



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 04:26 PM UTC

PDB ID : 3CTN / pdb_00003ctn
Title : STRUCTURE OF CALCIUM-SATURATED CARDIAC TROPONIN C,
NMR, 30 STRUCTURES
Authors : Sia, S.K.; Li, M.X.; Spyropoulos, L.; Gagne, S.M.; Liu, W.; Putkey, J.A.;
Sykes, B.D.
Deposited on : 1997-05-08

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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

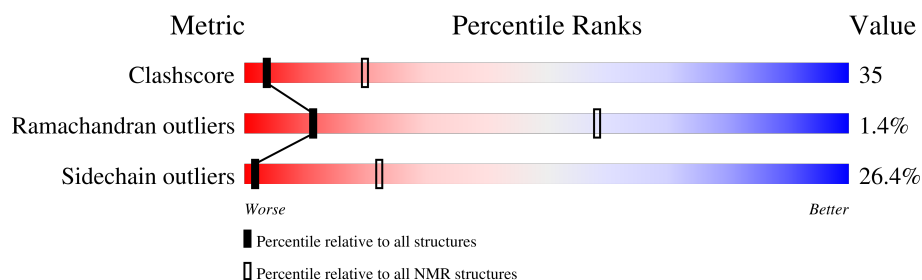
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	76	12% 61% . 24%

2 Ensemble composition and analysis

This entry contains 30 models. Model 18 is the overall representative, medoid model (most similar to other models).

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:96-A:123, A:129-A:158 (58)	0.56	18

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 7, 9, 10, 11, 13, 14, 18, 19, 22, 26, 27, 29, 30
2	1, 5, 12, 17, 20, 24
3	4, 15, 16, 23
4	3, 21, 25
5	6, 8
Single-model clusters	28

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1198 atoms, of which 579 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TROPONIN C.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1196	380	579	94	139	4	

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

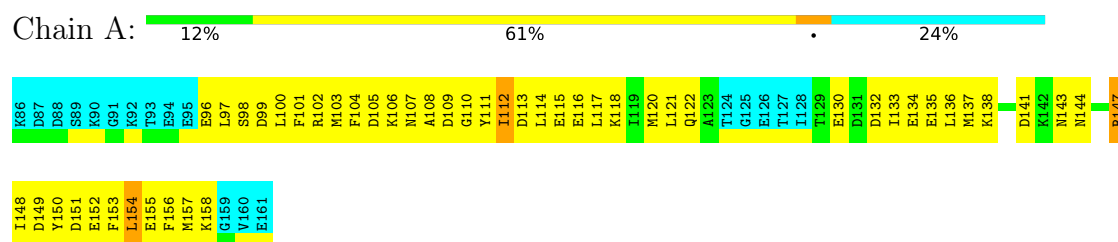
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

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: TROPONIN C

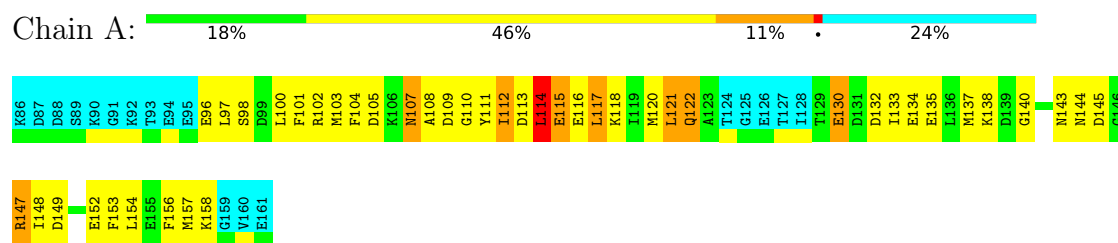


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

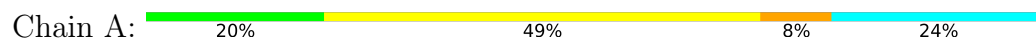
4.2.1 Score per residue for model 1

• Molecule 1: TROPONIN C



4.2.2 Score per residue for model 2

• Molecule 1: TROPONIN C

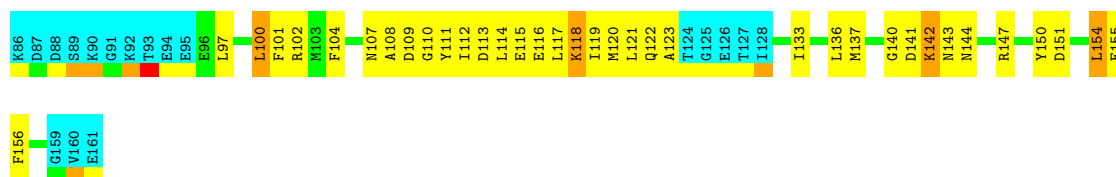




4.2.3 Score per residue for model 3

- Molecule 1: TROPONIN C

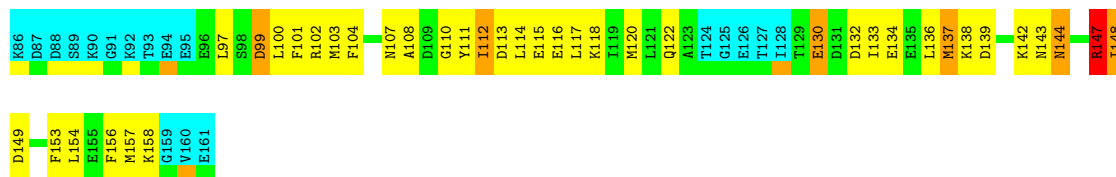
Chain A: 29% 42% 5% 24%



4.2.4 Score per residue for model 4

- Molecule 1: TROPONIN C

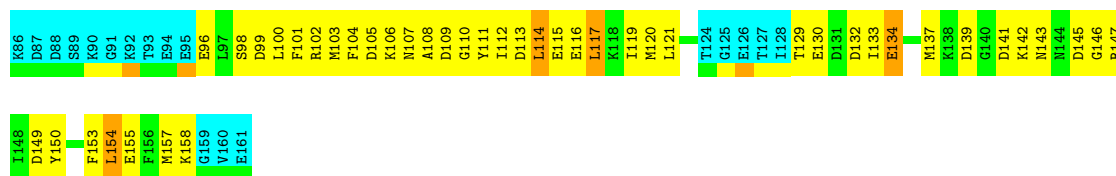
Chain A: 25% 42% 8% 24%



4.2.5 Score per residue for model 5

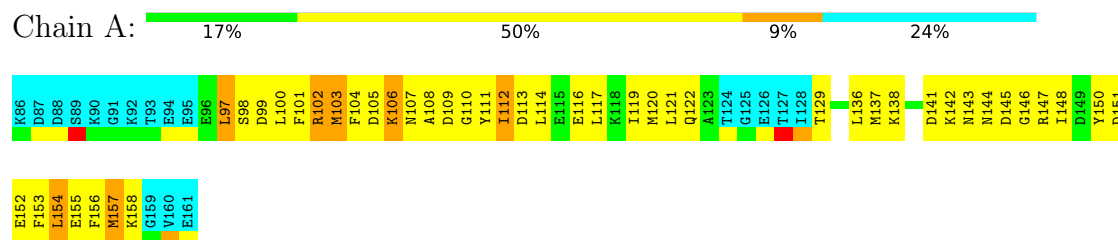
- Molecule 1: TROPONIN C

Chain A: 18% 53% 5% 24%



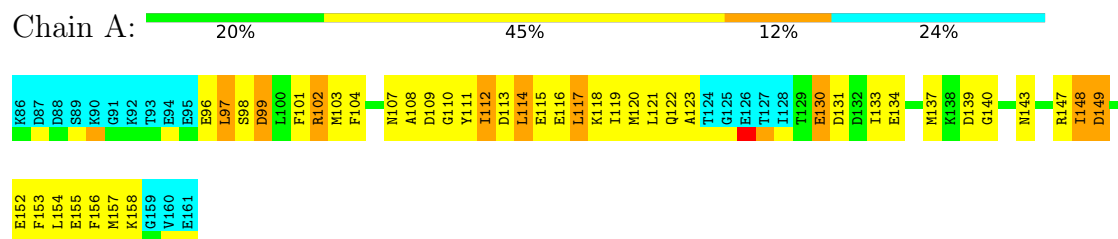
4.2.6 Score per residue for model 6

- Molecule 1: TROPONIN C



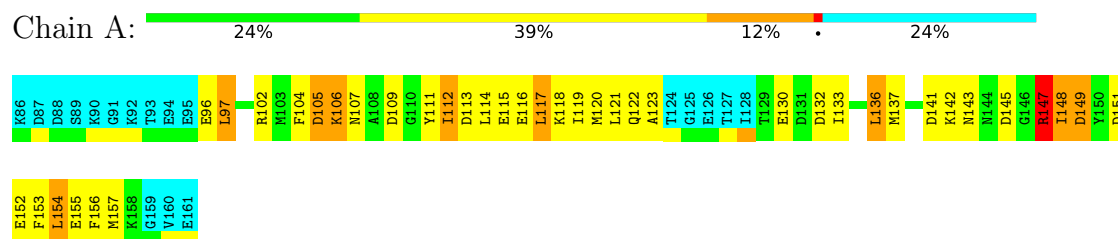
4.2.7 Score per residue for model 7

- Molecule 1: TROPONIN C



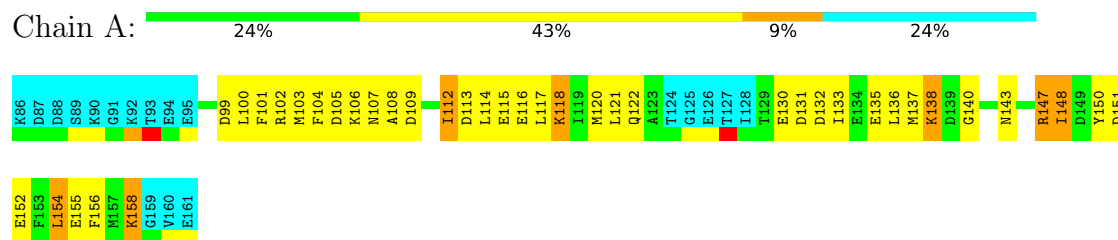
4.2.8 Score per residue for model 8

- Molecule 1: TROPONIN C



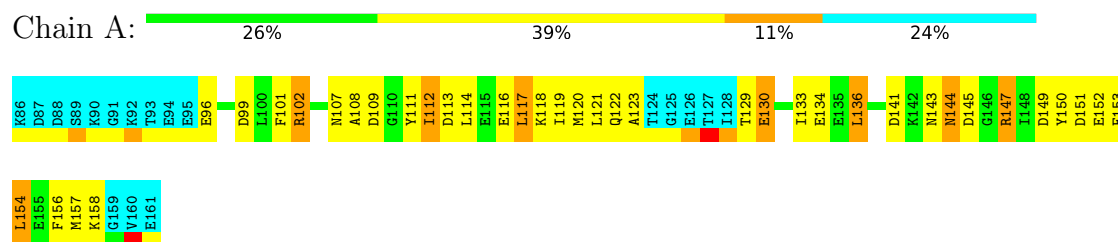
4.2.9 Score per residue for model 9

- Molecule 1: TROPONIN C



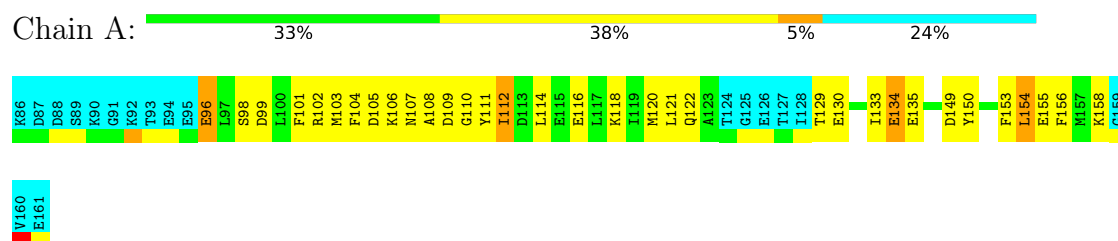
4.2.10 Score per residue for model 10

• Molecule 1: TROPONIN C



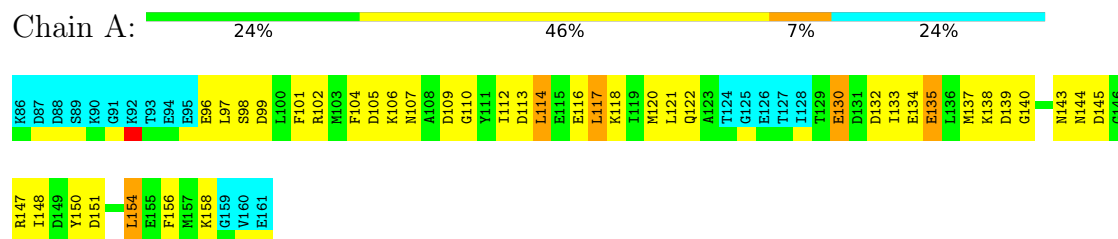
4.2.11 Score per residue for model 11

• Molecule 1: TROPONIN C



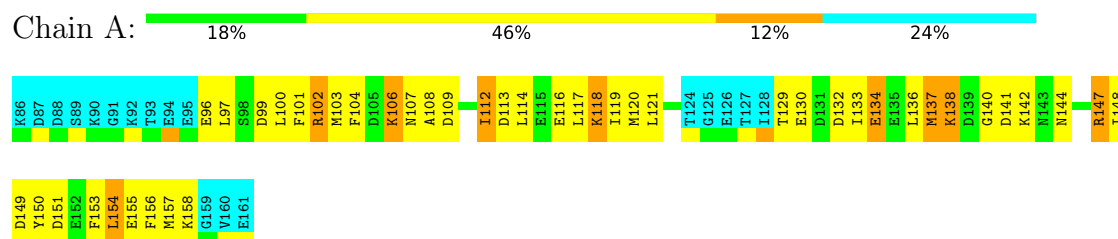
4.2.12 Score per residue for model 12

• Molecule 1: TROPONIN C



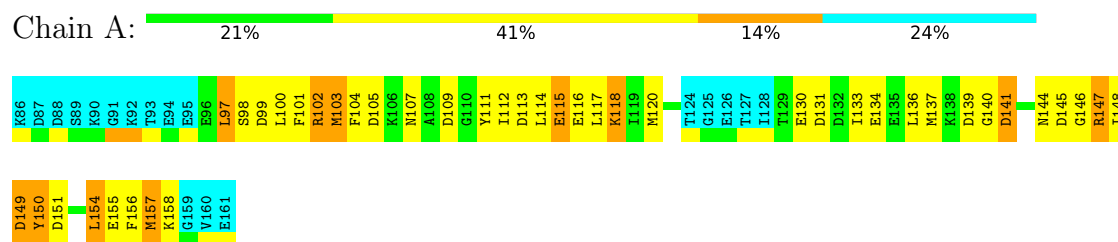
4.2.13 Score per residue for model 13

• Molecule 1: TROPONIN C



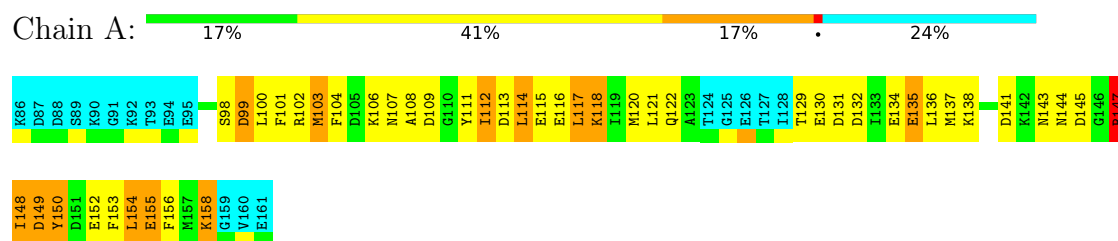
4.2.14 Score per residue for model 14

• Molecule 1: TROPONIN C



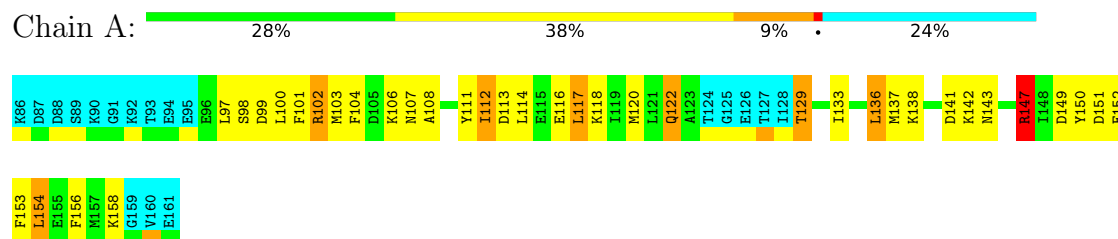
4.2.15 Score per residue for model 15

• Molecule 1: TROPONIN C



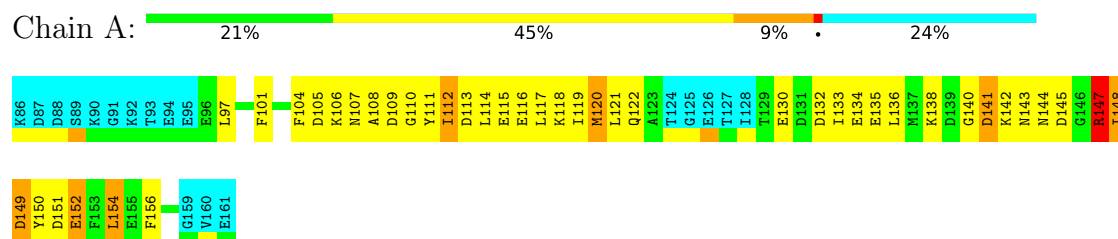
4.2.16 Score per residue for model 16

• Molecule 1: TROPONIN C



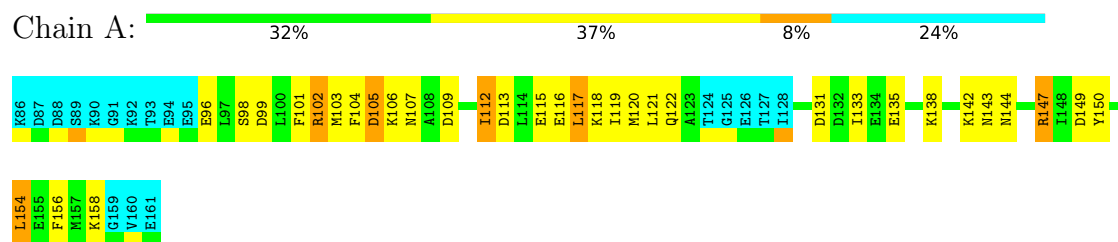
4.2.17 Score per residue for model 17

• Molecule 1: TROPONIN C



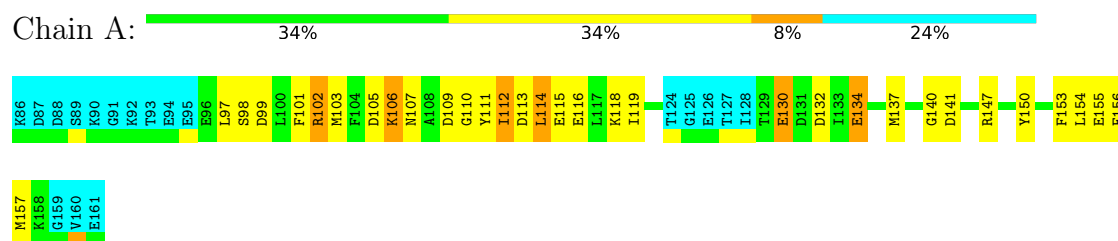
4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: TROPONIN C



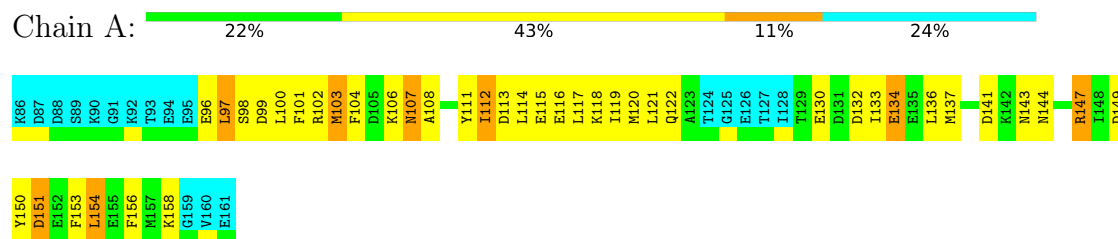
4.2.19 Score per residue for model 19

• Molecule 1: TROPONIN C



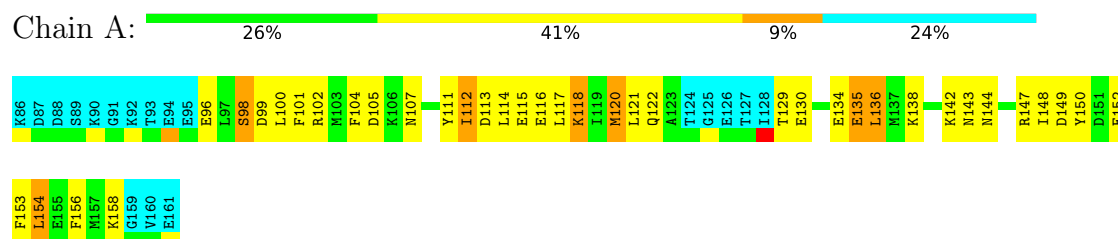
4.2.20 Score per residue for model 20

• Molecule 1: TROPONIN C



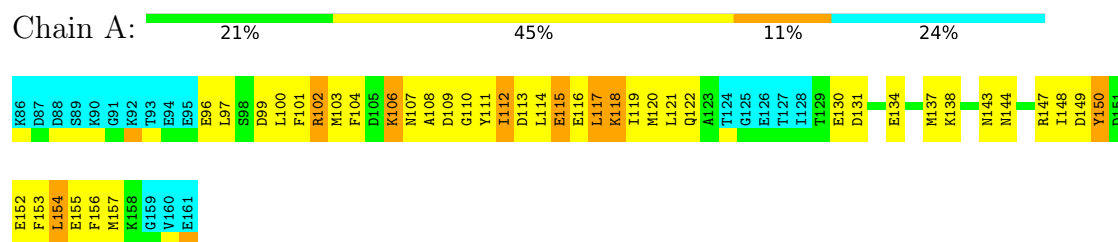
4.2.21 Score per residue for model 21

• Molecule 1: TROPONIN C



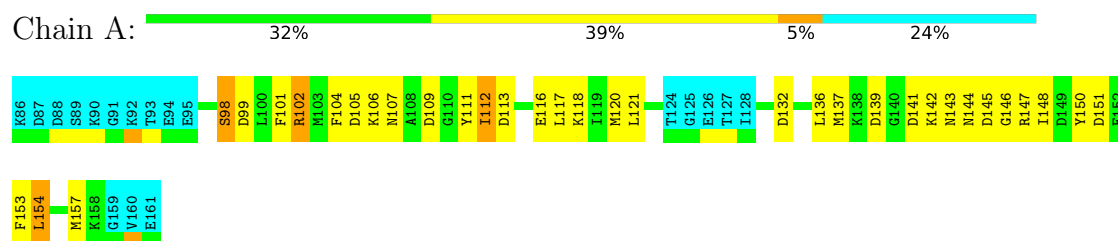
4.2.22 Score per residue for model 22

• Molecule 1: TROPONIN C



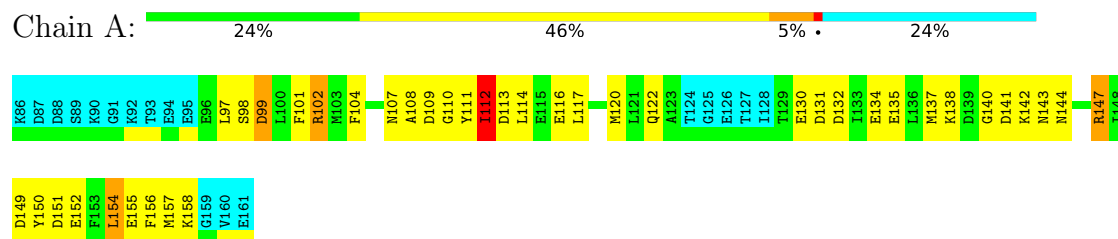
4.2.23 Score per residue for model 23

• Molecule 1: TROPONIN C



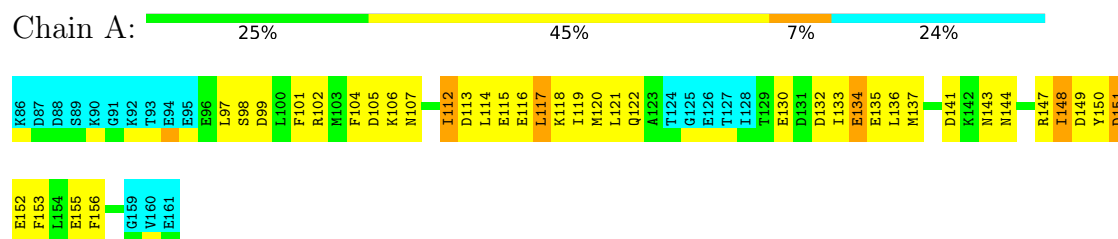
4.2.24 Score per residue for model 24

• Molecule 1: TROPONIN C



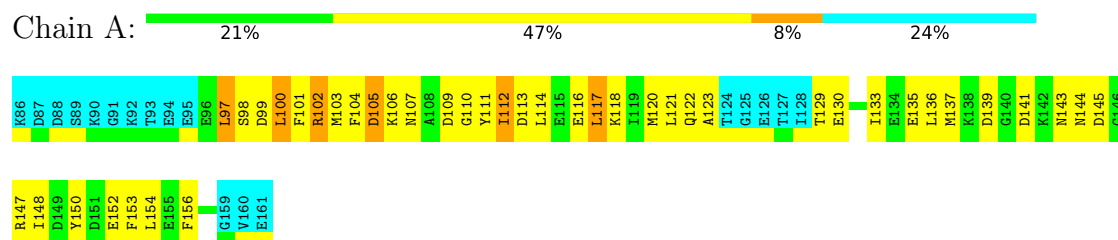
4.2.25 Score per residue for model 25

• Molecule 1: TROPONIN C



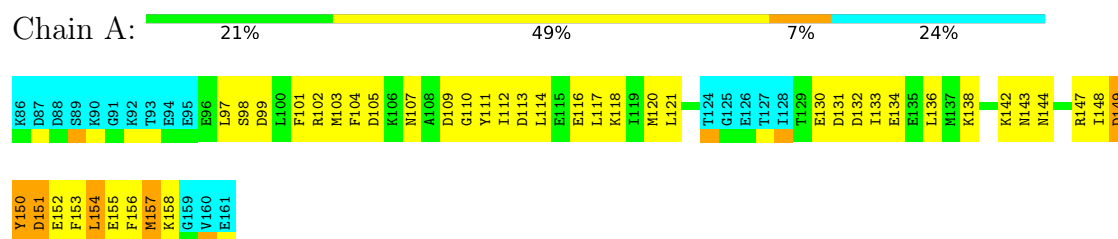
4.2.26 Score per residue for model 26

• Molecule 1: TROPONIN C



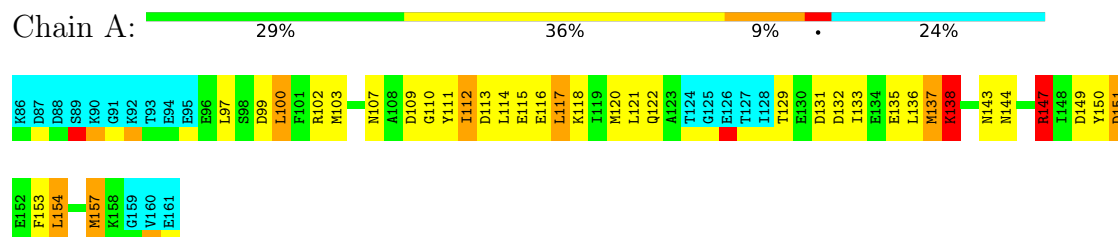
4.2.27 Score per residue for model 27

• Molecule 1: TROPONIN C



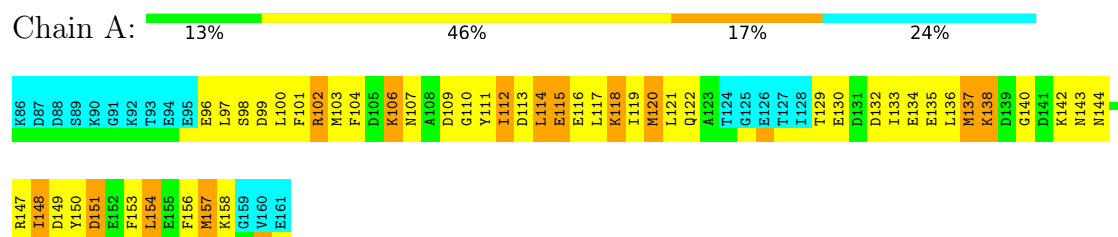
4.2.28 Score per residue for model 28

• Molecule 1: TROPONIN C



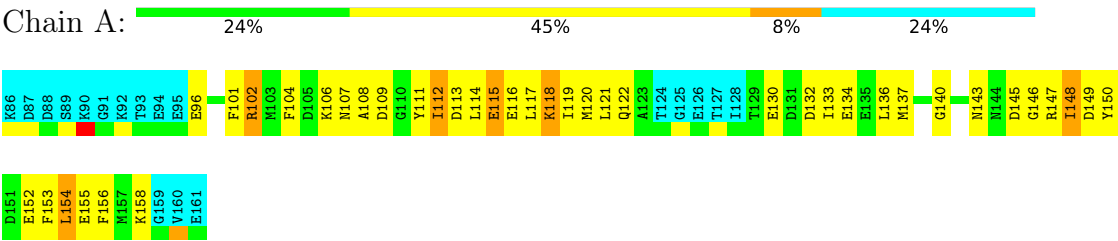
4.2.29 Score per residue for model 29

• Molecule 1: TROPONIN C



4.2.30 Score per residue for model 30

● Molecule 1: TROPONIN C



5 Refinement protocol and experimental data overview

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

Of the 35 calculated structures, 30 were deposited, based on the following criterion: *LOWEST TOTAL ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.44±0.01	0±0/489 (0.0± 0.0%)	1.56±0.02	0±0/653 (0.0± 0.1%)
All	All	1.44	0/14670 (0.0%)	1.56	4/19590 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.9±0.3
All	All	0	57

There are no bond-length outliers.

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	148	ILE	N-CA-CB	-5.34	104.73	111.46	1	3
1	A	112	ILE	N-CA-CB	-5.09	105.39	112.52	24	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	102	ARG	Sidechain	29
1	A	147	ARG	Sidechain	28

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	483	451	451	33±7
All	All	14550	13530	13530	978

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD13	1:A:137:MET:HE2	1.00	1.33	16	2
1:A:150:TYR:O	1:A:154:LEU:HD23	0.91	1.63	29	20
1:A:117:LEU:HD11	1:A:156:PHE:CZ	0.87	2.03	17	5
1:A:117:LEU:HD13	1:A:137:MET:SD	0.83	2.14	15	3
1:A:117:LEU:HD21	1:A:136:LEU:HD23	0.83	1.50	30	1
1:A:117:LEU:HD22	1:A:137:MET:SD	0.82	2.14	15	3
1:A:118:LYS:HG2	1:A:133:ILE:HD13	0.79	1.53	3	2
1:A:96:GLU:O	1:A:100:LEU:HD23	0.78	1.78	21	2
1:A:114:LEU:HD13	1:A:114:LEU:O	0.77	1.78	14	1
1:A:100:LEU:HD21	1:A:120:MET:HE2	0.77	1.57	29	1
1:A:136:LEU:HD22	1:A:156:PHE:CE1	0.76	2.16	16	1
1:A:118:LYS:HG2	1:A:133:ILE:HG21	0.76	1.55	1	4
1:A:118:LYS:HD3	1:A:133:ILE:HD13	0.76	1.58	30	2
1:A:97:LEU:HD21	1:A:157:MET:HB3	0.76	1.57	8	1
1:A:114:LEU:HD23	1:A:137:MET:CB	0.75	2.11	14	1
1:A:118:LYS:HB3	1:A:133:ILE:HG21	0.74	1.57	10	2
1:A:97:LEU:HD23	1:A:157:MET:SD	0.73	2.22	6	1
1:A:117:LEU:HD22	1:A:137:MET:HG2	0.73	1.58	16	3
1:A:118:LYS:CD	1:A:133:ILE:HD13	0.73	2.14	30	1
1:A:117:LEU:HD22	1:A:137:MET:HE2	0.72	1.61	1	3
1:A:137:MET:HE1	1:A:148:ILE:HD12	0.72	1.60	25	4
1:A:106:LYS:HE3	1:A:119:ILE:HD13	0.72	1.59	6	1
1:A:136:LEU:HD22	1:A:156:PHE:CZ	0.71	2.20	16	1
1:A:117:LEU:HD21	1:A:156:PHE:CZ	0.71	2.19	25	7
1:A:136:LEU:C	1:A:136:LEU:HD12	0.69	2.11	6	1
1:A:118:LYS:CG	1:A:133:ILE:HG21	0.68	2.17	1	3
1:A:117:LEU:O	1:A:117:LEU:HD13	0.68	1.87	26	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD23	1:A:114:LEU:O	0.66	1.90	20	7
1:A:153:PHE:CE1	1:A:157:MET:HE1	0.66	2.24	27	1
1:A:117:LEU:HD21	1:A:156:PHE:CE2	0.66	2.26	18	3
1:A:104:PHE:CB	1:A:120:MET:HE3	0.66	2.21	3	1
1:A:121:LEU:HD23	1:A:121:LEU:N	0.66	2.05	1	6
1:A:150:TYR:CE1	1:A:154:LEU:HD21	0.66	2.26	3	8
1:A:104:PHE:HB3	1:A:120:MET:HE3	0.65	1.65	3	1
1:A:153:PHE:CZ	1:A:157:MET:HE1	0.64	2.28	27	2
1:A:106:LYS:HD2	1:A:119:ILE:HG21	0.64	1.69	19	2
1:A:117:LEU:HD11	1:A:156:PHE:CE2	0.64	2.28	20	1
1:A:107:ASN:O	1:A:108:ALA:HB3	0.63	1.93	16	15
1:A:117:LEU:HD11	1:A:121:LEU:HD21	0.63	1.69	23	1
1:A:153:PHE:CZ	1:A:157:MET:HE3	0.62	2.28	6	1
1:A:111:TYR:N	1:A:111:TYR:CD1	0.62	2.68	26	19
1:A:114:LEU:HD13	1:A:114:LEU:C	0.62	2.18	14	1
1:A:114:LEU:HD21	1:A:133:ILE:HG22	0.62	1.71	20	5
1:A:97:LEU:HD23	1:A:153:PHE:CE1	0.62	2.29	8	1
1:A:118:LYS:CB	1:A:133:ILE:HG21	0.62	2.25	10	2
1:A:132:ASP:O	1:A:136:LEU:HD23	0.61	1.94	25	2
1:A:150:TYR:CZ	1:A:154:LEU:HD11	0.61	2.31	13	1
1:A:98:SER:CB	1:A:150:TYR:CE1	0.61	2.84	23	3
1:A:117:LEU:CD1	1:A:156:PHE:CZ	0.60	2.83	17	2
1:A:136:LEU:HD12	1:A:156:PHE:CE2	0.60	2.31	10	1
1:A:100:LEU:HD23	1:A:103:MET:HE3	0.59	1.72	2	3
1:A:118:LYS:HA	1:A:133:ILE:HD13	0.59	1.73	8	3
1:A:114:LEU:C	1:A:114:LEU:HD23	0.59	2.23	10	2
1:A:153:PHE:C	1:A:153:PHE:CD1	0.59	2.81	4	11
1:A:117:LEU:HD21	1:A:136:LEU:HD11	0.59	1.73	6	1
1:A:121:LEU:HD12	1:A:133:ILE:CD1	0.58	2.28	13	1
1:A:101:PHE:C	1:A:101:PHE:CD1	0.58	2.81	5	21
1:A:110:GLY:C	1:A:111:TYR:CD1	0.58	2.81	5	14
1:A:114:LEU:CD2	1:A:137:MET:CB	0.58	2.82	14	1
1:A:156:PHE:CD1	1:A:156:PHE:C	0.58	2.81	3	9
1:A:101:PHE:CZ	1:A:110:GLY:O	0.57	2.58	6	5
1:A:97:LEU:N	1:A:97:LEU:CD2	0.57	2.68	2	2
1:A:106:LYS:CD	1:A:119:ILE:HG21	0.57	2.28	19	1
1:A:118:LYS:HG3	1:A:133:ILE:HG21	0.57	1.77	26	1
1:A:103:MET:SD	1:A:104:PHE:CE2	0.56	2.98	29	2
1:A:153:PHE:CZ	1:A:157:MET:CE	0.56	2.87	27	3
1:A:153:PHE:CZ	1:A:157:MET:SD	0.56	2.99	29	3
1:A:106:LYS:CD	1:A:119:ILE:HD13	0.56	2.31	13	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD11	1:A:156:PHE:HZ	0.55	1.61	30	1
1:A:117:LEU:HD22	1:A:137:MET:CG	0.55	2.32	4	2
1:A:114:LEU:HD23	1:A:114:LEU:C	0.55	2.27	2	4
1:A:121:LEU:HD21	1:A:136:LEU:HD21	0.55	1.78	3	1
1:A:104:PHE:CG	1:A:120:MET:SD	0.55	3.00	4	4
1:A:136:LEU:HD12	1:A:156:PHE:CE1	0.55	2.37	8	1
1:A:114:LEU:CD2	1:A:133:ILE:HG22	0.55	2.32	12	1
1:A:97:LEU:CD2	1:A:157:MET:CB	0.55	2.85	14	1
1:A:140:GLY:HA3	1:A:156:PHE:CD2	0.54	2.37	9	6
1:A:107:ASN:CB	1:A:116:GLU:CD	0.54	2.81	13	10
1:A:118:LYS:HB2	1:A:133:ILE:HD13	0.54	1.77	10	2
1:A:104:PHE:CD2	1:A:120:MET:SD	0.54	3.01	14	2
1:A:111:TYR:CD1	1:A:111:TYR:N	0.53	2.75	5	5
1:A:118:LYS:HG3	1:A:133:ILE:HD13	0.53	1.79	7	3
1:A:117:LEU:C	1:A:117:LEU:CD1	0.53	2.80	26	1
1:A:99:ASP:O	1:A:103:MET:CB	0.53	2.57	7	9
1:A:120:MET:HE1	1:A:157:MET:HE1	0.53	1.79	28	1
1:A:106:LYS:HD3	1:A:119:ILE:HD13	0.53	1.79	8	3
1:A:107:ASN:CB	1:A:116:GLU:OE2	0.53	2.57	2	13
1:A:140:GLY:CA	1:A:156:PHE:CD1	0.53	2.92	7	4
1:A:113:ASP:OD1	1:A:116:GLU:CG	0.53	2.57	3	8
1:A:149:ASP:O	1:A:153:PHE:CB	0.53	2.57	4	4
1:A:106:LYS:CE	1:A:119:ILE:HG21	0.53	2.33	5	1
1:A:100:LEU:HD23	1:A:103:MET:CE	0.53	2.33	20	2
1:A:130:GLU:O	1:A:134:GLU:CG	0.53	2.57	7	17
1:A:101:PHE:CE1	1:A:112:ILE:HG13	0.52	2.39	6	2
1:A:137:MET:SD	1:A:148:ILE:CD1	0.52	2.97	8	2
1:A:121:LEU:HD11	1:A:136:LEU:CD2	0.52	2.34	20	1
1:A:115:GLU:O	1:A:118:LYS:CG	0.52	2.57	14	5
1:A:117:LEU:CD1	1:A:156:PHE:CE2	0.52	2.92	20	2
1:A:104:PHE:CD2	1:A:120:MET:HE3	0.52	2.40	2	1
1:A:104:PHE:O	1:A:106:LYS:N	0.52	2.43	8	6
1:A:104:PHE:CE1	1:A:120:MET:HA	0.52	2.40	7	14
1:A:117:LEU:O	1:A:117:LEU:CD1	0.52	2.58	26	1
1:A:104:PHE:CD1	1:A:120:MET:HA	0.51	2.40	7	12
1:A:132:ASP:OD1	1:A:132:ASP:N	0.51	2.44	8	1
1:A:112:ILE:HG23	1:A:116:GLU:CB	0.51	2.36	23	15
1:A:150:TYR:CE1	1:A:154:LEU:CD2	0.51	2.94	16	4
1:A:117:LEU:HD21	1:A:156:PHE:HZ	0.51	1.64	4	1
1:A:143:ASN:ND2	1:A:152:GLU:OE2	0.51	2.44	9	7
1:A:153:PHE:CE1	1:A:157:MET:CE	0.51	2.94	27	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:ILE:O	1:A:123:ALA:CB	0.51	2.59	7	2
1:A:113:ASP:OD1	1:A:115:GLU:N	0.50	2.45	25	3
1:A:104:PHE:CB	1:A:120:MET:HE2	0.50	2.36	13	1
1:A:136:LEU:HD12	1:A:156:PHE:CZ	0.50	2.41	10	1
1:A:104:PHE:CD1	1:A:120:MET:HG3	0.50	2.41	7	8
1:A:114:LEU:HD23	1:A:137:MET:CG	0.50	2.37	14	1
1:A:114:LEU:CD2	1:A:137:MET:HB2	0.50	2.37	14	1
1:A:114:LEU:O	1:A:114:LEU:CD2	0.50	2.58	1	2
1:A:112:ILE:CG2	1:A:116:GLU:HB2	0.50	2.37	22	15
1:A:119:ILE:O	1:A:123:ALA:HB2	0.50	2.06	10	2
1:A:117:LEU:CD2	1:A:133:ILE:HG23	0.50	2.37	30	2
1:A:145:ASP:OD2	1:A:147:ARG:CG	0.50	2.60	8	1
1:A:106:LYS:HD2	1:A:119:ILE:HD13	0.50	1.83	13	1
1:A:107:ASN:O	1:A:107:ASN:ND2	0.50	2.45	12	8
1:A:114:LEU:HD23	1:A:137:MET:HB2	0.50	1.83	14	1
1:A:114:LEU:CA	1:A:137:MET:SD	0.49	3.00	3	1
1:A:139:ASP:N	1:A:139:ASP:OD1	0.49	2.44	7	1
1:A:143:ASN:OD1	1:A:144:ASN:N	0.49	2.45	28	2
1:A:137:MET:HE1	1:A:148:ILE:CD1	0.49	2.34	25	1
1:A:145:ASP:OD1	1:A:146:GLY:N	0.49	2.44	6	5
1:A:117:LEU:HD13	1:A:117:LEU:C	0.49	2.31	26	1
1:A:111:TYR:CD2	1:A:149:ASP:HB3	0.49	2.42	22	2
1:A:131:ASP:OD1	1:A:132:ASP:N	0.49	2.46	28	1
1:A:111:TYR:CE2	1:A:149:ASP:HB3	0.49	2.43	2	8
1:A:153:PHE:O	1:A:154:LEU:C	0.49	2.56	21	7
1:A:118:LYS:HD3	1:A:133:ILE:HD12	0.49	1.85	9	1
1:A:112:ILE:HG23	1:A:116:GLU:HB3	0.49	1.85	13	5
1:A:104:PHE:CD1	1:A:120:MET:CB	0.48	2.96	7	1
1:A:107:ASN:OD1	1:A:109:ASP:CG	0.48	2.56	8	20
1:A:114:LEU:CB	1:A:137:MET:SD	0.48	3.01	3	1
1:A:114:LEU:CD2	1:A:114:LEU:N	0.48	2.76	6	3
1:A:114:LEU:C	1:A:114:LEU:CD2	0.48	2.86	10	2
1:A:113:ASP:O	1:A:114:LEU:C	0.48	2.56	1	3
1:A:143:ASN:CG	1:A:145:ASP:OD2	0.48	2.57	1	3
1:A:143:ASN:O	1:A:144:ASN:C	0.48	2.57	10	15
1:A:122:GLN:HG3	1:A:123:ALA:N	0.48	2.22	8	3
1:A:104:PHE:CD1	1:A:120:MET:CG	0.48	2.96	7	2
1:A:97:LEU:HD22	1:A:157:MET:HG3	0.48	1.85	1	1
1:A:97:LEU:O	1:A:153:PHE:CE1	0.48	2.66	8	1
1:A:115:GLU:HA	1:A:118:LYS:CD	0.48	2.39	29	1
1:A:104:PHE:CE1	1:A:120:MET:HG3	0.48	2.43	7	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD22	1:A:154:LEU:HA	0.48	1.86	8	1
1:A:97:LEU:HD23	1:A:100:LEU:HD12	0.48	1.85	1	1
1:A:137:MET:SD	1:A:148:ILE:HD11	0.48	2.49	26	3
1:A:135:GLU:OE1	1:A:138:LYS:NZ	0.48	2.47	12	1
1:A:136:LEU:HB3	1:A:156:PHE:CZ	0.48	2.44	15	1
1:A:113:ASP:OD1	1:A:116:GLU:OE2	0.47	2.32	12	6
1:A:100:LEU:HG	1:A:104:PHE:CD2	0.47	2.44	26	1
1:A:103:MET:SD	1:A:104:PHE:CD2	0.47	3.08	14	1
1:A:98:SER:CB	1:A:150:TYR:OH	0.47	2.62	15	1
1:A:113:ASP:O	1:A:115:GLU:N	0.47	2.47	1	1
1:A:113:ASP:OD1	1:A:116:GLU:CD	0.47	2.57	24	6
1:A:114:LEU:CD2	1:A:137:MET:HG2	0.47	2.40	6	3
1:A:153:PHE:CZ	1:A:157:MET:HE2	0.47	2.44	10	1
1:A:150:TYR:CZ	1:A:154:LEU:HD21	0.47	2.44	16	2
1:A:113:ASP:OD1	1:A:115:GLU:CB	0.47	2.62	22	2
1:A:113:ASP:OD2	1:A:116:GLU:OE2	0.47	2.33	7	15
1:A:117:LEU:CD2	1:A:137:MET:SD	0.47	2.98	15	2
1:A:114:LEU:CD1	1:A:137:MET:HG2	0.47	2.39	6	2
1:A:97:LEU:HD21	1:A:157:MET:CB	0.47	2.35	8	1
1:A:113:ASP:CG	1:A:116:GLU:OE2	0.47	2.57	10	4
1:A:98:SER:O	1:A:99:ASP:C	0.47	2.57	24	4
1:A:107:ASN:HB3	1:A:116:GLU:CD	0.47	2.35	15	14
1:A:98:SER:OG	1:A:99:ASP:N	0.47	2.47	16	3
1:A:155:GLU:O	1:A:156:PHE:C	0.47	2.57	27	3
1:A:140:GLY:O	1:A:152:GLU:CD	0.47	2.57	17	1
1:A:144:ASN:C	1:A:145:ASP:OD1	0.47	2.58	2	1
1:A:101:PHE:CE2	1:A:149:ASP:C	0.47	2.93	18	3
1:A:107:ASN:HB2	1:A:116:GLU:CD	0.47	2.35	13	7
1:A:130:GLU:O	1:A:134:GLU:CD	0.47	2.58	15	1
1:A:149:ASP:OD2	1:A:151:ASP:CG	0.47	2.58	24	1
1:A:106:LYS:HE3	1:A:119:ILE:HG21	0.47	1.86	25	1
1:A:107:ASN:OD1	1:A:109:ASP:OD1	0.47	2.33	26	6
1:A:107:ASN:OD1	1:A:109:ASP:OD2	0.47	2.33	18	2
1:A:114:LEU:C	1:A:114:LEU:CD1	0.47	2.88	14	1
1:A:143:ASN:CG	1:A:152:GLU:OE2	0.47	2.58	16	3
1:A:114:LEU:O	1:A:118:LYS:HG3	0.46	2.10	8	1
1:A:143:ASN:CG	1:A:152:GLU:OE1	0.46	2.59	24	3
1:A:143:ASN:OD1	1:A:152:GLU:OE1	0.46	2.33	6	5
1:A:114:LEU:O	1:A:118:LYS:CG	0.46	2.64	8	1
1:A:143:ASN:OD1	1:A:143:ASN:C	0.46	2.57	6	12
1:A:104:PHE:CB	1:A:120:MET:CE	0.46	2.93	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD22	1:A:137:MET:SD	0.46	2.50	16	2
1:A:143:ASN:OD1	1:A:145:ASP:OD1	0.46	2.34	10	1
1:A:131:ASP:O	1:A:135:GLU:OE1	0.46	2.34	15	1
1:A:136:LEU:HG	1:A:156:PHE:CE1	0.46	2.45	26	1
1:A:144:ASN:O	1:A:145:ASP:OD1	0.46	2.34	26	1
1:A:151:ASP:OD1	1:A:151:ASP:N	0.46	2.46	9	5
1:A:97:LEU:N	1:A:97:LEU:HD22	0.46	2.26	2	1
1:A:114:LEU:HD13	1:A:137:MET:HG3	0.46	1.88	16	1
1:A:112:ILE:O	1:A:147:ARG:HA	0.46	2.11	18	10
1:A:113:ASP:OD1	1:A:113:ASP:C	0.46	2.59	5	2
1:A:153:PHE:CD1	1:A:153:PHE:C	0.45	2.93	26	3
1:A:141:ASP:OD1	1:A:148:ILE:HG12	0.45	2.12	6	2
1:A:137:MET:O	1:A:138:LYS:C	0.45	2.59	24	5
1:A:149:ASP:OD1	1:A:149:ASP:N	0.45	2.49	15	1
1:A:149:ASP:OD1	1:A:152:GLU:CD	0.45	2.58	1	1
1:A:107:ASN:HB2	1:A:116:GLU:OE2	0.45	2.12	26	14
1:A:143:ASN:ND2	1:A:145:ASP:OD2	0.45	2.50	2	1
1:A:136:LEU:HD12	1:A:137:MET:N	0.45	2.26	6	1
1:A:156:PHE:CD1	1:A:156:PHE:O	0.45	2.70	11	1
1:A:99:ASP:N	1:A:99:ASP:OD1	0.45	2.49	12	1
1:A:118:LYS:CB	1:A:133:ILE:HD13	0.45	2.42	20	1
1:A:121:LEU:HD11	1:A:136:LEU:HD22	0.45	1.86	20	1
1:A:118:LYS:O	1:A:122:GLN:OE1	0.45	2.34	1	1
1:A:140:GLY:HA3	1:A:156:PHE:CD1	0.45	2.47	2	4
1:A:104:PHE:CB	1:A:120:MET:SD	0.45	3.04	27	2
1:A:149:ASP:O	1:A:153:PHE:HB2	0.45	2.12	1	3
1:A:141:ASP:OD1	1:A:148:ILE:CG1	0.45	2.65	6	2
1:A:145:ASP:OD1	1:A:147:ARG:O	0.45	2.35	15	1
1:A:98:SER:HB3	1:A:150:TYR:CE1	0.45	2.46	20	3
1:A:107:ASN:O	1:A:108:ALA:C	0.45	2.60	17	3
1:A:98:SER:HB2	1:A:150:TYR:CZ	0.45	2.47	25	1
1:A:105:ASP:O	1:A:106:LYS:C	0.45	2.59	6	1
1:A:107:ASN:O	1:A:108:ALA:CB	0.45	2.65	6	4
1:A:117:LEU:HD23	1:A:121:LEU:HD11	0.45	1.88	15	1
1:A:130:GLU:O	1:A:134:GLU:HG3	0.45	2.12	11	7
1:A:136:LEU:HG	1:A:156:PHE:CZ	0.45	2.47	20	1
1:A:141:ASP:OD1	1:A:143:ASN:OD1	0.45	2.35	24	1
1:A:121:LEU:HD11	1:A:136:LEU:HD23	0.44	1.88	17	1
1:A:149:ASP:O	1:A:153:PHE:HB3	0.44	2.12	13	4
1:A:99:ASP:O	1:A:103:MET:HB3	0.44	2.12	26	3
1:A:117:LEU:HG	1:A:120:MET:HE2	0.44	1.89	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD23	1:A:137:MET:HG2	0.44	1.89	14	1
1:A:98:SER:HB2	1:A:150:TYR:OH	0.44	2.13	15	2
1:A:135:GLU:OE2	1:A:136:LEU:N	0.44	2.50	21	1
1:A:117:LEU:HD13	1:A:137:MET:HE1	0.44	1.89	22	1
1:A:129:THR:HG22	1:A:130:GLU:H	0.44	1.72	2	1
1:A:122:GLN:CG	1:A:123:ALA:N	0.44	2.80	8	2
1:A:150:TYR:O	1:A:154:LEU:HD12	0.44	2.12	13	2
1:A:145:ASP:OD2	1:A:147:ARG:HG3	0.44	2.12	8	1
1:A:100:LEU:HD23	1:A:103:MET:HE2	0.44	1.90	6	1
1:A:117:LEU:CD1	1:A:137:MET:SD	0.44	2.98	15	1
1:A:114:LEU:CD2	1:A:137:MET:SD	0.44	3.06	16	1
1:A:145:ASP:OD1	1:A:145:ASP:C	0.44	2.60	12	2
1:A:98:SER:HA	1:A:150:TYR:CE1	0.44	2.46	21	1
1:A:118:LYS:HG3	1:A:119:ILE:N	0.44	2.28	20	3
1:A:117:LEU:CD2	1:A:137:MET:HG2	0.44	2.43	29	2
1:A:118:LYS:CD	1:A:133:ILE:CD1	0.44	2.94	30	1
1:A:115:GLU:O	1:A:118:LYS:HG2	0.44	2.13	21	4
1:A:110:GLY:C	1:A:111:TYR:CG	0.43	2.96	4	1
1:A:114:LEU:O	1:A:115:GLU:C	0.43	2.62	5	2
1:A:97:LEU:O	1:A:98:SER:C	0.43	2.61	26	3
1:A:148:ILE:CG2	1:A:153:PHE:HB2	0.43	2.42	2	5
1:A:119:ILE:HA	1:A:122:GLN:NE2	0.43	2.27	3	1
1:A:130:GLU:O	1:A:134:GLU:OE1	0.43	2.36	15	1
1:A:114:LEU:CD2	1:A:118:LYS:HE3	0.43	2.42	22	1
1:A:101:PHE:CD1	1:A:101:PHE:C	0.43	2.95	10	1
1:A:100:LEU:HG	1:A:104:PHE:CE2	0.43	2.47	26	1
1:A:143:ASN:ND2	1:A:152:GLU:CD	0.43	2.76	6	1
1:A:114:LEU:CD1	1:A:137:MET:HG3	0.43	2.44	16	1
1:A:141:ASP:O	1:A:144:ASN:ND2	0.43	2.52	24	1
1:A:118:LYS:HD3	1:A:133:ILE:CD1	0.43	2.39	30	2
1:A:145:ASP:C	1:A:145:ASP:OD1	0.43	2.59	17	1
1:A:98:SER:HB3	1:A:150:TYR:CZ	0.43	2.49	18	1
1:A:149:ASP:OD1	1:A:151:ASP:HB2	0.43	2.14	28	6
1:A:136:LEU:C	1:A:156:PHE:CZ	0.43	2.96	26	1
1:A:111:TYR:C	1:A:112:ILE:HG12	0.43	2.39	7	4
1:A:153:PHE:CZ	1:A:157:MET:HG3	0.43	2.48	5	1
1:A:131:ASP:OD1	1:A:131:ASP:C	0.43	2.60	7	2
1:A:114:LEU:HG	1:A:137:MET:CB	0.43	2.44	20	3
1:A:107:ASN:OD1	1:A:116:GLU:OE2	0.43	2.37	20	1
1:A:121:LEU:HD21	1:A:136:LEU:CD2	0.43	2.44	3	1
1:A:104:PHE:HB3	1:A:120:MET:CE	0.43	2.44	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ASP:HA	1:A:112:ILE:HD13	0.42	1.91	18	5
1:A:137:MET:HE2	1:A:148:ILE:HD12	0.42	1.91	13	1
1:A:118:LYS:HG3	1:A:133:ILE:CD1	0.42	2.44	13	2
1:A:137:MET:O	1:A:137:MET:SD	0.42	2.77	7	2
1:A:112:ILE:O	1:A:148:ILE:N	0.42	2.52	9	1
1:A:117:LEU:O	1:A:118:LYS:C	0.42	2.61	23	2
1:A:102:ARG:HG2	1:A:102:ARG:O	0.42	2.14	26	1
1:A:153:PHE:CD1	1:A:154:LEU:N	0.42	2.87	8	1
1:A:130:GLU:OE2	1:A:134:GLU:CD	0.42	2.62	19	1
1:A:140:GLY:CA	1:A:156:PHE:CG	0.42	3.02	24	1
1:A:100:LEU:O	1:A:104:PHE:N	0.42	2.53	4	1
1:A:101:PHE:CZ	1:A:149:ASP:HA	0.42	2.50	5	1
1:A:101:PHE:HE2	1:A:148:ILE:HG22	0.42	1.73	14	1
1:A:113:ASP:OD1	1:A:116:GLU:HG3	0.42	2.14	10	6
1:A:136:LEU:O	1:A:137:MET:C	0.42	2.62	29	3
1:A:136:LEU:C	1:A:136:LEU:CD1	0.42	2.81	6	1
1:A:114:LEU:CD2	1:A:137:MET:HG3	0.42	2.44	29	2
1:A:101:PHE:CE2	1:A:110:GLY:O	0.42	2.73	7	1
1:A:112:ILE:CG2	1:A:116:GLU:CB	0.42	2.97	23	3
1:A:140:GLY:HA3	1:A:156:PHE:CG	0.42	2.50	24	1
1:A:118:LYS:CG	1:A:133:ILE:HD13	0.42	2.44	30	1
1:A:121:LEU:CD1	1:A:133:ILE:HG12	0.42	2.45	3	1
1:A:97:LEU:HD22	1:A:157:MET:SD	0.42	2.55	27	1
1:A:142:LYS:HG3	1:A:155:GLU:OE1	0.41	2.15	3	1
1:A:136:LEU:O	1:A:156:PHE:CE2	0.41	2.73	15	1
1:A:97:LEU:HD22	1:A:154:LEU:HD13	0.41	1.90	20	1
1:A:107:ASN:HB3	1:A:116:GLU:OE2	0.41	2.15	23	2
1:A:139:ASP:OD1	1:A:139:ASP:N	0.41	2.53	4	1
1:A:109:ASP:OD1	1:A:109:ASP:N	0.41	2.54	10	2
1:A:114:LEU:HD21	1:A:137:MET:HG2	0.41	1.91	8	1
1:A:113:ASP:OD2	1:A:115:GLU:CB	0.41	2.67	19	1
1:A:100:LEU:HD22	1:A:157:MET:HE2	0.41	1.91	28	1
1:A:136:LEU:C	1:A:138:LYS:N	0.41	2.78	29	1
1:A:103:MET:O	1:A:103:MET:CG	0.41	2.68	2	1
1:A:105:ASP:HA	1:A:112:ILE:CD1	0.41	2.45	25	2
1:A:113:ASP:OD2	1:A:115:GLU:HB3	0.41	2.14	14	1
1:A:115:GLU:HA	1:A:118:LYS:CE	0.41	2.45	21	1
1:A:107:ASN:HB3	1:A:116:GLU:OE1	0.41	2.16	10	1
1:A:130:GLU:O	1:A:134:GLU:HB2	0.41	2.16	12	1
1:A:155:GLU:O	1:A:158:LYS:HB3	0.41	2.16	15	1
1:A:149:ASP:OD2	1:A:151:ASP:HB2	0.41	2.15	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:GLU:O	1:A:134:GLU:HG2	0.41	2.16	10	2
1:A:100:LEU:O	1:A:101:PHE:C	0.41	2.63	4	2
1:A:140:GLY:HA3	1:A:156:PHE:CE2	0.41	2.50	9	1
1:A:98:SER:CA	1:A:150:TYR:OH	0.41	2.68	15	1
1:A:136:LEU:O	1:A:156:PHE:CE1	0.41	2.74	26	1
1:A:99:ASP:O	1:A:103:MET:HB2	0.41	2.16	13	2
1:A:106:LYS:HG3	1:A:119:ILE:CD1	0.41	2.45	29	1
1:A:114:LEU:CD2	1:A:114:LEU:C	0.41	2.93	1	1
1:A:113:ASP:OD2	1:A:115:GLU:HB2	0.41	2.16	9	1
1:A:140:GLY:CA	1:A:156:PHE:CD2	0.41	3.04	9	1
1:A:156:PHE:C	1:A:156:PHE:CD1	0.41	2.99	12	3
1:A:98:SER:C	1:A:100:LEU:N	0.41	2.79	15	1
1:A:111:TYR:HA	1:A:148:ILE:O	0.41	2.16	21	1
1:A:101:PHE:CE1	1:A:110:GLY:O	0.41	2.74	29	1
1:A:141:ASP:CG	1:A:144:ASN:HA	0.41	2.41	13	3
1:A:148:ILE:HG12	1:A:152:GLU:OE2	0.41	2.15	17	1
1:A:147:ARG:NH1	1:A:147:ARG:HG3	0.41	2.31	23	1
1:A:113:ASP:C	1:A:115:GLU:N	0.41	2.77	1	1
1:A:120:MET:CE	1:A:157:MET:CE	0.41	2.99	4	1
1:A:121:LEU:CD1	1:A:133:ILE:HG23	0.41	2.46	9	1
1:A:150:TYR:O	1:A:154:LEU:CD1	0.40	2.69	2	1
1:A:155:GLU:HA	1:A:158:LYS:HB2	0.40	1.93	9	1
1:A:145:ASP:OD1	1:A:145:ASP:N	0.40	2.53	10	1
1:A:99:ASP:O	1:A:103:MET:HG3	0.40	2.16	19	1
1:A:137:MET:SD	1:A:137:MET:O	0.40	2.79	30	1
1:A:104:PHE:CG	1:A:120:MET:HE2	0.40	2.51	13	1
1:A:143:ASN:OD1	1:A:145:ASP:OD2	0.40	2.39	1	1
1:A:100:LEU:HD22	1:A:100:LEU:HA	0.40	1.77	3	1
1:A:145:ASP:OD2	1:A:147:ARG:O	0.40	2.38	10	1
1:A:141:ASP:HA	1:A:152:GLU:OE1	0.40	2.17	15	1
1:A:140:GLY:O	1:A:142:LYS:N	0.40	2.55	17	1
1:A:107:ASN:OD1	1:A:109:ASP:HB3	0.40	2.17	22	1
1:A:103:MET:HG2	1:A:103:MET:O	0.40	2.16	27	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	58/76 (76%)	51±2 (88±4%)	6±2 (11±4%)	1±1 (1±1%)	11	58
All	All	1740/2280 (76%)	1525 (88%)	190 (11%)	25 (1%)	11	58

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	105	ASP	12
1	A	141	ASP	3
1	A	158	LYS	3
1	A	144	ASN	3
1	A	138	LYS	2
1	A	114	LEU	1
1	A	147	ARG	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	53/68 (78%)	39±3 (74±6%)	14±3 (26±6%)	2	22
All	All	1590/2040 (78%)	1171 (74%)	419 (26%)	2	22

All 39 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	112	ILE	30
1	A	154	LEU	29
1	A	122	GLN	21
1	A	117	LEU	19
1	A	158	LYS	18
1	A	97	LEU	15
1	A	114	LEU	14
1	A	135	GLU	14
1	A	96	GLU	13
1	A	115	GLU	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	132	ASP	13
1	A	142	LYS	13
1	A	138	LYS	13
1	A	102	ARG	13
1	A	155	GLU	12
1	A	148	ILE	11
1	A	141	ASP	11
1	A	151	ASP	11
1	A	106	LYS	11
1	A	130	GLU	10
1	A	118	LYS	10
1	A	99	ASP	10
1	A	136	LEU	10
1	A	103	MET	8
1	A	100	LEU	8
1	A	157	MET	8
1	A	129	THR	7
1	A	147	ARG	7
1	A	134	GLU	7
1	A	149	ASP	7
1	A	131	ASP	6
1	A	150	TYR	6
1	A	139	ASP	5
1	A	137	MET	4
1	A	98	SER	4
1	A	120	MET	3
1	A	107	ASN	2
1	A	152	GLU	2
1	A	121	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

No chemical shift data were provided