



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:07 am GMT

PDB ID : 2MLE  
Title : NMR structure of the C-domain of troponin C bound to the anchoring region of troponin I  
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Deposited on : 2014-02-26

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

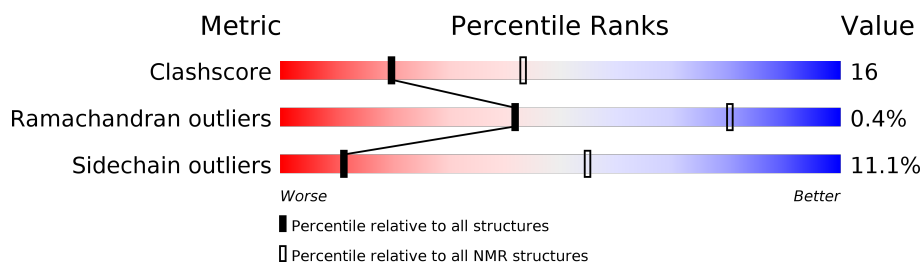
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 78%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	C	72	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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	C:94-C:157 (64)	0.68	14

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 1 single-model cluster was found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1130 atoms, of which 545 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	C	72	Total	C	H	N	O	S	0
			1128	360	545	88	130	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	MET	-	INITIATING METHIONINE	UNP P63316

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

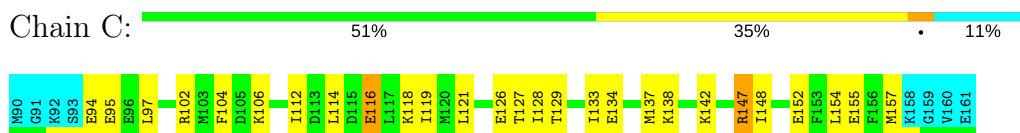
Mol	Chain	Residues	Atoms	
2	C	2	Total	Ca
			2	2

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

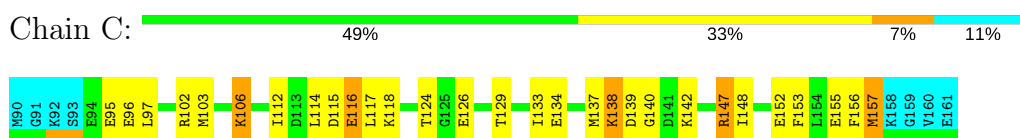


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

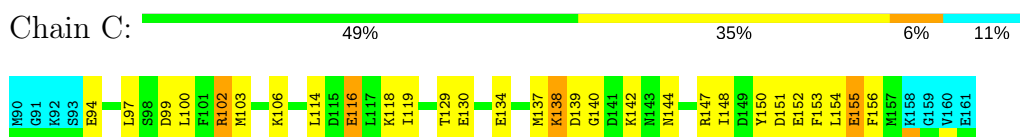
#### 4.2.1 Score per residue for model 1

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



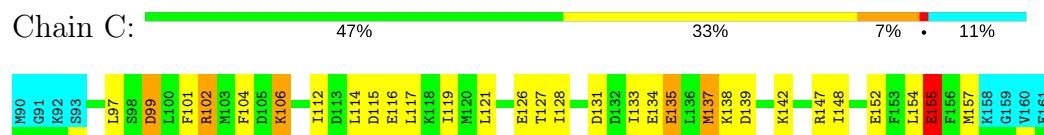
#### 4.2.2 Score per residue for model 2

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



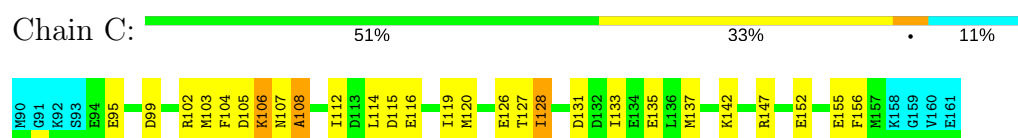
### 4.2.3 Score per residue for model 3

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



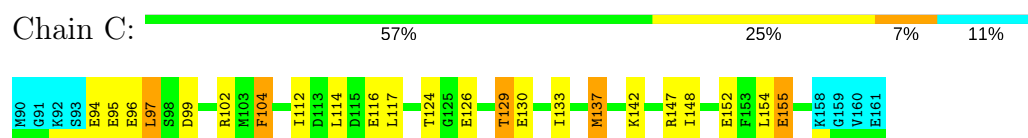
### 4.2.4 Score per residue for model 4

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



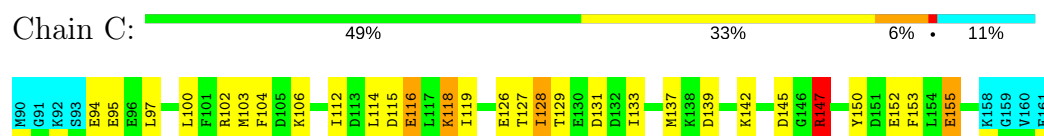
### 4.2.5 Score per residue for model 5

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



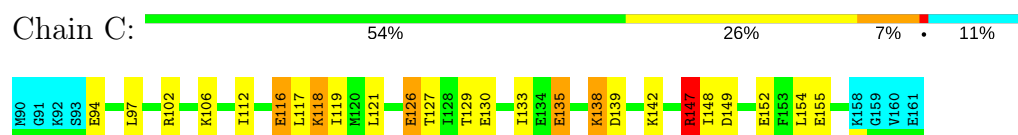
### 4.2.6 Score per residue for model 6

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



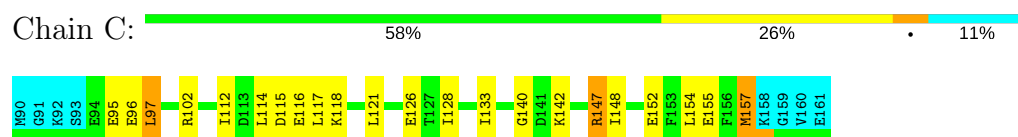
### 4.2.7 Score per residue for model 7

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



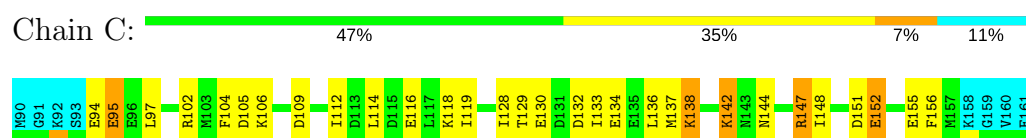
### 4.2.8 Score per residue for model 8

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



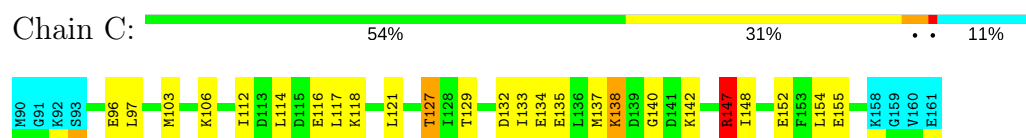
### 4.2.9 Score per residue for model 9

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



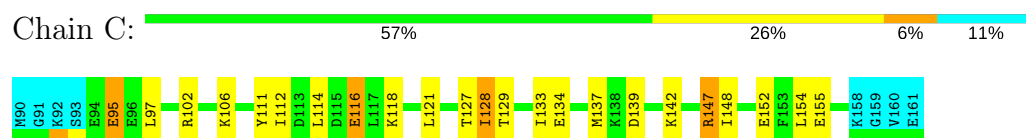
### 4.2.10 Score per residue for model 10

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



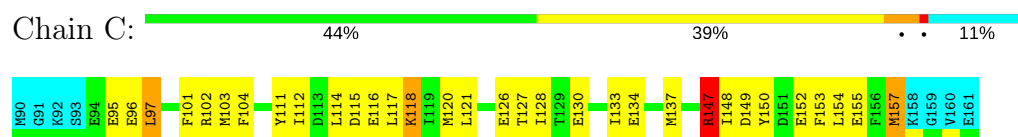
### 4.2.11 Score per residue for model 11

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



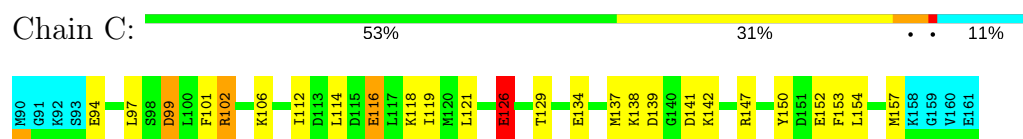
### 4.2.12 Score per residue for model 12

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



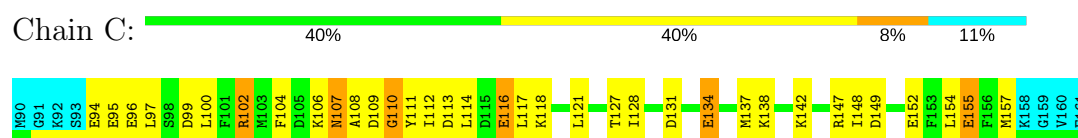
#### 4.2.13 Score per residue for model 13

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



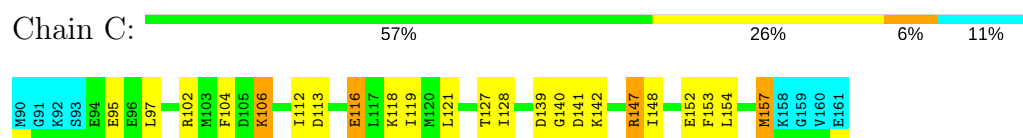
#### 4.2.14 Score per residue for model 14 (medoid)

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



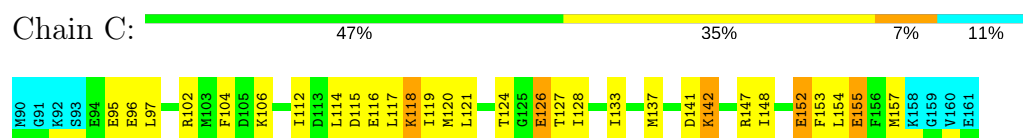
#### 4.2.15 Score per residue for model 15

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



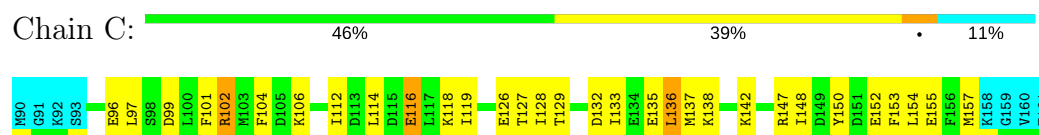
#### 4.2.16 Score per residue for model 16

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



#### 4.2.17 Score per residue for model 17

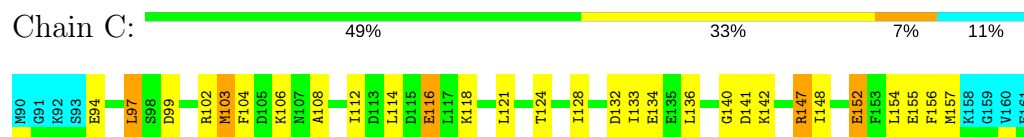
- Molecule 1: Troponin C, slow skeletal and cardiac muscles





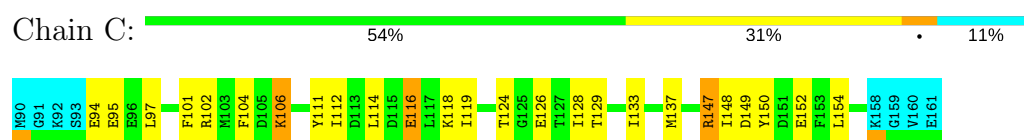
### 4.2.18 Score per residue for model 18

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



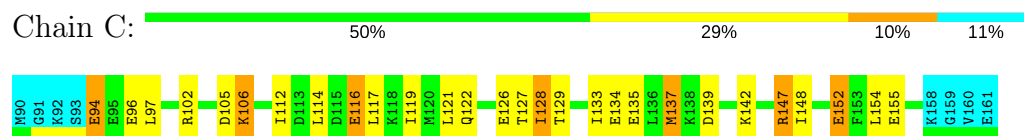
### 4.2.19 Score per residue for model 19

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



### 4.2.20 Score per residue for model 20

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



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	geometry optimization	
ProcheckNMR	refinement	
X-PLOR NIH	refinement	
X-PLOR NIH	geometry optimization	
CYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2mle_cs.str
Number of chemical shift lists	1
Total number of shifts	689
Number of shifts mapped to atoms	689
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 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	C	1.55±0.02	6±1/532 (1.2±0.2%)	1.17±0.02	0±0/713 (0.0±0.1%)
All	All	1.55	125/10640 (1.2%)	1.17	2/14260 (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	C	0.0±0.0	1.9±0.2
All	All	0	39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	152	GLU	CD-OE2	-9.17	1.15	1.25	2	20
1	C	116	GLU	CD-OE1	-8.79	1.16	1.25	1	19
1	C	116	GLU	CD-OE2	-8.73	1.16	1.25	18	20
1	C	152	GLU	CD-OE1	-7.42	1.17	1.25	4	19
1	C	95	GLU	CD-OE2	-6.73	1.18	1.25	5	7
1	C	135	GLU	CD-OE2	-6.36	1.18	1.25	17	5
1	C	155	GLU	CD-OE2	-6.17	1.18	1.25	14	6
1	C	96	GLU	CD-OE1	-5.82	1.19	1.25	1	1
1	C	94	GLU	CD-OE2	-5.80	1.19	1.25	13	7
1	C	134	GLU	CD-OE1	-5.49	1.19	1.25	12	1
1	C	110	GLY	N-CA	5.48	1.54	1.46	14	1
1	C	155	GLU	CD-OE1	-5.48	1.19	1.25	7	1
1	C	126	GLU	CD-OE2	-5.44	1.19	1.25	7	9
1	C	96	GLU	CD-OE2	-5.38	1.19	1.25	14	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	130	GLU	CD-OE1	-5.29	1.19	1.25	2	1
1	C	134	GLU	CD-OE2	-5.19	1.20	1.25	14	1
1	C	130	GLU	CD-OE2	-5.11	1.20	1.25	9	1
1	C	109	ASP	CG-OD1	-5.03	1.13	1.25	9	1

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	C	126	GLU	N-CA-CB	-5.22	101.19	110.60	17	1
1	C	150	TYR	N-CA-CB	-5.05	101.50	110.60	17	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	C	147	ARG	Sidechain	20
1	C	102	ARG	Sidechain	19

## 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	C	526	482	482	16±3
All	All	10560	9640	9640	315

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:97:LEU:HD22	1:C:154:LEU:HD13	1.06	1.24	18	11
1:C:97:LEU:HD22	1:C:154:LEU:HD21	0.89	1.43	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:114:LEU:HD21	1:C:137:MET:HB2	0.88	1.42	1	3
1:C:117:LEU:HD23	1:C:133:ILE:HG23	0.87	1.46	8	2
1:C:114:LEU:HD22	1:C:133:ILE:HG22	0.87	1.46	1	1
1:C:117:LEU:HD22	1:C:133:ILE:HG23	0.83	1.50	16	2
1:C:106:LYS:HE2	1:C:119:ILE:HD12	0.76	1.56	20	4
1:C:106:LYS:HE3	1:C:119:ILE:HD12	0.75	1.56	2	3
1:C:114:LEU:HD11	1:C:137:MET:SD	0.71	2.25	2	1
1:C:121:LEU:HB3	1:C:128:ILE:HG21	0.70	1.63	11	1
1:C:128:ILE:CG2	1:C:133:ILE:HD11	0.68	2.18	8	1
1:C:97:LEU:HD22	1:C:154:LEU:CD2	0.66	2.18	17	1
1:C:104:PHE:CE1	1:C:117:LEU:HD23	0.66	2.25	3	1
1:C:114:LEU:CD1	1:C:133:ILE:HG22	0.65	2.22	8	1
1:C:97:LEU:HD13	1:C:154:LEU:HD12	0.65	1.67	8	2
1:C:97:LEU:CD2	1:C:154:LEU:HD13	0.65	2.21	11	3
1:C:129:THR:O	1:C:133:ILE:HD12	0.64	1.92	9	3
1:C:114:LEU:HD13	1:C:137:MET:HG2	0.63	1.70	3	1
1:C:106:LYS:CE	1:C:119:ILE:HD12	0.63	2.23	20	5
1:C:121:LEU:HB3	1:C:128:ILE:HD13	0.63	1.68	15	1
1:C:114:LEU:HD12	1:C:133:ILE:HG22	0.63	1.71	8	2
1:C:112:ILE:HB	1:C:148:ILE:HB	0.62	1.72	15	16
1:C:128:ILE:CD1	1:C:133:ILE:HD11	0.62	2.24	3	1
1:C:117:LEU:HD11	1:C:148:ILE:HD11	0.62	1.70	3	1
1:C:147:ARG:CZ	1:C:147:ARG:HB3	0.61	2.25	10	1
1:C:124:THR:HG22	1:C:126:GLU:HG2	0.61	1.70	16	1
1:C:106:LYS:HG2	1:C:116:GLU:HG2	0.59	1.73	17	5
1:C:114:LEU:CD2	1:C:134:GLU:HA	0.59	2.27	18	2
1:C:104:PHE:CE2	1:C:112:ILE:HG21	0.59	2.32	5	1
1:C:128:ILE:HB	1:C:133:ILE:HD11	0.58	1.75	20	1
1:C:141:ASP:N	1:C:148:ILE:HD12	0.58	2.13	15	1
1:C:100:LEU:HD23	1:C:157:MET:HE2	0.57	1.74	14	1
1:C:104:PHE:HB3	1:C:112:ILE:HD12	0.57	1.76	12	2
1:C:139:ASP:O	1:C:142:LYS:HE3	0.57	1.99	1	1
1:C:106:LYS:CE	1:C:116:GLU:HG2	0.57	2.30	14	1
1:C:121:LEU:HD23	1:C:128:ILE:HG13	0.57	1.74	18	1
1:C:121:LEU:HD12	1:C:133:ILE:HG12	0.57	1.76	10	2
1:C:135:GLU:HA	1:C:138:LYS:CE	0.57	2.29	7	1
1:C:127:THR:HG22	1:C:132:ASP:HB3	0.56	1.77	10	1
1:C:140:GLY:C	1:C:148:ILE:HD12	0.56	2.20	15	4
1:C:114:LEU:HD13	1:C:137:MET:CG	0.56	2.30	3	2
1:C:97:LEU:HD12	1:C:157:MET:SD	0.56	2.41	8	1
1:C:97:LEU:HD21	1:C:154:LEU:HD13	0.55	1.76	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:106:LYS:CG	1:C:116:GLU:HG2	0.54	2.32	18	2
1:C:142:LYS:HE3	1:C:155:GLU:CD	0.54	2.23	5	2
1:C:115:ASP:HA	1:C:118:LYS:HG2	0.54	1.79	8	2
1:C:128:ILE:HD11	1:C:133:ILE:HD11	0.53	1.79	18	1
1:C:128:ILE:CG1	1:C:133:ILE:HD11	0.53	2.32	6	1
1:C:97:LEU:HD22	1:C:154:LEU:CD1	0.53	2.17	18	2
1:C:97:LEU:HD13	1:C:154:LEU:CD2	0.53	2.33	20	1
1:C:97:LEU:HB3	1:C:157:MET:SD	0.52	2.43	1	1
1:C:140:GLY:HA2	1:C:156:PHE:CD1	0.52	2.39	2	2
1:C:106:LYS:HE3	1:C:116:GLU:HG2	0.52	1.82	14	2
1:C:121:LEU:HB3	1:C:128:ILE:HD12	0.52	1.82	12	3
1:C:107:ASN:O	1:C:108:ALA:HB3	0.52	2.04	4	2
1:C:97:LEU:HD11	1:C:153:PHE:CD2	0.52	2.40	15	2
1:C:97:LEU:CD2	1:C:154:LEU:HD21	0.52	2.29	17	1
1:C:104:PHE:CZ	1:C:117:LEU:HD23	0.51	2.40	3	2
1:C:97:LEU:HG	1:C:150:TYR:CE1	0.51	2.41	2	2
1:C:135:GLU:HA	1:C:138:LYS:HE3	0.51	1.82	3	1
1:C:106:LYS:CD	1:C:119:ILE:HD12	0.51	2.34	17	1
1:C:104:PHE:CE1	1:C:112:ILE:HG23	0.51	2.41	15	1
1:C:94:GLU:HA	1:C:97:LEU:HD21	0.51	1.83	20	2
1:C:117:LEU:HD11	1:C:148:ILE:CD1	0.50	2.36	3	1
1:C:112:ILE:CD1	1:C:153:PHE:CD1	0.50	2.94	15	1
1:C:114:LEU:HD21	1:C:134:GLU:HA	0.50	1.82	10	1
1:C:100:LEU:HD23	1:C:157:MET:CE	0.50	2.36	14	1
1:C:135:GLU:HA	1:C:138:LYS:HE2	0.50	1.81	7	1
1:C:142:LYS:HD2	1:C:155:GLU:CB	0.50	2.36	10	1
1:C:134:GLU:O	1:C:138:LYS:HG2	0.50	2.07	14	1
1:C:127:THR:O	1:C:128:ILE:HD13	0.50	2.06	16	1
1:C:114:LEU:CD2	1:C:133:ILE:HG22	0.50	2.31	1	2
1:C:134:GLU:O	1:C:138:LYS:HE2	0.50	2.07	1	1
1:C:153:PHE:HA	1:C:156:PHE:HB3	0.50	1.83	2	2
1:C:114:LEU:HD21	1:C:137:MET:SD	0.50	2.47	20	3
1:C:137:MET:HE1	1:C:147:ARG:CA	0.49	2.37	19	1
1:C:117:LEU:HD23	1:C:133:ILE:CG2	0.49	2.36	12	1
1:C:112:ILE:HD12	1:C:153:PHE:CD2	0.49	2.41	6	1
1:C:138:LYS:N	1:C:138:LYS:HD3	0.49	2.21	2	1
1:C:114:LEU:HD21	1:C:137:MET:HG2	0.49	1.84	19	2
1:C:154:LEU:HA	1:C:157:MET:HE2	0.49	1.84	18	2
1:C:97:LEU:HD11	1:C:153:PHE:HD2	0.49	1.68	15	1
1:C:97:LEU:HD13	1:C:157:MET:SD	0.49	2.48	15	1
1:C:130:GLU:HA	1:C:133:ILE:HD12	0.49	1.84	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:115:ASP:O	1:C:119:ILE:HG12	0.49	2.07	16	3
1:C:128:ILE:HG13	1:C:133:ILE:HD11	0.49	1.85	6	1
1:C:99:ASP:O	1:C:102:ARG:HG2	0.49	2.07	13	3
1:C:142:LYS:HD2	1:C:142:LYS:N	0.49	2.23	9	2
1:C:109:ASP:O	1:C:111:TYR:N	0.49	2.46	14	1
1:C:115:ASP:HA	1:C:118:LYS:CG	0.49	2.38	16	1
1:C:118:LYS:HA	1:C:133:ILE:HD13	0.49	1.84	7	1
1:C:101:PHE:CE1	1:C:112:ILE:CD1	0.48	2.97	17	1
1:C:112:ILE:HD13	1:C:153:PHE:CD1	0.48	2.43	17	1
1:C:114:LEU:HG	1:C:137:MET:SD	0.48	2.48	14	2
1:C:97:LEU:HB2	1:C:154:LEU:HD11	0.48	1.84	17	1
1:C:114:LEU:C	1:C:114:LEU:HD13	0.48	2.27	6	1
1:C:117:LEU:HD12	1:C:137:MET:SD	0.48	2.48	14	1
1:C:115:ASP:O	1:C:118:LYS:HG3	0.48	2.09	6	3
1:C:124:THR:HG22	1:C:126:GLU:HG3	0.48	1.85	1	2
1:C:135:GLU:CA	1:C:138:LYS:HE3	0.48	2.38	3	1
1:C:147:ARG:HB2	1:C:147:ARG:CZ	0.48	2.39	7	1
1:C:134:GLU:O	1:C:138:LYS:HE3	0.47	2.08	10	2
1:C:121:LEU:HD11	1:C:126:GLU:OE2	0.47	2.09	13	1
1:C:152:GLU:O	1:C:156:PHE:HB2	0.47	2.10	18	1
1:C:142:LYS:HE3	1:C:155:GLU:CG	0.47	2.39	20	1
1:C:134:GLU:HG3	1:C:138:LYS:CE	0.47	2.40	9	2
1:C:121:LEU:HD23	1:C:128:ILE:CG1	0.47	2.39	18	1
1:C:137:MET:SD	1:C:147:ARG:HA	0.47	2.49	11	1
1:C:121:LEU:HD23	1:C:128:ILE:HG21	0.47	1.87	20	1
1:C:114:LEU:HD21	1:C:137:MET:CE	0.47	2.40	13	1
1:C:107:ASN:O	1:C:108:ALA:CB	0.47	2.62	4	1
1:C:114:LEU:HD21	1:C:137:MET:CG	0.47	2.40	19	1
1:C:114:LEU:HD23	1:C:117:LEU:HD12	0.47	1.87	1	1
1:C:99:ASP:HA	1:C:102:ARG:NH2	0.46	2.26	14	2
1:C:106:LYS:HG3	1:C:116:GLU:HA	0.46	1.88	1	1
1:C:139:ASP:O	1:C:142:LYS:HE2	0.46	2.11	2	2
1:C:103:MET:O	1:C:106:LYS:NZ	0.46	2.47	1	1
1:C:111:TYR:CB	1:C:147:ARG:HD2	0.46	2.41	19	1
1:C:115:ASP:HA	1:C:118:LYS:HG3	0.46	1.88	16	1
1:C:106:LYS:HE3	1:C:119:ILE:CD1	0.46	2.40	6	1
1:C:142:LYS:HD2	1:C:155:GLU:CG	0.46	2.41	8	1
1:C:106:LYS:CE	1:C:116:GLU:HA	0.46	2.41	17	1
1:C:139:ASP:O	1:C:142:LYS:NZ	0.46	2.45	6	5
1:C:121:LEU:HB3	1:C:128:ILE:CD1	0.46	2.41	12	3
1:C:142:LYS:HD2	1:C:155:GLU:HB3	0.46	1.88	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:114:LEU:HD21	1:C:137:MET:CB	0.46	2.41	20	1
1:C:101:PHE:CE1	1:C:150:TYR:HA	0.45	2.46	19	2
1:C:118:LYS:HE2	1:C:119:ILE:CG1	0.45	2.41	6	1
1:C:97:LEU:HD22	1:C:154:LEU:HB2	0.45	1.89	3	1
1:C:145:ASP:O	1:C:147:ARG:NH2	0.45	2.50	6	1
1:C:106:LYS:HE3	1:C:119:ILE:HG13	0.45	1.89	3	2
1:C:114:LEU:CD2	1:C:137:MET:HB2	0.45	2.41	5	2
1:C:106:LYS:HG3	1:C:116:GLU:CG	0.45	2.41	15	1
1:C:106:LYS:HE2	1:C:119:ILE:CD1	0.45	2.42	17	1
1:C:97:LEU:HA	1:C:100:LEU:CD2	0.44	2.42	6	1
1:C:129:THR:O	1:C:133:ILE:HG12	0.44	2.12	6	1
1:C:117:LEU:CD2	1:C:133:ILE:HG23	0.44	2.32	16	1
1:C:101:PHE:CZ	1:C:112:ILE:HG13	0.44	2.48	3	1
1:C:140:GLY:HA3	1:C:148:ILE:CD1	0.44	2.42	10	1
1:C:106:LYS:HE3	1:C:116:GLU:HA	0.44	1.88	13	1
1:C:121:LEU:HD22	1:C:126:GLU:HG3	0.44	1.89	7	1
1:C:114:LEU:HB2	1:C:137:MET:CE	0.44	2.42	17	1
1:C:111:TYR:HB3	1:C:147:ARG:HG3	0.44	1.90	11	2
1:C:106:LYS:HB3	1:C:116:GLU:HG2	0.44	1.89	19	1
1:C:121:LEU:HD22	1:C:126:GLU:CB	0.44	2.43	7	1
1:C:153:PHE:CE2	1:C:157:MET:SD	0.44	3.11	16	1
1:C:147:ARG:CZ	1:C:147:ARG:CB	0.44	2.96	10	1
1:C:132:ASP:O	1:C:136:LEU:HD13	0.44	2.13	9	1
1:C:106:LYS:CE	1:C:116:GLU:HG3	0.44	2.43	15	1
1:C:103:MET:HG3	1:C:104:PHE:N	0.44	2.28	18	1
1:C:128:ILE:CB	1:C:133:ILE:HD11	0.44	2.42	20	1
1:C:142:LYS:NZ	1:C:155:GLU:HB2	0.43	2.28	1	2
1:C:134:GLU:HG2	1:C:138:LYS:HE2	0.43	1.90	3	1
1:C:121:LEU:HD12	1:C:128:ILE:HG21	0.43	1.88	15	1
1:C:137:MET:SD	1:C:148:ILE:HG12	0.43	2.53	5	1
1:C:139:ASP:O	1:C:142:LYS:CE	0.43	2.65	2	4
1:C:101:PHE:CE1	1:C:112:ILE:HG12	0.43	2.49	19	2
1:C:97:LEU:HA	1:C:157:MET:HE3	0.43	1.88	14	1
1:C:135:GLU:CA	1:C:138:LYS:HE2	0.43	2.42	7	1
1:C:118:LYS:HG3	1:C:133:ILE:HD13	0.43	1.90	18	1
1:C:97:LEU:HD13	1:C:154:LEU:HD13	0.43	1.89	17	1
1:C:142:LYS:HG3	1:C:155:GLU:HG2	0.43	1.91	4	1
1:C:153:PHE:O	1:C:157:MET:HG2	0.42	2.14	13	1
1:C:114:LEU:HD23	1:C:137:MET:SD	0.42	2.54	6	1
1:C:131:ASP:HA	1:C:134:GLU:HB3	0.42	1.91	3	1
1:C:142:LYS:HD3	1:C:152:GLU:HA	0.42	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:132:ASP:O	1:C:136:LEU:HG	0.42	2.15	18	1
1:C:97:LEU:HD13	1:C:154:LEU:HA	0.42	1.91	12	1
1:C:100:LEU:HA	1:C:103:MET:HG2	0.42	1.92	6	2
1:C:134:GLU:O	1:C:138:LYS:HG3	0.42	2.14	13	1
1:C:147:ARG:HB3	1:C:147:ARG:CZ	0.42	2.44	20	1
1:C:112:ILE:HA	1:C:116:GLU:OE1	0.42	2.15	18	1
1:C:104:PHE:CB	1:C:112:ILE:HD12	0.42	2.44	16	1
1:C:94:GLU:HA	1:C:97:LEU:CD2	0.42	2.44	20	1
1:C:118:LYS:HE2	1:C:119:ILE:HG13	0.42	1.92	6	1
1:C:113:ASP:HB3	1:C:116:GLU:HG3	0.42	1.90	14	1
1:C:115:ASP:O	1:C:118:LYS:CG	0.42	2.68	8	1
1:C:121:LEU:HG	1:C:133:ILE:CD1	0.42	2.45	16	1
1:C:121:LEU:HD12	1:C:133:ILE:HD11	0.42	1.91	11	1
1:C:105:ASP:O	1:C:106:LYS:NZ	0.41	2.53	4	1
1:C:94:GLU:O	1:C:97:LEU:HB3	0.41	2.14	19	1
1:C:97:LEU:HD13	1:C:154:LEU:HD21	0.41	1.92	20	1
1:C:141:ASP:HA	1:C:152:GLU:OE2	0.41	2.15	16	1
1:C:128:ILE:HB	1:C:133:ILE:CG1	0.41	2.44	17	1
1:C:126:GLU:O	1:C:128:ILE:N	0.41	2.53	4	1
1:C:142:LYS:HB2	1:C:152:GLU:HG2	0.41	1.92	20	1
1:C:121:LEU:HB2	1:C:128:ILE:CD1	0.41	2.45	8	1
1:C:142:LYS:HD2	1:C:155:GLU:HG2	0.41	1.93	8	1
1:C:142:LYS:HG3	1:C:155:GLU:CG	0.41	2.46	4	1
1:C:134:GLU:O	1:C:137:MET:HB3	0.41	2.15	3	2
1:C:106:LYS:HG3	1:C:116:GLU:HG2	0.41	1.92	2	1
1:C:132:ASP:O	1:C:136:LEU:HD22	0.41	2.15	17	1
1:C:106:LYS:HG2	1:C:116:GLU:HA	0.41	1.92	20	1
1:C:104:PHE:HB3	1:C:112:ILE:HG12	0.41	1.92	17	1
1:C:111:TYR:CG	1:C:147:ARG:HD2	0.41	2.50	12	1
1:C:106:LYS:HG2	1:C:119:ILE:HD12	0.41	1.93	15	1
1:C:117:LEU:O	1:C:121:LEU:HG	0.41	2.16	7	1
1:C:112:ILE:O	1:C:148:ILE:N	0.41	2.48	19	1
1:C:130:GLU:CA	1:C:133:ILE:HD12	0.41	2.46	5	1
1:C:106:LYS:HE2	1:C:116:GLU:O	0.41	2.16	11	1
1:C:106:LYS:HG3	1:C:116:GLU:HG3	0.41	1.92	15	1
1:C:142:LYS:CE	1:C:155:GLU:HG3	0.40	2.47	8	1
1:C:106:LYS:HE3	1:C:116:GLU:HG3	0.40	1.93	15	1
1:C:97:LEU:HA	1:C:157:MET:CE	0.40	2.46	14	1
1:C:97:LEU:CD1	1:C:154:LEU:HA	0.40	2.46	12	1
1:C:129:THR:O	1:C:130:GLU:HB2	0.40	2.16	5	1
1:C:104:PHE:HB3	1:C:112:ILE:HG23	0.40	1.93	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:137:MET:HE1	1:C:147:ARG:HA	0.40	1.93	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	C	64/72 (89%)	63±1 (98±2%)	1±1 (2±2%)	0±1 (0±1%)	42	80
All	All	1280/1440 (89%)	1253 (98%)	22 (2%)	5 (0%)	42	80

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	108	ALA	2
1	C	128	ILE	1
1	C	127	THR	1
1	C	110	GLY	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	C	58/64 (91%)	52±2 (89±3%)	6±2 (11±3%)	11	55
All	All	1160/1280 (91%)	1031 (89%)	129 (11%)	11	55

All 35 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	C	118	LYS	13
1	C	127	THR	10
1	C	147	ARG	9
1	C	155	GLU	8
1	C	129	THR	8
1	C	106	LYS	7
1	C	138	LYS	6
1	C	128	ILE	5
1	C	99	ASP	5
1	C	103	MET	4
1	C	142	LYS	4
1	C	97	LEU	4
1	C	104	PHE	4
1	C	157	MET	4
1	C	149	ASP	4
1	C	131	ASP	3
1	C	137	MET	3
1	C	120	MET	3
1	C	105	ASP	2
1	C	144	ASN	2
1	C	141	ASP	2
1	C	151	ASP	2
1	C	156	PHE	2
1	C	126	GLU	2
1	C	134	GLU	2
1	C	124	THR	2
1	C	95	GLU	1
1	C	122	GLN	1
1	C	94	GLU	1
1	C	135	GLU	1
1	C	136	LEU	1
1	C	150	TYR	1
1	C	107	ASN	1
1	C	113	ASP	1
1	C	117	LEU	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 76% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mle\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	689
Number of shifts mapped to atoms	689
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	71	$-0.16 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	65	$0.03 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	70	$0.30 \pm 0.65$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 610 atoms were assigned a chemical shift out of a possible 786. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	254/320 (79%)	126/128 (98%)	64/128 (50%)	64/64 (100%)
Sidechain	339/414 (82%)	211/238 (89%)	128/162 (79%)	0/14 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	17/52 (33%)	17/28 (61%)	0/24 (0%)	0/0 (—%)
Overall	610/786 (78%)	354/394 (90%)	192/314 (61%)	64/78 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 669 atoms were assigned a chemical shift out of a possible 876. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	279/360 (78%)	138/144 (96%)	71/144 (49%)	70/72 (97%)
Sidechain	373/464 (80%)	231/268 (86%)	142/180 (79%)	0/16 (0%)
Aromatic	17/52 (33%)	17/28 (61%)	0/24 (0%)	0/0 (—%)
Overall	669/876 (76%)	386/440 (88%)	213/348 (61%)	70/88 (80%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain C:

