Full wwPDB NMR Structure Validation Report (i)

Feb 14, 2022 – 06:21 AM EST

PDB ID	:	1JC2
Title	:	COMPLEX OF THE C-DOMAIN OF TROPONIN C WITH RESIDUES 1-40 OF TROPONIN I
Authors	:	Mercier, P.; Spyracopoulos, L.; Sykes, B.D.
Deposited on	:	2001-06-07

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

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

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

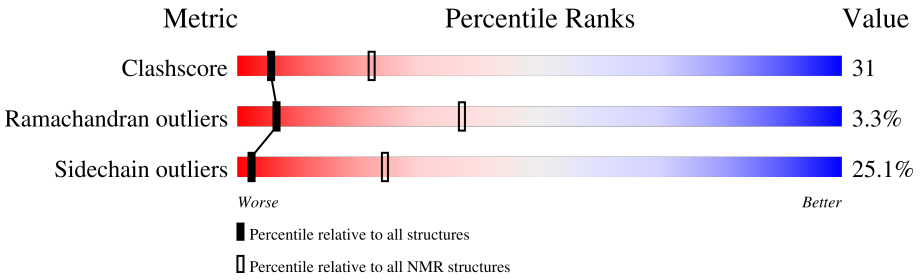
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	76	17% 58% 8% 16% •

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 30 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:96-A:158 (63)	0.52	30

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 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1164 atoms, of which 560 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TROPONIN C, SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	75	1162	369	560	97	132	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MET	-	cloning artifact	UNP P02588

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

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: TROPONIN C, SKELETAL MUSCLE

Chain A: 17% 58% 8% 16%

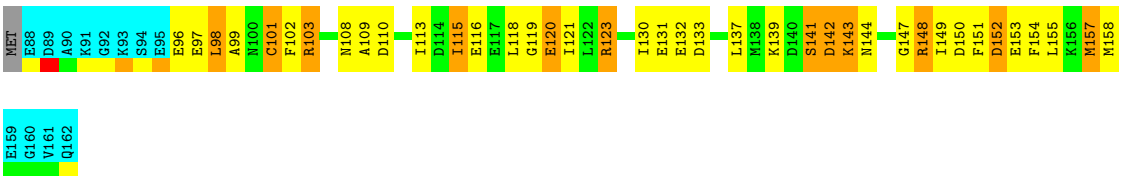
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: TROPONIN C, SKELETAL MUSCLE

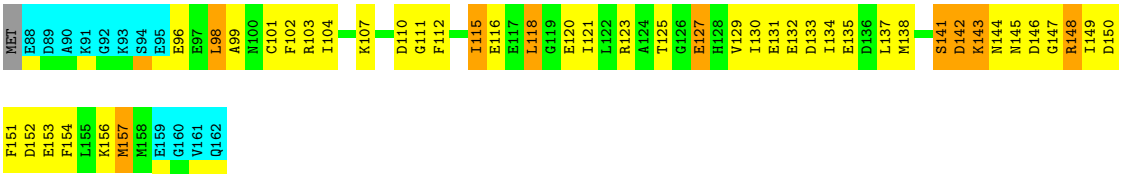
Chain A: 32% 36% 16% 16%



4.2.2 Score per residue for model 2

• Molecule 1: TROPONIN C, SKELETAL MUSCLE

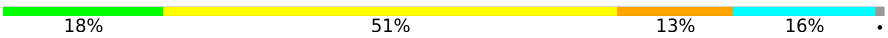
Chain A: 25% 46% 12% 16%

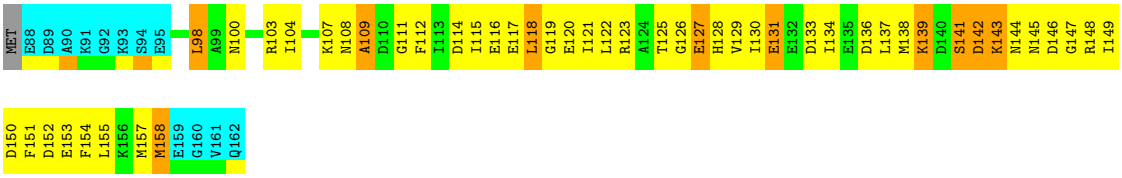


4.2.3 Score per residue for model 3

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A:

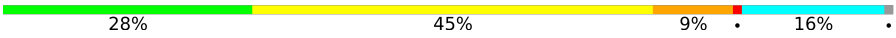


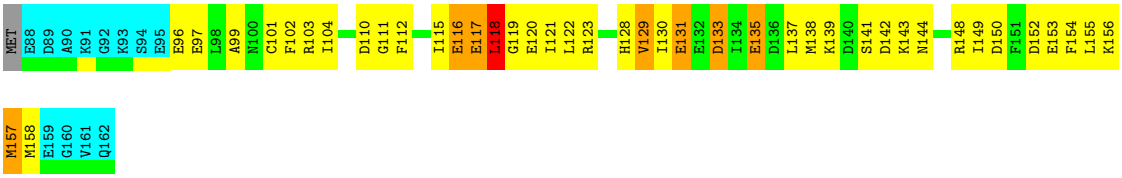


4.2.4 Score per residue for model 4

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A:

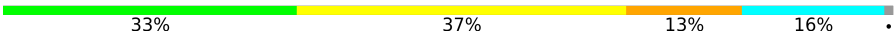


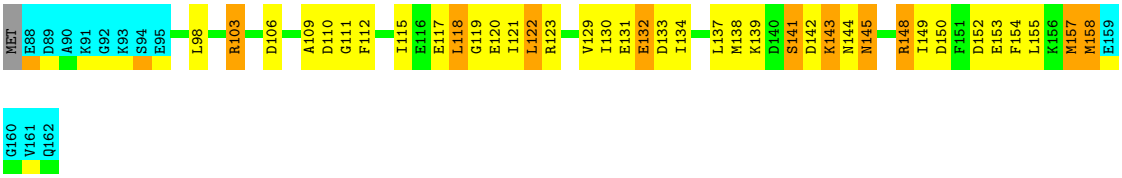


4.2.5 Score per residue for model 5

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 32% 38% 12% • 16% •

MET E88 D89 A90 K91 G92 K93 S94 E95 L98 C101 F102 R103 I104 F105 D106 K107 G111 F112 I115 E116 E117 L118 G119 E120 I121 L122 R123 A124 E127 H128 V129 I130 E131 E132 D133 K139 D140 S141 D142 K143 N144 N145 D146 G147 R148 I149 D150 F151 D152 E153 F154 L155 K156

M157 M158 E159 G160 V161 Q162

4.2.7 Score per residue for model 7

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 25% 46% 12% 16% •

MET E88 D89 A90 K91 G92 K93 S94 E95 E96 E97 L98 A99 N100 C101 F102 R103 K107 N108 A109 D110 G111 F112 I113 D114 I115 E116 E117 L118 G119 E120 I121 L122 R123 A124 E127 H128 E131 E132 D133 I134 M138 S141 D142 K143 N144 N145 D146 I149 D150 F151 D152 E153 F154

L155 K156 M157 M158 E159 G160 V161 Q162

4.2.8 Score per residue for model 8

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 28% 38% 17% 16% •

MET E88 D89 A90 K91 G92 K93 S94 E95 E96 E97 L98 C101 F102 R103 I104 F105 D106 K107 N108 A109 D110 G111 F112 I115 E116 E117 L118 G119 E120 R123 A124 T125 G126 E127 H128 E131 E132 D133 I134 E135 S141 D142 K143 N144 N145 D146 G147 R148 I149 D150 F151 D152 E153 F154

L155 K156 M157 M158 E159 G160 V161 Q162

4.2.9 Score per residue for model 9

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 29% 41% 12% • 16% •

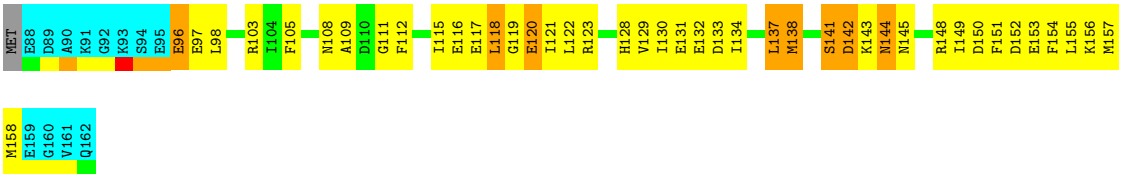
MET E88 D89 A90 K91 G92 K93 S94 E95 L98 A99 N100 C101 F102 R103 I104 F105 D106 K107 G111 F112 I115 E116 E117 L118 G119 E120 I121 L122 R123 E127 H128 V129 E132 D133 I134 E135 D136 L137 M138 K139 D140 S141 D142 K143 N144 N145 D146 G147 R148 I149 D150 F151 D152 E153

F154 L155 K156 M157 M158 E159 G160 V161 Q162

4.2.10 Score per residue for model 10

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

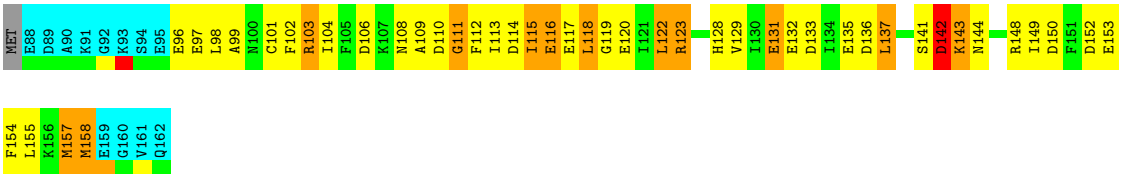
Chain A: 26% 46% 11% 16%



4.2.11 Score per residue for model 11

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 24% 42% 16% 16%



4.2.12 Score per residue for model 12

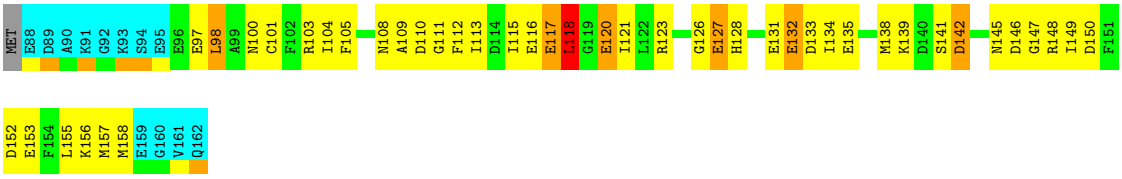
- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 20% 46% 17% 16%

4.2.13 Score per residue for model 13

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

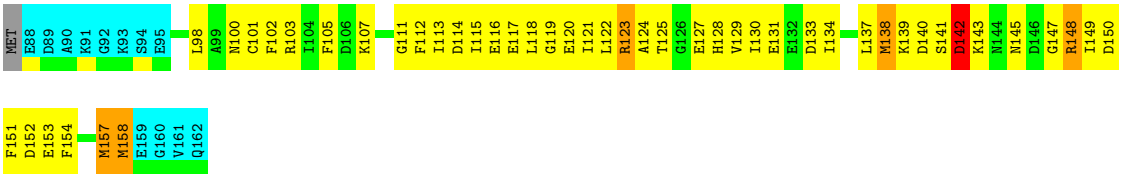
Chain A: 25% 49% 8% 16%



4.2.14 Score per residue for model 14

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

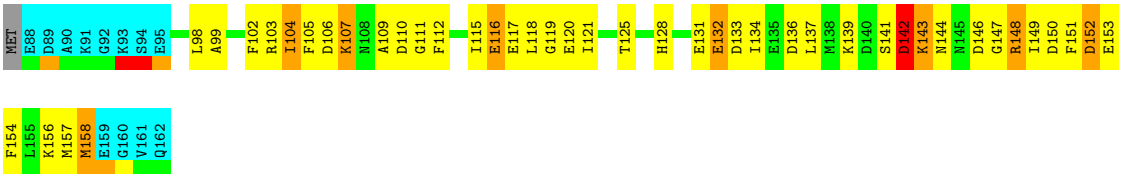
Chain A: 21% 54% 7% • 16% •



4.2.15 Score per residue for model 15

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

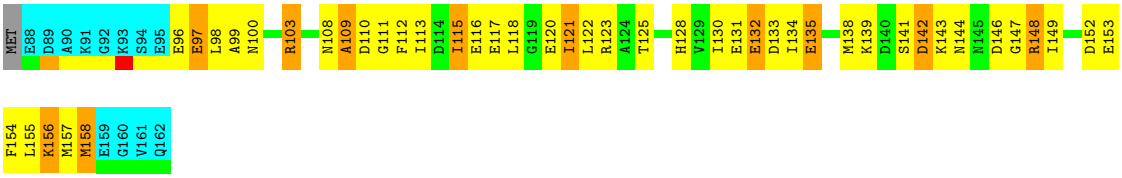
Chain A: 25% 46% 11% • 16% •



4.2.16 Score per residue for model 16

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 24% 45% 14% 16% •



4.2.17 Score per residue for model 17

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 30% 37% 16% 16% •

4.2.18 Score per residue for model 18

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 25% 38% 18% 16%

MET E88 D89 A90 K91 G92 K93 S94 E95 L98 A99 N100 C101 F102 R103 I104 F105 D106 K107 D110 G111 F112 I113 D114 I115 E116 E117 L118 G119 E120 I121 L122 R123 H128 V129 I130 E131 E132 D133 I134 M138 K139 D140 S141 D142 K143 D146 G147 R148 I149 D150 F151 D152 E153 F154 L155 K156 M157 M158 E159 G160 V161 Q162

4.2.19 Score per residue for model 19

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 29% 46% 8% 16%

MET E88 D89 A90 K91 G92 K93 S94 E95 E96 E97 L98 A99 N100 C101 F102 R103 I104 K107 N108 A109 D110 I115 E116 E117 L118 G119 E120 I121 L122 R123 H128 V129 I130 E131 E132 D133 I134 E135 D136 L137 D140 S141 D142 K143 D146 G147 R148 I149 D150 F151 D152 E153 F154 L155 K156 M157 M158 E159 G160 V161 Q162

4.2.20 Score per residue for model 20

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 38% 36% 9% 16%

MET E88 D89 A90 K91 G92 K93 S94 E95 E96 E97 L98 C101 F102 R103 I104 F105 G111 F112 I113 D114 I115 E116 E117 L118 G119 E120 I121 L122 R123 I130 E131 E132 D133 I134 E135 M138 S141 D142 K143 N144 N145 R148 I149 D150 F151 D152 E153 F154 L155 K156 M157 M158 E159 G160 V161 Q162

4.2.21 Score per residue for model 21

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 18% 54% 9% 16%

MET E88 D89 A90 K91 G92 K93 S94 E95 E96 E97 L98 A99 N100 C101 F102 R103 I104 F105 D106 K107 N108 A109 D110 G111 F112 I115 E116 E117 L118 G119 E120 I121 L122 R123 G126 E127 H128 V129 I130 E131 E132 D133 I134 E135 D136 L137 M138 K139 D140 S141 D142 K143 N144 N145 D146 G147 R148 I149 D152 E153 F154 L155 K156 M157 M158 E159 G160 V161 Q162

4.2.22 Score per residue for model 22

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 33% 41% 8% • 16% •

MET E88 D89 A90 K91 C92 K93 S94 E95 L98 F102 R103 D106 K107 N108 A109 D110 G111 F112 I113 L118 G119 E120 I121 L122 R123 V129 I130 E131 E132 D133 I134 E135 M138 S141 D142 K143 N144 N145 R148 I149 D150 F151 D152 E153 K156 M157 M158 E159 G160 V161

Q162

4.2.23 Score per residue for model 23

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 29% 42% 11% • 16% •

MET E88 D89 A90 K91 C92 K93 S94 E95 E96 A99 N100 C101 F102 R103 I104 F105 D106 K107 N108 A109 D110 G111 F112 I113 D114 I115 E116 E117 L118 G119 E120 I121 L122 R123 A124 T125 I130 E131 E132 D133 I134 E135 D136 L137 M138 S141 D142 K143 R148 I149 D150 F151 D152 E153 F154

L155 K156 M157 M158 E159 G160 V161 Q162

4.2.24 Score per residue for model 24

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 32% 39% 11% • 16% •

MET E88 D89 A90 K91 C92 K93 S94 E95 E96 E97 L98 C101 F102 R103 D106 K107 N108 A109 D110 G111 F112 I113 D114 I115 E116 E117 L118 G119 E120 I121 L122 R123 V129 I130 E131 E132 D133 I134 K139 D140 S141 D142 K143 N144 N145 R148 I149 D150 F151 D152 E153 F154 L155 K156

M157 M158 E159 G160 V161 Q162

4.2.25 Score per residue for model 25

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A: 25% 46% 11% • 16% •

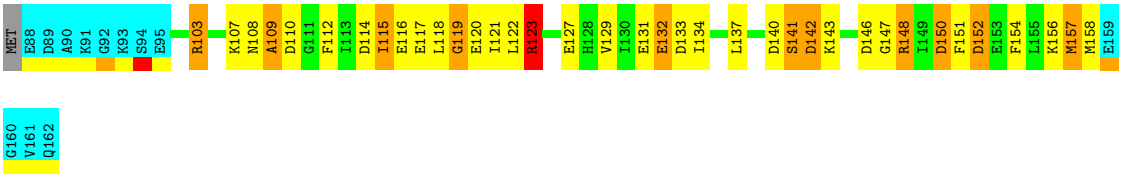
MET E88 D89 A90 K91 C92 K93 S94 E95 E96 E97 L98 A99 N100 C101 F102 R103 N108 A109 D110 G111 F112 I113 D114 I115 E116 G119 E120 I121 L122 R123 E127 H128 V129 I130 E131 E132 D133 I134 E135 D136 L137 M138 K139 D140 S141 D142 K143 D146 G147 R148 I149 D150 F151 D152 E153

F154 L155 K156 M157 M158 E159 G160 V161 Q162

4.2.26 Score per residue for model 26

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

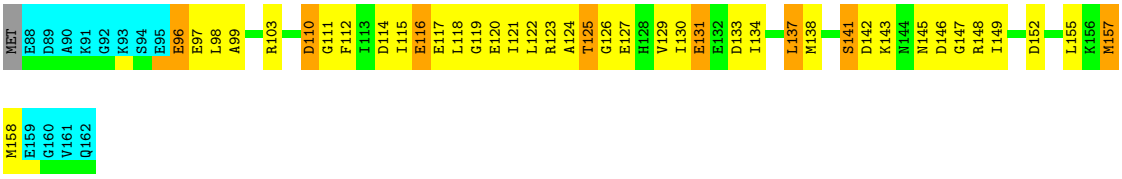
Chain A: 34% 33% 14% • 16% •



4.2.27 Score per residue for model 27

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

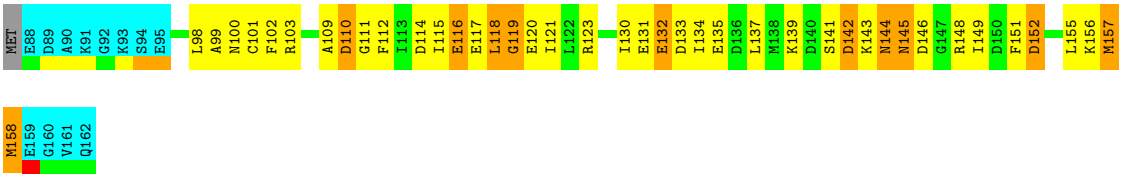
Chain A: 29% 43% 11% 16% •



4.2.28 Score per residue for model 28

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

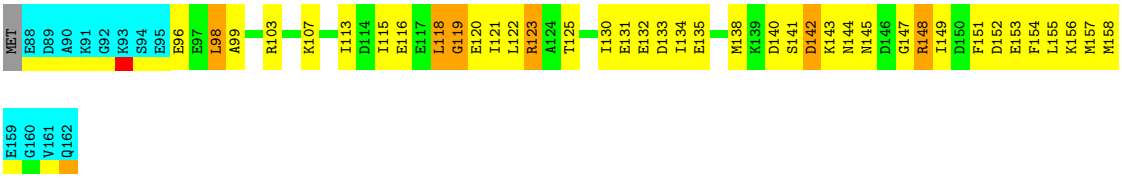
Chain A: 29% 39% 14% 16% •



4.2.29 Score per residue for model 29

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

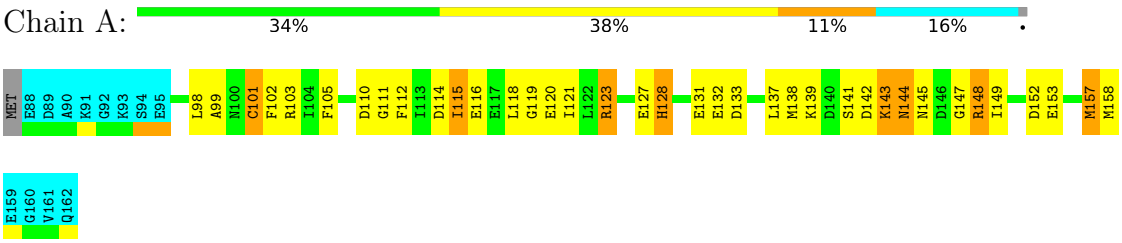
Chain A: 32% 43% 8% 16% •



4.2.30 Score per residue for model 30 (medoid)

- Molecule 1: TROPONIN C, SKELETAL MUSCLE

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 30 calculated structures, 30 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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

There are no covalent bond-length or bond-angle outliers.

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	2.9±0.4
All	All	0	86

There are no bond-length outliers.

There are no bond-angle outliers.

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	103	ARG	Sidechain	29
1	A	148	ARG	Sidechain	29
1	A	123	ARG	Sidechain	28

6.2 Too-close contacts (i)

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	513	479	479	31±6
All	All	15450	14370	14370	921

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:LEU:HD13	1:A:129:VAL:HG11	0.93	1.36	26	5
1:A:137:LEU:CD1	1:A:149:ILE:HD11	0.81	2.05	5	1
1:A:120:GLU:O	1:A:124:ALA:HB2	0.79	1.77	14	3
1:A:151:PHE:CE2	1:A:155:LEU:HD11	0.78	2.12	3	1
1:A:151:PHE:O	1:A:155:LEU:HD12	0.77	1.78	24	3
1:A:151:PHE:CD2	1:A:155:LEU:HD11	0.76	2.16	3	1
1:A:98:LEU:CD2	1:A:155:LEU:HD23	0.76	2.10	13	1
1:A:122:LEU:O	1:A:125:THR:HG22	0.74	1.82	16	4
1:A:98:LEU:HD23	1:A:155:LEU:HD23	0.73	1.61	13	1
1:A:105:PHE:CD2	1:A:121:ILE:HD13	0.72	2.19	14	2
1:A:127:GLU:O	1:A:129:VAL:HG23	0.72	1.84	27	3
1:A:131:GLU:OE1	1:A:134:ILE:HD12	0.69	1.87	22	1
1:A:98:LEU:HD23	1:A:154:PHE:CE1	0.69	2.22	2	1
1:A:154:PHE:HA	1:A:157:MET:HE3	0.69	1.63	10	1
1:A:105:PHE:O	1:A:121:ILE:HD11	0.68	1.89	20	3
1:A:115:ILE:HD11	1:A:135:GLU:HA	0.68	1.64	2	3
1:A:137:LEU:C	1:A:137:LEU:HD12	0.67	2.09	5	1
1:A:122:LEU:HB3	1:A:129:VAL:HG21	0.67	1.65	14	4
1:A:130:ILE:HD12	1:A:132:GLU:HB2	0.67	1.65	12	1
1:A:105:PHE:HB3	1:A:113:ILE:HD13	0.64	1.69	13	1
1:A:118:LEU:HG	1:A:137:LEU:HD21	0.64	1.69	5	1
1:A:117:GLU:O	1:A:121:ILE:HD12	0.64	1.93	14	3
1:A:118:LEU:HB3	1:A:134:ILE:HG23	0.63	1.71	27	11
1:A:151:PHE:CD1	1:A:152:ASP:N	0.63	2.66	24	5
1:A:102:PHE:CD2	1:A:151:PHE:CE1	0.63	2.87	6	1
1:A:149:ILE:HD13	1:A:157:MET:HE1	0.62	1.69	5	1
1:A:125:THR:HG23	1:A:127:GLU:HG3	0.62	1.69	14	1
1:A:122:LEU:HD22	1:A:129:VAL:HG21	0.62	1.70	17	2
1:A:105:PHE:CE2	1:A:121:ILE:HG21	0.62	2.30	14	1
1:A:108:ASN:O	1:A:109:ALA:HB3	0.61	1.95	12	4
1:A:138:MET:CE	1:A:149:ILE:HD12	0.60	2.26	22	6
1:A:118:LEU:O	1:A:122:LEU:HD12	0.59	1.95	4	2
1:A:151:PHE:CG	1:A:152:ASP:N	0.59	2.70	1	4
1:A:98:LEU:HD21	1:A:158:MET:HB3	0.58	1.74	21	3
1:A:127:GLU:O	1:A:128:HIS:CG	0.58	2.56	25	1
1:A:157:MET:CG	1:A:158:MET:N	0.58	2.66	5	19
1:A:111:GLY:O	1:A:112:PHE:CD1	0.57	2.56	23	11
1:A:128:HIS:CG	1:A:128:HIS:O	0.57	2.56	30	1
1:A:128:HIS:O	1:A:128:HIS:CD2	0.57	2.57	12	4
1:A:98:LEU:CD2	1:A:98:LEU:N	0.57	2.68	16	4
1:A:128:HIS:O	1:A:128:HIS:CG	0.57	2.57	18	5
1:A:108:ASN:O	1:A:109:ALA:HB2	0.57	1.99	26	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD23	1:A:122:LEU:HD12	0.56	1.74	7	1
1:A:149:ILE:HG21	1:A:157:MET:CE	0.56	2.30	10	1
1:A:118:LEU:HD12	1:A:134:ILE:HG23	0.56	1.78	12	1
1:A:110:ASP:O	1:A:112:PHE:CD2	0.56	2.59	2	3
1:A:129:VAL:HG12	1:A:134:ILE:CG1	0.55	2.30	10	1
1:A:122:LEU:HD13	1:A:129:VAL:CG1	0.55	2.23	26	1
1:A:111:GLY:C	1:A:112:PHE:CG	0.55	2.80	12	20
1:A:118:LEU:HD11	1:A:137:LEU:HD12	0.55	1.79	12	1
1:A:115:ILE:HG23	1:A:116:GLU:N	0.55	2.17	23	23
1:A:98:LEU:HD13	1:A:158:MET:CE	0.55	2.32	29	1
1:A:115:ILE:CG2	1:A:116:GLU:N	0.55	2.70	1	24
1:A:122:LEU:HD23	1:A:127:GLU:OE1	0.54	2.02	14	1
1:A:111:GLY:C	1:A:112:PHE:CD1	0.54	2.81	6	6
1:A:150:ASP:OD1	1:A:153:GLU:CG	0.54	2.56	12	8
1:A:141:SER:O	1:A:143:LYS:N	0.54	2.41	26	25
1:A:155:LEU:O	1:A:158:MET:CE	0.54	2.56	8	2
1:A:110:ASP:O	1:A:112:PHE:CE2	0.54	2.61	18	1
1:A:98:LEU:HD12	1:A:158:MET:CE	0.53	2.34	8	1
1:A:128:HIS:C	1:A:129:VAL:HG23	0.53	2.24	9	1
1:A:98:LEU:N	1:A:98:LEU:HD22	0.53	2.19	16	1
1:A:144:ASN:ND2	1:A:144:ASN:N	0.53	2.57	10	3
1:A:104:ILE:HD12	1:A:104:ILE:N	0.53	2.19	23	5
1:A:125:THR:HG23	1:A:127:GLU:H	0.52	1.63	27	1
1:A:122:LEU:O	1:A:125:THR:CG2	0.52	2.57	27	4
1:A:150:ASP:O	1:A:154:PHE:CB	0.52	2.58	1	6
1:A:110:ASP:OD1	1:A:111:GLY:N	0.52	2.42	5	5
1:A:142:ASP:OD2	1:A:148:ARG:N	0.52	2.42	24	2
1:A:119:GLY:HA2	1:A:134:ILE:HD13	0.52	1.79	25	4
1:A:120:GLU:CG	1:A:121:ILE:N	0.52	2.72	4	19
1:A:129:VAL:HG12	1:A:134:ILE:HG12	0.52	1.81	10	1
1:A:99:ALA:O	1:A:102:PHE:CB	0.52	2.57	17	7
1:A:122:LEU:HD22	1:A:129:VAL:HG11	0.52	1.80	11	1
1:A:147:GLY:O	1:A:148:ARG:CG	0.52	2.58	15	7
1:A:145:ASN:N	1:A:145:ASN:OD1	0.51	2.43	22	3
1:A:142:ASP:OD2	1:A:146:ASP:N	0.51	2.43	18	1
1:A:146:ASP:N	1:A:146:ASP:OD1	0.51	2.43	18	2
1:A:127:GLU:O	1:A:128:HIS:ND1	0.51	2.43	25	1
1:A:112:PHE:N	1:A:112:PHE:CD1	0.51	2.79	25	1
1:A:138:MET:O	1:A:142:ASP:N	0.51	2.44	12	8
1:A:127:GLU:O	1:A:129:VAL:N	0.51	2.43	21	2
1:A:120:GLU:HG3	1:A:121:ILE:N	0.51	2.21	12	13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:MET:HG3	1:A:158:MET:N	0.51	2.20	14	12
1:A:137:LEU:HD12	1:A:149:ILE:HD11	0.51	1.81	5	1
1:A:111:GLY:C	1:A:112:PHE:CD2	0.51	2.84	15	5
1:A:108:ASN:O	1:A:110:ASP:N	0.51	2.44	1	1
1:A:154:PHE:O	1:A:157:MET:N	0.51	2.44	12	1
1:A:120:GLU:O	1:A:124:ALA:CB	0.51	2.56	14	1
1:A:113:ILE:HG23	1:A:117:GLU:OE1	0.51	2.06	13	1
1:A:106:ASP:OD1	1:A:110:ASP:N	0.51	2.44	24	1
1:A:138:MET:HE3	1:A:149:ILE:HD12	0.51	1.82	20	1
1:A:144:ASN:ND2	1:A:146:ASP:OD2	0.51	2.44	15	1
1:A:150:ASP:OD1	1:A:153:GLU:N	0.50	2.42	22	6
1:A:118:LEU:HD12	1:A:122:LEU:HD12	0.50	1.82	10	2
1:A:150:ASP:OD1	1:A:152:ASP:N	0.50	2.44	26	1
1:A:143:LYS:N	1:A:153:GLU:OE2	0.50	2.44	7	2
1:A:128:HIS:O	1:A:128:HIS:ND1	0.50	2.43	11	2
1:A:150:ASP:OD1	1:A:151:PHE:N	0.50	2.44	26	1
1:A:120:GLU:OE1	1:A:121:ILE:N	0.50	2.45	1	3
1:A:110:ASP:OD1	1:A:112:PHE:N	0.50	2.43	13	5
1:A:157:MET:HG2	1:A:158:MET:N	0.50	2.22	25	2
1:A:106:ASP:OD1	1:A:109:ALA:N	0.50	2.45	22	2
1:A:138:MET:CE	1:A:149:ILE:CD1	0.50	2.89	22	1
1:A:144:ASN:ND2	1:A:153:GLU:OE2	0.50	2.45	12	12
1:A:112:PHE:CD1	1:A:112:PHE:N	0.50	2.80	27	3
1:A:118:LEU:HD21	1:A:137:LEU:HB3	0.49	1.84	14	2
1:A:147:GLY:C	1:A:148:ARG:CG	0.49	2.81	29	3
1:A:128:HIS:O	1:A:129:VAL:CB	0.49	2.61	9	1
1:A:149:ILE:HG22	1:A:154:PHE:HB2	0.49	1.84	10	1
1:A:105:PHE:O	1:A:107:LYS:N	0.49	2.45	15	4
1:A:122:LEU:CD1	1:A:129:VAL:HG11	0.49	2.25	26	1
1:A:154:PHE:CD2	1:A:157:MET:SD	0.49	3.06	29	1
1:A:98:LEU:HD13	1:A:158:MET:HE1	0.49	1.85	29	1
1:A:118:LEU:HD23	1:A:134:ILE:HG23	0.49	1.85	2	3
1:A:96:GLU:O	1:A:100:ASN:ND2	0.49	2.46	21	1
1:A:105:PHE:CZ	1:A:121:ILE:HG21	0.48	2.42	14	1
1:A:113:ILE:O	1:A:149:ILE:N	0.48	2.45	1	1
1:A:103:ARG:HG3	1:A:104:ILE:N	0.48	2.23	15	2
1:A:118:LEU:HD13	1:A:134:ILE:CG2	0.48	2.38	29	1
1:A:114:ASP:OD1	1:A:114:ASP:N	0.48	2.46	25	4
1:A:104:ILE:O	1:A:107:LYS:CD	0.48	2.62	21	1
1:A:111:GLY:O	1:A:112:PHE:CG	0.48	2.66	20	12
1:A:112:PHE:CB	1:A:148:ARG:HD2	0.48	2.39	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD13	1:A:134:ILE:HG23	0.48	1.84	29	2
1:A:149:ILE:CG2	1:A:150:ASP:N	0.48	2.76	14	2
1:A:141:SER:CB	1:A:149:ILE:HG12	0.48	2.39	17	24
1:A:138:MET:HE2	1:A:149:ILE:HD12	0.48	1.84	4	1
1:A:117:GLU:C	1:A:121:ILE:HD12	0.48	2.29	27	2
1:A:110:ASP:OD2	1:A:112:PHE:N	0.48	2.44	18	1
1:A:104:ILE:O	1:A:107:LYS:CE	0.48	2.61	21	1
1:A:110:ASP:OD1	1:A:110:ASP:N	0.48	2.46	22	1
1:A:98:LEU:HD11	1:A:158:MET:SD	0.47	2.49	15	1
1:A:129:VAL:CG1	1:A:133:ASP:HB3	0.47	2.39	4	1
1:A:131:GLU:OE1	1:A:131:GLU:CA	0.47	2.62	11	2
1:A:101:CYS:HA	1:A:104:ILE:HD13	0.47	1.85	23	1
1:A:104:ILE:N	1:A:104:ILE:CD1	0.47	2.77	11	2
1:A:105:PHE:O	1:A:121:ILE:CD1	0.47	2.63	6	2
1:A:110:ASP:N	1:A:110:ASP:OD1	0.47	2.46	11	2
1:A:114:ASP:OD2	1:A:116:GLU:N	0.47	2.43	24	1
1:A:155:LEU:O	1:A:158:MET:HE2	0.47	2.09	8	2
1:A:146:ASP:OD1	1:A:148:ARG:O	0.47	2.33	15	3
1:A:142:ASP:OD2	1:A:147:GLY:N	0.47	2.48	6	5
1:A:110:ASP:OD1	1:A:112:PHE:O	0.47	2.33	4	3
1:A:107:LYS:NZ	1:A:120:GLU:OE2	0.47	2.47	29	1
1:A:146:ASP:OD2	1:A:148:ARG:O	0.47	2.32	6	3
1:A:98:LEU:HD22	1:A:155:LEU:HD23	0.47	1.86	20	1
1:A:144:ASN:O	1:A:145:ASN:CB	0.47	2.63	8	4
1:A:154:PHE:CZ	1:A:158:MET:HG3	0.47	2.45	21	1
1:A:122:LEU:O	1:A:125:THR:HG23	0.47	2.10	29	1
1:A:154:PHE:CE2	1:A:157:MET:SD	0.47	3.07	29	1
1:A:138:MET:O	1:A:142:ASP:CB	0.47	2.63	7	4
1:A:119:GLY:O	1:A:123:ARG:CG	0.46	2.63	14	1
1:A:121:ILE:O	1:A:124:ALA:HB3	0.46	2.11	17	2
1:A:122:LEU:CD2	1:A:129:VAL:HG21	0.46	2.41	5	1
1:A:149:ILE:CG2	1:A:154:PHE:CA	0.46	2.93	10	1
1:A:98:LEU:HD22	1:A:154:PHE:HE1	0.46	1.71	5	1
1:A:137:LEU:CD1	1:A:149:ILE:CD1	0.46	2.86	5	1
1:A:146:ASP:OD1	1:A:147:GLY:N	0.46	2.48	8	3
1:A:150:ASP:N	1:A:153:GLU:OE1	0.46	2.47	11	1
1:A:115:ILE:HD11	1:A:135:GLU:HG2	0.46	1.87	11	3
1:A:128:HIS:O	1:A:129:VAL:HB	0.46	2.10	9	1
1:A:108:ASN:CG	1:A:109:ALA:N	0.46	2.68	24	2
1:A:138:MET:HE2	1:A:149:ILE:CD1	0.46	2.40	4	1
1:A:141:SER:O	1:A:142:ASP:C	0.46	2.54	27	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:GLY:O	1:A:148:ARG:HG2	0.46	2.11	15	4
1:A:150:ASP:OD2	1:A:153:GLU:OE2	0.46	2.34	10	2
1:A:118:LEU:CG	1:A:137:LEU:HD21	0.46	2.38	5	1
1:A:151:PHE:CD2	1:A:152:ASP:N	0.46	2.84	1	1
1:A:114:ASP:OD2	1:A:117:GLU:OE2	0.46	2.34	3	2
1:A:117:GLU:O	1:A:120:GLU:HG2	0.46	2.10	7	5
1:A:131:GLU:O	1:A:133:ASP:N	0.46	2.49	8	1
1:A:106:ASP:OD1	1:A:117:GLU:OE1	0.46	2.33	11	1
1:A:102:PHE:CZ	1:A:151:PHE:CE1	0.46	3.04	12	1
1:A:131:GLU:O	1:A:132:GLU:C	0.46	2.55	20	20
1:A:154:PHE:HA	1:A:157:MET:HG2	0.46	1.88	2	3
1:A:125:THR:OG1	1:A:126:GLY:N	0.46	2.49	8	2
1:A:106:ASP:OD2	1:A:110:ASP:CA	0.46	2.64	11	1
1:A:150:ASP:OD1	1:A:153:GLU:CB	0.45	2.64	15	3
1:A:150:ASP:O	1:A:154:PHE:HB3	0.45	2.11	14	1
1:A:112:PHE:HB2	1:A:148:ARG:CD	0.45	2.41	5	1
1:A:103:ARG:CG	1:A:104:ILE:HD12	0.45	2.42	15	1
1:A:98:LEU:N	1:A:98:LEU:CD2	0.45	2.78	24	1
1:A:154:PHE:O	1:A:157:MET:SD	0.45	2.74	6	3
1:A:144:ASN:O	1:A:144:ASN:CG	0.45	2.55	9	1
1:A:98:LEU:HD11	1:A:158:MET:CE	0.45	2.41	15	1
1:A:128:HIS:CG	1:A:129:VAL:N	0.45	2.82	9	1
1:A:108:ASN:OD1	1:A:110:ASP:OD2	0.45	2.34	13	1
1:A:145:ASN:O	1:A:147:GLY:N	0.45	2.49	8	1
1:A:98:LEU:CD1	1:A:158:MET:HB3	0.45	2.42	10	1
1:A:118:LEU:HD11	1:A:137:LEU:CD1	0.45	2.41	12	1
1:A:110:ASP:OD2	1:A:112:PHE:O	0.45	2.33	25	3
1:A:153:GLU:O	1:A:157:MET:HG2	0.45	2.11	6	3
1:A:141:SER:OG	1:A:153:GLU:O	0.45	2.34	20	1
1:A:154:PHE:O	1:A:157:MET:CG	0.45	2.65	2	3
1:A:99:ALA:O	1:A:102:PHE:HB3	0.45	2.12	19	6
1:A:157:MET:O	1:A:158:MET:C	0.45	2.56	8	2
1:A:127:GLU:O	1:A:128:HIS:C	0.45	2.54	25	2
1:A:142:ASP:OD1	1:A:146:ASP:OD1	0.45	2.34	21	2
1:A:130:ILE:O	1:A:131:GLU:C	0.45	2.56	28	16
1:A:154:PHE:O	1:A:155:LEU:C	0.45	2.55	29	12
1:A:118:LEU:HB3	1:A:134:ILE:CG2	0.45	2.41	15	9
1:A:147:GLY:O	1:A:148:ARG:HG3	0.45	2.12	8	4
1:A:105:PHE:HB3	1:A:113:ILE:CD1	0.45	2.42	13	1
1:A:119:GLY:O	1:A:123:ARG:HG2	0.45	2.12	14	1
1:A:154:PHE:O	1:A:157:MET:HG3	0.44	2.13	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:GLY:O	1:A:128:HIS:N	0.44	2.51	3	1
1:A:99:ALA:O	1:A:102:PHE:HB2	0.44	2.13	18	2
1:A:98:LEU:O	1:A:99:ALA:C	0.44	2.56	29	11
1:A:117:GLU:O	1:A:119:GLY:N	0.44	2.50	4	1
1:A:146:ASP:OD1	1:A:148:ARG:N	0.44	2.45	16	1
1:A:121:ILE:HG22	1:A:122:LEU:N	0.44	2.26	25	1
1:A:118:LEU:O	1:A:122:LEU:CD1	0.44	2.64	4	1
1:A:135:GLU:OE1	1:A:135:GLU:CA	0.44	2.65	4	1
1:A:113:ILE:HG23	1:A:117:GLU:HB3	0.44	1.89	13	2
1:A:121:ILE:O	1:A:125:THR:HG23	0.44	2.12	15	2
1:A:153:GLU:O	1:A:157:MET:CG	0.44	2.66	6	3
1:A:119:GLY:HA2	1:A:134:ILE:CD1	0.44	2.43	3	2
1:A:135:GLU:OE1	1:A:135:GLU:HA	0.44	2.12	4	1
1:A:142:ASP:OD1	1:A:145:ASN:N	0.44	2.51	27	3
1:A:114:ASP:OD2	1:A:116:GLU:HB2	0.44	2.13	17	1
1:A:150:ASP:O	1:A:154:PHE:HB2	0.44	2.12	1	6
1:A:113:ILE:O	1:A:148:ARG:HA	0.44	2.13	29	4
1:A:116:GLU:O	1:A:119:GLY:N	0.44	2.50	14	1
1:A:117:GLU:O	1:A:120:GLU:CG	0.43	2.66	7	1
1:A:119:GLY:O	1:A:123:ARG:HG3	0.43	2.14	26	1
1:A:141:SER:HB3	1:A:149:ILE:HG12	0.43	1.90	20	17
1:A:150:ASP:OD1	1:A:150:ASP:C	0.43	2.57	22	6
1:A:118:LEU:HD22	1:A:134:ILE:HG23	0.43	1.89	7	1
1:A:96:GLU:O	1:A:99:ALA:HB3	0.43	2.13	1	1
1:A:138:MET:O	1:A:142:ASP:HB2	0.43	2.13	7	3
1:A:151:PHE:O	1:A:155:LEU:CD1	0.43	2.60	24	2
1:A:118:LEU:O	1:A:119:GLY:C	0.43	2.57	29	2
1:A:122:LEU:O	1:A:125:THR:OG1	0.43	2.35	29	1
1:A:120:GLU:O	1:A:121:ILE:C	0.43	2.57	13	4
1:A:146:ASP:O	1:A:147:GLY:C	0.43	2.57	13	3
1:A:106:ASP:OD2	1:A:109:ALA:HA	0.43	2.13	5	1
1:A:154:PHE:CD1	1:A:154:PHE:C	0.43	2.92	2	1
1:A:108:ASN:O	1:A:109:ALA:C	0.43	2.57	17	5
1:A:122:LEU:HD12	1:A:122:LEU:H	0.43	1.72	4	1
1:A:119:GLY:O	1:A:120:GLU:C	0.43	2.57	28	13
1:A:146:ASP:OD1	1:A:146:ASP:C	0.43	2.57	7	4
1:A:102:PHE:CE1	1:A:113:ILE:HD11	0.43	2.49	22	1
1:A:137:LEU:HD12	1:A:157:MET:HE3	0.43	1.88	4	1
1:A:136:ASP:OD1	1:A:136:ASP:C	0.43	2.57	21	2
1:A:141:SER:HB3	1:A:149:ILE:CG1	0.43	2.43	12	1
1:A:108:ASN:OD1	1:A:110:ASP:CG	0.43	2.57	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:GLU:C	1:A:128:HIS:ND1	0.43	2.72	25	1
1:A:116:GLU:HG3	1:A:117:GLU:N	0.43	2.29	3	1
1:A:137:LEU:CD1	1:A:137:LEU:C	0.43	2.80	5	1
1:A:145:ASN:O	1:A:146:ASP:C	0.43	2.57	8	1
1:A:123:ARG:NH1	1:A:123:ARG:HG2	0.43	2.29	25	1
1:A:101:CYS:O	1:A:102:PHE:C	0.42	2.57	14	8
1:A:114:ASP:OD1	1:A:114:ASP:C	0.42	2.58	11	1
1:A:156:LYS:O	1:A:157:MET:C	0.42	2.57	2	2
1:A:142:ASP:OD1	1:A:146:ASP:N	0.42	2.42	17	1
1:A:117:GLU:O	1:A:118:LEU:C	0.42	2.56	4	3
1:A:157:MET:SD	1:A:157:MET:C	0.42	2.97	4	1
1:A:118:LEU:CD1	1:A:137:LEU:CD2	0.42	2.98	5	1
1:A:118:LEU:CD1	1:A:137:LEU:HD21	0.42	2.44	5	1
1:A:114:ASP:OD1	1:A:116:GLU:N	0.42	2.52	12	1
1:A:98:LEU:HD13	1:A:155:LEU:CD2	0.42	2.44	28	1
1:A:142:ASP:CG	1:A:146:ASP:OD1	0.42	2.57	3	1
1:A:98:LEU:O	1:A:101:CYS:N	0.42	2.51	11	1
1:A:157:MET:HG2	1:A:158:MET:SD	0.42	2.54	11	1
1:A:131:GLU:O	1:A:135:GLU:HG3	0.42	2.14	12	2
1:A:105:PHE:O	1:A:106:ASP:C	0.42	2.57	18	1
1:A:106:ASP:OD1	1:A:108:ASN:O	0.42	2.37	23	1
1:A:98:LEU:HD23	1:A:154:PHE:HE1	0.42	1.70	2	1
1:A:131:GLU:O	1:A:135:GLU:OE1	0.42	2.37	8	1
1:A:113:ILE:CD1	1:A:154:PHE:CD1	0.42	3.03	11	1
1:A:150:ASP:OD1	1:A:153:GLU:HB2	0.42	2.15	15	4
1:A:153:GLU:O	1:A:154:PHE:C	0.42	2.57	21	3
1:A:103:ARG:CG	1:A:104:ILE:N	0.42	2.83	15	1
1:A:115:ILE:CD1	1:A:135:GLU:HG2	0.42	2.44	23	1
1:A:127:GLU:HB3	1:A:129:VAL:CG2	0.42	2.44	2	1
1:A:130:ILE:CD1	1:A:132:GLU:HB2	0.42	2.44	10	1
1:A:116:GLU:O	1:A:117:GLU:C	0.42	2.57	14	1
1:A:108:ASN:ND2	1:A:110:ASP:OD2	0.42	2.50	19	1
1:A:106:ASP:CG	1:A:110:ASP:N	0.42	2.73	24	1
1:A:114:ASP:OD1	1:A:116:GLU:CG	0.42	2.68	3	1
1:A:106:ASP:OD2	1:A:110:ASP:N	0.42	2.53	5	1
1:A:108:ASN:HB3	1:A:110:ASP:OD1	0.42	2.14	7	1
1:A:115:ILE:CD1	1:A:135:GLU:HA	0.42	2.45	19	2
1:A:150:ASP:OD1	1:A:153:GLU:CD	0.42	2.57	12	3
1:A:114:ASP:OD2	1:A:116:GLU:CG	0.42	2.67	23	1
1:A:127:GLU:O	1:A:128:HIS:HB3	0.41	2.15	9	1
1:A:138:MET:O	1:A:139:LYS:C	0.41	2.58	25	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD12	1:A:122:LEU:HD11	0.41	1.91	4	1
1:A:102:PHE:HA	1:A:154:PHE:CE2	0.41	2.50	7	1
1:A:149:ILE:HG23	1:A:154:PHE:N	0.41	2.30	10	1
1:A:150:ASP:O	1:A:151:PHE:C	0.41	2.58	10	1
1:A:113:ILE:HD12	1:A:113:ILE:N	0.41	2.30	12	1
1:A:126:GLY:O	1:A:127:GLU:OE2	0.41	2.37	13	1
1:A:106:ASP:O	1:A:109:ALA:N	0.41	2.47	15	1
1:A:98:LEU:HD12	1:A:158:MET:HE1	0.41	1.91	8	1
1:A:108:ASN:O	1:A:109:ALA:CB	0.41	2.66	26	2
1:A:142:ASP:OD1	1:A:148:ARG:O	0.41	2.37	26	1
1:A:150:ASP:OD1	1:A:153:GLU:HG3	0.41	2.15	10	1
1:A:137:LEU:O	1:A:141:SER:HB2	0.41	2.15	10	2
1:A:100:ASN:O	1:A:101:CYS:C	0.41	2.57	28	1
1:A:142:ASP:HA	1:A:153:GLU:OE2	0.41	2.16	8	1
1:A:101:CYS:O	1:A:104:ILE:HB	0.41	2.16	19	1
1:A:146:ASP:O	1:A:146:ASP:CG	0.41	2.59	25	1
1:A:114:ASP:N	1:A:114:ASP:OD1	0.41	2.53	28	1
1:A:108:ASN:O	1:A:108:ASN:OD1	0.41	2.39	16	1
1:A:138:MET:SD	1:A:147:GLY:C	0.41	2.99	3	1
1:A:101:CYS:SG	1:A:105:PHE:CE2	0.41	3.03	8	1
1:A:98:LEU:HB3	1:A:154:PHE:CZ	0.41	2.51	9	1
1:A:144:ASN:O	1:A:144:ASN:OD1	0.41	2.38	9	1
1:A:108:ASN:O	1:A:109:ALA:O	0.41	2.39	16	1
1:A:118:LEU:CD2	1:A:122:LEU:HD12	0.41	2.46	18	1
1:A:142:ASP:OD2	1:A:146:ASP:OD1	0.41	2.38	27	1
1:A:113:ILE:O	1:A:148:ARG:CA	0.41	2.69	29	1
1:A:135:GLU:O	1:A:136:ASP:C	0.41	2.59	23	2
1:A:150:ASP:C	1:A:150:ASP:OD1	0.41	2.58	18	1
1:A:106:ASP:OD1	1:A:110:ASP:OD1	0.41	2.38	23	1
1:A:129:VAL:HG12	1:A:133:ASP:HB3	0.41	1.93	24	1
1:A:106:ASP:OD1	1:A:109:ALA:CA	0.40	2.69	12	1
1:A:100:ASN:O	1:A:104:ILE:HG12	0.40	2.16	3	1
1:A:108:ASN:HB2	1:A:110:ASP:OD2	0.40	2.16	7	1
1:A:150:ASP:N	1:A:150:ASP:OD1	0.40	2.53	8	1
1:A:114:ASP:OD1	1:A:117:GLU:HB2	0.40	2.16	18	1
1:A:123:ARG:NH1	1:A:129:VAL:O	0.40	2.55	22	1
1:A:103:ARG:HG2	1:A:104:ILE:HD12	0.40	1.93	23	1
1:A:136:ASP:O	1:A:139:LYS:HB2	0.40	2.16	3	1
1:A:112:PHE:CB	1:A:148:ARG:CD	0.40	2.99	5	1
1:A:134:ILE:O	1:A:137:LEU:HG	0.40	2.16	5	1
1:A:117:GLU:O	1:A:121:ILE:HG13	0.40	2.17	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ASP:CG	1:A:110:ASP:CA	0.40	2.89	24	1
1:A:150:ASP:OD1	1:A:150:ASP:N	0.40	2.54	1	1
1:A:149:ILE:HG22	1:A:150:ASP:N	0.40	2.30	14	1
1:A:149:ILE:HA	1:A:153:GLU:OE1	0.40	2.17	15	1
1:A:158:MET:CE	1:A:158:MET:C	0.40	2.90	15	1
1:A:108:ASN:OD1	1:A:108:ASN:C	0.40	2.59	19	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	63/76 (83%)	52±2 (83±4%)	8±2 (13±4%)	2±1 (3±2%)	6 37
All	All	1890/2280 (83%)	1575 (83%)	252 (13%)	63 (3%)	6 37

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	142	ASP	29
1	A	109	ALA	6
1	A	119	GLY	6
1	A	145	ASN	4
1	A	118	LEU	2
1	A	129	VAL	2
1	A	126	GLY	2
1	A	106	ASP	2
1	A	128	HIS	2
1	A	111	GLY	2
1	A	125	THR	2
1	A	127	GLU	1
1	A	158	MET	1
1	A	132	GLU	1
1	A	121	ILE	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	56/66 (85%)	42±2 (75±3%)	14±2 (25±3%)	2 24
All	All	1680/1980 (85%)	1258 (75%)	422 (25%)	2 24

All 43 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	133	ASP	30
1	A	152	ASP	26
1	A	118	LEU	23
1	A	157	MET	20
1	A	141	SER	17
1	A	143	LYS	17
1	A	132	GLU	15
1	A	158	MET	15
1	A	156	LYS	15
1	A	139	LYS	14
1	A	101	CYS	13
1	A	103	ARG	13
1	A	137	LEU	13
1	A	97	GLU	12
1	A	116	GLU	12
1	A	138	MET	12
1	A	98	LEU	11
1	A	115	ILE	11
1	A	123	ARG	11
1	A	107	LYS	11
1	A	96	GLU	10
1	A	145	ASN	9
1	A	151	PHE	8
1	A	131	GLU	8
1	A	128	HIS	8
1	A	142	ASP	8
1	A	120	GLU	7
1	A	135	GLU	7
1	A	144	ASN	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	100	ASN	6
1	A	140	ASP	6
1	A	122	LEU	5
1	A	127	GLU	4
1	A	117	GLU	4
1	A	110	ASP	3
1	A	105	PHE	2
1	A	148	ARG	2
1	A	154	PHE	2
1	A	114	ASP	2
1	A	146	ASP	1
1	A	104	ILE	1
1	A	136	ASP	1
1	A	150	ASP	1

6.3.3 RNA (i)

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 monosaccharides 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 (i)

No chemical shift data were provided