Full wwPDB NMR Structure Validation Report

Feb 17, 2022 – 11:57 AM EST

PDB ID	:	1OZS
Title	:	C-domain of human cardiac troponin C in complex with the inhibitory region of human cardiac troponin I
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Deposited on	:	2003-04-09

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

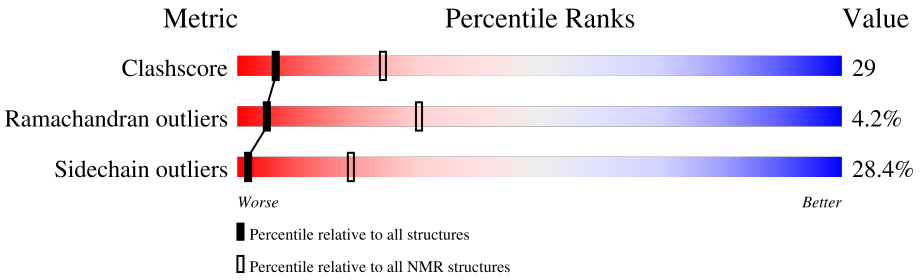
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	73	44% 45% 5% 5%
2	B	20	10% 20% 5% 65%

2 Ensemble composition and analysis

This entry contains 30 models. Model 13 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:93-A:161, B:132-B:138 (76)	0.59	13

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1532 atoms, of which 760 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms						Trace
1	A	73	Total	C	H	N	O	S	0
			1150	366	558	90	131	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	cloning artifact	UNP P63316

- Molecule 2 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					Trace
2	B	20	Total	C	H	N	O	0
			380	113	202	39	26	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Ca
			2	2

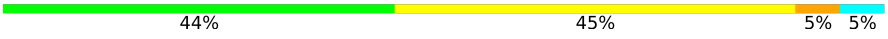
4 Residue-property plots

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.

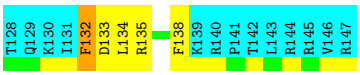
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



• Molecule 2: Troponin I, cardiac muscle

Chain B:



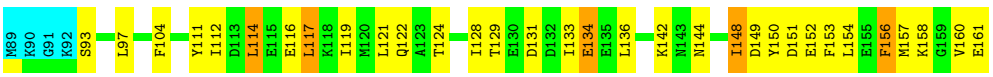
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

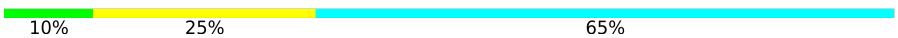
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

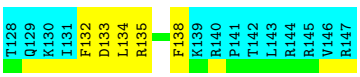
Chain A:



• Molecule 2: Troponin I, cardiac muscle

Chain B:

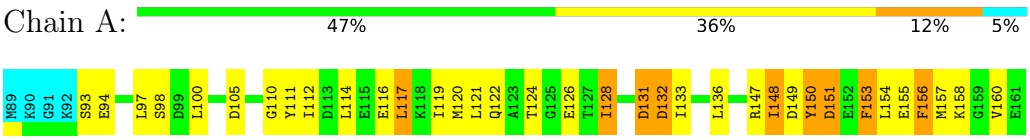




4.2.2 Score per residue for model 2

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



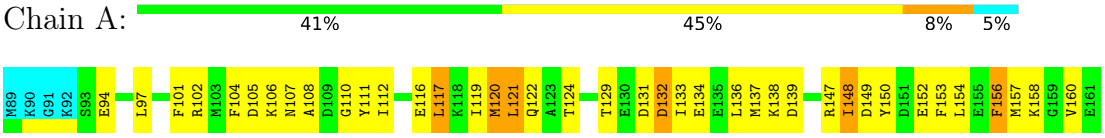
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.3 Score per residue for model 3

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



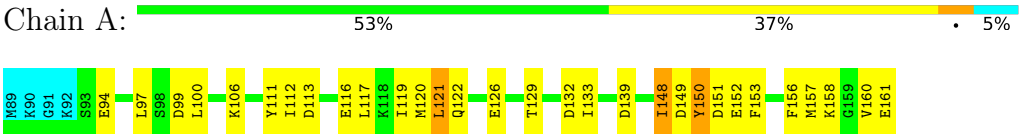
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.4 Score per residue for model 4

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



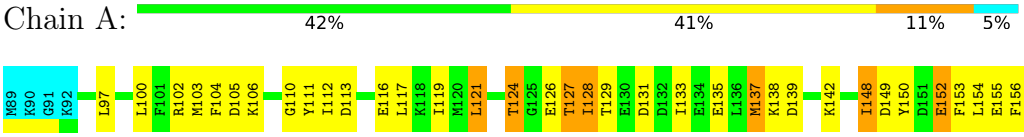
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



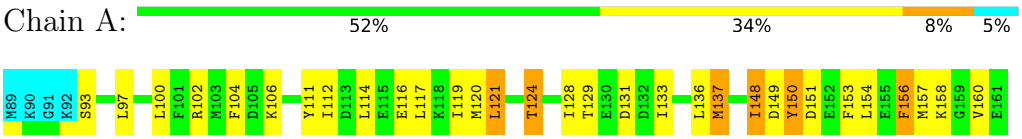
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.6 Score per residue for model 6

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



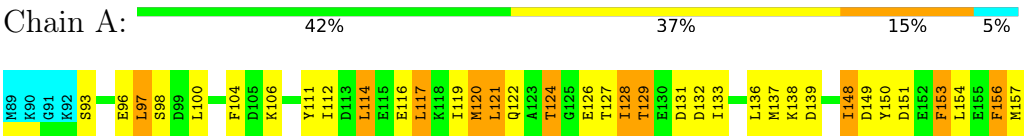
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.7 Score per residue for model 7

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



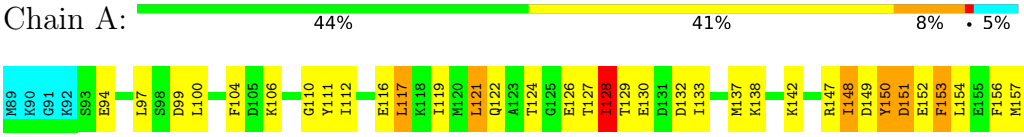
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.8 Score per residue for model 8

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



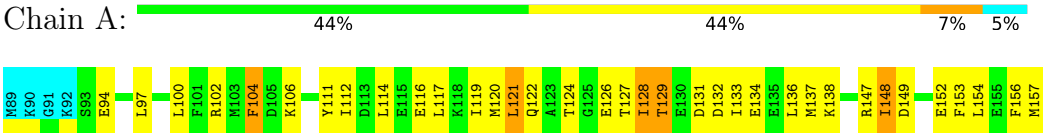
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.9 Score per residue for model 9

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



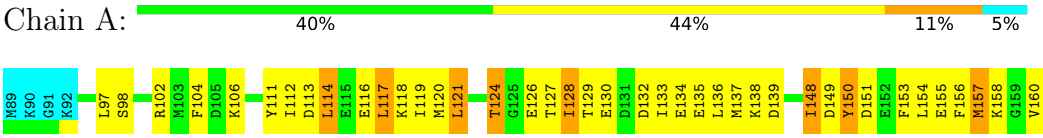
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.10 Score per residue for model 10

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



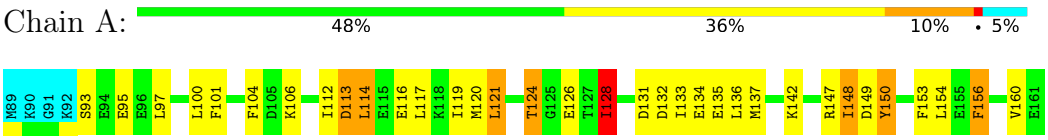
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.11 Score per residue for model 11

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



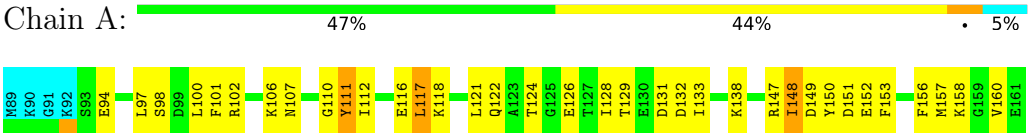
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



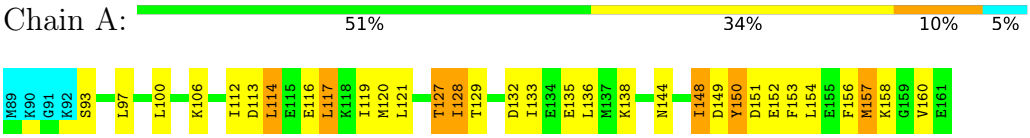
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



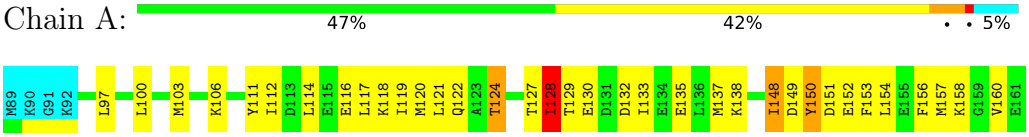
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



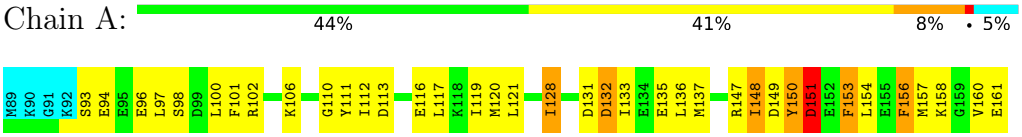
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



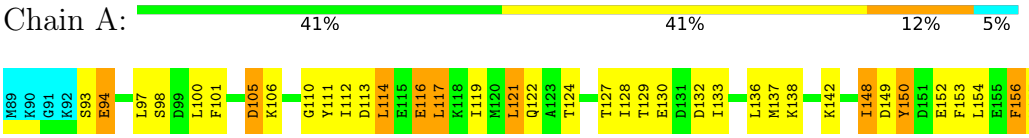
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.16 Score per residue for model 16

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



• Molecule 2: Troponin I, cardiac muscle

Chain B:

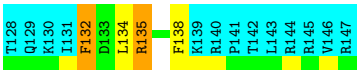
4.2.17 Score per residue for model 17

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:

• Molecule 2: Troponin I, cardiac muscle

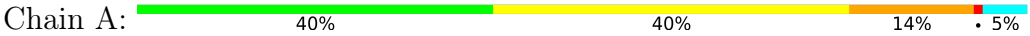
Chain B:

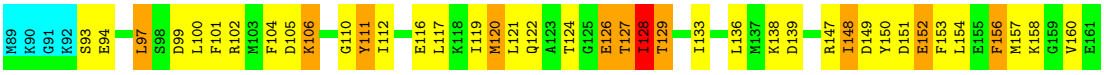


4.2.18 Score per residue for model 18

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

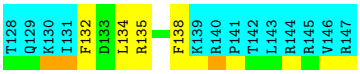
Chain A:





• Molecule 2: Troponin I, cardiac muscle

Chain B:



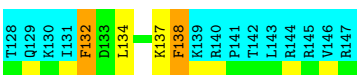
4.2.19 Score per residue for model 19

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:

• Molecule 2: Troponin I, cardiac muscle

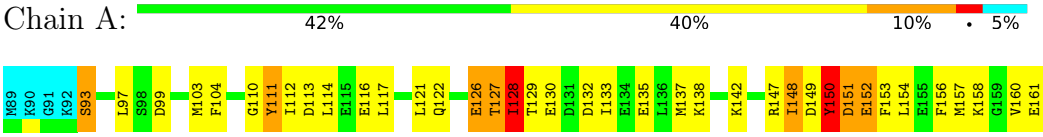
Chain B:



4.2.20 Score per residue for model 20

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



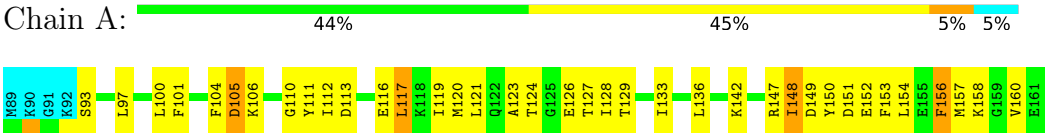
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.21 Score per residue for model 21

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



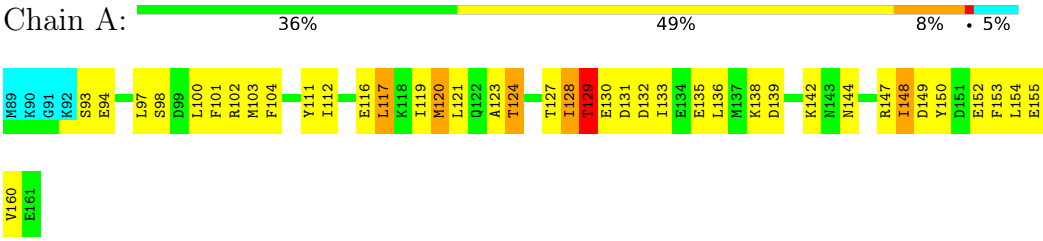
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.22 Score per residue for model 22

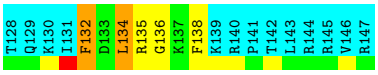
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



• Molecule 2: Troponin I, cardiac muscle

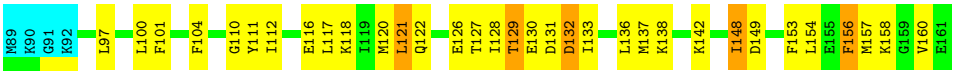
Chain B:



4.2.23 Score per residue for model 23

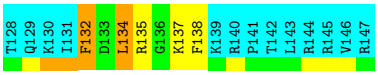
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



• Molecule 2: Troponin I, cardiac muscle

Chain B:



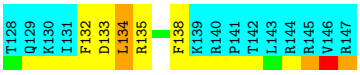
4.2.24 Score per residue for model 24

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:

• Molecule 2: Troponin I, cardiac muscle

Chain B:



4.2.25 Score per residue for model 25

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:

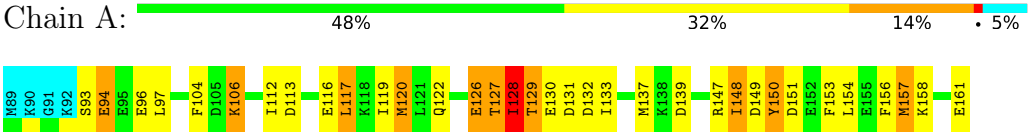
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.26 Score per residue for model 26

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



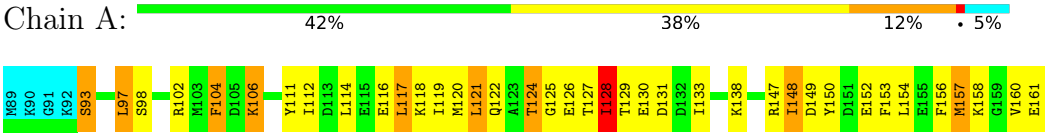
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.27 Score per residue for model 27

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



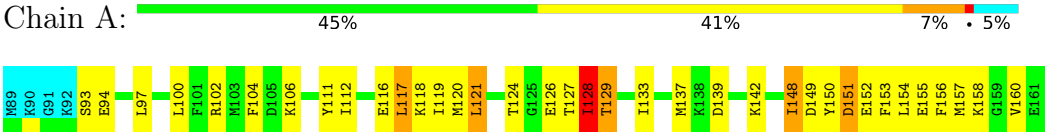
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.28 Score per residue for model 28

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



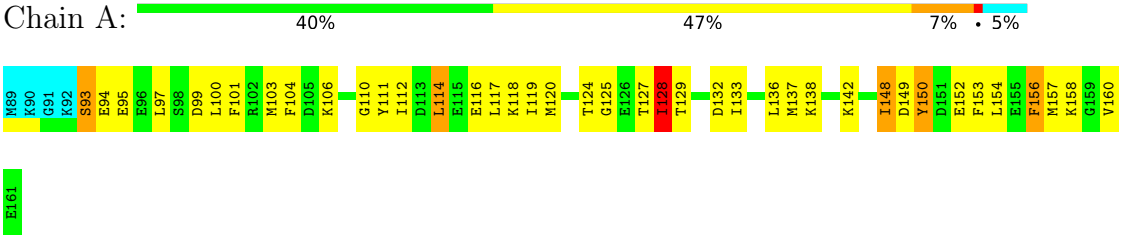
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.29 Score per residue for model 29

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



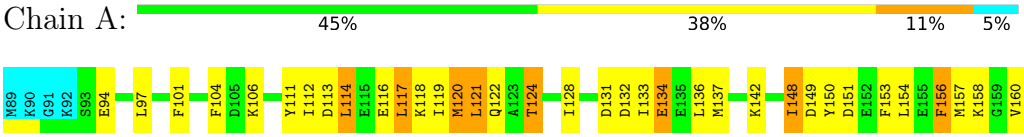
• Molecule 2: Troponin I, cardiac muscle

Chain B:

4.2.30 Score per residue for model 30

• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



• Molecule 2: Troponin I, cardiac muscle

Chain B:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *100 structures calculated using CNS simulated annealing protocol starting from extended structures.*

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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	562	518	518	31±5
2	B	62	62	62	8±3
All	All	18780	17400	17400	1033

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HD21	1:A:129:THR:HG22	0.93	1.40	12	1
1:A:121:LEU:HD11	1:A:133:ILE:HD11	0.93	1.35	4	3
1:A:150:TYR:CE1	1:A:154:LEU:HD21	0.85	2.06	30	14
2:B:132:PHE:O	2:B:134:LEU:HD12	0.84	1.72	3	5
1:A:121:LEU:HD12	1:A:133:ILE:HD11	0.82	1.48	24	2
1:A:97:LEU:HD22	1:A:153:PHE:CZ	0.81	2.11	25	5
1:A:121:LEU:CD2	1:A:129:THR:HG22	0.81	2.06	12	2
1:A:127:THR:O	1:A:129:THR:HG23	0.80	1.77	7	4
1:A:121:LEU:HD22	1:A:133:ILE:HD13	0.80	1.53	13	1
1:A:124:THR:HG22	2:B:132:PHE:CD1	0.80	2.11	21	1
1:A:100:LEU:HD13	2:B:138:PHE:CE1	0.79	2.13	24	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD23	1:A:100:LEU:HD12	0.79	1.52	25	4
1:A:97:LEU:HD23	1:A:100:LEU:HD23	0.79	1.54	14	2
1:A:148:ILE:HD13	1:A:149:ASP:N	0.77	1.94	3	28
1:A:97:LEU:HD21	1:A:157:MET:CG	0.77	2.09	16	12
1:A:126:GLU:O	1:A:129:THR:HG23	0.76	1.79	12	1
1:A:148:ILE:HD11	1:A:153:PHE:N	0.76	1.95	26	26
1:A:117:LEU:CB	1:A:133:ILE:HG23	0.76	2.10	20	4
1:A:127:THR:HG23	1:A:128:ILE:HG12	0.76	1.56	24	1
1:A:160:VAL:HG13	2:B:135:ARG:CG	0.75	2.10	23	6
1:A:97:LEU:HD11	1:A:157:MET:CG	0.75	2.12	23	6
1:A:97:LEU:HD23	1:A:153:PHE:CZ	0.74	2.17	27	9
1:A:117:LEU:HB3	1:A:133:ILE:HG23	0.74	1.59	20	16
1:A:104:PHE:HA	1:A:119:ILE:HD13	0.74	1.59	21	3
1:A:121:LEU:CD1	1:A:133:ILE:HD11	0.73	2.12	4	3
1:A:160:VAL:HG22	2:B:135:ARG:HG3	0.73	1.58	22	19
1:A:121:LEU:HD23	1:A:128:ILE:HG12	0.73	1.59	2	1
1:A:121:LEU:HD21	1:A:128:ILE:CG1	0.73	2.13	11	4
1:A:128:ILE:HG22	1:A:132:ASP:CB	0.73	2.14	13	1
1:A:100:LEU:HD13	1:A:157:MET:CE	0.73	2.14	18	1
1:A:114:LEU:HD13	1:A:117:LEU:HD12	0.72	1.61	17	1
1:A:160:VAL:HG21	2:B:138:PHE:CB	0.72	2.13	2	10
1:A:136:LEU:HD11	1:A:156:PHE:CZ	0.72	2.18	18	17
1:A:121:LEU:HD21	1:A:132:ASP:HB3	0.72	1.60	2	3
1:A:114:LEU:HD21	1:A:134:GLU:HG2	0.72	1.61	10	3
1:A:100:LEU:HD13	1:A:157:MET:HE1	0.72	1.62	18	1
1:A:121:LEU:HD13	1:A:124:THR:HG23	0.71	1.62	27	1
1:A:112:ILE:HG23	1:A:116:GLU:HB3	0.71	1.63	26	13
2:B:133:ASP:C	2:B:134:LEU:HD12	0.71	2.05	20	4
1:A:123:ALA:HB1	2:B:133:ASP:HB2	0.71	1.63	21	1
1:A:160:VAL:HG22	2:B:135:ARG:HA	0.71	1.63	10	12
1:A:160:VAL:HG13	2:B:135:ARG:HG2	0.70	1.62	23	3
1:A:97:LEU:HD11	1:A:157:MET:SD	0.70	2.26	21	4
1:A:97:LEU:HD13	1:A:154:LEU:HD22	0.70	1.64	21	15
1:A:114:LEU:HD21	1:A:134:GLU:CG	0.70	2.16	10	2
1:A:97:LEU:HD13	1:A:154:LEU:HA	0.70	1.63	22	9
1:A:97:LEU:HD23	1:A:100:LEU:CD1	0.69	2.17	9	4
1:A:117:LEU:HD13	1:A:120:MET:HG3	0.69	1.63	22	4
1:A:121:LEU:HD21	1:A:128:ILE:HD12	0.68	1.63	5	2
1:A:121:LEU:HD13	1:A:124:THR:OG1	0.68	1.87	30	4
1:A:160:VAL:HG21	2:B:138:PHE:HB2	0.68	1.65	17	6
1:A:160:VAL:HG13	2:B:135:ARG:HG3	0.68	1.64	24	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:THR:O	1:A:128:ILE:HD11	0.68	1.88	28	1
1:A:113:ASP:O	1:A:117:LEU:HD23	0.68	1.88	20	3
1:A:121:LEU:HD22	1:A:133:ILE:CD1	0.67	2.19	13	2
1:A:121:LEU:HD11	1:A:128:ILE:HG13	0.67	1.66	6	5
1:A:127:THR:O	1:A:128:ILE:HG23	0.67	1.89	8	3
1:A:128:ILE:HD12	1:A:132:ASP:HB2	0.67	1.65	24	1
1:A:114:LEU:HD23	1:A:133:ILE:CG2	0.67	2.19	11	1
1:A:117:LEU:HD11	1:A:136:LEU:HG	0.67	1.66	7	3
1:A:117:LEU:HD11	1:A:137:MET:SD	0.67	2.29	19	1
1:A:136:LEU:HD12	1:A:136:LEU:O	0.67	1.90	10	7
1:A:106:LYS:CD	1:A:119:ILE:HD11	0.66	2.20	27	1
1:A:121:LEU:CD2	1:A:128:ILE:HD12	0.66	2.21	5	2
1:A:117:LEU:HD11	1:A:137:MET:CG	0.66	2.20	6	1
1:A:112:ILE:HG23	1:A:116:GLU:CB	0.66	2.21	18	28
1:A:121:LEU:O	1:A:121:LEU:HD13	0.66	1.90	5	1
1:A:121:LEU:HD11	1:A:128:ILE:HG12	0.66	1.68	11	3
1:A:97:LEU:HD21	1:A:157:MET:HG3	0.66	1.66	25	10
1:A:112:ILE:HG23	1:A:116:GLU:HB2	0.65	1.68	19	15
1:A:157:MET:O	1:A:160:VAL:HG23	0.65	1.90	23	13
1:A:136:LEU:HD21	2:B:134:LEU:HD21	0.65	1.67	13	3
1:A:97:LEU:HD21	1:A:157:MET:HG2	0.65	1.67	15	16
1:A:148:ILE:HD11	1:A:153:PHE:CA	0.65	2.20	17	3
1:A:124:THR:HG23	2:B:132:PHE:CD1	0.65	2.26	10	1
1:A:100:LEU:HD13	2:B:138:PHE:CE2	0.65	2.27	17	3
1:A:123:ALA:HB1	2:B:133:ASP:CB	0.64	2.22	21	1
1:A:112:ILE:HG22	1:A:117:LEU:HD12	0.64	1.68	18	1
1:A:121:LEU:HD11	1:A:129:THR:HA	0.64	1.69	24	1
1:A:121:LEU:HD21	1:A:129:THR:CG2	0.64	2.20	12	1
1:A:121:LEU:HD22	1:A:133:ILE:HG12	0.63	1.68	1	1
1:A:121:LEU:HD23	1:A:128:ILE:CG1	0.63	2.23	2	2
1:A:120:MET:SD	2:B:134:LEU:HD21	0.63	2.33	15	2
1:A:121:LEU:HD12	1:A:122:GLN:N	0.63	2.09	14	1
1:A:97:LEU:HD11	1:A:157:MET:HG2	0.62	1.71	12	14
1:A:97:LEU:HA	1:A:100:LEU:HD12	0.62	1.71	29	4
1:A:106:LYS:HD3	1:A:119:ILE:HD11	0.62	1.71	26	1
1:A:117:LEU:O	1:A:117:LEU:HD13	0.62	1.95	12	1
1:A:148:ILE:HD13	1:A:148:ILE:C	0.62	2.15	6	16
1:A:121:LEU:HD22	1:A:121:LEU:O	0.62	1.94	16	1
1:A:128:ILE:HD12	1:A:132:ASP:HB3	0.62	1.72	26	1
1:A:121:LEU:HD12	1:A:129:THR:HG23	0.61	1.69	5	1
1:A:114:LEU:HA	1:A:117:LEU:HD12	0.61	1.72	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD11	1:A:137:MET:HG2	0.61	1.69	6	1
1:A:128:ILE:H	1:A:128:ILE:HD13	0.61	1.56	7	1
1:A:121:LEU:HD11	1:A:136:LEU:HD23	0.61	1.72	13	1
1:A:117:LEU:HD23	1:A:133:ILE:HG23	0.61	1.71	4	2
1:A:124:THR:HG22	2:B:132:PHE:CG	0.61	2.31	21	1
1:A:121:LEU:HD21	1:A:128:ILE:HG12	0.61	1.72	28	2
1:A:117:LEU:HD12	1:A:133:ILE:HG23	0.61	1.70	28	1
1:A:104:PHE:CD2	1:A:112:ILE:HD13	0.60	2.31	24	1
1:A:121:LEU:HD13	1:A:133:ILE:HG13	0.60	1.73	20	3
1:A:117:LEU:HD23	1:A:120:MET:HE1	0.60	1.73	14	1
2:B:132:PHE:CD1	2:B:134:LEU:HD22	0.60	2.31	22	1
1:A:128:ILE:HD12	1:A:132:ASP:CB	0.60	2.26	24	3
2:B:132:PHE:CE1	2:B:134:LEU:HD11	0.59	2.32	24	1
1:A:114:LEU:HD21	1:A:134:GLU:HG3	0.59	1.73	11	1
1:A:121:LEU:CD1	1:A:129:THR:HG22	0.59	2.28	4	1
1:A:121:LEU:HD11	1:A:128:ILE:CG1	0.59	2.27	25	3
1:A:97:LEU:CB	1:A:154:LEU:HD22	0.59	2.28	5	15
1:A:121:LEU:HD21	1:A:128:ILE:HG13	0.59	1.72	11	1
1:A:124:THR:HG21	1:A:128:ILE:HD11	0.59	1.72	12	4
1:A:128:ILE:HG22	1:A:132:ASP:CG	0.59	2.17	13	1
1:A:154:LEU:HD23	1:A:154:LEU:N	0.59	2.12	29	10
1:A:148:ILE:HD11	1:A:152:GLU:C	0.59	2.18	21	17
2:B:132:PHE:CE2	2:B:134:LEU:HD11	0.59	2.32	3	5
1:A:126:GLU:O	1:A:127:THR:HG22	0.58	1.97	8	3
1:A:100:LEU:HD12	2:B:138:PHE:CE2	0.58	2.32	15	1
1:A:128:ILE:HD11	1:A:133:ILE:HG12	0.58	1.74	26	1
1:A:117:LEU:HD13	1:A:137:MET:HE3	0.58	1.75	5	1
1:A:121:LEU:HD21	1:A:133:ILE:CD1	0.58	2.28	7	1
1:A:121:LEU:HD13	1:A:124:THR:HG1	0.58	1.59	6	3
1:A:123:ALA:HB3	2:B:134:LEU:CD1	0.58	2.28	22	1
1:A:117:LEU:HD13	1:A:137:MET:CE	0.58	2.28	5	1
1:A:121:LEU:CD1	1:A:129:THR:HG23	0.58	2.28	5	1
1:A:121:LEU:HD12	1:A:133:ILE:CD1	0.58	2.25	24	2
1:A:160:VAL:HG21	2:B:138:PHE:HB3	0.57	1.76	2	5
1:A:126:GLU:CG	1:A:128:ILE:HD12	0.57	2.29	25	2
1:A:114:LEU:O	1:A:133:ILE:HG21	0.57	1.99	7	1
1:A:97:LEU:CD2	1:A:100:LEU:HD23	0.57	2.27	14	1
1:A:128:ILE:N	1:A:128:ILE:HD13	0.57	2.13	25	3
1:A:121:LEU:HD11	1:A:133:ILE:CD1	0.57	2.23	4	2
1:A:118:LYS:HA	1:A:133:ILE:HD12	0.57	1.76	10	2
1:A:117:LEU:HD21	1:A:136:LEU:HB3	0.57	1.77	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:GLU:O	1:A:128:ILE:HD13	0.57	2.00	28	2
1:A:121:LEU:HD12	1:A:129:THR:HG22	0.57	1.77	4	2
1:A:114:LEU:HD23	1:A:134:GLU:CG	0.57	2.30	9	1
1:A:124:THR:HG21	2:B:132:PHE:CD2	0.56	2.35	5	2
1:A:124:THR:HG23	2:B:134:LEU:HD13	0.56	1.76	22	1
1:A:121:LEU:HD21	1:A:128:ILE:CD1	0.56	2.31	5	1
1:A:114:LEU:HD13	1:A:114:LEU:N	0.56	2.15	19	3
1:A:126:GLU:C	1:A:128:ILE:HD13	0.56	2.20	11	2
1:A:114:LEU:HD23	1:A:133:ILE:HG22	0.56	1.76	11	2
1:A:124:THR:HG21	2:B:132:PHE:CE2	0.56	2.36	5	6
1:A:120:MET:SD	1:A:136:LEU:HD21	0.56	2.41	18	2
1:A:114:LEU:HD23	1:A:134:GLU:HG3	0.55	1.76	9	1
1:A:97:LEU:HD13	1:A:154:LEU:CB	0.55	2.31	29	3
1:A:117:LEU:HD21	1:A:137:MET:SD	0.55	2.41	15	1
1:A:113:ASP:O	1:A:117:LEU:HD12	0.55	2.02	21	1
2:B:134:LEU:HD12	2:B:134:LEU:N	0.54	2.17	2	13
1:A:100:LEU:HD21	2:B:138:PHE:CE1	0.54	2.37	5	1
1:A:117:LEU:HD13	1:A:133:ILE:O	0.54	2.02	6	2
2:B:132:PHE:CD1	2:B:132:PHE:N	0.54	2.74	4	13
1:A:117:LEU:HD13	1:A:120:MET:CE	0.54	2.33	15	1
1:A:121:LEU:HD21	1:A:133:ILE:HD13	0.54	1.79	7	1
1:A:128:ILE:HG22	1:A:129:THR:HG22	0.54	1.80	17	2
1:A:124:THR:HG23	1:A:126:GLU:H	0.53	1.63	9	1
2:B:132:PHE:CD1	2:B:134:LEU:CD1	0.53	2.91	24	1
1:A:121:LEU:HD11	1:A:132:ASP:HB3	0.53	1.80	3	2
1:A:97:LEU:HD11	1:A:157:MET:HG3	0.53	1.80	14	3
1:A:121:LEU:HD22	1:A:129:THR:HG22	0.53	1.79	24	1
1:A:97:LEU:HD13	1:A:154:LEU:HB3	0.53	1.80	2	3
1:A:121:LEU:HD21	1:A:132:ASP:HB2	0.53	1.79	3	1
1:A:111:TYR:HA	1:A:148:ILE:O	0.53	2.04	3	15
1:A:117:LEU:HD12	1:A:133:ILE:HA	0.53	1.79	12	1
1:A:97:LEU:CD2	1:A:100:LEU:HD12	0.53	2.32	22	1
2:B:132:PHE:H	2:B:134:LEU:HD12	0.53	1.65	26	1
1:A:120:MET:HB3	2:B:134:LEU:HD21	0.52	1.81	23	1
1:A:123:ALA:HB3	2:B:134:LEU:HD11	0.52	1.81	22	1
1:A:128:ILE:HG21	1:A:132:ASP:CG	0.52	2.25	23	1
1:A:121:LEU:HG	1:A:129:THR:HG22	0.52	1.81	28	1
1:A:148:ILE:HG23	1:A:148:ILE:O	0.51	2.05	6	4
1:A:126:GLU:HG2	1:A:128:ILE:HD12	0.51	1.80	25	2
1:A:101:PHE:CD1	1:A:153:PHE:CD2	0.51	2.99	22	9
1:A:112:ILE:HB	1:A:148:ILE:CG2	0.51	2.36	17	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:HD13	2:B:138:PHE:HE2	0.51	1.66	11	2
1:A:116:GLU:O	1:A:119:ILE:HD12	0.51	2.05	6	21
1:A:136:LEU:CD2	2:B:134:LEU:HD21	0.51	2.35	17	2
2:B:132:PHE:CE2	2:B:134:LEU:CD1	0.51	2.94	28	12
1:A:121:LEU:HD22	1:A:133:ILE:CG1	0.51	2.34	1	1
1:A:121:LEU:C	1:A:121:LEU:HD13	0.50	2.27	16	1
1:A:127:THR:HG23	1:A:128:ILE:CG1	0.50	2.33	24	1
1:A:100:LEU:HD12	1:A:157:MET:SD	0.49	2.47	8	1
1:A:150:TYR:CD1	1:A:154:LEU:HD21	0.49	2.42	29	2
1:A:160:VAL:HG22	2:B:135:ARG:CG	0.49	2.35	11	4
1:A:97:LEU:HD22	1:A:154:LEU:HA	0.49	1.84	7	5
1:A:129:THR:O	1:A:131:ASP:N	0.49	2.44	26	2
1:A:124:THR:HG21	2:B:132:PHE:HB2	0.49	1.84	14	1
1:A:93:SER:O	1:A:97:LEU:HD12	0.49	2.06	20	1
1:A:97:LEU:HD23	1:A:153:PHE:CE1	0.49	2.43	18	4
1:A:124:THR:HB	1:A:128:ILE:HD11	0.48	1.84	5	1
2:B:132:PHE:CD1	2:B:134:LEU:HD11	0.48	2.43	24	1
1:A:121:LEU:HD23	1:A:128:ILE:HD11	0.48	1.85	16	1
1:A:160:VAL:HG11	2:B:138:PHE:O	0.48	2.08	17	1
1:A:124:THR:HG23	2:B:132:PHE:CG	0.48	2.43	10	1
1:A:101:PHE:CD2	1:A:150:TYR:CE2	0.48	3.01	29	2
1:A:148:ILE:HD13	1:A:149:ASP:O	0.48	2.09	18	10
2:B:132:PHE:CD2	2:B:134:LEU:HD13	0.48	2.43	8	5
1:A:121:LEU:HD11	1:A:128:ILE:CD1	0.48	2.38	28	1
1:A:121:LEU:HD21	1:A:132:ASP:CB	0.48	2.35	2	1
1:A:116:GLU:CA	1:A:119:ILE:HD12	0.48	2.38	15	2
1:A:136:LEU:HD11	1:A:156:PHE:HZ	0.48	1.68	10	1
1:A:127:THR:O	1:A:129:THR:N	0.48	2.46	13	1
1:A:127:THR:HG23	1:A:127:THR:O	0.48	2.07	20	1
1:A:104:PHE:O	1:A:119:ILE:HD13	0.48	2.08	18	1
1:A:148:ILE:HD11	1:A:152:GLU:HB2	0.48	1.86	1	3
1:A:128:ILE:HG21	1:A:132:ASP:OD2	0.48	2.08	8	1
2:B:132:PHE:CD1	2:B:134:LEU:HD13	0.48	2.43	21	1
1:A:127:THR:HG22	1:A:128:ILE:N	0.47	2.24	19	3
1:A:97:LEU:CD1	1:A:154:LEU:HD22	0.47	2.39	5	5
1:A:121:LEU:HD23	1:A:129:THR:HA	0.47	1.86	1	1
1:A:127:THR:O	1:A:128:ILE:HD13	0.47	2.08	17	2
1:A:117:LEU:HD11	1:A:137:MET:HB2	0.47	1.85	23	2
1:A:121:LEU:HD12	1:A:129:THR:CG2	0.47	2.39	5	2
1:A:124:THR:HG23	2:B:133:ASP:HB3	0.47	1.86	7	1
1:A:117:LEU:HD21	1:A:137:MET:N	0.47	2.24	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ILE:HD13	1:A:132:ASP:HB3	0.47	1.86	15	1
1:A:121:LEU:HD22	1:A:124:THR:CG2	0.47	2.40	16	1
1:A:121:LEU:HD11	1:A:128:ILE:HD11	0.47	1.86	28	1
1:A:149:ASP:O	1:A:151:ASP:N	0.47	2.47	24	10
1:A:104:PHE:CA	1:A:119:ILE:HD13	0.47	2.38	21	2
1:A:112:ILE:O	1:A:148:ILE:HG22	0.47	2.10	21	1
1:A:128:ILE:HD13	1:A:132:ASP:CB	0.46	2.41	29	1
1:A:107:ASN:O	1:A:108:ALA:HB3	0.46	2.10	3	1
1:A:121:LEU:HD13	1:A:128:ILE:HG13	0.46	1.87	7	1
1:A:157:MET:CE	2:B:138:PHE:CE1	0.46	2.99	18	1
1:A:124:THR:HG23	2:B:134:LEU:CD1	0.46	2.40	22	1
1:A:157:MET:CE	2:B:138:PHE:CE2	0.46	2.99	4	2
1:A:120:MET:O	2:B:134:LEU:HD21	0.45	2.12	22	1
1:A:153:PHE:CD1	1:A:153:PHE:O	0.45	2.70	12	14
1:A:148:ILE:C	1:A:148:ILE:CD1	0.45	2.83	6	3
1:A:120:MET:HB2	2:B:134:LEU:HD21	0.45	1.87	3	2
1:A:121:LEU:HD21	1:A:128:ILE:HD11	0.45	1.89	25	1
1:A:156:PHE:HE2	2:B:134:LEU:HD23	0.45	1.72	16	3
1:A:120:MET:HG3	1:A:121:LEU:HD12	0.45	1.88	13	1
2:B:134:LEU:O	2:B:138:PHE:CD2	0.45	2.70	23	4
1:A:121:LEU:O	1:A:124:THR:HG22	0.45	2.11	16	2
1:A:136:LEU:HD21	2:B:134:LEU:CD2	0.44	2.42	25	2
1:A:150:TYR:HD1	1:A:154:LEU:HD21	0.44	1.72	29	3
1:A:128:ILE:HG22	1:A:132:ASP:HB2	0.44	1.88	13	1
1:A:97:LEU:CD2	1:A:153:PHE:CZ	0.44	2.99	14	2
1:A:126:GLU:O	1:A:127:THR:CG2	0.44	2.64	8	2
1:A:104:PHE:CZ	1:A:120:MET:CE	0.44	3.00	25	2
1:A:128:ILE:HG12	1:A:128:ILE:O	0.44	2.12	11	1
1:A:116:GLU:HA	1:A:119:ILE:HD12	0.44	1.89	15	1
1:A:126:GLU:CB	1:A:128:ILE:CD1	0.44	2.96	18	1
2:B:132:PHE:O	2:B:132:PHE:CD2	0.44	2.71	3	5
1:A:117:LEU:HD21	1:A:136:LEU:HG	0.44	1.89	2	1
1:A:148:ILE:CD1	1:A:149:ASP:O	0.44	2.65	3	1
2:B:134:LEU:N	2:B:134:LEU:CD1	0.44	2.81	8	5
1:A:148:ILE:HD11	1:A:153:PHE:HA	0.44	1.89	17	2
1:A:96:GLU:O	1:A:100:LEU:HD13	0.44	2.13	7	1
1:A:94:GLU:CG	1:A:154:LEU:HD13	0.44	2.42	16	2
1:A:117:LEU:CD2	1:A:133:ILE:HG23	0.43	2.40	4	1
1:A:117:LEU:HD22	1:A:133:ILE:O	0.43	2.13	27	2
1:A:104:PHE:CE2	1:A:120:MET:HE3	0.43	2.48	3	1
1:A:105:ASP:O	1:A:106:LYS:CG	0.43	2.66	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:MET:CE	2:B:138:PHE:CD1	0.43	3.01	18	1
1:A:101:PHE:CZ	1:A:150:TYR:N	0.43	2.86	21	1
1:A:117:LEU:HD13	1:A:120:MET:SD	0.43	2.53	24	1
2:B:134:LEU:CD1	2:B:134:LEU:N	0.43	2.82	6	6
2:B:132:PHE:CZ	2:B:134:LEU:CD1	0.43	3.02	28	1
1:A:160:VAL:HG13	2:B:135:ARG:O	0.43	2.14	27	1
1:A:117:LEU:HB2	1:A:133:ILE:HG23	0.43	1.84	20	1
1:A:120:MET:CB	2:B:134:LEU:HD21	0.43	2.44	3	1
1:A:97:LEU:HB2	1:A:154:LEU:HD22	0.43	1.91	13	1
1:A:128:ILE:HG21	1:A:132:ASP:OD1	0.43	2.14	23	1
1:A:110:GLY:O	1:A:111:TYR:CD1	0.43	2.72	3	12
1:A:117:LEU:HD21	1:A:136:LEU:CG	0.43	2.44	2	1
1:A:121:LEU:HD21	1:A:133:ILE:HD11	0.43	1.90	14	1
1:A:97:LEU:HA	1:A:100:LEU:HD22	0.43	1.90	4	1
1:A:124:THR:CG2	2:B:132:PHE:CD1	0.43	3.00	10	1
1:A:118:LYS:HG2	1:A:121:LEU:HD11	0.43	1.89	14	1
1:A:129:THR:HG23	1:A:132:ASP:H	0.43	1.74	14	1
1:A:94:GLU:HG3	1:A:154:LEU:HD13	0.43	1.90	16	1
1:A:124:THR:HG23	1:A:125:GLY:N	0.43	2.28	29	2
2:B:133:ASP:O	2:B:134:LEU:C	0.43	2.56	24	1
1:A:128:ILE:HD13	1:A:128:ILE:N	0.42	2.28	11	1
1:A:121:LEU:HD13	1:A:124:THR:CG2	0.42	2.44	19	1
2:B:132:PHE:CZ	2:B:134:LEU:HD11	0.42	2.49	24	1
1:A:121:LEU:HB2	1:A:133:ILE:HD11	0.42	1.91	23	2
1:A:128:ILE:HD11	2:B:132:PHE:HE2	0.42	1.73	24	1
1:A:157:MET:HA	1:A:160:VAL:HG23	0.42	1.91	9	4
2:B:132:PHE:O	2:B:133:ASP:C	0.42	2.57	24	1
1:A:117:LEU:HD23	1:A:137:MET:SD	0.42	2.55	7	2
1:A:132:ASP:OD2	2:B:132:PHE:CZ	0.42	2.73	11	1
1:A:105:ASP:O	1:A:106:LYS:CB	0.42	2.67	18	1
2:B:133:ASP:O	2:B:138:PHE:CZ	0.42	2.72	21	1
2:B:134:LEU:O	2:B:138:PHE:CD1	0.42	2.73	4	3
1:A:128:ILE:HB	1:A:132:ASP:CB	0.42	2.44	7	1
1:A:124:THR:CB	1:A:128:ILE:HD11	0.41	2.45	6	1
1:A:128:ILE:N	1:A:128:ILE:CD1	0.41	2.83	25	1
1:A:121:LEU:HD13	1:A:125:GLY:H	0.41	1.75	27	1
2:B:132:PHE:CE2	2:B:134:LEU:HD13	0.41	2.50	28	1
2:B:133:ASP:O	2:B:138:PHE:CE1	0.41	2.73	14	1
1:A:128:ILE:C	1:A:129:THR:HG22	0.41	2.35	22	1
1:A:111:TYR:CE2	1:A:149:ASP:OD1	0.41	2.74	28	1
1:A:120:MET:HB2	2:B:134:LEU:HD11	0.41	1.91	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:ASP:O	1:A:117:LEU:HD13	0.41	2.15	25	1
1:A:112:ILE:N	1:A:148:ILE:O	0.41	2.50	28	1
2:B:136:GLY:O	2:B:138:PHE:N	0.41	2.52	15	1
1:A:97:LEU:HD23	1:A:100:LEU:HD13	0.41	1.92	9	1
1:A:111:TYR:CE1	1:A:149:ASP:OD2	0.41	2.73	9	1
1:A:149:ASP:O	1:A:150:TYR:C	0.41	2.59	16	1
1:A:121:LEU:HD13	1:A:133:ILE:CG1	0.41	2.41	20	1
1:A:121:LEU:HD23	1:A:133:ILE:HG12	0.41	1.92	28	1
1:A:97:LEU:CD2	1:A:157:MET:CG	0.41	2.99	4	1
1:A:157:MET:O	1:A:160:VAL:N	0.41	2.51	16	2
1:A:153:PHE:O	1:A:156:PHE:HB2	0.41	2.15	11	1
1:A:128:ILE:HG21	1:A:132:ASP:HB2	0.41	1.91	19	1
1:A:132:ASP:OD2	2:B:132:PHE:CE1	0.41	2.74	20	1
1:A:153:PHE:O	1:A:153:PHE:CD1	0.41	2.74	28	1
2:B:134:LEU:N	2:B:134:LEU:HD12	0.41	2.31	28	1
1:A:124:THR:HG23	1:A:128:ILE:HD11	0.41	1.92	2	1
1:A:104:PHE:CZ	1:A:120:MET:HE2	0.41	2.51	25	2
1:A:96:GLU:CB	2:B:138:PHE:CE1	0.41	3.03	15	1
2:B:133:ASP:O	2:B:138:PHE:CE2	0.41	2.74	21	1
1:A:97:LEU:HB3	1:A:154:LEU:HD22	0.41	1.93	29	1
1:A:124:THR:CG2	2:B:133:ASP:CB	0.40	2.99	7	1
1:A:121:LEU:HD13	1:A:133:ILE:CD1	0.40	2.45	9	2
1:A:101:PHE:HB2	1:A:153:PHE:CE2	0.40	2.52	17	1
1:A:126:GLU:O	1:A:127:THR:HB	0.40	2.17	24	1
1:A:160:VAL:HG13	2:B:136:GLY:H	0.40	1.75	7	1
1:A:104:PHE:CB	1:A:112:ILE:HD13	0.40	2.46	22	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	68/73 (93%)	56±2 (82±3%)	9±2 (13±3%)	3±1 (4±2%)	5	30
2	B	7/20 (35%)	4±1 (59±19%)	3±1 (37±16%)	0±0 (4±7%)	5	29
All	All	2250/2790 (81%)	1805 (80%)	350 (16%)	95 (4%)	5	30

All 15 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	150	TYR	15
1	A	128	ILE	15
1	A	129	THR	14
1	A	93	SER	9
1	A	127	THR	8
1	A	151	ASP	7
1	A	105	ASP	5
1	A	131	ASP	4
1	A	126	GLU	4
2	B	132	PHE	3
2	B	137	LYS	3
1	A	130	GLU	3
2	B	136	GLY	2
1	A	94	GLU	2
2	B	135	ARG	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	61/65 (94%)	44±4 (72±6%)	17±4 (28±6%)	2	19
2	B	6/19 (32%)	4±1 (71±13%)	2±1 (29±13%)	1	17
All	All	2010/2520 (80%)	1440 (72%)	570 (28%)	2	19

All 55 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	148	ILE	30
1	A	156	PHE	29
1	A	158	LYS	28
1	A	106	LYS	22
2	B	132	PHE	21
1	A	122	GLN	18
1	A	138	LYS	18

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Mol	Chain	Res	Type	Models (Total)
1	A	117	LEU	17
1	A	128	ILE	17
1	A	121	LEU	17
1	A	104	PHE	16
1	A	147	ARG	15
1	A	94	GLU	14
1	A	102	ARG	14
1	A	120	MET	14
1	A	93	SER	13
1	A	142	LYS	13
1	A	124	THR	13
1	A	114	LEU	12
1	A	137	MET	12
2	B	133	ASP	11
1	A	131	ASP	11
1	A	132	ASP	11
1	A	150	TYR	11
1	A	126	GLU	10
1	A	139	ASP	10
1	A	111	TYR	10
1	A	135	GLU	10
1	A	161	GLU	9
1	A	113	ASP	9
1	A	98	SER	8
1	A	130	GLU	8
1	A	151	ASP	8
1	A	155	GLU	7
2	B	137	LYS	7
1	A	99	ASP	7
2	B	138	PHE	6
1	A	103	MET	6
1	A	118	LYS	6
1	A	129	THR	5
1	A	157	MET	5
2	B	134	LEU	5
1	A	127	THR	5
1	A	134	GLU	4
1	A	144	ASN	4
1	A	153	PHE	4
1	A	152	GLU	3
2	B	135	ARG	3
1	A	97	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	95	GLU	3
1	A	105	ASP	2
1	A	116	GLU	2
1	A	96	GLU	2
1	A	100	LEU	1
1	A	107	ASN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

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

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided