



Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2022 – 06:03 PM EST

PDB ID : 1SCV
Title : NMR STRUCTURE OF THE C TERMINAL DOMAIN OF CARDIAC TROPONIN C BOUND TO THE N TERMINAL DOMAIN OF CARDIAC TROPONIN I
Authors : Finley, N.L.; Howarth, J.W.; Rosevear, P.R.
Deposited on : 2004-02-12

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:

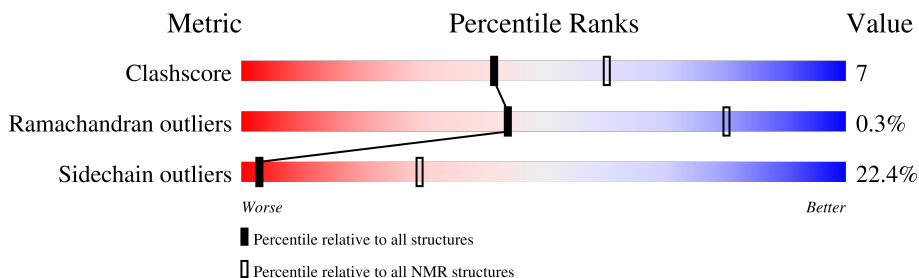
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	81	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 7 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:94-A:160 (67)	0.35	3

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1282 atoms, of which 624 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1280	404	624	102	143	7	0

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

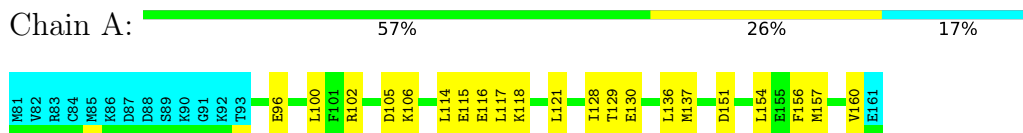
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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

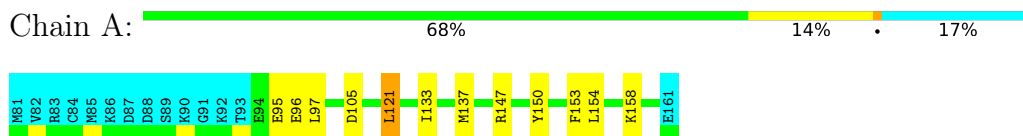


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

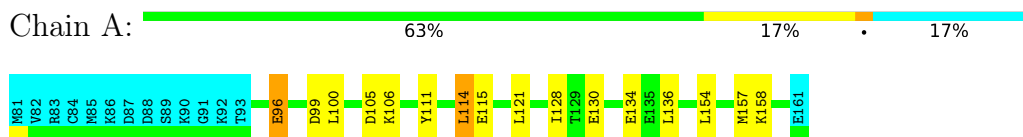
4.2.1 Score per residue for model 1

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



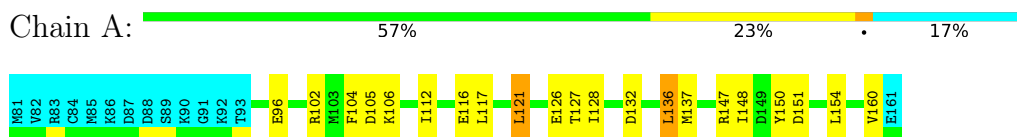
4.2.2 Score per residue for model 2

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



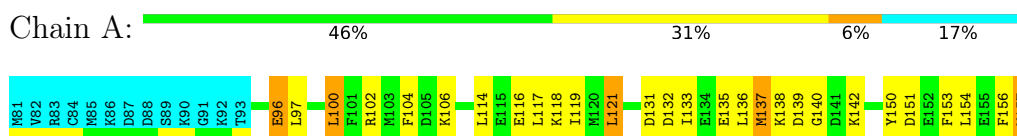
4.2.3 Score per residue for model 3 (medoid)

- 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



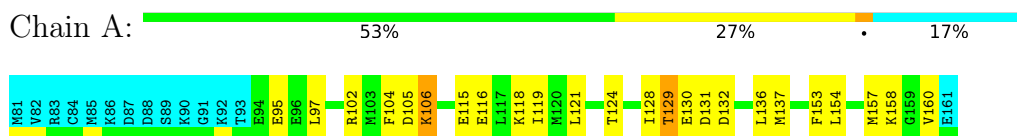
4.2.5 Score per residue for model 5

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



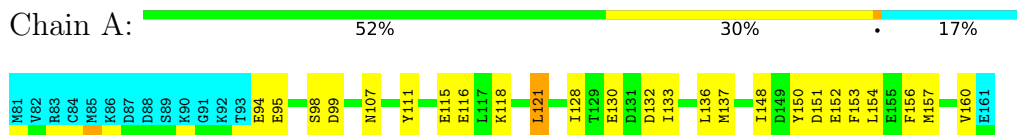
4.2.6 Score per residue for model 6

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



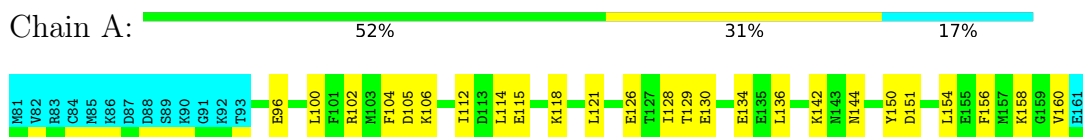
4.2.7 Score per residue for model 7

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



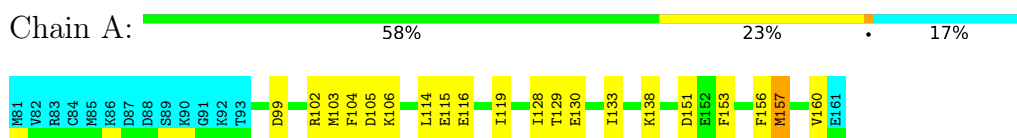
4.2.8 Score per residue for model 8

- 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



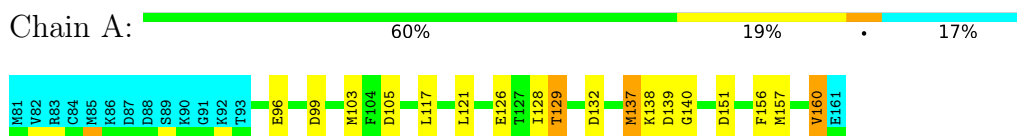
4.2.10 Score per residue for model 10

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



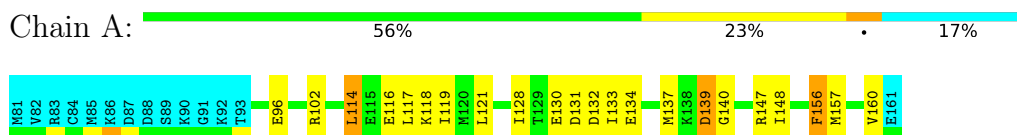
4.2.11 Score per residue for model 11

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



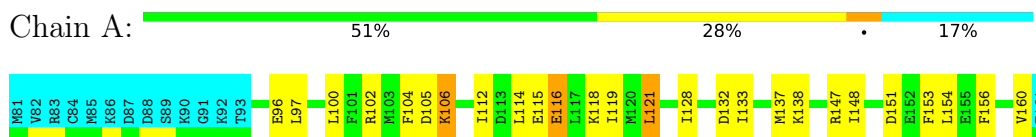
4.2.12 Score per residue for model 12

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



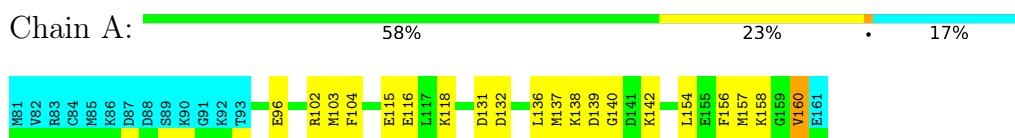
4.2.13 Score per residue for model 13

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



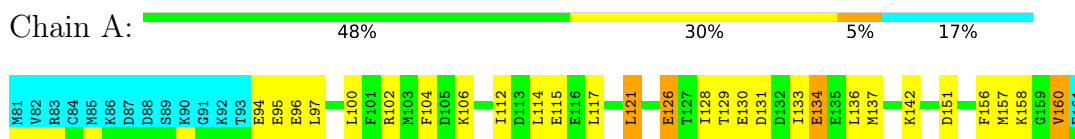
4.2.14 Score per residue for model 14

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



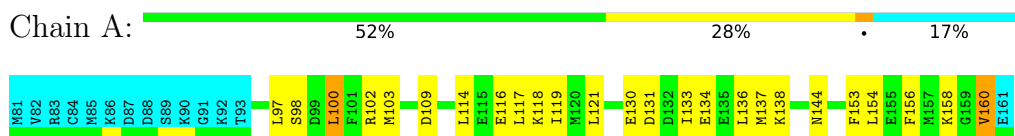
4.2.15 Score per residue for model 15

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



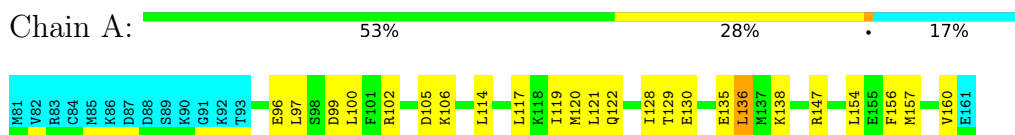
4.2.16 Score per residue for model 16

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



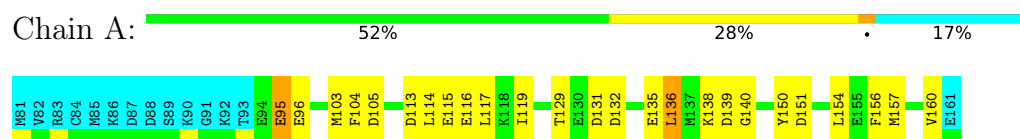
4.2.17 Score per residue for model 17

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



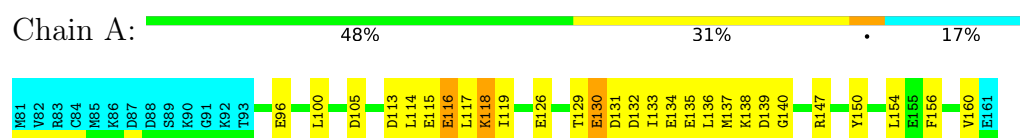
4.2.18 Score per residue for model 18

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



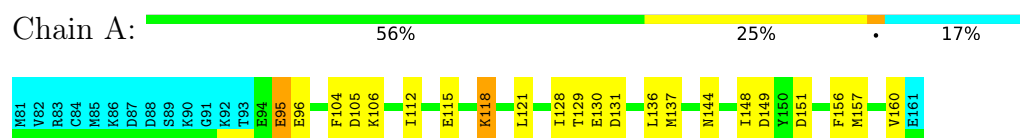
4.2.19 Score per residue for model 19

- 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: *DGSA*.

Of the 20 calculated structures, 20 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	refinement	1.0
CNX	refinement	1.0

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.

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 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	547	509	509	8±4
All	All	10980	10180	10179	155

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD13	1:A:117:LEU:HD12	0.81	1.54	4	1
1:A:156:PHE:O	1:A:160:VAL:HG22	0.73	1.84	9	9
1:A:121:LEU:HD21	1:A:128:ILE:HB	0.71	1.61	2	1
1:A:117:LEU:HD11	1:A:137:MET:HG2	0.70	1.60	19	2
1:A:118:LYS:HG2	1:A:133:ILE:HD13	0.69	1.62	19	1
1:A:106:LYS:CD	1:A:119:ILE:HG21	0.69	2.18	6	1
1:A:117:LEU:HD22	1:A:137:MET:SD	0.68	2.28	10	3
1:A:150:TYR:CZ	1:A:154:LEU:HD21	0.67	2.24	4	2
1:A:156:PHE:CE1	1:A:160:VAL:HG11	0.66	2.25	11	2
1:A:114:LEU:HD21	1:A:134:GLU:HG2	0.65	1.67	2	1
1:A:150:TYR:CE2	1:A:154:LEU:HD11	0.65	2.27	4	1
1:A:117:LEU:O	1:A:121:LEU:HD12	0.64	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:GLU:HA	1:A:119:ILE:HD12	0.64	1.69	16	7
1:A:150:TYR:O	1:A:154:LEU:HD23	0.62	1.93	1	5
1:A:126:GLU:OE1	1:A:128:ILE:HD11	0.62	1.93	3	1
1:A:96:GLU:OE2	1:A:100:LEU:HD13	0.62	1.94	4	1
1:A:121:LEU:HD11	1:A:128:ILE:CG1	0.61	2.25	2	1
1:A:114:LEU:HA	1:A:117:LEU:HD12	0.60	1.71	4	2
1:A:121:LEU:HD12	1:A:122:GLN:N	0.60	2.11	17	2
1:A:112:ILE:HG23	1:A:116:GLU:HB3	0.60	1.73	13	1
1:A:121:LEU:HD13	1:A:133:ILE:HD12	0.60	1.73	13	1
1:A:104:PHE:HB3	1:A:112:ILE:HD13	0.60	1.74	20	5
1:A:156:PHE:O	1:A:160:VAL:HG13	0.60	1.95	14	4
1:A:121:LEU:HD13	1:A:133:ILE:HG12	0.58	1.75	7	3
1:A:117:LEU:HD23	1:A:133:ILE:HG22	0.58	1.74	16	1
1:A:128:ILE:HG21	1:A:133:ILE:CD1	0.58	2.28	13	1
1:A:147:ARG:O	1:A:148:ILE:HD13	0.58	1.99	12	3
1:A:97:LEU:HD21	1:A:157:MET:HG2	0.58	1.75	4	1
1:A:133:ILE:HA	1:A:136:LEU:HD13	0.57	1.75	19	1
1:A:150:TYR:O	1:A:154:LEU:HD13	0.57	2.00	7	2
1:A:117:LEU:HD23	1:A:133:ILE:HG23	0.57	1.77	12	2
1:A:106:LYS:HD3	1:A:119:ILE:HG21	0.57	1.75	6	2
1:A:128:ILE:HG21	1:A:133:ILE:HD11	0.56	1.77	13	1
1:A:114:LEU:HD13	1:A:117:LEU:CD1	0.55	2.29	4	1
1:A:150:TYR:CD2	1:A:154:LEU:HD11	0.55	2.36	4	1
1:A:117:LEU:HD23	1:A:133:ILE:CG2	0.55	2.31	16	3
1:A:121:LEU:HD23	1:A:128:ILE:HD13	0.55	1.79	12	2
1:A:117:LEU:O	1:A:121:LEU:HD23	0.55	2.00	16	1
1:A:150:TYR:CE1	1:A:154:LEU:HD21	0.54	2.37	10	1
1:A:121:LEU:HD23	1:A:128:ILE:HG13	0.53	1.80	3	1
1:A:117:LEU:HD11	1:A:137:MET:CG	0.53	2.32	19	2
1:A:121:LEU:HD12	1:A:128:ILE:HG13	0.53	1.81	6	1
1:A:97:LEU:HD22	1:A:157:MET:HG3	0.53	1.80	17	1
1:A:118:LYS:HG3	1:A:133:ILE:HD13	0.52	1.82	4	1
1:A:106:LYS:HD2	1:A:119:ILE:HG21	0.52	1.82	6	2
1:A:121:LEU:CD2	1:A:128:ILE:HG21	0.51	2.35	3	1
1:A:94:GLU:HA	1:A:97:LEU:HD12	0.51	1.83	15	1
1:A:97:LEU:HD22	1:A:153:PHE:CE2	0.51	2.41	4	5
1:A:121:LEU:HD12	1:A:128:ILE:HG12	0.51	1.82	15	1
1:A:121:LEU:HD11	1:A:128:ILE:HG12	0.50	1.83	2	1
1:A:96:GLU:CD	1:A:100:LEU:HD13	0.50	2.28	4	1
1:A:129:THR:HG22	1:A:132:ASP:OD2	0.49	2.07	18	1
1:A:121:LEU:CD2	1:A:128:ILE:HD13	0.48	2.38	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LYS:CG	1:A:133:ILE:HD13	0.48	2.39	4	1
1:A:130:GLU:HA	1:A:133:ILE:HD12	0.47	1.86	7	2
1:A:96:GLU:OE2	1:A:100:LEU:HD11	0.47	2.09	2	1
1:A:117:LEU:HD22	1:A:137:MET:HG2	0.47	1.86	11	1
1:A:121:LEU:HD12	1:A:121:LEU:C	0.47	2.30	17	1
1:A:117:LEU:HD21	1:A:136:LEU:HD22	0.47	1.87	3	1
1:A:140:GLY:CA	1:A:156:PHE:CD2	0.47	2.98	12	1
1:A:156:PHE:CE1	1:A:160:VAL:HG13	0.46	2.45	17	1
1:A:128:ILE:HG22	1:A:129:THR:N	0.46	2.26	20	7
1:A:153:PHE:CZ	1:A:157:MET:CG	0.45	2.99	9	1
1:A:114:LEU:HD22	1:A:137:MET:HG3	0.45	1.87	13	1
1:A:117:LEU:HD22	1:A:137:MET:CG	0.45	2.42	16	1
1:A:150:TYR:CE1	1:A:154:LEU:HD11	0.45	2.47	7	1
1:A:139:ASP:OD2	1:A:156:PHE:CE1	0.44	2.71	12	2
1:A:140:GLY:CA	1:A:156:PHE:CE2	0.44	3.01	12	1
1:A:117:LEU:HD21	1:A:136:LEU:HB3	0.44	1.90	17	2
1:A:153:PHE:CE1	1:A:157:MET:CG	0.43	3.00	7	1
1:A:156:PHE:CD1	1:A:160:VAL:HG11	0.43	2.48	15	1
1:A:114:LEU:HD21	1:A:134:GLU:HA	0.43	1.89	15	1
1:A:148:ILE:HG22	1:A:149:ASP:N	0.43	2.28	20	1
1:A:139:ASP:OD2	1:A:156:PHE:CZ	0.43	2.72	12	2
1:A:128:ILE:CG2	1:A:133:ILE:HD11	0.42	2.42	13	1
1:A:112:ILE:HG22	1:A:113:ASP:N	0.42	2.29	10	1
1:A:114:LEU:HD22	1:A:137:MET:SD	0.42	2.53	16	1
1:A:150:TYR:CE1	1:A:154:LEU:CD2	0.42	3.03	3	1
1:A:115:GLU:O	1:A:118:LYS:CG	0.42	2.68	20	1
1:A:100:LEU:O	1:A:103:MET:CG	0.42	2.67	16	1
1:A:111:TYR:CD1	1:A:111:TYR:N	0.42	2.88	2	2
1:A:139:ASP:OD1	1:A:140:GLY:N	0.42	2.53	4	5
1:A:156:PHE:CE1	1:A:160:VAL:CG1	0.42	3.02	11	2
1:A:148:ILE:HG23	1:A:152:GLU:HB2	0.42	1.92	7	1
1:A:121:LEU:HD22	1:A:128:ILE:HG21	0.41	1.91	7	1
1:A:129:THR:O	1:A:133:ILE:HD12	0.41	2.15	9	1
1:A:126:GLU:CD	1:A:128:ILE:HD11	0.41	2.37	3	1
1:A:153:PHE:CZ	1:A:157:MET:HG3	0.40	2.51	9	1
1:A:98:SER:CA	1:A:150:TYR:CE1	0.40	3.05	5	1
1:A:114:LEU:HD11	1:A:134:GLU:HA	0.40	1.91	12	1
1:A:121:LEU:HD11	1:A:128:ILE:CD1	0.40	2.46	2	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	67/81 (83%)	61±1 (91±2%)	6±1 (9±2%)	0±0 (0±1%)	44	80
All	All	1340/1620 (83%)	1216 (91%)	120 (9%)	4 (0%)	44	80

All 3 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	138	LYS	2
1	A	124	THR	1
1	A	126	GLU	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	60/73 (82%)	47±3 (78±5%)	13±3 (22±5%)	3	29
All	All	1200/1460 (82%)	931 (78%)	269 (22%)	3	29

All 42 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	96	GLU	15
1	A	105	ASP	14
1	A	136	LEU	14
1	A	157	MET	12
1	A	151	ASP	12
1	A	102	ARG	11
1	A	106	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	115	GLU	10
1	A	130	GLU	10
1	A	132	ASP	9
1	A	160	VAL	9
1	A	100	LEU	9
1	A	131	ASP	9
1	A	118	LYS	9
1	A	121	LEU	8
1	A	137	MET	8
1	A	158	LYS	8
1	A	114	LEU	7
1	A	154	LEU	7
1	A	138	LYS	7
1	A	95	GLU	6
1	A	99	ASP	6
1	A	116	GLU	6
1	A	104	PHE	5
1	A	135	GLU	5
1	A	134	GLU	5
1	A	142	LYS	4
1	A	129	THR	4
1	A	126	GLU	4
1	A	103	MET	4
1	A	147	ARG	3
1	A	98	SER	3
1	A	120	MET	3
1	A	144	ASN	3
1	A	109	ASP	2
1	A	113	ASP	2
1	A	127	THR	1
1	A	124	THR	1
1	A	94	GLU	1
1	A	107	ASN	1
1	A	139	ASP	1
1	A	156	PHE	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 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

No chemical shift data were provided