



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:32 PM UTC

PDB ID : 2RR8 / pdb_00002rr8
BMRB ID : 11175
Title : Solution structure of calponin homology domain of IQGAP1
Authors : Umemoto, R.; Nishida, N.; Ogino, S.; Shimada, I.
Deposited on : 2010-06-09

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

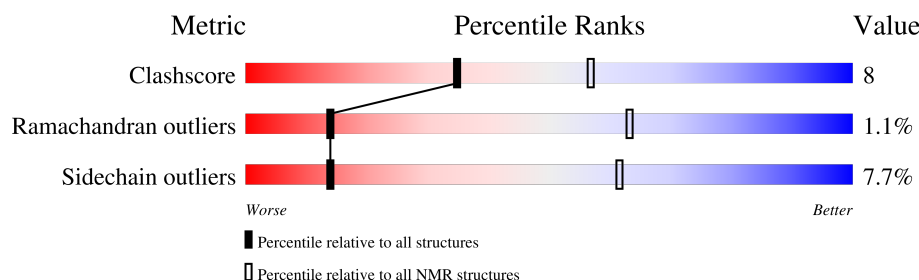
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	190	

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:37-A:202 (166)	1.20	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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3078 atoms, of which 1532 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called IQGAP1 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	190	Total	C	H	N	O	S	0
			3078	989	1532	258	289	10	

There are 5 discrepancies between the modelled and reference sequences:

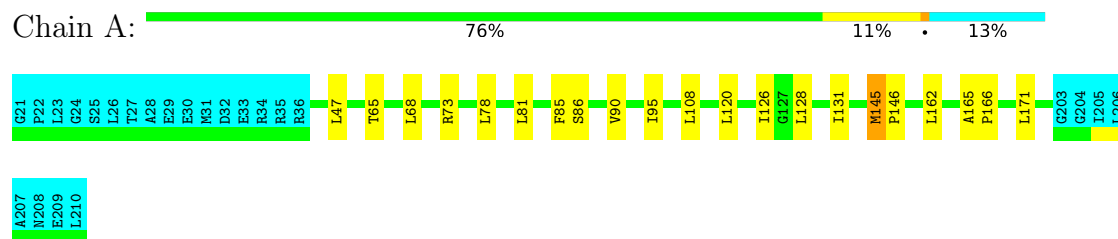
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP Q6P1N4
A	22	PRO	-	expression tag	UNP Q6P1N4
A	23	LEU	-	expression tag	UNP Q6P1N4
A	24	GLY	-	expression tag	UNP Q6P1N4
A	25	SER	-	expression tag	UNP Q6P1N4

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: IQGAP1 protein

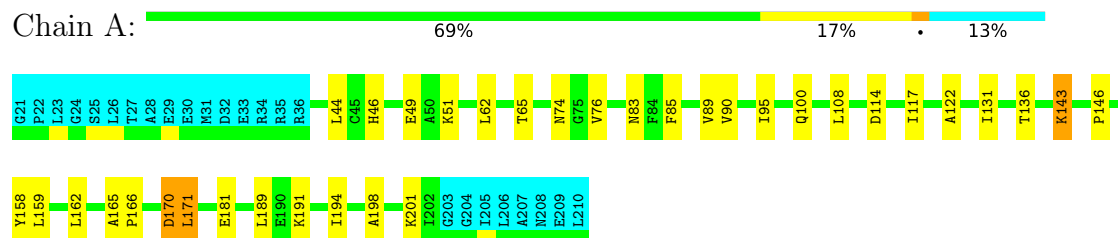


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

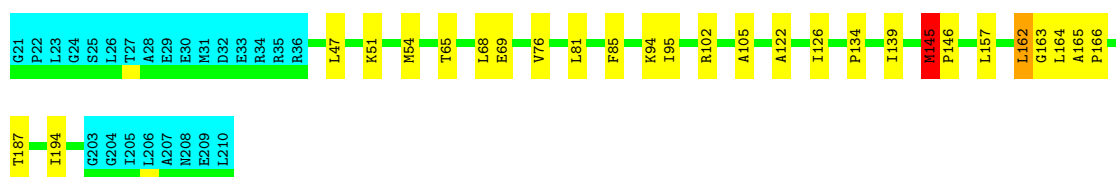
- Molecule 1: IQGAP1 protein



4.2.2 Score per residue for model 2

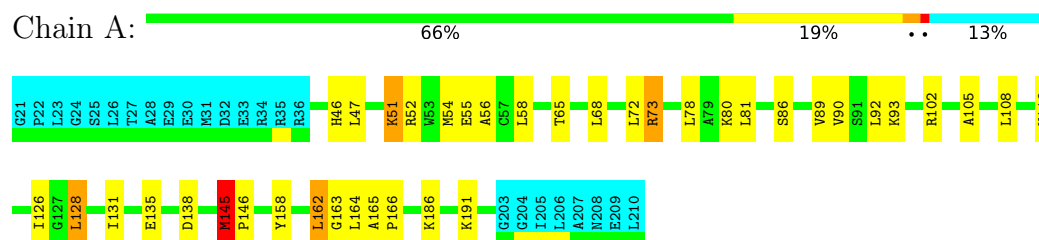
- Molecule 1: IQGAP1 protein





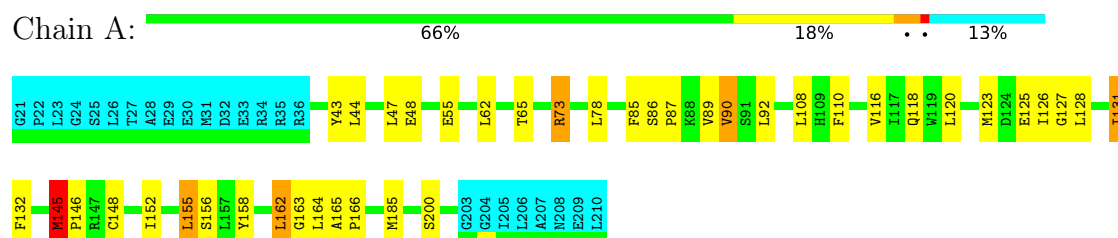
4.2.3 Score per residue for model 3

- Molecule 1: IQGAP1 protein



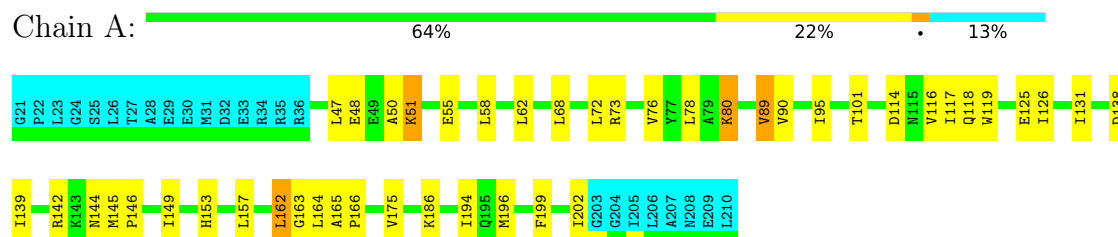
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: IQGAP1 protein



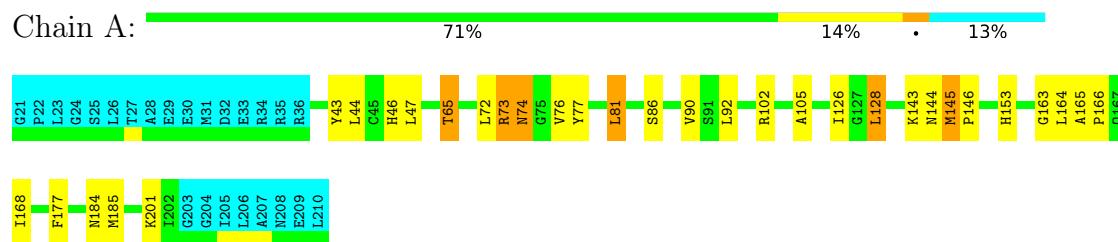
4.2.5 Score per residue for model 5

- Molecule 1: IQGAP1 protein



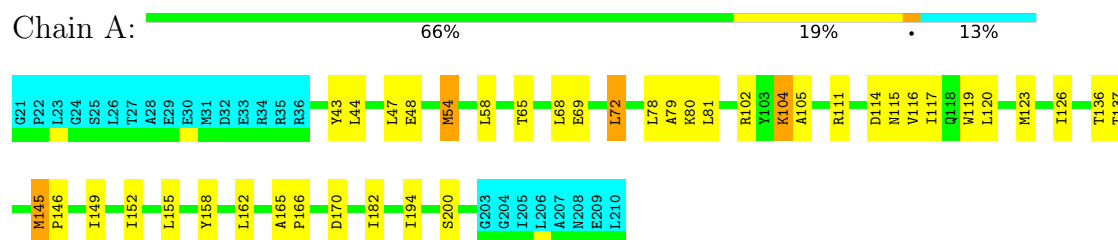
4.2.6 Score per residue for model 6

- Molecule 1: IQGAP1 protein



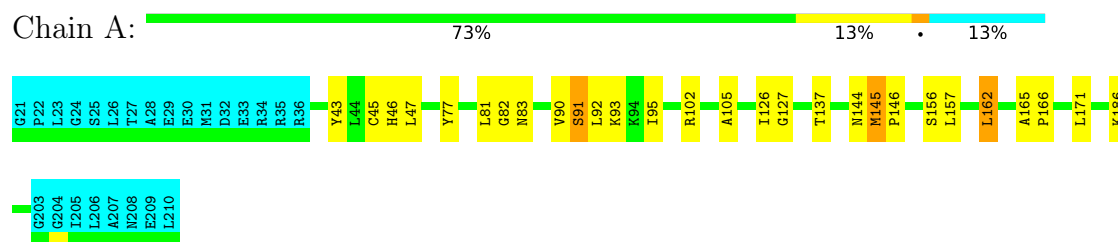
4.2.7 Score per residue for model 7

- Molecule 1: IQGAP1 protein



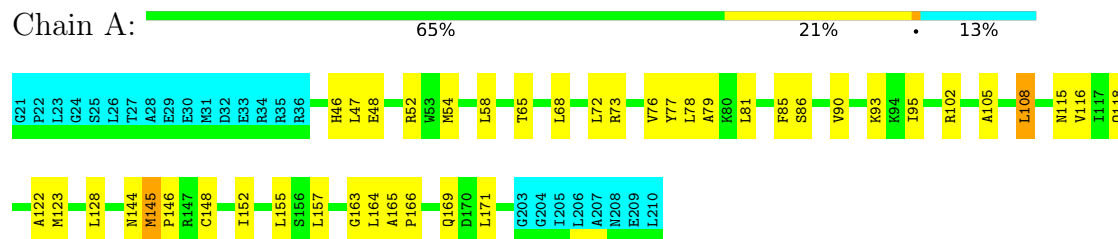
4.2.8 Score per residue for model 8

- Molecule 1: IQGAP1 protein



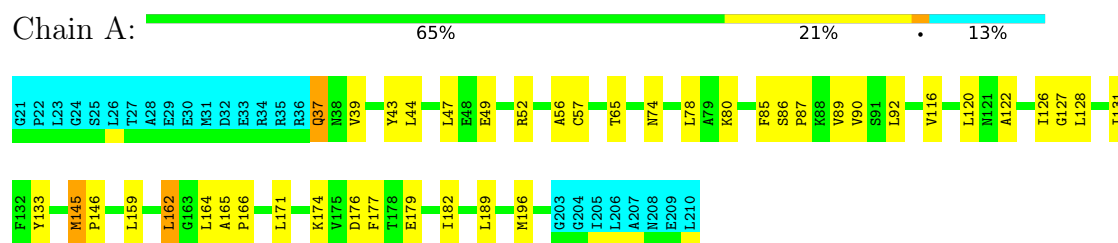
4.2.9 Score per residue for model 9

- Molecule 1: IQGAP1 protein

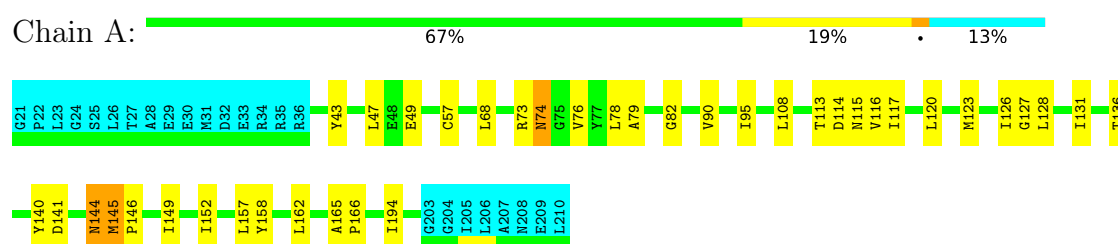


4.2.10 Score per residue for model 10

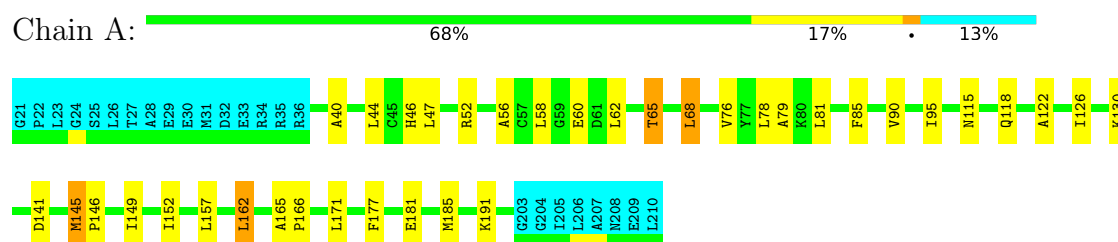
- Molecule 1: IQGAP1 protein



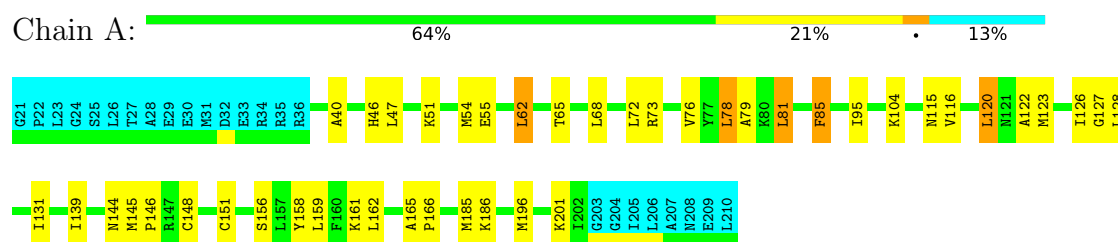
- Molecule 1: IQGAP1 protein



- Molecule 1: IQGAP1 protein

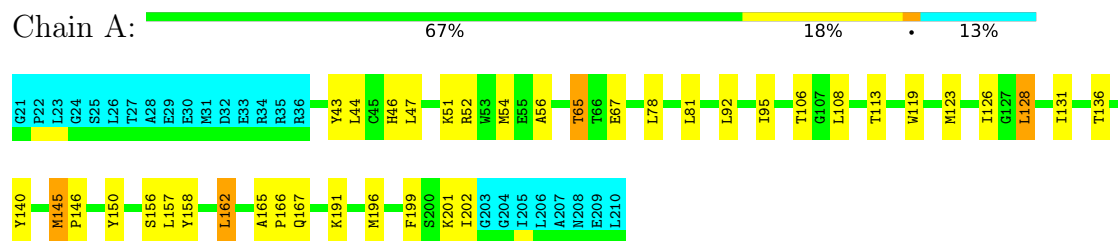


- Molecule 1: IQGAP1 protein



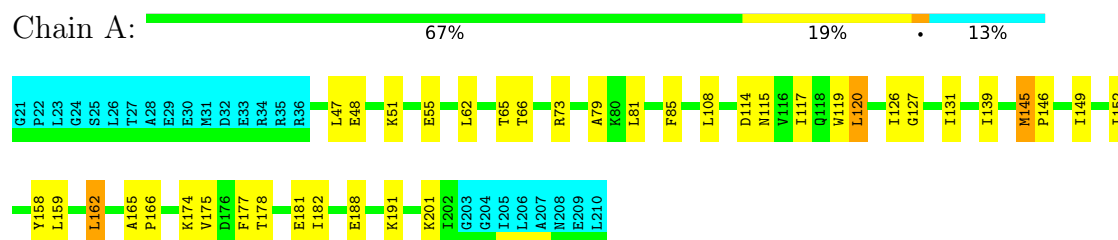
4.2.14 Score per residue for model 14

- Molecule 1: IQGAP1 protein



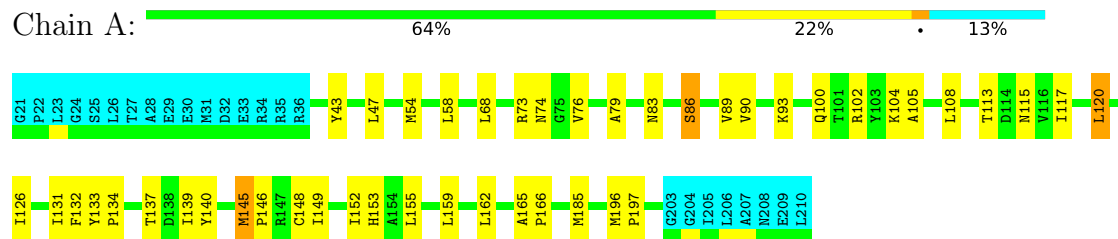
4.2.15 Score per residue for model 15

- Molecule 1: IQGAP1 protein



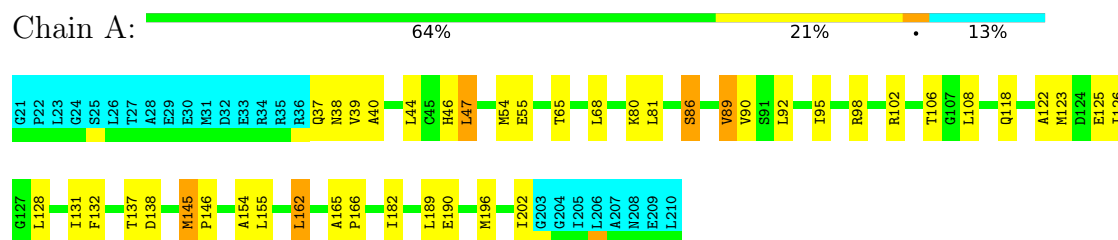
4.2.16 Score per residue for model 16

- Molecule 1: IQGAP1 protein



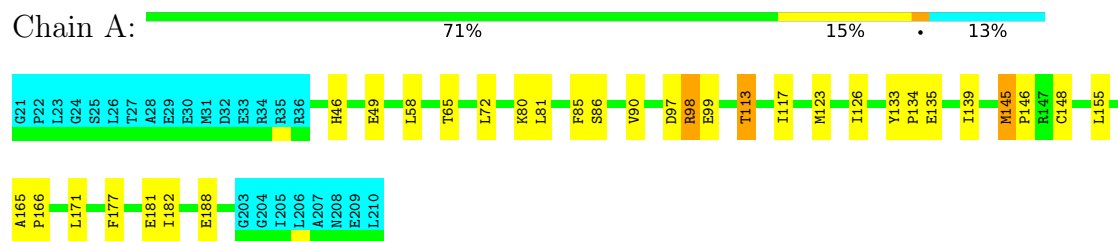
4.2.17 Score per residue for model 17

- Molecule 1: IQGAP1 protein



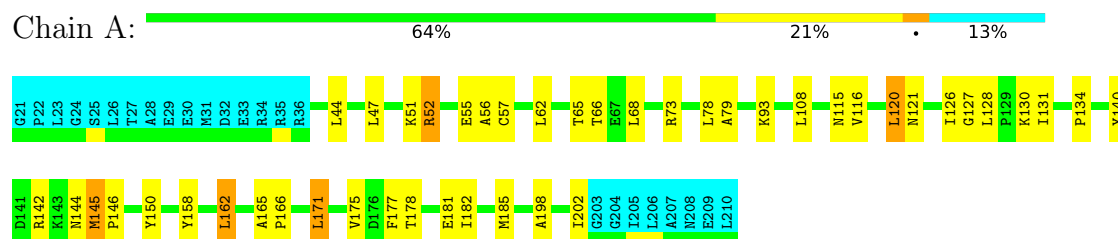
4.2.18 Score per residue for model 18

- Molecule 1: IQGAP1 protein



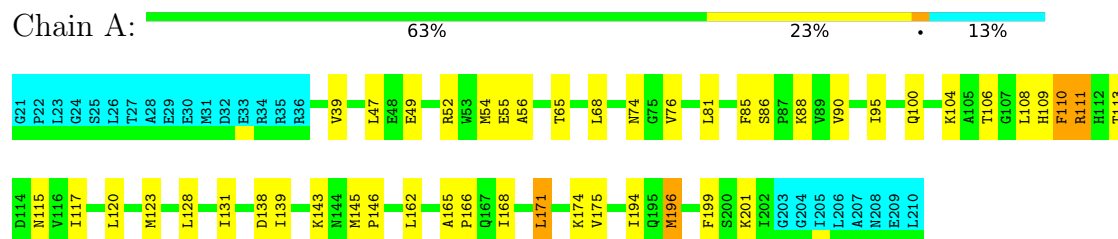
4.2.19 Score per residue for model 19

- Molecule 1: IQGAP1 protein



4.2.20 Score per residue for model 20

- Molecule 1: IQGAP1 protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	2.1

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	2093
Number of shifts mapped to atoms	2093
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	1367	1354	1354	22±5
All	All	27340	27080	27080	437

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:VAL:HG13	1:A:95:ILE:HG21	0.96	1.37	5	2
1:A:126:ILE:HG21	1:A:162:LEU:HD22	0.90	1.42	13	2
1:A:123:MET:HE1	1:A:155:LEU:HD21	0.89	1.43	7	1
1:A:159:LEU:HD13	1:A:162:LEU:HD11	0.87	1.45	15	1
1:A:159:LEU:HD12	1:A:162:LEU:HD11	0.86	1.48	10	1
1:A:47:LEU:HD23	1:A:65:THR:HG22	0.81	1.50	12	1
1:A:47:LEU:HD22	1:A:68:LEU:HD23	0.76	1.56	3	7
1:A:126:ILE:HD11	1:A:162:LEU:HD13	0.76	1.58	7	5
1:A:76:VAL:HG13	1:A:95:ILE:HG23	0.73	1.61	12	4
1:A:126:ILE:HD13	1:A:162:LEU:HD13	0.71	1.63	19	1
1:A:108:LEU:HD13	1:A:140:TYR:CD2	0.68	2.24	19	1
1:A:73:ARG:HD2	1:A:108:LEU:HD13	0.66	1.66	3	1
1:A:47:LEU:HB3	1:A:65:THR:HG23	0.65	1.67	17	3
1:A:90:VAL:HG12	1:A:118:GLN:HB3	0.65	1.68	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:HD13	1:A:158:TYR:CE1	0.65	2.27	19	1
1:A:73:ARG:HG2	1:A:145:MET:HE1	0.64	1.69	6	2
1:A:123:MET:CE	1:A:155:LEU:HD21	0.64	2.23	7	1
1:A:108:LEU:HD13	1:A:140:TYR:CE2	0.64	2.28	11	2
1:A:44:LEU:HD22	1:A:177:PHE:CE2	0.64	2.28	10	2
1:A:43:TYR:CD2	1:A:185:MET:HE3	0.63	2.28	6	3
1:A:76:VAL:HG13	1:A:95:ILE:CG2	0.63	2.22	20	4
1:A:85:PHE:CE1	1:A:155:LEU:HD21	0.63	2.29	18	1
1:A:131:ILE:HD11	1:A:132:PHE:CE2	0.63	2.29	4	2
1:A:43:TYR:CE2	1:A:47:LEU:HD11	0.62	2.30	8	6
1:A:73:ARG:O	1:A:108:LEU:HD11	0.62	1.95	9	1
1:A:43:TYR:CZ	1:A:47:LEU:HD11	0.62	2.30	11	3
1:A:116:VAL:CG1	1:A:136:THR:HG23	0.61	2.25	11	1
1:A:120:LEU:HD11	1:A:133:TYR:CE1	0.61	2.30	16	1
1:A:146:PRO:HG3	1:A:194:ILE:HG21	0.61	1.70	5	2
1:A:86:SER:O	1:A:90:VAL:HG22	0.61	1.96	6	8
1:A:163:GLY:C	1:A:164:LEU:HD22	0.61	2.21	4	4
1:A:44:LEU:HG	1:A:185:MET:HE2	0.60	1.72	6	2
1:A:76:VAL:HG23	1:A:95:ILE:CG2	0.60	2.26	1	1
1:A:126:ILE:CG2	1:A:162:LEU:HD22	0.60	2.26	4	1
1:A:44:LEU:HD13	1:A:177:PHE:CD2	0.60	2.32	10	1
1:A:163:GLY:C	1:A:164:LEU:HD12	0.60	2.21	5	2
1:A:158:TYR:CE1	1:A:162:LEU:HD21	0.59	2.33	14	2
1:A:131:ILE:HD11	1:A:132:PHE:CZ	0.59	2.33	4	1
1:A:78:LEU:HG	1:A:116:VAL:HG22	0.59	1.74	13	8
1:A:51:LYS:NZ	1:A:68:LEU:HD22	0.58	2.13	13	1
1:A:126:ILE:HG21	1:A:162:LEU:CD2	0.58	2.28	11	1
1:A:126:ILE:HG13	1:A:162:LEU:HD21	0.58	1.75	5	1
1:A:54:MET:HE3	1:A:81:LEU:CD2	0.58	2.28	13	1
1:A:73:ARG:CG	1:A:145:MET:HE1	0.58	2.29	6	1
1:A:114:ASP:HA	1:A:117:ILE:HD12	0.58	1.73	7	4
1:A:149:ILE:HA	1:A:152:ILE:HD12	0.58	1.76	15	3
1:A:148:CYS:O	1:A:152:ILE:HD12	0.57	1.99	9	2
1:A:170:ASP:C	1:A:171:LEU:HD13	0.57	2.24	1	1
1:A:123:MET:HB3	1:A:128:LEU:HD12	0.57	1.75	9	2
1:A:74:ASN:CG	1:A:76:VAL:HG12	0.56	2.24	1	1
1:A:58:LEU:HD11	1:A:81:LEU:HA	0.56	1.76	12	1
1:A:126:ILE:CG1	1:A:162:LEU:HD21	0.56	2.30	5	1
1:A:128:LEU:HD23	1:A:133:TYR:CE1	0.56	2.36	10	1
1:A:154:ALA:HB2	1:A:202:ILE:HG21	0.56	1.77	17	1
1:A:134:PRO:HG2	1:A:139:ILE:HD11	0.56	1.76	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LEU:HD13	1:A:162:LEU:CD1	0.56	2.27	15	1
1:A:85:PHE:CE2	1:A:159:LEU:HD13	0.56	2.36	13	1
1:A:113:THR:HG23	1:A:140:TYR:CE2	0.56	2.36	14	2
1:A:123:MET:HB2	1:A:128:LEU:HD12	0.56	1.76	20	1
1:A:146:PRO:HG3	1:A:194:ILE:HG23	0.56	1.75	1	1
1:A:116:VAL:CG1	1:A:139:ILE:HD12	0.56	2.31	5	1
1:A:77:TYR:O	1:A:81:LEU:HD23	0.56	2.01	9	3
1:A:123:MET:HE3	1:A:133:TYR:HB3	0.56	1.75	18	1
1:A:120:LEU:O	1:A:120:LEU:HD13	0.55	2.01	7	3
1:A:189:LEU:HD22	1:A:196:MET:HG3	0.55	1.77	10	1
1:A:81:LEU:HD21	1:A:85:PHE:CE2	0.55	2.36	15	1
1:A:74:ASN:HB2	1:A:76:VAL:HG22	0.55	1.77	6	1
1:A:74:ASN:HB3	1:A:76:VAL:HG22	0.55	1.77	16	1
1:A:85:PHE:CE1	1:A:122:ALA:HB1	0.55	2.37	10	2
1:A:89:VAL:HG23	1:A:125:GLU:OE1	0.55	2.01	5	1
1:A:78:LEU:HD21	1:A:139:ILE:HD13	0.55	1.79	13	1
1:A:44:LEU:HD11	1:A:181:GLU:HG3	0.55	1.79	12	2
1:A:178:THR:O	1:A:182:ILE:HD12	0.54	2.02	19	2
1:A:95:ILE:HD13	1:A:98:ARG:NH1	0.54	2.18	17	1
1:A:90:VAL:HG12	1:A:118:GLN:CB	0.54	2.32	17	2
1:A:82:GLY:C	1:A:90:VAL:HG21	0.54	2.26	8	2
1:A:91:SER:C	1:A:92:LEU:HD23	0.54	2.28	8	1
1:A:58:LEU:HD11	1:A:80:LYS:CG	0.54	2.32	5	1
1:A:126:ILE:CD1	1:A:162:LEU:HD13	0.54	2.32	17	5
1:A:126:ILE:HG22	1:A:162:LEU:HD22	0.54	1.78	4	1
1:A:158:TYR:O	1:A:162:LEU:HD12	0.54	2.03	4	2
1:A:120:LEU:HD21	1:A:133:TYR:CD1	0.53	2.38	16	1
1:A:47:LEU:CB	1:A:65:THR:HG22	0.53	2.34	6	1
1:A:49:GLU:OE1	1:A:171:LEU:HD12	0.53	2.04	18	1
1:A:153:HIS:CE1	1:A:168:ILE:HD13	0.53	2.38	6	1
1:A:73:ARG:O	1:A:139:ILE:HG22	0.53	2.03	15	1
1:A:73:ARG:HD3	1:A:108:LEU:HD12	0.53	1.79	9	1
1:A:37:GLN:NE2	1:A:182:ILE:HG21	0.53	2.18	10	1
1:A:126:ILE:HD11	1:A:162:LEU:HD22	0.53	1.81	7	1
1:A:44:LEU:O	1:A:65:THR:HG21	0.53	2.04	14	1
1:A:146:PRO:HG2	1:A:194:ILE:HG21	0.53	1.81	7	2
1:A:126:ILE:CD1	1:A:162:LEU:HD22	0.53	2.34	7	1
1:A:73:ARG:CD	1:A:108:LEU:HD12	0.52	2.34	9	1
1:A:86:SER:OG	1:A:122:ALA:HB1	0.52	2.04	17	1
1:A:120:LEU:HD21	1:A:134:PRO:HD2	0.52	1.82	19	1
1:A:54:MET:HE1	1:A:81:LEU:HD22	0.52	1.81	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:THR:O	1:A:117:ILE:HD12	0.52	2.04	11	4
1:A:126:ILE:HD12	1:A:158:TYR:CE1	0.52	2.40	7	1
1:A:134:PRO:CG	1:A:139:ILE:HD11	0.52	2.35	2	3
1:A:128:LEU:HD11	1:A:158:TYR:CE2	0.52	2.40	13	1
1:A:171:LEU:HD13	1:A:171:LEU:N	0.51	2.19	1	1
1:A:55:GLU:CB	1:A:62:LEU:HD13	0.51	2.35	5	2
1:A:44:LEU:HD12	1:A:182:ILE:HG12	0.51	1.82	17	3
1:A:126:ILE:HD11	1:A:162:LEU:CD1	0.51	2.33	7	1
1:A:37:GLN:HB3	1:A:40:ALA:HB3	0.51	1.82	17	1
1:A:120:LEU:HA	1:A:123:MET:HE3	0.51	1.82	4	2
1:A:54:MET:HB2	1:A:81:LEU:HD21	0.51	1.80	14	1
1:A:157:LEU:HD21	1:A:202:ILE:HG22	0.51	1.82	5	1
1:A:65:THR:HA	1:A:68:LEU:HD23	0.51	1.82	12	1
1:A:40:ALA:HB1	1:A:185:MET:HB2	0.51	1.83	13	2
1:A:47:LEU:CD2	1:A:68:LEU:HD23	0.51	2.36	16	2
1:A:85:PHE:HB2	1:A:159:LEU:HD11	0.50	1.83	1	1
1:A:73:ARG:HD2	1:A:108:LEU:HD11	0.50	1.81	4	1
1:A:198:ALA:HB3	1:A:201:LYS:CG	0.50	2.36	1	1
1:A:47:LEU:CB	1:A:65:THR:HG23	0.50	2.37	9	8
1:A:60:GLU:OE2	1:A:62:LEU:HD11	0.50	2.06	12	1
1:A:145:MET:N	1:A:146:PRO:HD2	0.50	2.22	13	17
1:A:78:LEU:HD12	1:A:119:TRP:CE3	0.50	2.41	14	2
1:A:116:VAL:HG11	1:A:139:ILE:HD12	0.50	1.83	5	1
1:A:44:LEU:HD13	1:A:177:PHE:CG	0.50	2.41	12	2
1:A:156:SER:OG	1:A:157:LEU:HD12	0.50	2.06	14	2
1:A:79:ALA:HB2	1:A:115:ASN:HB3	0.50	1.84	7	8
1:A:79:ALA:HB2	1:A:115:ASN:CB	0.50	2.37	11	3
1:A:47:LEU:HD22	1:A:185:MET:HE1	0.49	1.84	4	1
1:A:54:MET:SD	1:A:81:LEU:HD13	0.49	2.47	20	2
1:A:126:ILE:HG21	1:A:162:LEU:HD13	0.49	1.84	4	1
1:A:58:LEU:HD22	1:A:80:LYS:HE2	0.49	1.85	3	2
1:A:87:PRO:HB2	1:A:92:LEU:HD12	0.49	1.84	4	1
1:A:123:MET:HB3	1:A:128:LEU:HD22	0.49	1.83	4	1
1:A:83:ASN:HB2	1:A:90:VAL:HG21	0.49	1.85	1	1
1:A:126:ILE:HD12	1:A:162:LEU:CD2	0.49	2.37	3	4
1:A:123:MET:HG2	1:A:155:LEU:HD11	0.49	1.85	4	1
1:A:66:THR:HG22	1:A:181:GLU:CD	0.49	2.32	15	1
1:A:48:GLU:OE1	1:A:175:VAL:HG11	0.49	2.06	15	1
1:A:81:LEU:HD12	1:A:119:TRP:HE1	0.48	1.68	15	1
1:A:51:LYS:HG2	1:A:62:LEU:HD22	0.48	1.85	1	1
1:A:149:ILE:HG22	1:A:153:HIS:CD2	0.48	2.43	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ILE:HD11	1:A:132:PHE:CE1	0.48	2.44	16	1
1:A:97:ASP:O	1:A:98:ARG:C	0.48	2.57	18	1
1:A:66:THR:HG22	1:A:181:GLU:OE1	0.48	2.08	19	1
1:A:123:MET:HB3	1:A:128:LEU:HD23	0.47	1.85	14	1
1:A:54:MET:CE	1:A:72:LEU:HD21	0.47	2.39	7	2
1:A:76:VAL:HG21	1:A:100:GLN:NE2	0.47	2.25	16	1
1:A:139:ILE:HG23	1:A:145:MET:SD	0.47	2.49	5	1
1:A:149:ILE:HD13	1:A:152:ILE:HD12	0.47	1.84	12	1
1:A:171:LEU:HD23	1:A:174:LYS:CB	0.47	2.39	20	1
1:A:79:ALA:HB3	1:A:95:ILE:CD1	0.47	2.40	9	1
1:A:76:VAL:HG23	1:A:95:ILE:HG21	0.47	1.86	1	1
1:A:126:ILE:HD12	1:A:162:LEU:HD11	0.47	1.87	5	1
1:A:55:GLU:OE1	1:A:62:LEU:HD11	0.47	2.09	13	1
1:A:163:GLY:O	1:A:164:LEU:HD22	0.47	2.08	3	2
1:A:108:LEU:HD13	1:A:140:TYR:CZ	0.47	2.45	11	1
1:A:196:MET:HE3	1:A:197:PRO:HD2	0.47	1.86	16	1
1:A:81:LEU:C	1:A:81:LEU:HD13	0.47	2.35	15	1
1:A:145:MET:CB	1:A:146:PRO:CD	0.46	2.93	2	9
1:A:83:ASN:OD1	1:A:90:VAL:HG21	0.46	2.11	16	1
1:A:126:ILE:CG2	1:A:128:LEU:HD12	0.46	2.41	6	2
1:A:54:MET:HG3	1:A:81:LEU:HD13	0.46	1.88	3	1
1:A:128:LEU:HD13	1:A:158:TYR:CZ	0.46	2.45	19	1
1:A:87:PRO:O	1:A:92:LEU:HD21	0.46	2.11	10	1
1:A:126:ILE:HG22	1:A:128:LEU:HD12	0.46	1.88	6	1
1:A:81:LEU:HD22	1:A:119:TRP:HE1	0.45	1.70	7	1
1:A:144:ASN:ND2	1:A:194:ILE:HD13	0.45	2.26	11	1
1:A:189:LEU:HD12	1:A:189:LEU:O	0.45	2.12	1	2
1:A:169:GLN:NE2	1:A:171:LEU:HD11	0.45	2.26	9	1
1:A:146:PRO:CG	1:A:194:ILE:HG21	0.45	2.41	2	1
1:A:90:VAL:HG13	1:A:118:GLN:HB3	0.45	1.87	12	1
1:A:51:LYS:O	1:A:62:LEU:HD12	0.45	2.11	15	1
1:A:51:LYS:HB3	1:A:68:LEU:HD13	0.45	1.89	5	1
1:A:123:MET:CB	1:A:128:LEU:HD12	0.45	2.41	9	3
1:A:95:ILE:HD13	1:A:98:ARG:HH11	0.44	1.71	17	1
1:A:171:LEU:HD12	1:A:175:VAL:HG11	0.44	1.88	19	1
1:A:158:TYR:CZ	1:A:162:LEU:HD11	0.44	2.47	4	1
1:A:39:VAL:HG21	1:A:196:MET:HB2	0.44	1.89	10	1
1:A:39:VAL:HG13	1:A:196:MET:SD	0.44	2.53	20	1
1:A:85:PHE:CZ	1:A:122:ALA:HB1	0.44	2.47	12	2
1:A:44:LEU:HA	1:A:47:LEU:HD12	0.44	1.88	6	1
1:A:116:VAL:HB	1:A:136:THR:HG23	0.44	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:ALA:HB1	1:A:166:PRO:HD2	0.44	1.90	16	20
1:A:102:ARG:O	1:A:105:ALA:HB3	0.44	2.13	3	7
1:A:145:MET:N	1:A:146:PRO:CD	0.44	2.81	5	5
1:A:40:ALA:HB1	1:A:185:MET:CB	0.44	2.43	13	1
1:A:72:LEU:HD21	1:A:148:CYS:SG	0.44	2.53	18	1
1:A:55:GLU:HB3	1:A:62:LEU:HD13	0.43	1.88	5	1
1:A:74:ASN:HA	1:A:108:LEU:HD21	0.43	1.89	20	1
1:A:171:LEU:HD23	1:A:174:LYS:HB2	0.43	1.90	20	1
1:A:52:ARG:O	1:A:56:ALA:HB2	0.43	2.14	19	6
1:A:92:LEU:O	1:A:93:LYS:C	0.43	2.61	3	1
1:A:149:ILE:HG22	1:A:153:HIS:HD2	0.43	1.73	16	1
1:A:126:ILE:CD1	1:A:162:LEU:HD11	0.43	2.42	8	2
1:A:157:LEU:HD21	1:A:202:ILE:CG2	0.43	2.43	5	1
1:A:123:MET:CG	1:A:128:LEU:HD12	0.43	2.44	17	1
1:A:154:ALA:HB2	1:A:202:ILE:CG2	0.43	2.43	17	1
1:A:126:ILE:CG2	1:A:128:LEU:HD22	0.43	2.44	14	1
1:A:128:LEU:HD13	1:A:158:TYR:CE2	0.43	2.49	11	1
1:A:55:GLU:CD	1:A:62:LEU:HD21	0.43	2.39	13	1
1:A:139:ILE:HG23	1:A:145:MET:HE3	0.43	1.90	20	1
1:A:177:PHE:HB2	1:A:182:ILE:HD11	0.43	1.90	15	2
1:A:54:MET:HE3	1:A:81:LEU:HD12	0.43	1.89	17	1
1:A:123:MET:HE3	1:A:151:CYS:SG	0.43	2.54	13	1
1:A:110:PHE:O	1:A:111:ARG:CB	0.43	2.67	20	1
1:A:48:GLU:OE2	1:A:175:VAL:HG21	0.43	2.14	5	1
1:A:43:TYR:CD2	1:A:47:LEU:HD11	0.43	2.48	7	1
1:A:51:LYS:HB3	1:A:68:LEU:HD11	0.42	1.90	3	1
1:A:113:THR:HG23	1:A:140:TYR:CD2	0.42	2.49	14	1
1:A:150:TYR:CE1	1:A:202:ILE:HD11	0.42	2.48	19	2
1:A:83:ASN:ND2	1:A:92:LEU:HD22	0.42	2.29	8	1
1:A:108:LEU:HD21	1:A:140:TYR:CE2	0.42	2.49	16	1
1:A:49:GLU:HG3	1:A:168:ILE:HD11	0.42	1.91	20	1
1:A:69:GLU:HB2	1:A:145:MET:HE3	0.42	1.91	7	1
1:A:169:GLN:CD	1:A:171:LEU:HD11	0.42	2.39	9	1
1:A:79:ALA:HB2	1:A:115:ASN:CG	0.42	2.40	11	1
1:A:44:LEU:HD22	1:A:177:PHE:CE1	0.42	2.50	6	1
1:A:123:MET:CB	1:A:128:LEU:HD13	0.42	2.44	3	1
1:A:120:LEU:HD23	1:A:120:LEU:O	0.42	2.15	20	2
1:A:74:ASN:O	1:A:78:LEU:HD23	0.42	2.15	11	1
1:A:73:ARG:HH11	1:A:108:LEU:HD22	0.42	1.75	3	1
1:A:72:LEU:HD22	1:A:149:ILE:CD1	0.42	2.45	5	1
1:A:58:LEU:CD1	1:A:81:LEU:HD22	0.42	2.45	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:HD11	1:A:81:LEU:HD22	0.42	1.91	9	1
1:A:47:LEU:HD21	1:A:68:LEU:CB	0.42	2.45	12	1
1:A:55:GLU:CD	1:A:62:LEU:HD22	0.42	2.40	19	1
1:A:145:MET:HB3	1:A:146:PRO:HD3	0.42	1.92	10	5
1:A:131:ILE:HD12	1:A:131:ILE:O	0.42	2.15	16	1
1:A:128:LEU:HD21	1:A:158:TYR:CD1	0.41	2.50	13	1
1:A:38:ASN:OD1	1:A:39:VAL:HG23	0.41	2.15	17	1
1:A:158:TYR:CD1	1:A:162:LEU:HD21	0.41	2.49	14	1
1:A:51:LYS:HB2	1:A:68:LEU:HD21	0.41	1.90	19	1
1:A:54:MET:HE2	1:A:72:LEU:HD21	0.41	1.92	7	1
1:A:85:PHE:HE1	1:A:122:ALA:HB1	0.41	1.76	13	1
1:A:171:LEU:HD22	1:A:175:VAL:CG1	0.41	2.45	20	1
1:A:148:CYS:C	1:A:152:ILE:HD12	0.41	2.40	4	1
1:A:51:LYS:HZ2	1:A:68:LEU:HD22	0.41	1.71	13	1
1:A:158:TYR:O	1:A:162:LEU:HD23	0.41	2.16	1	1
1:A:51:LYS:CB	1:A:68:LEU:HD13	0.41	2.46	5	1
1:A:150:TYR:CD1	1:A:202:ILE:HD11	0.41	2.50	19	1
1:A:126:ILE:HG12	1:A:162:LEU:HD13	0.41	1.93	11	1
1:A:89:VAL:HG11	1:A:122:ALA:HA	0.41	1.93	1	2
1:A:158:TYR:CD2	1:A:162:LEU:HD21	0.41	2.51	15	1
1:A:50:ALA:HB2	1:A:153:HIS:NE2	0.41	2.31	5	1
1:A:47:LEU:HG	1:A:68:LEU:HD23	0.40	1.93	5	1
1:A:92:LEU:HD12	1:A:95:ILE:HD12	0.40	1.93	14	1
1:A:76:VAL:HG23	1:A:95:ILE:HG23	0.40	1.91	1	1
1:A:81:LEU:HD13	1:A:81:LEU:O	0.40	2.16	15	1
1:A:47:LEU:HD23	1:A:65:THR:O	0.40	2.16	17	1
1:A:158:TYR:CD1	1:A:158:TYR:C	0.40	2.99	14	1
1:A:85:PHE:HE2	1:A:159:LEU:HD13	0.40	1.73	13	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	166/190 (87%)	149±3 (90±2%)	16±3 (9±2%)	2±1 (1±1%)	14	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3320/3800 (87%)	2973 (90%)	312 (9%)	35 (1%)	14	63

All 10 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	145	MET	14
1	A	127	GLY	7
1	A	89	VAL	6
1	A	199	PHE	2
1	A	143	LYS	1
1	A	90	VAL	1
1	A	95	ILE	1
1	A	156	SER	1
1	A	58	LEU	1
1	A	198	ALA	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	148/166 (89%)	137±3 (92±2%)	11±3 (8±2%)	14	61
All	All	2960/3320 (89%)	2733 (92%)	227 (8%)	14	61

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	162	LEU	12
1	A	46	HIS	10
1	A	65	THR	8
1	A	73	ARG	7
1	A	144	ASN	7
1	A	171	LEU	6
1	A	120	LEU	6
1	A	108	LEU	5
1	A	191	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	145	MET	5
1	A	196	MET	5
1	A	51	LYS	4
1	A	157	LEU	4
1	A	55	GLU	4
1	A	72	LEU	4
1	A	138	ASP	4
1	A	186	LYS	4
1	A	155	LEU	4
1	A	80	LYS	4
1	A	104	LYS	4
1	A	137	THR	4
1	A	93	LYS	4
1	A	201	LYS	4
1	A	49	GLU	3
1	A	143	LYS	3
1	A	128	LEU	3
1	A	48	GLU	3
1	A	85	PHE	3
1	A	74	ASN	3
1	A	81	LEU	3
1	A	57	CYS	3
1	A	68	LEU	3
1	A	106	THR	3
1	A	100	GLN	2
1	A	136	THR	2
1	A	170	ASP	2
1	A	135	GLU	2
1	A	110	PHE	2
1	A	125	GLU	2
1	A	200	SER	2
1	A	142	ARG	2
1	A	92	LEU	2
1	A	54	MET	2
1	A	111	ARG	2
1	A	52	ARG	2
1	A	174	LYS	2
1	A	141	ASP	2
1	A	78	LEU	2
1	A	130	LYS	2
1	A	188	GLU	2
1	A	86	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	47	LEU	2
1	A	69	GLU	1
1	A	94	LYS	1
1	A	187	THR	1
1	A	131	ILE	1
1	A	156	SER	1
1	A	101	THR	1
1	A	199	PHE	1
1	A	184	ASN	1
1	A	45	CYS	1
1	A	91	SER	1
1	A	37	GLN	1
1	A	164	LEU	1
1	A	176	ASP	1
1	A	179	GLU	1
1	A	114	ASP	1
1	A	62	LEU	1
1	A	148	CYS	1
1	A	161	LYS	1
1	A	67	GLU	1
1	A	167	GLN	1
1	A	58	LEU	1
1	A	159	LEU	1
1	A	102	ARG	1
1	A	189	LEU	1
1	A	190	GLU	1
1	A	98	ARG	1
1	A	99	GLU	1
1	A	113	THR	1
1	A	126	ILE	1
1	A	181	GLU	1
1	A	121	ASN	1
1	A	185	MET	1
1	A	88	LYS	1
1	A	109	HIS	1
1	A	115	ASN	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 79% for the well-defined parts and 78% 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	2093
Number of shifts mapped to atoms	2093
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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	1.90 ± 0.12	Should be checked
$^{13}\text{C}_\beta$	177	2.91 ± 0.05	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	167	0.55 ± 0.30	None needed (imprecise)

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 79%, i.e. 1856 atoms were assigned a chemical shift out of a possible 2357. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	637/823 (77%)	323/333 (97%)	166/332 (50%)	148/158 (94%)
Sidechain	1119/1313 (85%)	745/851 (88%)	364/414 (88%)	10/48 (21%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	100/221 (45%)	51/107 (48%)	47/108 (44%)	2/6 (33%)
Overall	1856/2357 (79%)	1119/1291 (87%)	577/854 (68%)	160/212 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 2093 atoms were assigned a chemical shift out of a possible 2673. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	726/945 (77%)	369/384 (96%)	190/380 (50%)	167/181 (92%)
Sidechain	1267/1507 (84%)	842/976 (86%)	414/473 (88%)	11/58 (19%)
Aromatic	100/221 (45%)	51/107 (48%)	47/108 (44%)	2/6 (33%)
Overall	2093/2673 (78%)	1262/1467 (86%)	651/961 (68%)	180/245 (73%)

7.1.4 Statistically unusual chemical shifts ⓘ

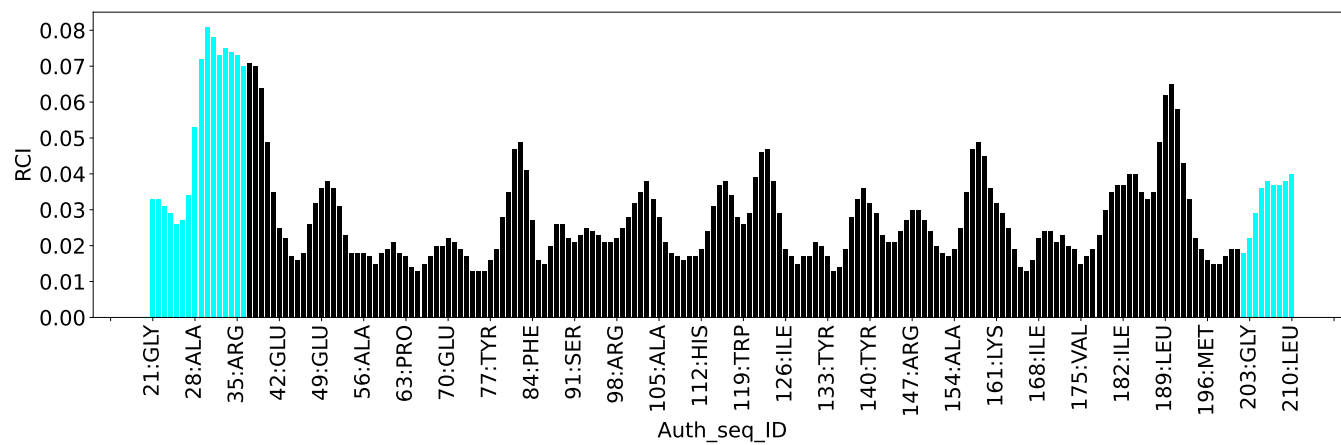
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	146	PRO	CD	19.91	45.11 – 55.58	-29.1
1	A	156	SER	HB3	1.77	2.49 – 5.20	-7.7
1	A	156	SER	HB2	2.26	2.61 – 5.13	-6.4
1	A	57	CYS	HB3	0.60	0.69 – 5.10	-5.2

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	1468
Intra-residue ($ i-j =0$)	259
Sequential ($ i-j =1$)	419
Medium range ($ i-j >1$ and $ i-j <5$)	385
Long range ($ i-j \geq 5$)	405
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	7.7
Number of long range restraints per residue ¹	2.1

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)	0.8	0.2
0.2-0.5 (Medium)	0.5	0.4
>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 ⓘ

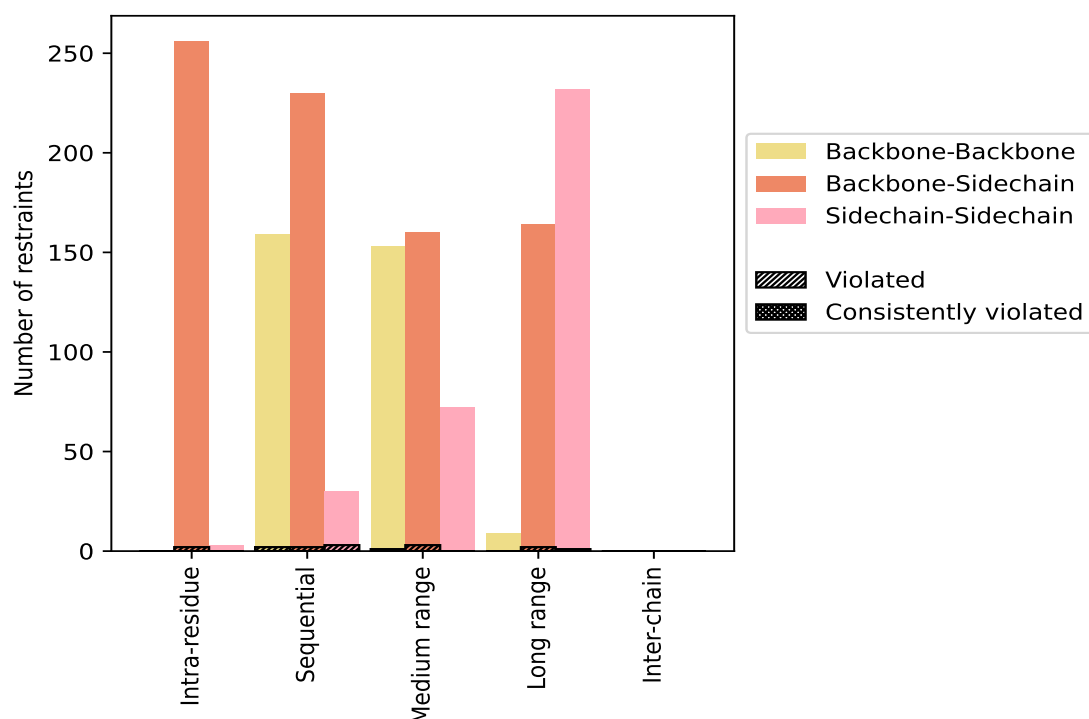
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	259	17.6	2	0.8	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	256	17.4	2	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	3	0.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	419	28.5	7	1.7	0.5	0	0.0	0.0
Backbone-Backbone	159	10.8	2	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	230	15.7	2	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	30	2.0	3	10.0	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	385	26.2	4	1.0	0.3	0	0.0	0.0
Backbone-Backbone	153	10.4	1	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	160	10.9	3	1.9	0.2	0	0.0	0.0
Sidechain-Sidechain	72	4.9	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	405	27.6	3	0.7	0.2	0	0.0	0.0
Backbone-Backbone	9	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	164	11.2	2	1.2	0.1	0	0.0	0.0
Sidechain-Sidechain	232	15.8	1	0.4	0.1	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	1468	100.0	16	1.1	1.1	0	0.0	0.0
Backbone-Backbone	321	21.9	3	0.9	0.2	0	0.0	0.0
Backbone-Sidechain	810	55.2	9	1.1	0.6	0	0.0	0.0
Sidechain-Sidechain	337	23.0	4	1.2	0.3	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	1	0	0	1	0.23	0.23	0.0	0.23
2	0	1	0	0	0	1	0.25	0.25	0.0	0.25
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	1	0	1	0	2	0.12	0.15	0.02	0.12
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	1	0	0	1	0.13	0.13	0.0	0.13
8	0	2	0	0	0	2	0.25	0.39	0.14	0.25
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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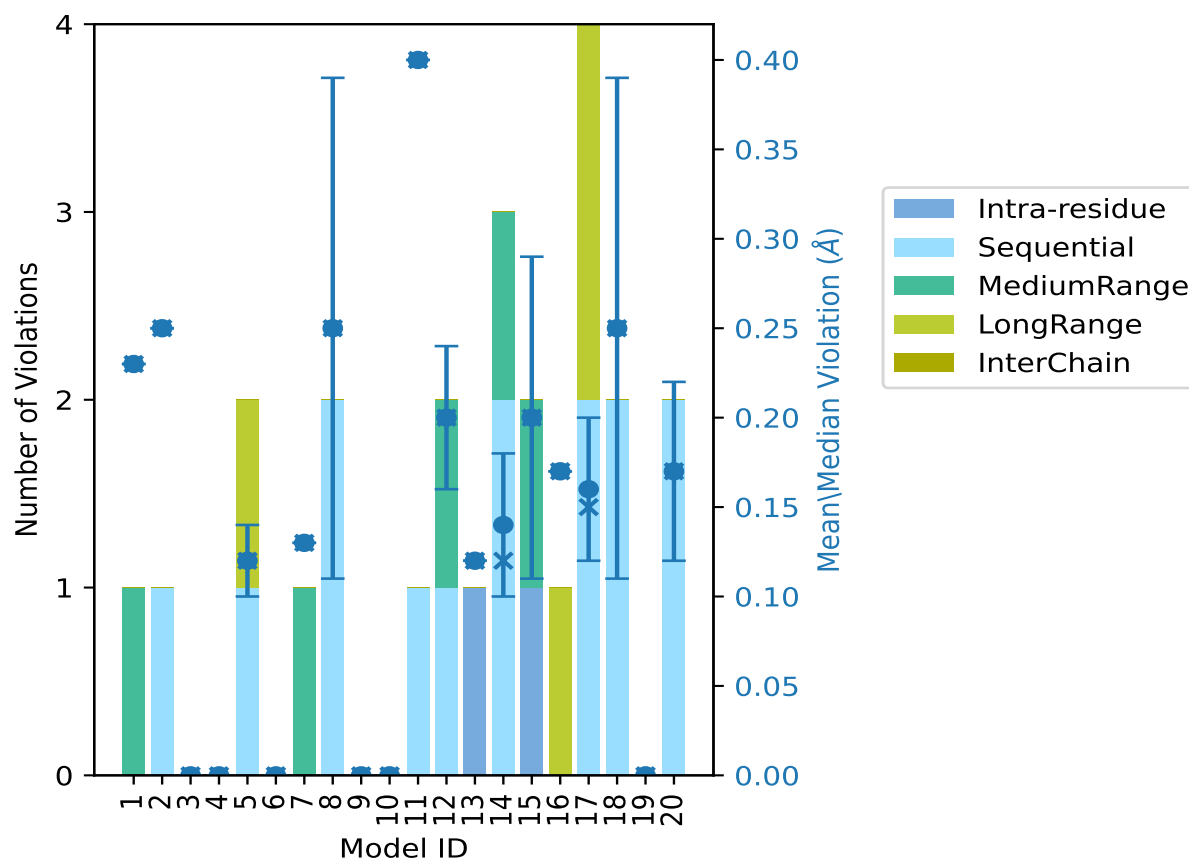
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	0	0	0	1	0.4	0.4	0.0	0.4
12	0	1	1	0	0	2	0.2	0.23	0.04	0.2
13	1	0	0	0	0	1	0.12	0.12	0.0	0.12
14	0	2	1	0	0	3	0.14	0.2	0.04	0.12
15	1	0	1	0	0	2	0.2	0.29	0.09	0.2
16	0	0	0	1	0	1	0.17	0.17	0.0	0.17
17	0	2	0	2	0	4	0.16	0.23	0.04	0.15
18	0	2	0	0	0	2	0.25	0.39	0.14	0.25
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	2	0	0	0	2	0.17	0.22	0.05	0.17

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 ⓘ



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

9.3 Distance violation statistics for the ensemble

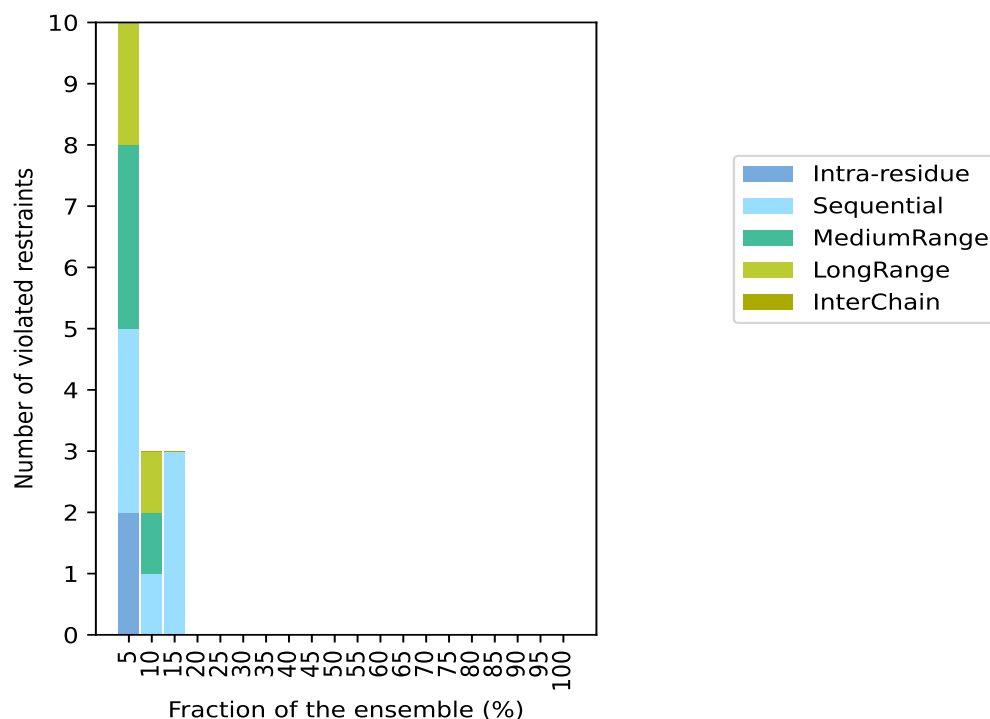
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1452(IR:257, SQ:412, MR:381, LR:402, IC:0) restraints are 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	%
2	3	3	2	0	10	1	5.0
0	1	1	1	0	3	2	10.0
0	3	0	0	0	3	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	0	0	0	0	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

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

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

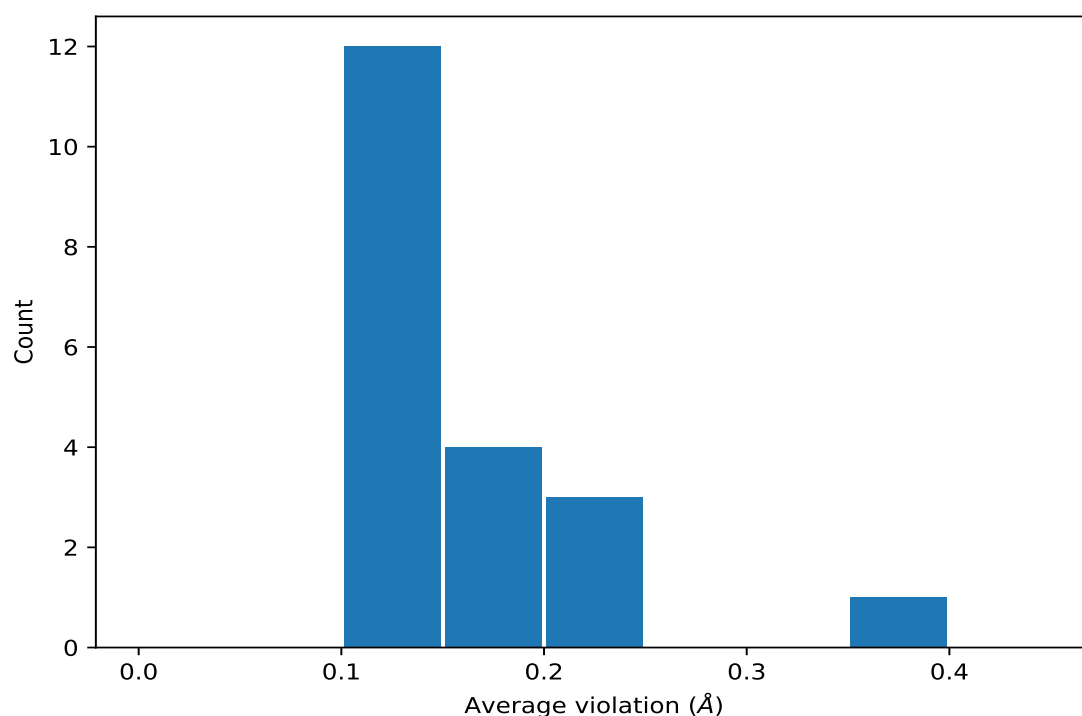
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,327)	1:209:A:GLU:H	1:210:A:LEU:H	3	0.39	0.0	0.39
(1,87)	1:105:A:ALA:HB1	1:106:A:THR:HB	3	0.22	0.01	0.22
(1,87)	1:105:A:ALA:HB2	1:106:A:THR:HB	3	0.22	0.01	0.22
(1,87)	1:105:A:ALA:HB3	1:106:A:THR:HB	3	0.22	0.01	0.22
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG21	3	0.12	0.02	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG22	3	0.12	0.02	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG23	3	0.12	0.02	0.11
(1,1093)	1:54:A:MET:HB2	1:55:A:GLU:HG2	2	0.17	0.06	0.17
(1,1093)	1:54:A:MET:HB2	1:55:A:GLU:HG3	2	0.17	0.06	0.17
(1,1093)	1:54:A:MET:HB3	1:55:A:GLU:HG2	2	0.17	0.06	0.17
(1,1093)	1:54:A:MET:HB3	1:55:A:GLU:HG3	2	0.17	0.06	0.17
(1,196)	1:126:A:ILE:HD11	1:158:A:TYR:HD1	2	0.15	0.02	0.15
(1,196)	1:126:A:ILE:HD11	1:158:A:TYR:HD2	2	0.15	0.02	0.15
(1,196)	1:126:A:ILE:HD12	1:158:A:TYR:HD1	2	0.15	0.02	0.15
(1,196)	1:126:A:ILE:HD12	1:158:A:TYR:HD2	2	0.15	0.02	0.15
(1,196)	1:126:A:ILE:HD13	1:158:A:TYR:HD1	2	0.15	0.02	0.15

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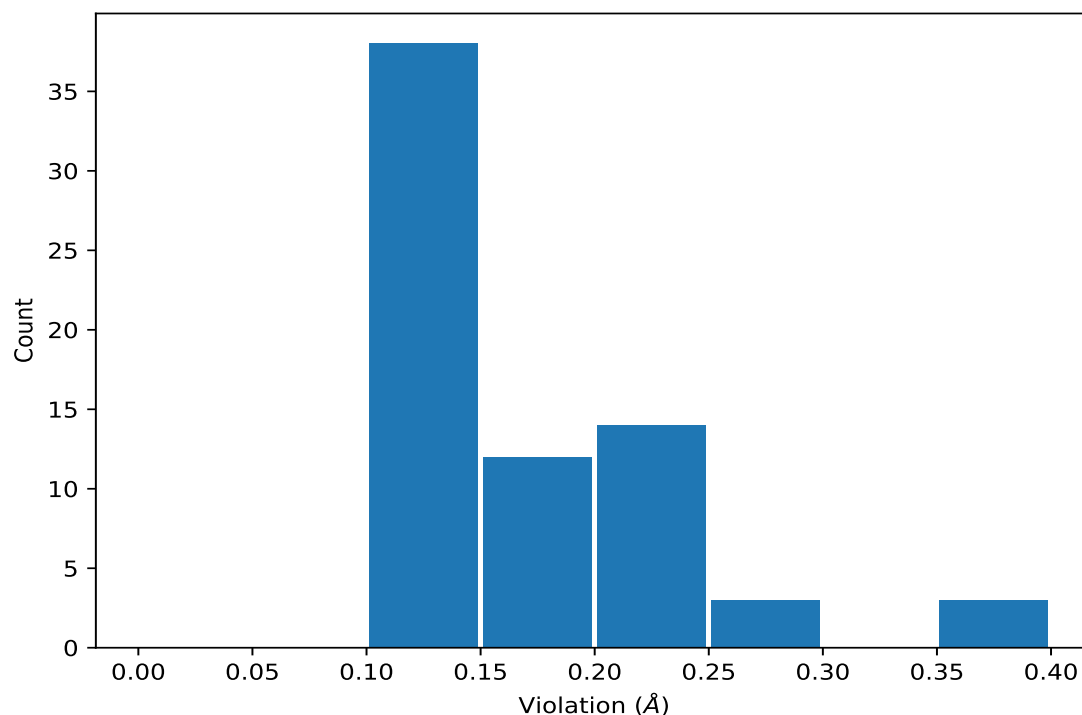
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,196)	1:126:A:ILE:HD13	1:158:A:TYR:HD2	2	0.15	0.02	0.15
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD11	2	0.12	0.01	0.12
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD12	2	0.12	0.01	0.12
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD13	2	0.12	0.01	0.12

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)
(1,327)	1:209:A:GLU:H	1:210:A:LEU:H	11	0.4
(1,327)	1:209:A:GLU:H	1:210:A:LEU:H	8	0.39
(1,327)	1:209:A:GLU:H	1:210:A:LEU:H	18	0.39
(1,1441)	1:191:A:LYS:HA	1:191:A:LYS:HG2	15	0.29
(1,1441)	1:191:A:LYS:HA	1:191:A:LYS:HG3	15	0.29
(1,527)	1:187:A:THR:HB	1:188:A:GLU:H	2	0.25
(1,1093)	1:54:A:MET:HB2	1:55:A:GLU:HG2	12	0.23
(1,1093)	1:54:A:MET:HB2	1:55:A:GLU:HG3	12	0.23
(1,1093)	1:54:A:MET:HB3	1:55:A:GLU:HG2	12	0.23
(1,1093)	1:54:A:MET:HB3	1:55:A:GLU:HG3	12	0.23
(1,362)	1:141:A:ASP:H	1:143:A:LYS:H	1	0.23
(1,87)	1:105:A:ALA:HB1	1:106:A:THR:HB	17	0.23
(1,87)	1:105:A:ALA:HB2	1:106:A:THR:HB	17	0.23
(1,87)	1:105:A:ALA:HB3	1:106:A:THR:HB	17	0.23
(1,87)	1:105:A:ALA:HB1	1:106:A:THR:HB	20	0.22
(1,87)	1:105:A:ALA:HB2	1:106:A:THR:HB	20	0.22
(1,87)	1:105:A:ALA:HB3	1:106:A:THR:HB	20	0.22
(1,87)	1:105:A:ALA:HB1	1:106:A:THR:HB	14	0.2
(1,87)	1:105:A:ALA:HB2	1:106:A:THR:HB	14	0.2
(1,87)	1:105:A:ALA:HB3	1:106:A:THR:HB	14	0.2
(1,196)	1:126:A:ILE:HD11	1:158:A:TYR:HD1	16	0.17
(1,196)	1:126:A:ILE:HD11	1:158:A:TYR:HD2	16	0.17
(1,196)	1:126:A:ILE:HD12	1:158:A:TYR:HD1	16	0.17
(1,196)	1:126:A:ILE:HD12	1:158:A:TYR:HD2	16	0.17
(1,196)	1:126:A:ILE:HD13	1:158:A:TYR:HD1	16	0.17
(1,196)	1:126:A:ILE:HD13	1:158:A:TYR:HD2	16	0.17
(1,1182)	1:78:A:LEU:HD11	1:81:A:LEU:H	12	0.16
(1,1182)	1:78:A:LEU:HD12	1:81:A:LEU:H	12	0.16
(1,1182)	1:78:A:LEU:HD13	1:81:A:LEU:H	12	0.16
(1,1182)	1:78:A:LEU:HD21	1:81:A:LEU:H	12	0.16
(1,1182)	1:78:A:LEU:HD22	1:81:A:LEU:H	12	0.16
(1,1182)	1:78:A:LEU:HD23	1:81:A:LEU:H	12	0.16
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG21	17	0.15
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG22	17	0.15
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG23	17	0.15
(1,741)	1:126:A:ILE:H	1:162:A:LEU:HD21	5	0.15
(1,741)	1:126:A:ILE:H	1:162:A:LEU:HD22	5	0.15
(1,741)	1:126:A:ILE:H	1:162:A:LEU:HD23	5	0.15
(1,152)	1:139:A:ILE:HA	1:145:A:MET:HE1	17	0.14
(1,152)	1:139:A:ILE:HA	1:145:A:MET:HE2	17	0.14
(1,152)	1:139:A:ILE:HA	1:145:A:MET:HE3	17	0.14
(1,196)	1:126:A:ILE:HD11	1:158:A:TYR:HD1	17	0.13
(1,196)	1:126:A:ILE:HD11	1:158:A:TYR:HD2	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:126:A:ILE:HD12	1:158:A:TYR:HD1	17	0.13
(1,196)	1:126:A:ILE:HD12	1:158:A:TYR:HD2	17	0.13
(1,196)	1:126:A:ILE:HD13	1:158:A:TYR:HD1	17	0.13
(1,196)	1:126:A:ILE:HD13	1:158:A:TYR:HD2	17	0.13
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD11	7	0.13
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD12	7	0.13
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD13	7	0.13
(1,1290)	1:126:A:ILE:H	1:128:A:LEU:HB2	14	0.12
(1,1290)	1:126:A:ILE:H	1:128:A:LEU:HB3	14	0.12
(1,1264)	1:111:A:ARG:HD2	1:112:A:HIS:HE1	20	0.12
(1,1264)	1:111:A:ARG:HD3	1:112:A:HIS:HE1	20	0.12
(1,559)	1:85:A:PHE:H	1:85:A:PHE:HD1	13	0.12
(1,559)	1:85:A:PHE:H	1:85:A:PHE:HD2	13	0.12
(1,1093)	1:54:A:MET:HB2	1:55:A:GLU:HG2	14	0.11
(1,1093)	1:54:A:MET:HB2	1:55:A:GLU:HG3	14	0.11
(1,1093)	1:54:A:MET:HB3	1:55:A:GLU:HG2	14	0.11
(1,1093)	1:54:A:MET:HB3	1:55:A:GLU:HG3	14	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG21	8	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG22	8	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG23	8	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG21	18	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG22	18	0.11
(1,874)	1:138:A:ASP:H	1:139:A:ILE:HG23	18	0.11
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD11	15	0.11
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD12	15	0.11
(1,65)	1:75:A:GLY:HA3	1:78:A:LEU:HD13	15	0.11
(1,807)	1:147:A:ARG:H	1:148:A:CYS:HA	5	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found