37	10	2
1:A:130:ALA:HB3	1:A:185:ASP:O	0.50	2.07	3	5
1:A:183:ALA:O	1:A:187:THR:CG2	0.49	2.61	2	10
1:A:174:LEU:O	1:A:178:LEU:HD12	0.49	2.07	5	2
1:A:220:GLY:O	1:A:223:ALA:HB3	0.49	2.07	7	10
1:A:190:GLY:HA3	1:A:195:ARG:HB3	0.49	1.85	4	4
1:A:177:ALA:O	1:A:181:LEU:HD12	0.49	2.08	9	5
1:A:133:VAL:HG12	1:A:134:ASN:O	0.49	2.07	8	8
1:A:60:ILE:CD1	1:A:75:LEU:HD21	0.49	2.37	4	1
1:A:73:ALA:HB3	1:A:79:VAL:HG21	0.49	1.85	6	1
1:A:150:VAL:HG21	1:A:220:GLY:HA3	0.49	1.83	6	2
1:A:60:ILE:HG13	1:A:75:LEU:HD21	0.48	1.85	9	2
1:A:51:LYS:NZ	1:A:52:VAL:HG23	0.48	2.24	2	1
1:A:56:PHE:O	1:A:60:ILE:HG23	0.47	2.09	1	1
1:A:25:VAL:O	1:A:29:ILE:HG12	0.47	2.10	5	10
1:A:79:VAL:HG23	1:A:149:LEU:HD23	0.47	1.85	4	2
1:A:54:LEU:C	1:A:54:LEU:HD13	0.47	2.34	2	2
1:A:73:ALA:HB1	1:A:76:ASN:HB2	0.47	1.86	7	2
1:A:133:VAL:HG13	1:A:138:GLY:N	0.47	2.25	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:VAL:O	1:A:186:TYR:O	0.47	2.33	3	10
1:A:168:ALA:N	1:A:169:PRO:CD	0.46	2.78	7	9
1:A:56:PHE:O	1:A:60:ILE:HD13	0.46	2.10	6	2
1:A:149:LEU:HD13	1:A:191:ILE:CD1	0.46	2.40	8	1
1:A:129:LEU:HD22	1:A:129:LEU:H	0.46	1.71	8	1
1:A:50:VAL:HG13	1:A:51:LYS:CE	0.46	2.40	5	2
1:A:22:THR:CG2	1:A:108:ALA:HB2	0.45	2.41	1	10
1:A:24:PHE:CE2	1:A:25:VAL:HG12	0.45	2.46	5	1
1:A:70:ILE:O	1:A:70:ILE:HG23	0.45	2.12	6	1
1:A:133:VAL:CG1	1:A:134:ASN:O	0.45	2.65	6	10
1:A:182:LEU:N	1:A:182:LEU:CD1	0.45	2.79	7	2
1:A:24:PHE:CE1	1:A:56:PHE:CD1	0.45	3.04	4	1
1:A:180:HIS:HA	1:A:184:ILE:HD13	0.45	1.87	4	1
1:A:101:GLN:CD	1:A:101:GLN:C	0.45	2.85	4	3
1:A:77:PRO:HG3	1:A:194:ALA:HB2	0.45	1.88	1	3
1:A:219:GLY:O	1:A:222:LEU:CD1	0.45	2.64	10	7
1:A:180:HIS:CD2	1:A:191:ILE:HD11	0.45	2.46	10	1
1:A:212:PHE:CD2	1:A:212:PHE:N	0.44	2.83	5	1
1:A:150:VAL:HG21	1:A:220:GLY:CA	0.44	2.42	6	2
1:A:211:ILE:HD12	1:A:212:PHE:N	0.44	2.26	9	1
1:A:218:ILE:O	1:A:222:LEU:CG	0.44	2.65	4	7
1:A:75:LEU:HD13	1:A:75:LEU:H	0.44	1.71	6	1
1:A:70:ILE:HG22	1:A:70:ILE:O	0.44	2.12	1	2
1:A:129:LEU:HD22	1:A:129:LEU:N	0.44	2.27	8	1
1:A:63:LEU:HD13	1:A:75:LEU:HD22	0.44	1.88	2	1
1:A:20:ALA:HB1	1:A:75:LEU:CB	0.44	2.42	8	3
1:A:129:LEU:HD11	1:A:135:SER:N	0.44	2.27	7	5
1:A:148:GLN:CD	1:A:148:GLN:C	0.44	2.86	7	1
1:A:133:VAL:HG13	1:A:137:GLN:C	0.43	2.38	8	1
1:A:145:GLY:O	1:A:148:GLN:CG	0.43	2.67	7	2
1:A:78:ALA:HB2	1:A:193:PRO:CD	0.43	2.44	5	1
1:A:133:VAL:C	1:A:134:ASN:O	0.43	2.60	8	1
1:A:75:LEU:CD2	1:A:75:LEU:C	0.43	2.91	6	1
1:A:63:LEU:HD22	1:A:75:LEU:HD23	0.43	1.90	2	1
1:A:170:LEU:HD12	1:A:170:LEU:C	0.43	2.38	7	1
1:A:73:ALA:HB1	1:A:75:LEU:HD22	0.43	1.90	6	1
1:A:214:VAL:HG13	1:A:215:GLY:N	0.43	2.29	3	7
1:A:148:GLN:HG3	1:A:149:LEU:N	0.43	2.28	6	1
1:A:133:VAL:CG1	1:A:138:GLY:N	0.42	2.82	4	10
1:A:146:THR:HG21	1:A:216:PRO:CB	0.42	2.44	5	1
1:A:77:PRO:HD3	1:A:194:ALA:HB2	0.42	1.90	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:214:VAL:HG22	1:A:218:ILE:HD12	0.42	1.90	8	1
1:A:180:HIS:O	1:A:184:ILE:HB	0.42	2.15	4	2
1:A:187:THR:OG1	1:A:189:CYS:CB	0.42	2.68	9	3
1:A:156:THR:CB	1:A:168:ALA:HB1	0.42	2.44	6	1
1:A:197:PHE:HA	1:A:200:ALA:CB	0.42	2.42	1	3
1:A:101:GLN:CD	1:A:102:CYS:N	0.42	2.78	3	1
1:A:147:LEU:HD12	1:A:223:ALA:HB2	0.42	1.90	5	3
1:A:106:ILE:HD11	1:A:197:PHE:CE2	0.42	2.50	9	1
1:A:62:THR:O	1:A:63:LEU:C	0.42	2.63	1	4
1:A:79:VAL:HG21	1:A:153:VAL:HG21	0.42	1.92	10	1
1:A:60:ILE:HG13	1:A:61:ALA:N	0.41	2.29	1	1
1:A:179:GLY:O	1:A:191:ILE:HD11	0.41	2.15	1	2
1:A:145:GLY:O	1:A:148:GLN:HG2	0.41	2.15	5	2
1:A:75:LEU:H	1:A:75:LEU:CD1	0.41	2.28	7	1
1:A:129:LEU:HD13	1:A:187:THR:O	0.41	2.15	5	3
1:A:73:ALA:HB1	1:A:75:LEU:HD13	0.41	1.91	7	1
1:A:138:GLY:HA2	1:A:141:ILE:HB	0.41	1.92	8	2
1:A:173:GLY:O	1:A:174:LEU:C	0.41	2.64	3	3
1:A:97:TYR:CD2	1:A:97:TYR:C	0.41	2.99	6	1
1:A:135:SER:O	1:A:211:ILE:HD13	0.41	2.16	8	1
1:A:138:GLY:O	1:A:142:GLU:CB	0.41	2.69	1	1
1:A:22:THR:HG23	1:A:108:ALA:CB	0.41	2.43	6	1
1:A:133:VAL:CG2	1:A:141:ILE:HD13	0.41	2.46	8	1
1:A:211:ILE:HD12	1:A:211:ILE:C	0.41	2.40	9	1
1:A:80:THR:HG21	1:A:97:TYR:CG	0.41	2.51	6	1
1:A:22:THR:HG23	1:A:108:ALA:CA	0.40	2.46	5	1
1:A:145:GLY:O	1:A:148:GLN:HG3	0.40	2.16	7	1
1:A:182:LEU:HD23	1:A:182:LEU:N	0.40	2.31	10	1
1:A:21:THR:O	1:A:25:VAL:HG22	0.40	2.15	5	1
1:A:21:THR:HG22	1:A:105:ALA:HB2	0.40	1.94	1	1
1:A:168:ALA:N	1:A:169:PRO:HD2	0.40	2.32	2	1
1:A:144:ILE:HG23	1:A:145:GLY:N	0.40	2.31	3	1
1:A:56:PHE:N	1:A:56:PHE:CD1	0.40	2.90	7	1
1:A:20:ALA:HB1	1:A:75:LEU:CA	0.40	2.47	1	1
1:A:24:PHE:CD1	1:A:24:PHE:C	0.40	2.96	4	1

6.3 Torsion angles

6.3.1 Protein backbone

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	165/292 (57%)	158±1 (96±1%)	7±1 (4±1%)	0±0 (0±0%)	49	83
All	All	1650/2920 (57%)	1581 (96%)	68 (4%)	1 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	190	GLY	1

6.3.2 Protein sidechains

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	120/235 (51%)	72±4 (60±3%)	48±4 (40±3%)	0	5
All	All	1200/2350 (51%)	724 (60%)	476 (40%)	0	5

All 90 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	18	PHE	10
1	A	21	THR	10
1	A	22	THR	10
1	A	23	LEU	10
1	A	28	SER	10
1	A	60	ILE	10
1	A	63	LEU	10
1	A	141	ILE	10
1	A	175	SER	10
1	A	181	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	182	LEU	10
1	A	187	THR	10
1	A	79	VAL	9
1	A	98	ILE	9
1	A	133	VAL	9
1	A	149	LEU	9
1	A	156	THR	9
1	A	191	ILE	9
1	A	74	HIS	8
1	A	185	ASP	8
1	A	186	TYR	8
1	A	226	ILE	8
1	A	67	VAL	8
1	A	174	LEU	8
1	A	115	ILE	7
1	A	154	LEU	7
1	A	196	SER	7
1	A	222	LEU	7
1	A	27	ILE	7
1	A	83	LEU	7
1	A	225	LEU	7
1	A	65	GLN	6
1	A	96	MET	6
1	A	147	LEU	6
1	A	152	CYS	6
1	A	153	VAL	6
1	A	195	ARG	6
1	A	199	SER	6
1	A	14	VAL	6
1	A	151	LEU	6
1	A	75	LEU	6
1	A	81	LEU	6
1	A	84	LEU	6
1	A	134	ASN	6
1	A	17	GLU	5
1	A	71	SER	5
1	A	129	LEU	5
1	A	58	LEU	5
1	A	95	LEU	5
1	A	102	CYS	5
1	A	109	THR	4
1	A	112	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	201	VAL	4
1	A	211	ILE	4
1	A	59	SER	4
1	A	70	ILE	4
1	A	101	GLN	4
1	A	135	SER	4
1	A	148	GLN	4
1	A	116	THR	4
1	A	25	VAL	3
1	A	48	ASP	3
1	A	51	LYS	3
1	A	113	SER	3
1	A	80	THR	3
1	A	127	ASN	3
1	A	227	TYR	3
1	A	69	HIS	3
1	A	99	ILE	2
1	A	137	GLN	2
1	A	126	ARG	2
1	A	50	VAL	2
1	A	66	SER	2
1	A	76	ASN	2
1	A	24	PHE	2
1	A	139	LEU	2
1	A	172	ILE	2
1	A	217	PHE	2
1	A	170	LEU	2
1	A	131	ASP	1
1	A	178	LEU	1
1	A	52	VAL	1
1	A	31	SER	1
1	A	213	TRP	1
1	A	180	HIS	1
1	A	128	ASP	1
1	A	192	ASN	1
1	A	54	LEU	1
1	A	184	ILE	1
1	A	144	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 37% for the well-defined parts and 24% 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	951
Number of shifts mapped to atoms	951
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	190	-1.24 ± 0.13	Should be checked
$^{13}\text{C}_\beta$	158	0.37 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	189	-0.72 ± 0.10	Should be applied
^{15}N	189	0.66 ± 0.30	Should be applied

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 37%, i.e. 800 atoms were assigned a chemical shift out of a possible 2145. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	475/838 (57%)	0/347 (0%)	319/330 (97%)	156/161 (97%)
Sidechain	316/1176 (27%)	0/797 (0%)	303/357 (85%)	13/22 (59%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	9/131 (7%)	0/65 (0%)	6/61 (10%)	3/5 (60%)
Overall	800/2145 (37%)	0/1209 (0%)	628/748 (84%)	172/188 (91%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 24%, i.e. 941 atoms were assigned a chemical shift out of a possible 3883. 0 out of 59 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	563/1473 (38%)	0/604 (0%)	379/584 (65%)	184/285 (65%)
Sidechain	369/2111 (17%)	0/1399 (0%)	354/649 (55%)	15/63 (24%)
Aromatic	9/299 (3%)	0/153 (0%)	6/132 (5%)	3/14 (21%)
Overall	941/3883 (24%)	0/2156 (0%)	739/1365 (54%)	202/362 (56%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ

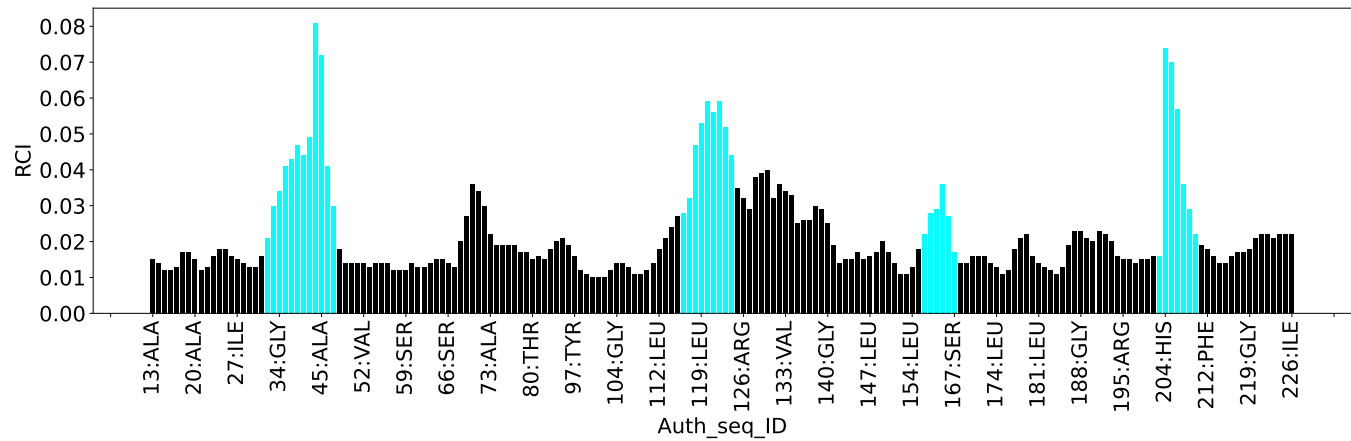
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	190	GLY	N	130.13	91.59 – 127.52	5.7

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	183
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	130
Long range ($ i-j \geq 5$)	53
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	354
Number of unmapped restraints	0
Number of restraints per residue	1.8
Number of long range restraints per residue ¹	0.2

¹Long 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)	32.9	0.2
0.2-0.5 (Medium)	8.8	0.35
>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. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

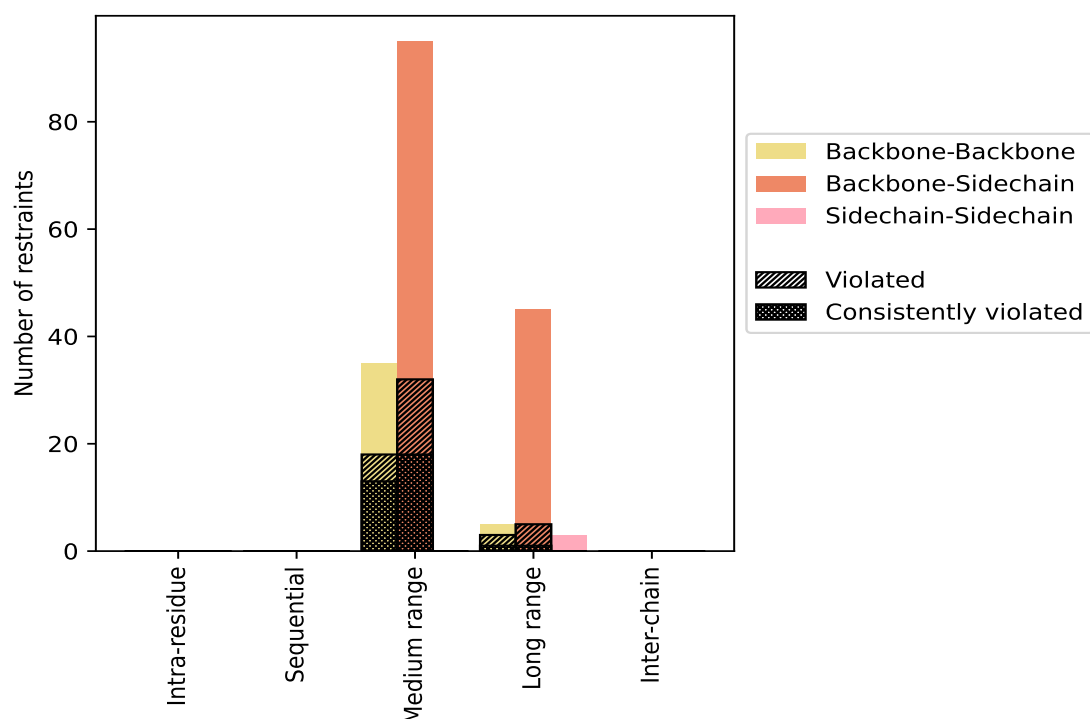
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	130	71.0	50	38.5	27.3	31	23.8	16.9
Backbone-Backbone	35	19.1	18	51.4	9.8	13	37.1	7.1
Backbone-Sidechain	95	51.9	32	33.7	17.5	18	18.9	9.8
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	53	29.0	8	15.1	4.4	2	3.8	1.1
Backbone-Backbone	5	2.7	3	60.0	1.6	1	20.0	0.5
Backbone-Sidechain	45	24.6	5	11.1	2.7	1	2.2	0.5
Sidechain-Sidechain	3	1.6	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	183	100.0	58	31.7	31.7	33	18.0	18.0
Backbone-Backbone	40	21.9	21	52.5	11.5	14	35.0	7.7
Backbone-Sidechain	140	76.5	37	26.4	20.2	19	13.6	10.4
Sidechain-Sidechain	3	1.6	0	0.0	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 [i](#)



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

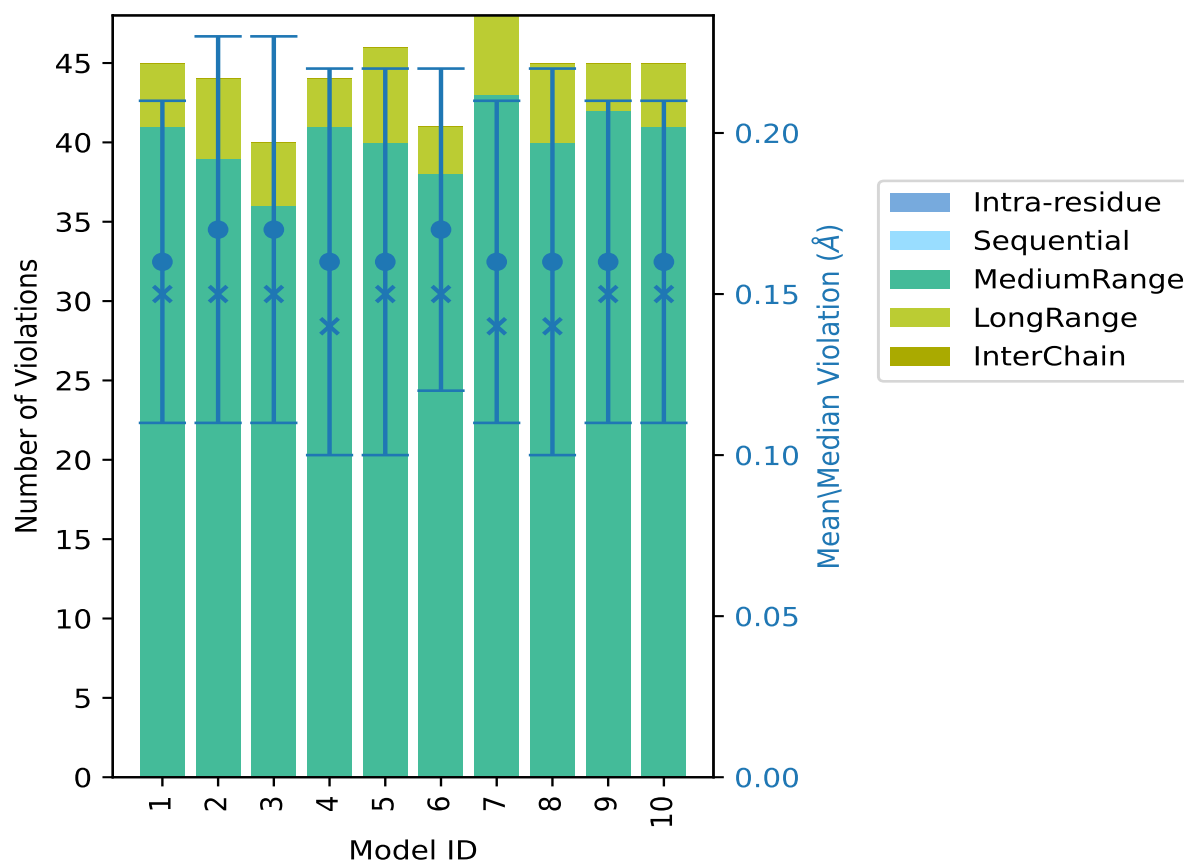
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	41	4	0	45	0.16	0.33	0.05	0.15
2	0	0	39	5	0	44	0.17	0.35	0.06	0.15
3	0	0	36	4	0	40	0.17	0.35	0.06	0.15
4	0	0	41	3	0	44	0.16	0.33	0.06	0.14
5	0	0	40	6	0	46	0.16	0.33	0.06	0.15
6	0	0	38	3	0	41	0.17	0.32	0.05	0.15
7	0	0	43	5	0	48	0.16	0.31	0.05	0.14
8	0	0	40	5	0	45	0.16	0.34	0.06	0.14
9	0	0	42	3	0	45	0.16	0.33	0.05	0.15
10	0	0	41	4	0	45	0.16	0.32	0.05	0.15

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

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 125(IR:0, SQ:0, MR:80, LR:45, 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	0	6	2	0	8	1	10.0
0	0	1	0	0	1	2	20.0
0	0	1	1	0	2	3	30.0

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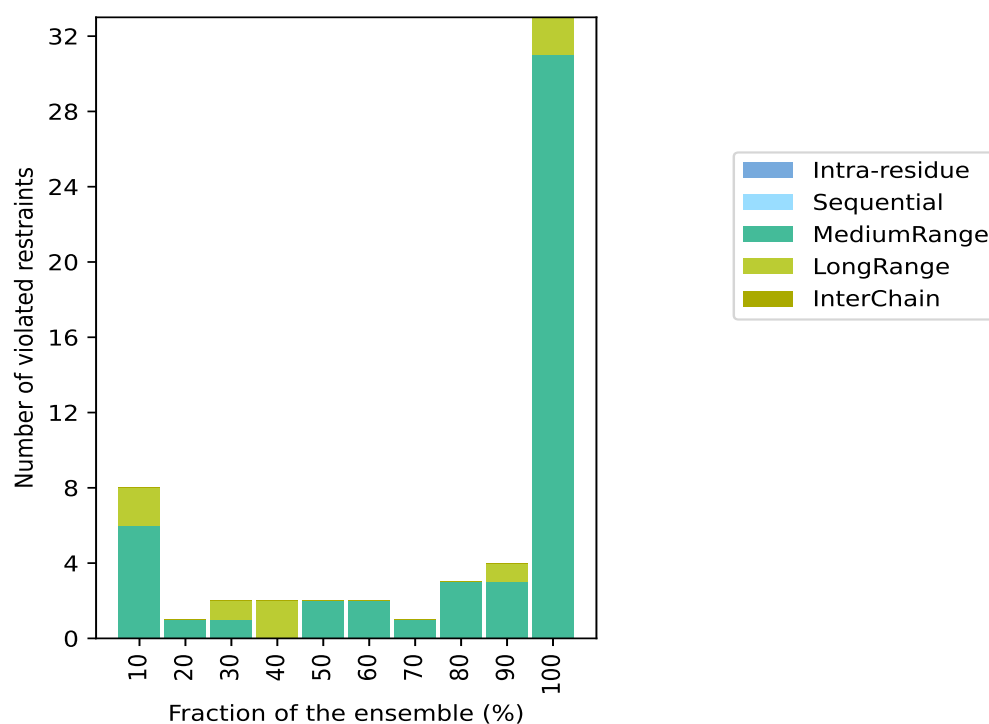
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	2	0	2	4	40.0
0	0	2	0	0	2	5	50.0
0	0	2	0	0	2	6	60.0
0	0	1	0	0	1	7	70.0
0	0	3	0	0	3	8	80.0
0	0	3	1	0	4	9	90.0
0	0	31	2	0	33	10	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

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

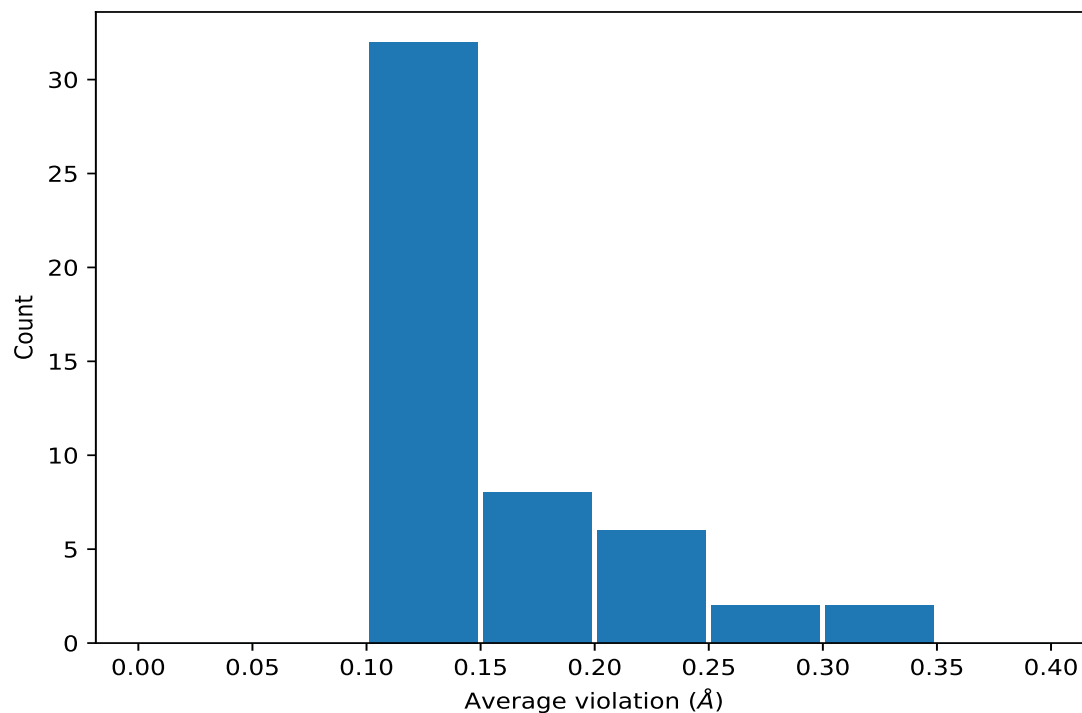


9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	10	0.32	0.01	0.32
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	10	0.31	0.01	0.31
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	10	0.3	0.01	0.3
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	10	0.26	0.06	0.23
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	10	0.24	0.01	0.24
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	10	0.23	0.01	0.23
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	10	0.23	0.01	0.23
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	10	0.21	0.01	0.21
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	10	0.21	0.01	0.21
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	10	0.2	0.04	0.18
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	10	0.19	0.01	0.19
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	10	0.19	0.01	0.19
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	10	0.18	0.01	0.18
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	10	0.17	0.01	0.17
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	10	0.17	0.01	0.17

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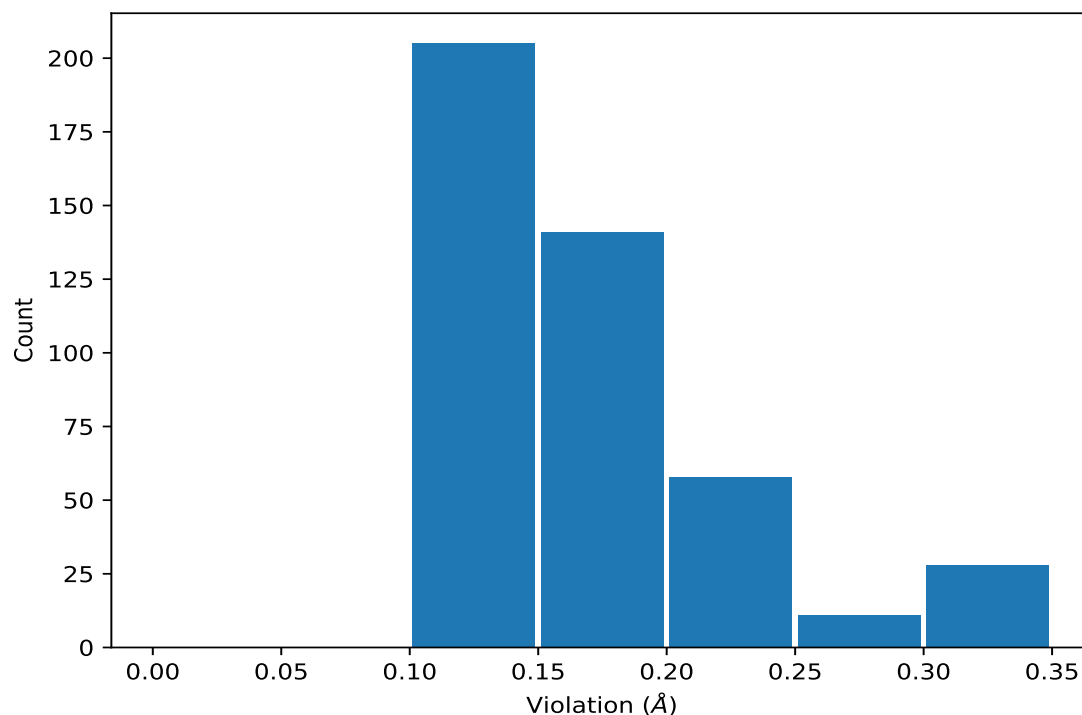
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	10	0.16	0.0	0.16
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	10	0.16	0.01	0.16
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	10	0.16	0.01	0.16
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	10	0.15	0.01	0.15
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	10	0.15	0.01	0.15
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	10	0.15	0.01	0.15
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	10	0.15	0.01	0.15
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	10	0.15	0.01	0.15
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	10	0.15	0.01	0.15
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	10	0.15	0.01	0.14
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	10	0.14	0.0	0.14
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	10	0.14	0.02	0.15
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	10	0.13	0.02	0.14
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	10	0.13	0.01	0.13
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	10	0.13	0.03	0.12
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	10	0.12	0.01	0.12
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	10	0.12	0.01	0.12
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	10	0.11	0.0	0.11
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	9	0.13	0.01	0.13
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	9	0.12	0.01	0.12
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	9	0.11	0.01	0.11
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	9	0.11	0.0	0.11
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	8	0.12	0.01	0.12
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	8	0.12	0.01	0.11
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	8	0.11	0.01	0.12
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	7	0.12	0.0	0.12
(1,36)	1:34:A:GLY:C	1:36:A:LYS:CG	6	0.12	0.02	0.12
(1,134)	1:178:A:LEU:C	1:180:A:HIS:CB	6	0.11	0.0	0.11
(1,45)	1:144:A:ILE:C	1:148:A:GLN:CB	5	0.12	0.01	0.11
(1,56)	1:142:A:GLU:C	1:145:A:GLY:CA	5	0.11	0.0	0.11
(1,149)	1:75:A:LEU:C	1:20:A:ALA:CB	4	0.11	0.01	0.11
(1,23)	1:176:A:VAL:C	1:149:A:LEU:CD1	4	0.1	0.0	0.1
(1,143)	1:195:A:ARG:C	1:190:A:GLY:CA	3	0.12	0.01	0.12
(1,121)	1:113:A:SER:C	1:115:A:ILE:CB	3	0.1	0.0	0.1
(1,103)	1:139:A:LEU:C	1:143:A:ILE:CB	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	2	0.35
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	3	0.35
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	8	0.34
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	1	0.33
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	4	0.33
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	8	0.33
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	9	0.33
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	3	0.33
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	5	0.33
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	6	0.32
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	4	0.32
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	10	0.32
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	2	0.31
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	3	0.31
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	7	0.31
(1,129)	1:200:A:ALA:C	1:197:A:PHE:CA	10	0.31
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	6	0.31
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	8	0.31
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	9	0.31
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	4	0.31
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	6	0.31
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	1	0.3
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	2	0.3
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	3	0.3
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	5	0.3
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	7	0.3
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	10	0.3
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	1	0.29
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	2	0.29
(1,112)	1:188:A:GLY:C	1:190:A:GLY:CA	7	0.29
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	8	0.29
(1,92)	1:136:A:GLY:C	1:133:A:VAL:CG1	9	0.29
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	4	0.26
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	2	0.26
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	8	0.26
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	8	0.25
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	10	0.25
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	3	0.25
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	6	0.24
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	1	0.24
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	3	0.24
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	7	0.24
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	9	0.24
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	4	0.24
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	1	0.23
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	2	0.23
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	5	0.23
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	7	0.23
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	10	0.23
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	1	0.23
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	5	0.23
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	7	0.23
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	9	0.23
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	6	0.23
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	2	0.23
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	5	0.23
(1,35)	1:185:A:ASP:C	1:187:A:THR:CG2	6	0.23
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	1	0.23
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	2	0.23
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	3	0.23
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	5	0.23
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	6	0.23
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	7	0.23
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	10	0.23
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	1	0.22
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	1	0.22
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	4	0.22
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	6	0.22
(1,102)	1:218:A:ILE:C	1:222:A:LEU:CA	9	0.22
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	3	0.22
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	4	0.22
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	10	0.22
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	1	0.22
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	9	0.22
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	8	0.22
(1,14)	1:135:A:SER:C	1:137:A:GLN:CB	9	0.22
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	4	0.21
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	6	0.21
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	7	0.21
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	8	0.21
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	9	0.21
(1,86)	1:175:A:SER:C	1:173:A:GLY:CA	8	0.21
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	3	0.21
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	5	0.21
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	7	0.21
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	8	0.21
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	2	0.2
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	7	0.2
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	8	0.2
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	4	0.2
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	5	0.2
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	10	0.2
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	2	0.2
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	10	0.2
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	3	0.19
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	5	0.19
(1,151)	1:189:A:CYS:C	1:187:A:THR:CB	10	0.19
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	4	0.19
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	9	0.19
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	10	0.19
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	5	0.19
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	2	0.19
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	3	0.19
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	6	0.19
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	7	0.19
(1,49)	1:176:A:VAL:C	1:178:A:LEU:CB	4	0.19
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	6	0.18
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	9	0.18
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	1	0.18
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	3	0.18
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	5	0.18
(1,117)	1:103:A:VAL:C	1:101:A:GLN:CA	6	0.18
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	6	0.18
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	1	0.18
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	6	0.18
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	8	0.18
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	1	0.18
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	3	0.18
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	4	0.18
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	5	0.18
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	7	0.18
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	8	0.18
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	10	0.18
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	1	0.18
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	4	0.18
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	5	0.18
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	6	0.18
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	7	0.18
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	9	0.18
(1,6)	1:220:A:GLY:C	1:222:A:LEU:CG	10	0.18
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	5	0.17
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	4	0.17
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	2	0.17
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	3	0.17
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	4	0.17
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	7	0.17
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	9	0.17
(1,81)	1:189:A:CYS:C	1:184:A:ILE:CB	8	0.17
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	5	0.17
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	7	0.17
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	1	0.17
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	2	0.17
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	3	0.17
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	5	0.17
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	10	0.17
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	2	0.17
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	9	0.17
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	2	0.17
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	6	0.17
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	9	0.17
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	6	0.17
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	10	0.17
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	1	0.16
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	2	0.16
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	4	0.16
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	10	0.16
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	1	0.16
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	2	0.16
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	8	0.16
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	9	0.16
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	5	0.16
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	7	0.16
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	3	0.16
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	5	0.16
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	10	0.16
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	2	0.16
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	8	0.16
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	10	0.16
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	1	0.16
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	4	0.16
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	7	0.16
(1,70)	1:65:A:GLN:C	1:62:A:THR:CA	9	0.16
(1,69)	1:103:A:VAL:C	1:18:A:PHE:CA	6	0.16
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	1	0.16
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	3	0.16
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	5	0.16
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	7	0.16
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	8	0.16
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	9	0.16
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	10	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	1	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	2	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	3	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	4	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	5	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	6	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	7	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	8	0.16
(1,7)	1:222:A:LEU:C	1:224:A:VAL:CB	9	0.16
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	3	0.15
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	5	0.15
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	7	0.15
(1,176)	1:18:A:PHE:C	1:20:A:ALA:CB	8	0.15
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	4	0.15
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	6	0.15
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	7	0.15
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	9	0.15
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	10	0.15
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	1	0.15
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	2	0.15
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	5	0.15
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	6	0.15
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	5	0.15
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	6	0.15
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	8	0.15
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	10	0.15
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	2	0.15
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	9	0.15
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	1	0.15
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	2	0.15
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	8	0.15
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	3	0.15
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	6	0.15
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	7	0.15
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	10	0.15
(1,84)	1:15:A:VAL:C	1:19:A:LEU:CA	6	0.15
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	2	0.15
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	10	0.15
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	5	0.15
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	6	0.15
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	9	0.15
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	10	0.15
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	2	0.15
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	5	0.15
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	9	0.15
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	10	0.15
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	1	0.15
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	3	0.15
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	4	0.15
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	5	0.15
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	9	0.15
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	2	0.15
(1,174)	1:15:A:VAL:C	1:13:A:ALA:CA	3	0.14
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	7	0.14
(1,143)	1:195:A:ARG:C	1:190:A:GLY:CA	3	0.14
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	4	0.14
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	10	0.14
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	1	0.14
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	2	0.14
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	3	0.14
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	9	0.14
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	1	0.14
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	3	0.14
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	6	0.14
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	8	0.14
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	10	0.14
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	4	0.14
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	7	0.14
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	1	0.14
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	4	0.14
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	5	0.14
(1,90)	1:96:A:MET:C	1:94:A:ALA:CA	9	0.14
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	3	0.14
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	6	0.14
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	8	0.14
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	1	0.14
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	9	0.14
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	10	0.14
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	2	0.14
(1,36)	1:34:A:GLY:C	1:36:A:LYS:CG	1	0.14
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	1	0.14
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	3	0.14
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	4	0.14
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	6	0.14
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	7	0.14
(1,26)	1:59:A:SER:C	1:61:A:ALA:CB	8	0.14
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	7	0.14
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	8	0.14
(1,24)	1:15:A:VAL:C	1:17:A:GLU:CB	10	0.14
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	1	0.14
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	2	0.14
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	6	0.14
(1,19)	1:178:A:LEU:C	1:181:A:LEU:CG	4	0.14
(1,17)	1:137:A:GLN:C	1:141:A:ILE:CB	7	0.14
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	6	0.13
(1,149)	1:75:A:LEU:C	1:20:A:ALA:CB	8	0.13
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	3	0.13
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	8	0.13
(1,130)	1:51:A:LYS:C	1:55:A:ALA:CA	7	0.13
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	5	0.13
(1,126)	1:73:A:ALA:C	1:75:A:LEU:CG	7	0.13
(1,98)	1:27:A:ILE:C	1:29:A:ILE:CG1	4	0.13
(1,96)	1:61:A:ALA:C	1:63:A:LEU:CB	9	0.13
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	6	0.13
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	9	0.13
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	6	0.13
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	7	0.13
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	10	0.13
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	3	0.13
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	4	0.13
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	8	0.13
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	1	0.13
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	1	0.13
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	4	0.13
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	8	0.13
(1,45)	1:144:A:ILE:C	1:148:A:GLN:CB	7	0.13
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	7	0.13
(1,36)	1:34:A:GLY:C	1:36:A:LYS:CG	7	0.13
(1,36)	1:34:A:GLY:C	1:36:A:LYS:CG	8	0.13
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	7	0.13
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	10	0.13
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	1	0.13
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	5	0.13
(1,177)	1:24:A:PHE:C	1:28:A:SER:CA	5	0.12
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	3	0.12
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	4	0.12
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	8	0.12
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	9	0.12
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	7	0.12
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	9	0.12
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	2	0.12
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	3	0.12
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	4	0.12
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	9	0.12
(1,143)	1:195:A:ARG:C	1:190:A:GLY:CA	10	0.12
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	1	0.12
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	7	0.12
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	2	0.12
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	4	0.12
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	5	0.12
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	6	0.12
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	7	0.12
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	1	0.12
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	3	0.12
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	10	0.12
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	2	0.12
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	4	0.12
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	5	0.12
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	9	0.12
(1,79)	1:192:A:ASN:C	1:190:A:GLY:CA	4	0.12
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	6	0.12
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	7	0.12
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	4	0.12
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	5	0.12
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	8	0.12
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	6	0.12
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	7	0.12
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	10	0.12
(1,54)	1:222:A:LEU:C	1:226:A:ILE:CB	10	0.12
(1,45)	1:144:A:ILE:C	1:148:A:GLN:CB	9	0.12
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	1	0.12
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	4	0.12
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	5	0.12
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	9	0.12
(1,42)	1:218:A:ILE:C	1:222:A:LEU:CD1	10	0.12
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	8	0.12
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	4	0.12
(1,172)	1:178:A:LEU:C	1:182:A:LEU:CG	7	0.11
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	1	0.11
(1,168)	1:219:A:GLY:C	1:223:A:ALA:CB	8	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	1	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	2	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	3	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	4	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	5	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	6	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	8	0.11
(1,152)	1:62:A:THR:C	1:64:A:ALA:CB	10	0.11
(1,149)	1:75:A:LEU:C	1:20:A:ALA:CB	3	0.11
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	6	0.11
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	10	0.11
(1,143)	1:195:A:ARG:C	1:190:A:GLY:CA	5	0.11
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	1	0.11
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	2	0.11
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	4	0.11
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	7	0.11
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	9	0.11
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	10	0.11
(1,134)	1:178:A:LEU:C	1:180:A:HIS:CB	5	0.11
(1,134)	1:178:A:LEU:C	1:180:A:HIS:CB	7	0.11
(1,134)	1:178:A:LEU:C	1:180:A:HIS:CB	8	0.11
(1,134)	1:178:A:LEU:C	1:180:A:HIS:CB	10	0.11
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	2	0.11
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	4	0.11
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	6	0.11
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	8	0.11
(1,121)	1:113:A:SER:C	1:115:A:ILE:CB	2	0.11
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	3	0.11
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	9	0.11
(1,109)	1:58:A:LEU:C	1:60:A:ILE:CB	10	0.11
(1,103)	1:139:A:LEU:C	1:143:A:ILE:CB	4	0.11
(1,103)	1:139:A:LEU:C	1:143:A:ILE:CB	5	0.11
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	2	0.11
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	4	0.11
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	7	0.11
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	8	0.11
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	1	0.11
(1,85)	1:175:A:SER:C	1:179:A:GLY:CA	3	0.11
(1,73)	1:103:A:VAL:C	1:106:A:ILE:CG1	2	0.11
(1,67)	1:134:A:ASN:C	1:187:A:THR:CA	5	0.11
(1,61)	1:141:A:ILE:C	1:138:A:GLY:CA	7	0.11
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	2	0.11
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	3	0.11
(1,60)	1:36:A:LYS:C	1:34:A:GLY:CA	5	0.11
(1,56)	1:142:A:GLU:C	1:145:A:GLY:CA	2	0.11
(1,56)	1:142:A:GLU:C	1:145:A:GLY:CA	3	0.11
(1,56)	1:142:A:GLU:C	1:145:A:GLY:CA	8	0.11
(1,45)	1:144:A:ILE:C	1:148:A:GLN:CB	1	0.11
(1,45)	1:144:A:ILE:C	1:148:A:GLN:CB	6	0.11
(1,45)	1:144:A:ILE:C	1:148:A:GLN:CB	10	0.11
(1,36)	1:34:A:GLY:C	1:36:A:LYS:CG	2	0.11
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	4	0.11
(1,20)	1:214:A:VAL:C	1:216:A:PRO:CG	5	0.11
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	7	0.11
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	8	0.11
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	9	0.11
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	10	0.11
(1,170)	1:75:A:LEU:C	1:73:A:ALA:CB	2	0.1
(1,149)	1:75:A:LEU:C	1:20:A:ALA:CB	2	0.1
(1,149)	1:75:A:LEU:C	1:20:A:ALA:CB	7	0.1
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	1	0.1
(1,145)	1:185:A:ASP:C	1:188:A:GLY:CA	8	0.1
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	3	0.1
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	5	0.1
(1,141)	1:72:A:GLY:C	1:74:A:HIS:CB	8	0.1
(1,138)	1:146:A:THR:C	1:148:A:GLN:CG	7	0.1
(1,134)	1:178:A:LEU:C	1:180:A:HIS:CB	1	0.1
(1,134)	1:178:A:LEU:C	1:180:A:HIS:CB	9	0.1
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	9	0.1
(1,127)	1:190:A:GLY:C	1:183:A:ALA:CB	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:197:A:PHE:C	1:106:A:ILE:CG1	5	0.1
(1,121)	1:113:A:SER:C	1:115:A:ILE:CB	4	0.1
(1,121)	1:113:A:SER:C	1:115:A:ILE:CB	9	0.1
(1,88)	1:17:A:GLU:C	1:19:A:LEU:CB	5	0.1
(1,56)	1:142:A:GLU:C	1:145:A:GLY:CA	4	0.1
(1,56)	1:142:A:GLU:C	1:145:A:GLY:CA	10	0.1
(1,36)	1:34:A:GLY:C	1:36:A:LYS:CG	5	0.1
(1,36)	1:34:A:GLY:C	1:36:A:LYS:CG	9	0.1
(1,23)	1:176:A:VAL:C	1:149:A:LEU:CD1	1	0.1
(1,23)	1:176:A:VAL:C	1:149:A:LEU:CD1	2	0.1
(1,23)	1:176:A:VAL:C	1:149:A:LEU:CD1	7	0.1
(1,23)	1:176:A:VAL:C	1:149:A:LEU:CD1	8	0.1
(1,8)	1:142:A:GLU:C	1:146:A:THR:CA	6	0.1

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

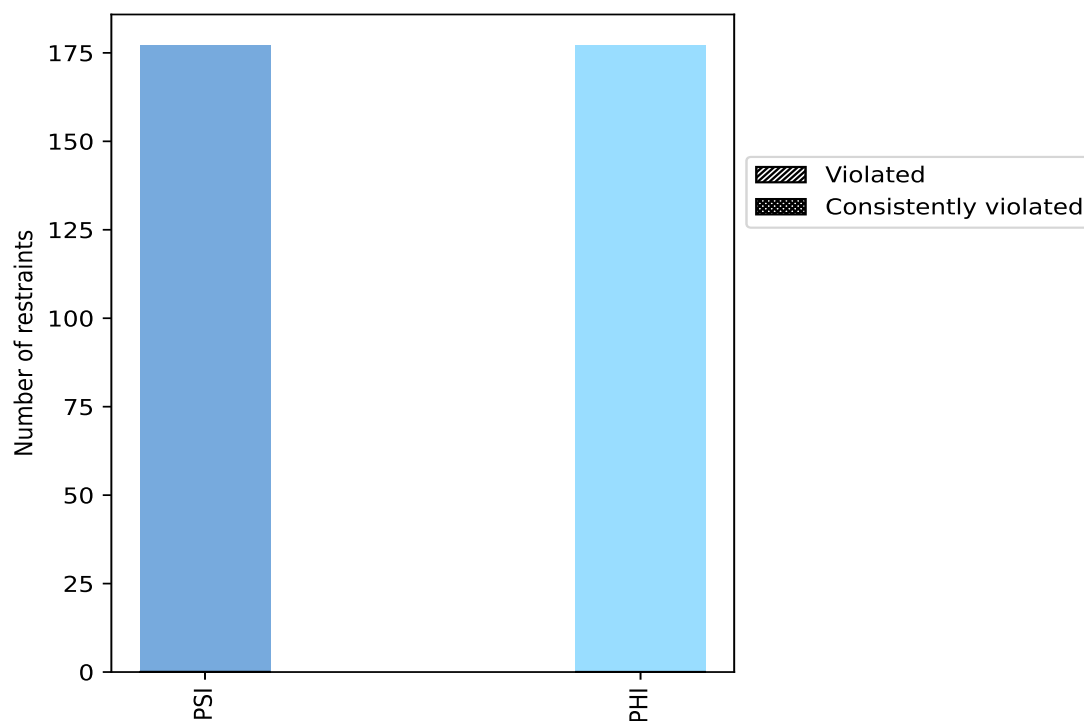
10.1 Summary of dihedral-angle violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	177	50.0	0	0.0	0.0	0	0.0	0.0
PHI	177	50.0	0	0.0	0.0	0	0.0	0.0
Total	354	100.0	0	0.0	0.0	0	0.0	0.0

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

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



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

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

No violations found

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

No violations found

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

No violations found

10.5 All violated dihedral-angle restraints [i](#)

No violations found