Full wwPDB NMR Structure Validation Report (i)

Oct 11, 2021 – 04:57 AM EDT

PDB ID	:	2JT0
Title	:	Solution structure of F104W cardiac troponin C
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Deposited on	:	2007-07-17

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:

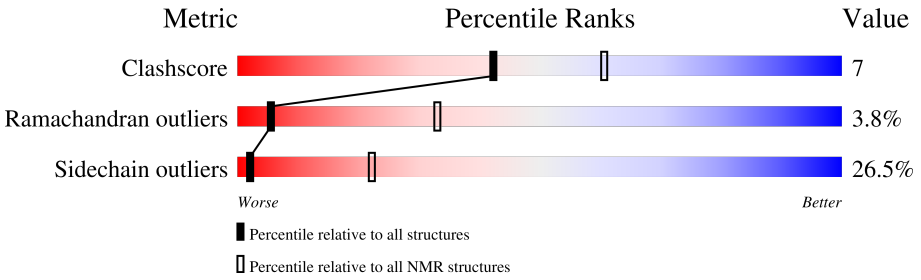
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	161	65% 28% • 6%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 1 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:2-A:86 (85)	0.96	1
2	A:93-A:158 (66)	0.52	4

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 and 4 single-model clusters were found.

Cluster number	Models
1	8, 10
2	6, 9
3	1, 5
Single-model clusters	2; 3; 4; 7

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2495 atoms, of which 1212 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	161	2495	795	1212	197	280	11	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	CYS	engineered mutation	UNP P63316
A	84	SER	CYS	engineered mutation	UNP P63316
A	104	TRP	PHE	engineered mutation	UNP P63316

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

Chain A: 65% 28% • 6%

M1 Y5 V9 L12 F24 F27 V28 L29 D33 G34 S35 I36 S37 T38 L41 M45 Q50 T53 L57 M60 V64 V72 D75 V79 M80 M81 S84 M85 K86 D87 D88 S89 K90 G91 K92 S93 L97 S98 D99 L100 K106

N107 L117 M120 L121 I128 D132 I133 E134 E135 L136 K142 D149 Y150 D151 L154 E155 F156 M157 K158 G159 V160 E161

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 (medoid)

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

Chain A: 61% 28% 5% 6%

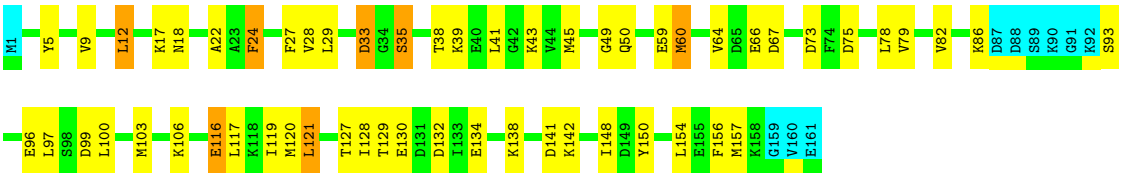
M1 A8 V9 E10 Q11 L12 Q16 F24 F27 V28 L29 E32 S37 T38 L41 V44 M45 R46 G49 Q50 N51 L57 Q58 E59 M60 I61 D62 E66 D67 V72 D73 F74 D75 V79 M80 M81 V82 R83 S84 M85 K86 D87 D88 S89 K90 G91 K92

S93 E94 E95 E96 L97 S98 D99 L100 K106 N107 A108 L121 I128 D132 L136 M137 D141 D151 E152 F153 L154 M157 K158 G159 V160 E161

4.2.2 Score per residue for model 2

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

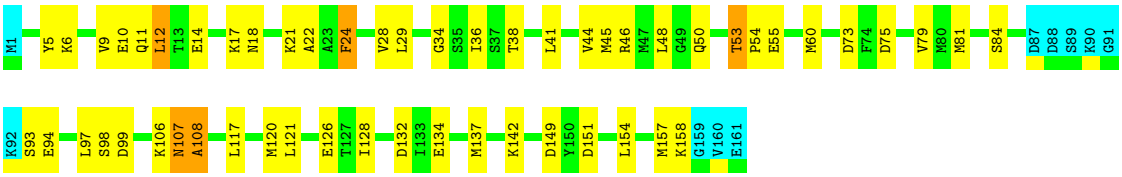
Chain A: 59% 30% • 6%



4.2.3 Score per residue for model 3

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

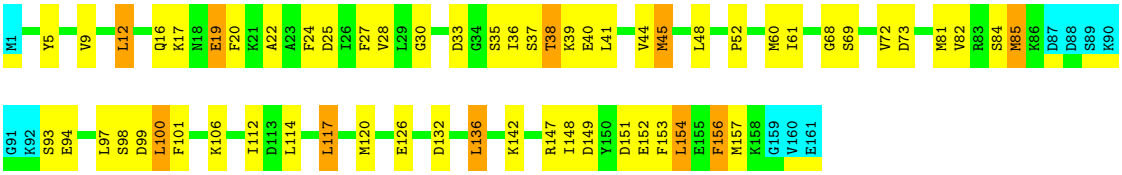
Chain A: 60% 30% • 6%



4.2.4 Score per residue for model 4

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

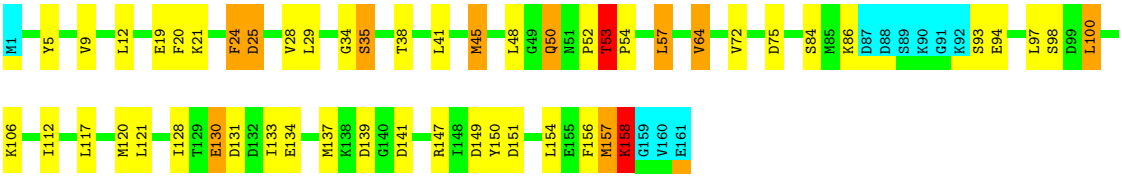
Chain A: 57% 31% 6% 6%



4.2.5 Score per residue for model 5

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

Chain A: 61% 25% 6% • 6%



4.2.6 Score per residue for model 6

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

Chain A: 61% 30% • 6%

M1 D2 Y5 V9 L12 N18 E19 F24 F27 V28 L29 G30 D33 G34 S35 I36 S37 T38 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 E55 M60 E66 V72 D73 F74 D75 E76 F77 L78 V79 S84 M85 K86 D87 D88

S89 K90 G91 K92 L97 S98 D99 L100 F101 R102 K106 L117 L121 D132 I133 E134 E135 L136 K142 N143 N144 D149 Y150 D151 L154 M157 K158 G159 V160 E161

4.2.7 Score per residue for model 7

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

Chain A: 55% 34% • • 6%

M1 D2 Y5 A8 V9 E10 Q11 L12 Q16 F20 K21 F24 D25 I26 F27 V28 L29 G30 G34 S35 T38 K39 E40 L41 Q50 P54 E55 E56 L57 Q58 E59 M60 I61 V64 D65 E66 D67 G68 S69 V72 D75 V79 M80 M81 V82 D87

D88 S89 K90 G91 K92 S93 E94 E95 E96 L97 S98 D99 L100 M103 K106 L114 L117 M120 L121 E126 T129 E130 E134 E135 L136 D141 K142 N143 N144 D145 Y150 D151 E152 F153 L154 M157 K158 G159 V160 E161

4.2.8 Score per residue for model 8

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

Chain A: 58% 33% • 6%

M1 I4 Y5 V9 E10 Q11 L12 E15 E19 F24 F27 V28 L29 S35 I36 S37 L41 G42 K43 V44 M45 L48 L57 Q58 E59 M60 E63 V64 S69 V72 D75 V79 M80 M81 V82 R83 S84 M85 K86 D87 D88 S89 K90 G91 K92

S93 E94 E95 E96 L97 S98 D99 L100 K106 N107 G110 D113 L117 M120 L121 Q122 T127 I128 T129 E134 E135 L136 M137 K142 D149 Y150 D151 E152 F153 L154 M157 K158 G159 V160 E161

4.2.9 Score per residue for model 9

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

Chain A: 58% 30% 6% 6%

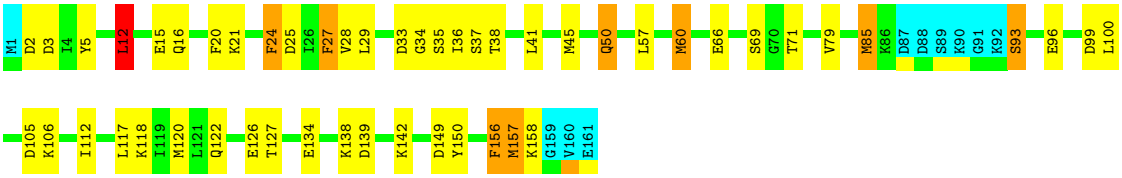
M1 Y5 K6 V9 L12 T13 E14 K17 F24 V28 L29 D33 G34 S35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 Q50 T53 P54 E55 E56 L57 V64 D65 V72 D73 F74 D75 V79 M80 M81 S84 M85 K86 D87 D88 S89 K90

G91 K92 S93 E94 E95 E96 L97 S98 D99 L100 K106 I112 D115 E116 L117 L121 Q122 E126 T127 I128 T129 E130 D131 D132 I133 E134 M137 K142 Y150 F153 L154 M157 K158 G159 V160 E161

4.2.10 Score per residue for model 10

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

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 10 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
CYANA	structure solution	
CYANA	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	1211	1143	1143	17±5
All	All	12110	11430	11430	170

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:53:THR:N	1:A:54:PRO:HD2	0.87	1.84	6	4
1:A:41:LEU:HD12	1:A:72:VAL:HG22	0.78	1.56	4	2
1:A:53:THR:N	1:A:54:PRO:CD	0.78	2.45	6	1
1:A:41:LEU:HD13	1:A:72:VAL:HG21	0.76	1.55	1	4
1:A:52:PRO:O	1:A:53:THR:HB	0.76	1.80	6	1
1:A:24:PHE:CE2	1:A:28:VAL:HG11	0.68	2.23	10	5
1:A:48:LEU:HD21	1:A:77:PHE:CZ	0.68	2.24	6	1
1:A:52:PRO:O	1:A:53:THR:CB	0.67	2.41	6	1
1:A:27:PHE:CD2	1:A:36:ILE:HD11	0.67	2.24	10	1
1:A:97:LEU:HD12	1:A:154:LEU:HD23	0.66	1.66	8	1
1:A:41:LEU:HD13	1:A:72:VAL:HG22	0.65	1.67	5	1
1:A:97:LEU:CD1	1:A:154:LEU:HD13	0.64	2.23	9	2
1:A:97:LEU:HD13	1:A:154:LEU:HD13	0.62	1.70	9	1
1:A:157:MET:O	1:A:158:LYS:C	0.61	2.38	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PHE:O	1:A:28:VAL:HG22	0.60	1.96	10	2
1:A:12:LEU:HD21	1:A:85:MET:CE	0.60	2.26	4	2
1:A:121:LEU:HD22	1:A:133:ILE:HD11	0.60	1.70	5	1
1:A:41:LEU:HD12	1:A:72:VAL:CG2	0.60	2.25	4	1
1:A:53:THR:HG22	1:A:54:PRO:HD3	0.60	1.74	6	1
1:A:41:LEU:HD21	1:A:64:VAL:HG11	0.59	1.75	7	1
1:A:5:TYR:O	1:A:9:VAL:HG23	0.59	1.97	2	8
1:A:38:THR:HB	1:A:61:ILE:HD13	0.59	1.75	4	1
1:A:8:ALA:HB1	1:A:82:VAL:HG21	0.59	1.74	7	2
1:A:75:ASP:O	1:A:79:VAL:HG23	0.59	1.97	6	7
1:A:154:LEU:HD12	1:A:154:LEU:O	0.58	1.98	9	2
1:A:12:LEU:HD21	1:A:85:MET:HE1	0.58	1.76	4	1
1:A:100:LEU:HD23	1:A:153:PHE:CZ	0.58	2.33	1	1
1:A:53:THR:CG2	1:A:54:PRO:HD3	0.57	2.30	6	1
1:A:41:LEU:CD1	1:A:72:VAL:HG22	0.57	2.29	6	1
1:A:54:PRO:HA	1:A:57:LEU:HD23	0.56	1.77	5	1
1:A:121:LEU:HD23	1:A:122:GLN:N	0.56	2.15	9	1
1:A:5:TYR:CB	1:A:79:VAL:HG23	0.56	2.30	10	1
1:A:97:LEU:HD22	1:A:154:LEU:CD2	0.56	2.31	3	1
1:A:121:LEU:HB3	1:A:127:THR:HG23	0.56	1.77	8	1
1:A:82:VAL:HG23	1:A:85:MET:CE	0.55	2.32	8	2
1:A:117:LEU:CD1	1:A:136:LEU:HD22	0.55	2.30	7	1
1:A:24:PHE:CE1	1:A:28:VAL:HG11	0.55	2.37	8	3
1:A:45:MET:HA	1:A:48:LEU:HD12	0.54	1.77	5	3
1:A:97:LEU:HD13	1:A:154:LEU:CD2	0.54	2.33	3	1
1:A:12:LEU:HD11	1:A:82:VAL:HG22	0.54	1.80	2	1
1:A:121:LEU:HD22	1:A:127:THR:HA	0.54	1.78	8	1
1:A:57:LEU:HD12	1:A:60:MET:HG3	0.53	1.79	10	1
1:A:121:LEU:HD12	1:A:126:GLU:O	0.53	2.03	7	1
1:A:130:GLU:HA	1:A:133:ILE:HD12	0.53	1.81	5	1
1:A:107:ASN:O	1:A:108:ALA:HB2	0.53	2.03	3	2
1:A:141:ASP:HB2	1:A:148:ILE:HD11	0.53	1.81	2	1
1:A:5:TYR:CG	1:A:79:VAL:HG13	0.53	2.39	3	1
1:A:97:LEU:HG	1:A:154:LEU:HD13	0.52	1.80	4	1
1:A:151:ASP:HA	1:A:154:LEU:HD12	0.52	1.81	8	1
1:A:97:LEU:HD22	1:A:154:LEU:HB2	0.52	1.80	9	1
1:A:48:LEU:HD13	1:A:81:MET:SD	0.52	2.44	4	2
1:A:127:THR:O	1:A:128:ILE:HD13	0.52	2.05	2	2
1:A:36:ILE:HD13	1:A:44:VAL:HG11	0.52	1.82	4	2
1:A:53:THR:H	1:A:54:PRO:HD2	0.52	1.57	6	2
1:A:41:LEU:CD2	1:A:64:VAL:HG11	0.51	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:CD2	1:A:57:LEU:HD11	0.51	2.35	5	1
1:A:150:TYR:CE1	1:A:154:LEU:HD21	0.51	2.40	2	3
1:A:52:PRO:C	1:A:53:THR:HG22	0.50	2.27	5	1
1:A:12:LEU:HD13	1:A:16:GLN:CD	0.49	2.27	1	1
1:A:117:LEU:CD1	1:A:136:LEU:HD12	0.49	2.37	4	1
1:A:97:LEU:HG	1:A:154:LEU:HD22	0.49	1.84	6	3
1:A:53:THR:HG23	1:A:54:PRO:CD	0.49	2.37	5	1
1:A:58:GLN:HA	1:A:61:ILE:HD12	0.48	1.84	7	1
1:A:24:PHE:CD2	1:A:28:VAL:HG11	0.48	2.43	10	1
1:A:100:LEU:HD23	1:A:153:PHE:HE2	0.48	1.69	9	1
1:A:41:LEU:HD13	1:A:60:MET:SD	0.47	2.48	2	1
1:A:100:LEU:HD22	1:A:157:MET:SD	0.47	2.49	1	1
1:A:41:LEU:HD13	1:A:72:VAL:CG2	0.47	2.38	7	3
1:A:41:LEU:O	1:A:44:VAL:HG22	0.47	2.09	1	1
1:A:150:TYR:CD1	1:A:154:LEU:HD21	0.47	2.45	6	2
1:A:117:LEU:HD11	1:A:136:LEU:HD12	0.47	1.86	4	1
1:A:60:MET:O	1:A:64:VAL:HG22	0.47	2.09	7	1
1:A:148:ILE:HG23	1:A:152:GLU:HB3	0.47	1.86	4	1
1:A:38:THR:HG21	1:A:65:ASP:OD2	0.47	2.10	9	1
1:A:116:GLU:HA	1:A:119:ILE:HD12	0.46	1.87	2	1
1:A:41:LEU:HD23	1:A:57:LEU:HD11	0.46	1.86	5	1
1:A:60:MET:O	1:A:64:VAL:HG13	0.46	2.10	7	1
1:A:12:LEU:HD22	1:A:16:GLN:HG3	0.46	1.87	4	1
1:A:28:VAL:HG23	1:A:30:GLY:H	0.46	1.69	4	3
1:A:28:VAL:HG12	1:A:34:GLY:HA3	0.46	1.87	7	2
1:A:8:ALA:CB	1:A:82:VAL:HG21	0.46	2.41	1	1
1:A:53:THR:CB	1:A:54:PRO:CD	0.45	2.94	3	3
1:A:57:LEU:HD11	1:A:61:ILE:HD11	0.45	1.87	1	1
1:A:121:LEU:HD13	1:A:127:THR:HA	0.45	1.87	2	1
1:A:78:LEU:O	1:A:82:VAL:HG23	0.45	2.10	2	1
1:A:41:LEU:HD23	1:A:57:LEU:HD21	0.45	1.88	9	1
1:A:97:LEU:HD13	1:A:154:LEU:HD21	0.45	1.88	5	1
1:A:100:LEU:HD23	1:A:153:PHE:CE2	0.44	2.47	9	1
1:A:101:PHE:CE1	1:A:112:ILE:HD11	0.44	2.47	4	1
1:A:18:ASN:O	1:A:22:ALA:HB2	0.44	2.12	3	2
1:A:12:LEU:HD12	1:A:16:GLN:HB3	0.43	1.90	7	1
1:A:57:LEU:O	1:A:57:LEU:HD12	0.43	2.13	8	1
1:A:52:PRO:C	1:A:53:THR:CG2	0.43	2.86	5	1
1:A:128:ILE:HG22	1:A:129:THR:HG23	0.43	1.90	8	1
1:A:132:ASP:O	1:A:136:LEU:HD23	0.43	2.14	4	2
1:A:53:THR:HG23	1:A:54:PRO:HD3	0.43	1.89	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD11	1:A:85:MET:CE	0.43	2.43	10	1
1:A:154:LEU:HD12	1:A:154:LEU:C	0.42	2.33	9	1
1:A:25:ASP:HA	1:A:28:VAL:HG22	0.42	1.91	5	3
1:A:117:LEU:HD12	1:A:136:LEU:HD22	0.42	1.92	7	1
1:A:150:TYR:O	1:A:153:PHE:CD1	0.41	2.73	8	1
1:A:53:THR:OG1	1:A:54:PRO:HD3	0.41	2.15	5	1
1:A:54:PRO:O	1:A:57:LEU:HD23	0.41	2.16	7	1
1:A:107:ASN:ND2	1:A:107:ASN:N	0.41	2.68	8	1
1:A:97:LEU:HD13	1:A:154:LEU:HD22	0.41	1.93	3	1
1:A:117:LEU:HD11	1:A:136:LEU:HD22	0.41	1.93	7	1
1:A:154:LEU:C	1:A:154:LEU:HD12	0.41	2.35	1	1
1:A:19:GLU:O	1:A:22:ALA:HB3	0.41	2.16	4	1
1:A:64:VAL:HG12	1:A:64:VAL:O	0.41	2.16	5	1
1:A:105:ASP:HB2	1:A:112:ILE:HD13	0.40	1.93	10	1
1:A:117:LEU:HD12	1:A:136:LEU:HD13	0.40	1.92	7	1
1:A:53:THR:CG2	1:A:54:PRO:CD	0.40	2.98	6	1
1:A:142:LYS:N	1:A:142:LYS:CD	0.40	2.85	7	1
1:A:57:LEU:HD12	1:A:57:LEU:O	0.40	2.16	10	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	151/161 (94%)	132±3 (87±2%)	13±2 (9±2%)	6±1 (4±1%)	5	33
All	All	1510/1610 (94%)	1318 (87%)	134 (9%)	58 (4%)	5	33

All 24 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	12	LEU	10
1	A	50	GLN	6
1	A	35	SER	4
1	A	64	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	34	GLY	4
1	A	69	SER	4
1	A	128	ILE	3
1	A	49	GLY	2
1	A	67	ASP	2
1	A	107	ASN	2
1	A	108	ALA	2
1	A	93	SER	2
1	A	53	THR	2
1	A	33	ASP	1
1	A	129	THR	1
1	A	52	PRO	1
1	A	68	GLY	1
1	A	86	LYS	1
1	A	158	LYS	1
1	A	2	ASP	1
1	A	66	GLU	1
1	A	145	ASP	1
1	A	110	GLY	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	134/142 (94%)	98±3 (74±2%)	36±3 (26±2%)	2 22
All	All	1340/1420 (94%)	985 (74%)	355 (26%)	2 22

All 97 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	24	PHE	10
1	A	106	LYS	10
1	A	157	MET	10
1	A	29	LEU	9
1	A	117	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	38	THR	8
1	A	93	SER	8
1	A	99	ASP	8
1	A	100	LEU	8
1	A	134	GLU	8
1	A	142	LYS	8
1	A	27	PHE	7
1	A	60	MET	7
1	A	84	SER	7
1	A	98	SER	7
1	A	45	MET	7
1	A	120	MET	7
1	A	37	SER	6
1	A	50	GLN	6
1	A	35	SER	6
1	A	149	ASP	6
1	A	73	ASP	5
1	A	94	GLU	5
1	A	121	LEU	5
1	A	137	MET	5
1	A	151	ASP	5
1	A	158	LYS	5
1	A	33	ASP	5
1	A	46	ARG	4
1	A	66	GLU	4
1	A	81	MET	4
1	A	95	GLU	4
1	A	132	ASP	4
1	A	17	LYS	4
1	A	43	LYS	4
1	A	86	LYS	4
1	A	130	GLU	4
1	A	21	LYS	4
1	A	55	GLU	4
1	A	19	GLU	4
1	A	20	PHE	4
1	A	10	GLU	3
1	A	59	GLU	3
1	A	85	MET	3
1	A	136	LEU	3
1	A	141	ASP	3
1	A	154	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	39	LYS	3
1	A	12	LEU	3
1	A	41	LEU	3
1	A	53	THR	3
1	A	126	GLU	3
1	A	156	PHE	3
1	A	150	TYR	3
1	A	122	GLN	3
1	A	16	GLN	2
1	A	67	ASP	2
1	A	96	GLU	2
1	A	103	MET	2
1	A	138	LYS	2
1	A	6	LYS	2
1	A	11	GLN	2
1	A	14	GLU	2
1	A	40	GLU	2
1	A	114	LEU	2
1	A	147	ARG	2
1	A	153	PHE	2
1	A	25	ASP	2
1	A	57	LEU	2
1	A	112	ILE	2
1	A	139	ASP	2
1	A	143	ASN	2
1	A	2	ASP	2
1	A	152	GLU	2
1	A	15	GLU	2
1	A	64	VAL	2
1	A	127	THR	2
1	A	32	GLU	1
1	A	51	ASN	1
1	A	62	ASP	1
1	A	116	GLU	1
1	A	75	ASP	1
1	A	131	ASP	1
1	A	18	ASN	1
1	A	102	ARG	1
1	A	144	ASN	1
1	A	65	ASP	1
1	A	129	THR	1
1	A	4	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	63	GLU	1
1	A	107	ASN	1
1	A	113	ASP	1
1	A	74	PHE	1
1	A	115	ASP	1
1	A	3	ASP	1
1	A	71	THR	1
1	A	118	LYS	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)

There are no ligands in this entry.

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