Full wwPDB NMR Structure Validation Report (i)

May 31, 2020 – 11:40 am BST

PDB ID	:	6OQH
Title	:	Solution NMR structure of a quiet outer membrane protein G Nanopore (OmpG mutant: Delta-L6-D215)
Authors	:	Sanganna Gari, R.R.; Seelheim, P.; Liang, B.; Tamm, L.K.
Deposited on	:	2019-04-26

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

We welcome your comments at *validation@mail.wwpdb.org*
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 (1)) were used in the production of this report:

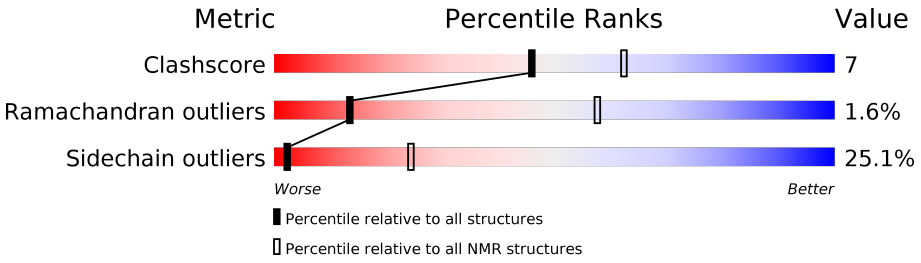
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 38%.

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	271	43% 22% 35%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:5-A:15, A:29-A:51, A:66-A:95, A:107-A:137, A:149-A:177, A:188-A:212, A:228-A:246, A:263-A:271 (177)	0.87	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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 7, 8, 9, 10
2	2, 6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4238 atoms, of which 2003 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Outer membrane protein G.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	271	4238	1419	2003	372	439	5	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P76045
A	?	-	TRP	deletion	UNP P76045
A	?	-	ASP	deletion	UNP P76045
A	?	-	TRP	deletion	UNP P76045
A	?	-	GLN	deletion	UNP P76045
A	?	-	ASP	deletion	UNP P76045
A	?	-	ASP	deletion	UNP P76045
A	?	-	ILE	deletion	UNP P76045
A	?	-	GLU	deletion	UNP P76045
A	219	GLY	ARG	conflict	UNP P76045

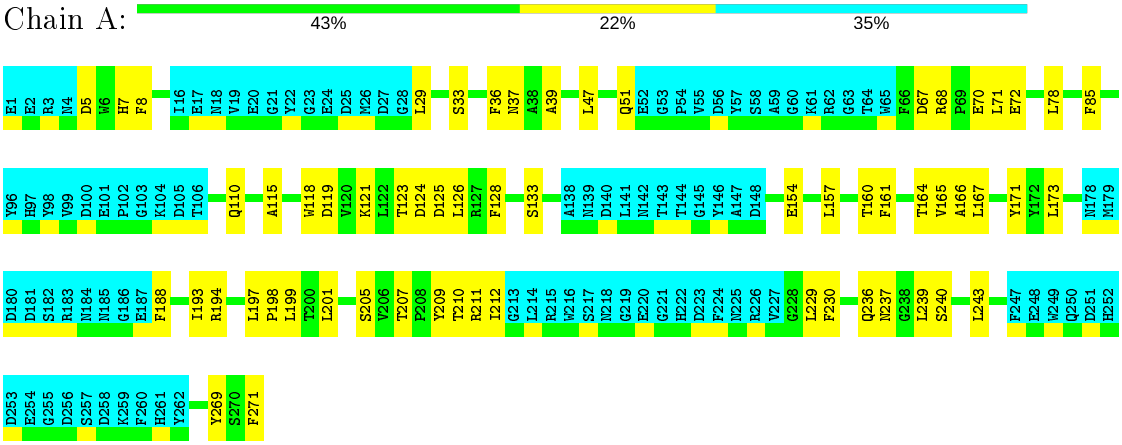
4 Residue-property plots (i)

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: Outer membrane protein G

Chain A:



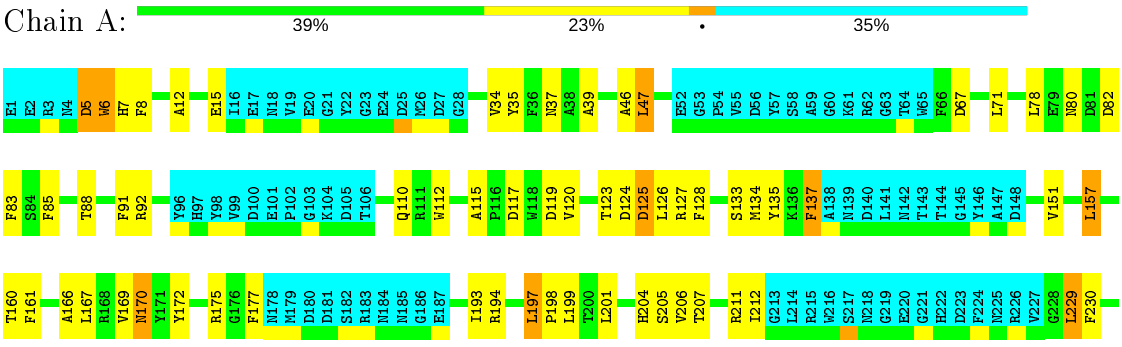
4.2 Scores per residue for each member of the ensemble

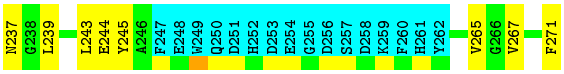
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Outer membrane protein G

Chain A:

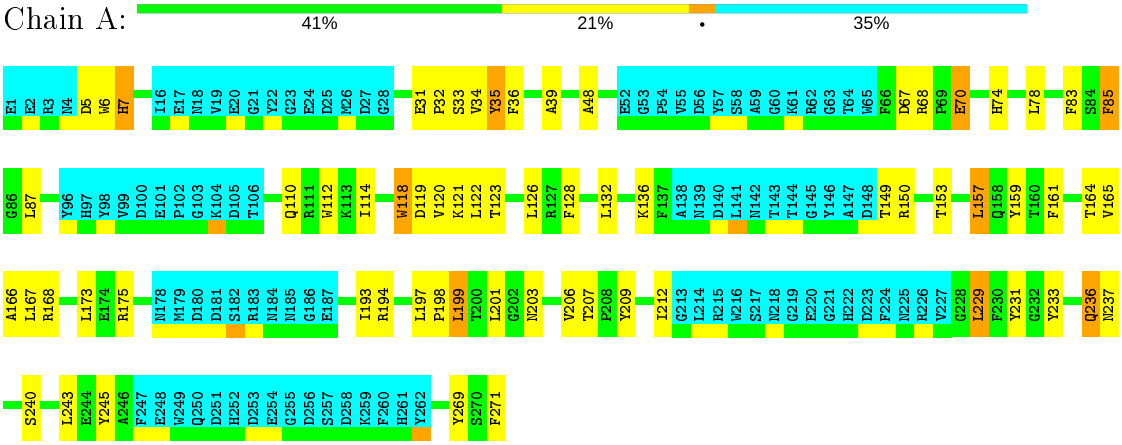




4.2.2 Score per residue for model 2

• Molecule 1: Outer membrane protein G

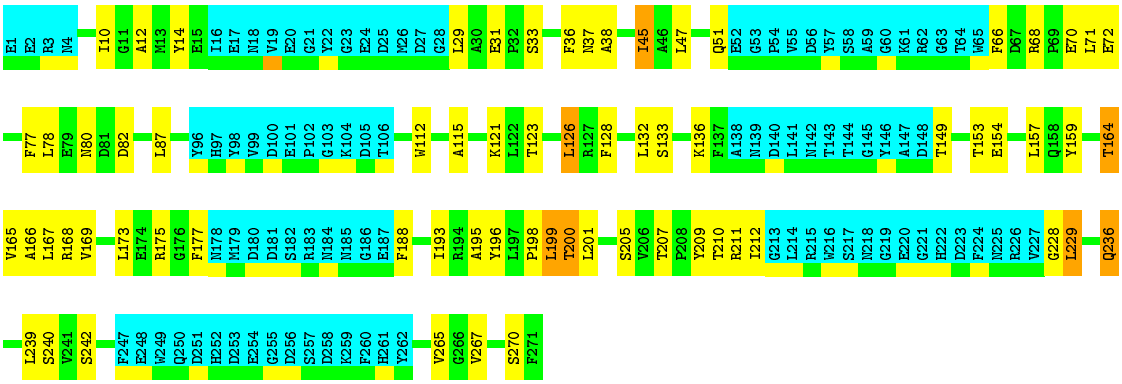
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Outer membrane protein G

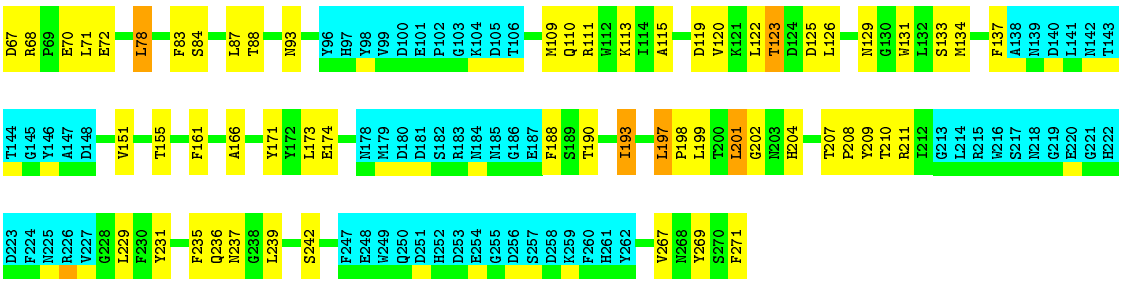
Chain A:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Outer membrane protein G

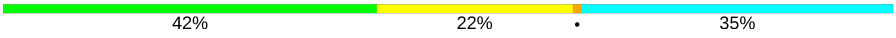
Chain A:

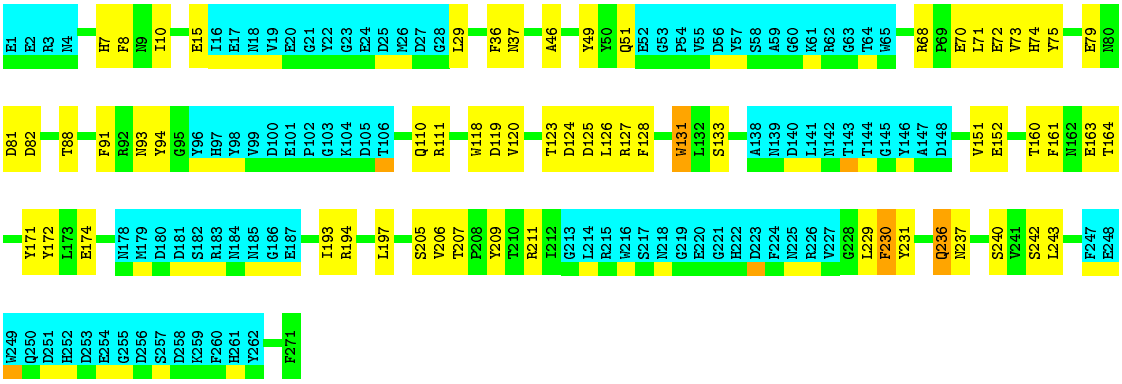


4.2.5 Score per residue for model 5

- Molecule 1: Outer membrane protein G

Chain A:

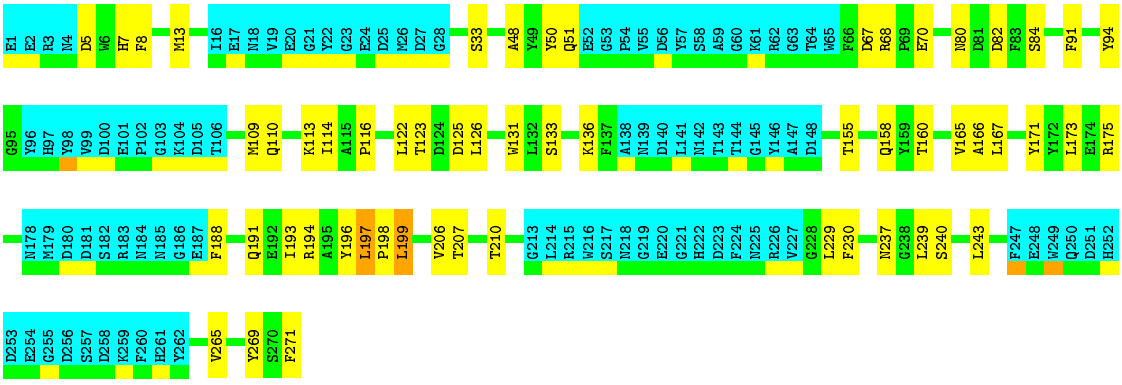




4.2.6 Score per residue for model 6

- Molecule 1: Outer membrane protein G

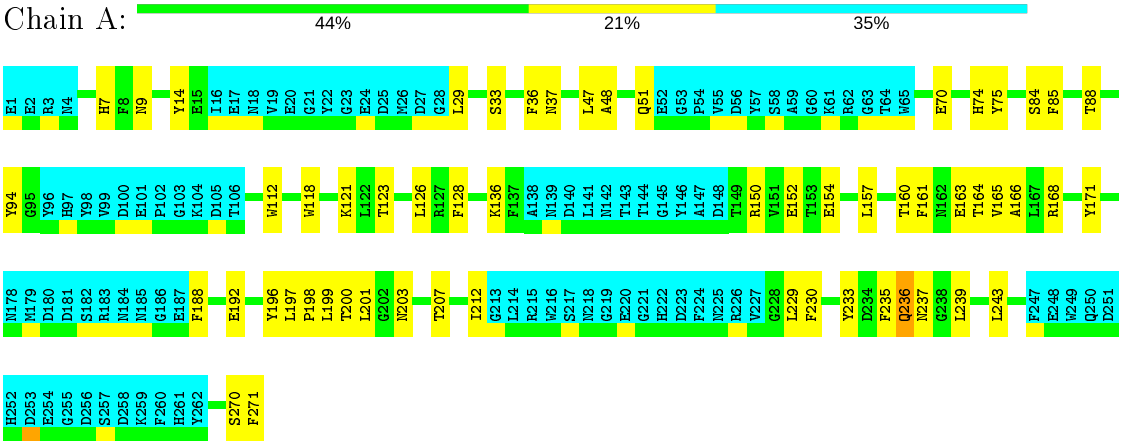
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Outer membrane protein G

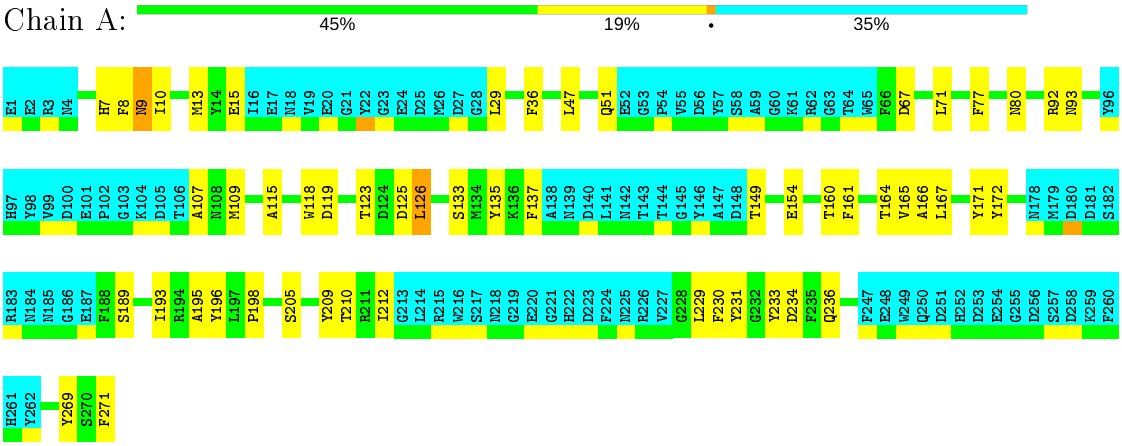
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Outer membrane protein G

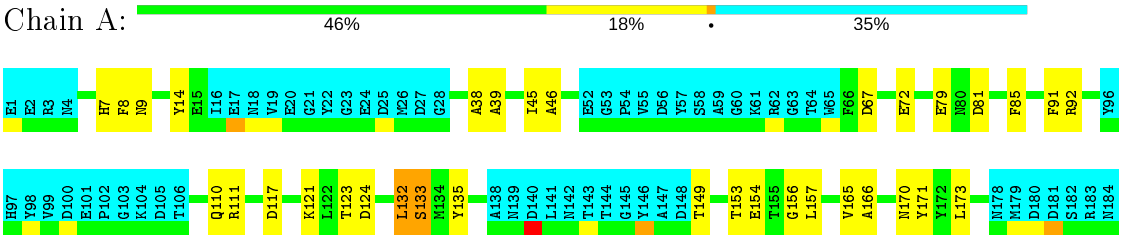
Chain A:

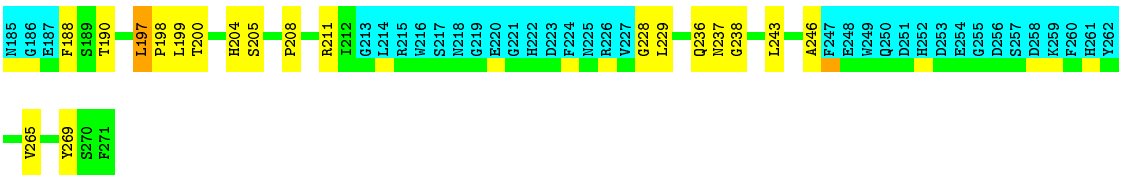


4.2.9 Score per residue for model 9

• Molecule 1: Outer membrane protein G

Chain A:

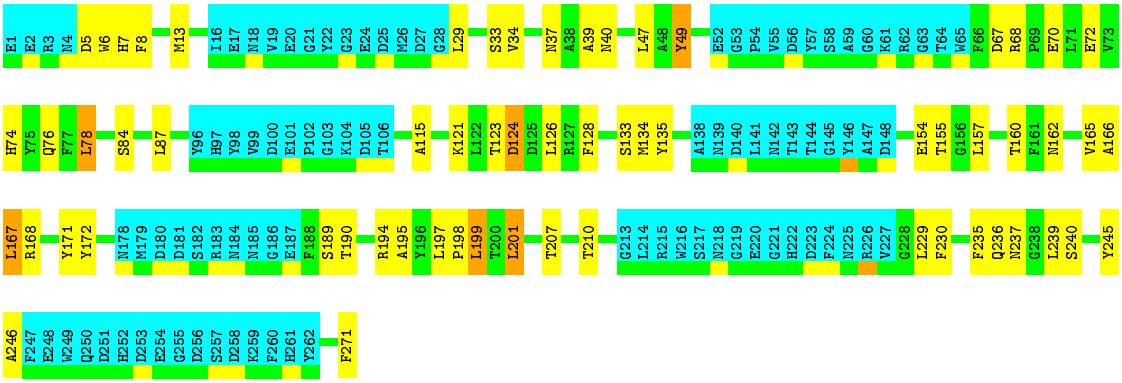




4.2.10 Score per residue for model 10

- Molecule 1: Outer membrane protein G

Chain A: 42% 21% 35%



5 Refinement protocol and experimental data overview

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

Of the 200 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
CNS	structure calculation	1.2

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1199
Number of shifts mapped to atoms	1199
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1473	1367	1364	19±5
All	All	14730	13670	13640	187

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:83:PHE:CE1	1:A:120:VAL:HG13	0.78	2.12	1	1
1:A:128:PHE:CE2	1:A:157:LEU:HD11	0.74	2.18	1	1
1:A:165:VAL:HG12	1:A:199:LEU:HD23	0.74	1.58	9	1
1:A:83:PHE:CE2	1:A:120:VAL:HG13	0.72	2.19	2	2
1:A:239:LEU:HD23	1:A:269:TYR:CD2	0.71	2.20	6	1
1:A:166:ALA:HB3	1:A:198:PRO:HG2	0.70	1.60	7	8
1:A:239:LEU:HD12	1:A:269:TYR:CD1	0.70	2.20	4	1
1:A:74:HIS:CD2	1:A:88:THR:HG22	0.70	2.22	5	1
1:A:239:LEU:HD23	1:A:240:SER:N	0.68	2.02	3	1
1:A:132:LEU:CD2	1:A:153:THR:HG23	0.67	2.19	9	2
1:A:87:LEU:HD12	1:A:114:ILE:HD11	0.67	1.65	2	1
1:A:126:LEU:HD23	1:A:157:LEU:HD21	0.66	1.68	3	1
1:A:7:HIS:HB3	1:A:39:ALA:HB3	0.65	1.66	4	1
1:A:126:LEU:CD2	1:A:157:LEU:HD11	0.65	2.20	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LYS:HG3	1:A:149:THR:HG23	0.64	1.70	3	1
1:A:122:LEU:HB3	1:A:126:LEU:HD22	0.63	1.70	2	1
1:A:160:THR:HG23	1:A:166:ALA:HB2	0.63	1.68	6	2
1:A:198:PRO:HA	1:A:207:THR:HG23	0.63	1.70	6	1
1:A:7:HIS:HB2	1:A:39:ALA:HB3	0.62	1.71	10	3
1:A:9:ASN:O	1:A:10:ILE:HD13	0.62	1.95	8	1
1:A:48:ALA:HB3	1:A:70:GLU:HB3	0.62	1.72	6	3
1:A:126:LEU:CD2	1:A:157:LEU:HD21	0.61	2.25	3	1
1:A:125:ASP:C	1:A:126:LEU:HD12	0.60	2.16	6	1
1:A:128:PHE:CD2	1:A:157:LEU:HD21	0.60	2.32	1	1
1:A:128:PHE:CZ	1:A:157:LEU:HD12	0.59	2.33	3	1
1:A:195:ALA:HB3	1:A:210:THR:O	0.59	1.98	10	1
1:A:134:MET:SD	1:A:151:VAL:HG12	0.59	2.38	4	1
1:A:128:PHE:CD2	1:A:157:LEU:HD11	0.58	2.32	1	1
1:A:37:ASN:OD1	1:A:46:ALA:HB2	0.58	1.97	5	2
1:A:165:VAL:HG12	1:A:199:LEU:CD2	0.58	2.28	9	2
1:A:197:LEU:HD12	1:A:197:LEU:N	0.58	2.13	10	1
1:A:14:TYR:HB2	1:A:265:VAL:HG23	0.58	1.74	3	2
1:A:208:PRO:HB3	1:A:229:LEU:HD23	0.58	1.76	9	1
1:A:229:LEU:HD13	1:A:230:PHE:N	0.57	2.15	1	1
1:A:173:LEU:HD12	1:A:191:GLN:HA	0.57	1.75	6	1
1:A:115:ALA:HB2	1:A:133:SER:HA	0.57	1.76	8	4
1:A:48:ALA:HB3	1:A:70:GLU:CB	0.57	2.29	6	4
1:A:38:ALA:HB3	1:A:45:ILE:HG13	0.57	1.77	9	1
1:A:193:ILE:HD11	1:A:212:ILE:HD11	0.56	1.75	2	1
1:A:206:VAL:HG13	1:A:230:PHE:O	0.56	2.00	6	2
1:A:165:VAL:HG23	1:A:199:LEU:HG	0.56	1.77	6	1
1:A:201:LEU:N	1:A:201:LEU:HD23	0.56	2.15	10	1
1:A:83:PHE:CZ	1:A:120:VAL:HG13	0.56	2.35	1	1
1:A:134:MET:HG3	1:A:151:VAL:HG12	0.56	1.75	1	1
1:A:165:VAL:HG12	1:A:199:LEU:HG	0.56	1.76	3	1
1:A:46:ALA:HB3	1:A:72:GLU:HB3	0.56	1.78	9	3
1:A:7:HIS:O	1:A:39:ALA:HB3	0.56	2.00	1	1
1:A:193:ILE:N	1:A:193:ILE:HD13	0.56	2.14	4	1
1:A:167:LEU:HD12	1:A:197:LEU:HB3	0.56	1.78	6	1
1:A:125:ASP:O	1:A:126:LEU:HD23	0.55	2.01	1	1
1:A:193:ILE:HD12	1:A:212:ILE:HD11	0.55	1.78	1	1
1:A:197:LEU:O	1:A:199:LEU:HD12	0.54	2.03	9	1
1:A:38:ALA:HB3	1:A:45:ILE:CG1	0.54	2.32	9	1
1:A:239:LEU:HD12	1:A:269:TYR:CE1	0.54	2.38	4	1
1:A:157:LEU:N	1:A:157:LEU:HD12	0.54	2.18	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:198:PRO:HA	1:A:207:THR:HG22	0.53	1.80	7	2
1:A:10:ILE:HG22	1:A:36:PHE:CE1	0.53	2.38	5	1
1:A:128:PHE:CE2	1:A:157:LEU:HD21	0.53	2.39	1	1
1:A:160:THR:HG23	1:A:166:ALA:CB	0.52	2.33	6	1
1:A:128:PHE:CG	1:A:157:LEU:HD21	0.52	2.39	1	1
1:A:204:HIS:CD2	1:A:206:VAL:HG13	0.52	2.39	1	1
1:A:228:GLY:O	1:A:229:LEU:HD12	0.52	2.05	3	1
1:A:132:LEU:HD23	1:A:153:THR:HG23	0.52	1.80	2	1
1:A:88:THR:OG1	1:A:115:ALA:HB3	0.51	2.05	4	1
1:A:122:LEU:CB	1:A:126:LEU:HD22	0.51	2.35	2	1
1:A:196:TYR:HB2	1:A:207:THR:HG22	0.51	1.82	3	1
1:A:38:ALA:HB3	1:A:45:ILE:HG23	0.51	1.82	3	1
1:A:193:ILE:H	1:A:193:ILE:HD13	0.51	1.65	4	1
1:A:123:THR:HG23	1:A:125:ASP:H	0.50	1.65	8	1
1:A:34:VAL:HG23	1:A:49:TYR:HB2	0.50	1.82	10	1
1:A:164:THR:HG22	1:A:200:THR:O	0.50	2.05	3	1
1:A:239:LEU:HD23	1:A:240:SER:H	0.50	1.65	3	1
1:A:132:LEU:HD13	1:A:133:SER:H	0.50	1.67	9	1
1:A:34:VAL:HG11	1:A:36:PHE:CZ	0.50	2.40	2	1
1:A:85:PHE:CZ	1:A:118:TRP:CD1	0.50	3.00	2	1
1:A:125:ASP:OD2	1:A:126:LEU:HD12	0.49	2.07	5	1
1:A:269:TYR:CE1	1:A:271:PHE:CE2	0.49	3.00	2	1
1:A:12:ALA:HB3	1:A:267:VAL:CG2	0.49	2.38	4	2
1:A:164:THR:HG23	1:A:165:VAL:HG12	0.49	1.85	7	1
1:A:107:ALA:HB3	1:A:109:MET:CE	0.48	2.37	8	1
1:A:243:LEU:HD11	1:A:265:VAL:HG13	0.48	1.85	1	1
1:A:128:PHE:CD1	1:A:157:LEU:HD12	0.48	2.44	2	1
1:A:167:LEU:HD21	1:A:197:LEU:HD23	0.48	1.85	10	1
1:A:114:ILE:HG23	1:A:114:ILE:O	0.48	2.08	2	1
1:A:165:VAL:HG13	1:A:199:LEU:CD1	0.48	2.39	10	1
1:A:164:THR:HG23	1:A:165:VAL:HG22	0.47	1.85	2	1
1:A:197:LEU:HD11	1:A:208:PRO:HG2	0.47	1.84	4	1
1:A:12:ALA:HB3	1:A:267:VAL:HG22	0.47	1.84	1	2
1:A:124:ASP:CB	1:A:126:LEU:HD23	0.47	2.39	10	1
1:A:243:LEU:HG	1:A:265:VAL:HG12	0.47	1.87	6	1
1:A:115:ALA:HB2	1:A:133:SER:CA	0.47	2.39	8	1
1:A:228:GLY:CA	1:A:246:ALA:HB2	0.47	2.40	9	1
1:A:159:TYR:CD1	1:A:161:PHE:CE2	0.46	3.03	2	1
1:A:171:TYR:CE2	1:A:193:ILE:HG22	0.46	2.45	6	1
1:A:198:PRO:CA	1:A:207:THR:HG23	0.46	2.40	6	1
1:A:124:ASP:HB2	1:A:126:LEU:HD23	0.46	1.86	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:PHE:CE2	1:A:118:TRP:CZ3	0.46	3.03	7	1
1:A:7:HIS:CB	1:A:39:ALA:HB3	0.46	2.41	2	1
1:A:38:ALA:HB3	1:A:45:ILE:CG2	0.46	2.41	3	1
1:A:201:LEU:HD13	1:A:202:GLY:N	0.46	2.25	4	1
1:A:239:LEU:HD23	1:A:239:LEU:C	0.46	2.31	7	1
1:A:75:TYR:CD1	1:A:75:TYR:N	0.45	2.84	5	1
1:A:135:TYR:CD2	1:A:135:TYR:N	0.45	2.84	8	2
1:A:171:TYR:CD1	1:A:193:ILE:HG22	0.45	2.47	5	1
1:A:85:PHE:CZ	1:A:118:TRP:CH2	0.45	3.05	7	1
1:A:164:THR:O	1:A:164:THR:HG22	0.45	2.11	8	1
1:A:195:ALA:HB3	1:A:210:THR:OG1	0.45	2.11	8	1
1:A:196:TYR:CD2	1:A:196:TYR:N	0.44	2.85	6	1
1:A:123:THR:HG22	1:A:126:LEU:HB2	0.44	1.88	8	1
1:A:193:ILE:HD11	1:A:212:ILE:HD12	0.44	1.89	8	1
1:A:196:TYR:N	1:A:196:TYR:CD1	0.44	2.85	8	1
1:A:47:LEU:HD23	1:A:71:LEU:HG	0.44	1.88	3	1
1:A:10:ILE:HD12	1:A:10:ILE:N	0.44	2.28	4	1
1:A:155:THR:HG23	1:A:171:TYR:HB2	0.43	1.89	6	1
1:A:91:PHE:N	1:A:91:PHE:CD2	0.43	2.85	6	1
1:A:169:VAL:HG23	1:A:195:ALA:HB2	0.43	1.88	3	1
1:A:47:LEU:HB3	1:A:71:LEU:HD23	0.43	1.90	1	1
1:A:193:ILE:HD11	1:A:212:ILE:CD1	0.43	2.44	2	1
1:A:122:LEU:O	1:A:123:THR:HG23	0.43	2.14	4	1
1:A:126:LEU:HD23	1:A:157:LEU:HD11	0.43	1.87	3	1
1:A:131:TRP:N	1:A:131:TRP:CD1	0.43	2.85	5	1
1:A:164:THR:O	1:A:165:VAL:HG13	0.43	2.14	8	1
1:A:206:VAL:HG23	1:A:206:VAL:O	0.43	2.14	1	1
1:A:206:VAL:CG1	1:A:229:LEU:HD12	0.43	2.44	2	1
1:A:199:LEU:HD23	1:A:200:THR:N	0.42	2.29	7	1
1:A:91:PHE:CD1	1:A:92:ARG:N	0.42	2.87	9	1
1:A:165:VAL:HG22	1:A:199:LEU:CD2	0.42	2.44	10	1
1:A:66:PHE:CD1	1:A:66:PHE:N	0.42	2.87	3	1
1:A:169:VAL:HG12	1:A:170:ASN:N	0.42	2.29	1	1
1:A:156:GLY:C	1:A:157:LEU:HD12	0.42	2.35	9	1
1:A:165:VAL:HG13	1:A:199:LEU:HD11	0.42	1.90	10	1
1:A:34:VAL:HG12	1:A:35:TYR:N	0.42	2.30	1	2
1:A:198:PRO:O	1:A:199:LEU:HD23	0.42	2.14	4	1
1:A:151:VAL:HG22	1:A:152:GLU:N	0.42	2.30	5	1
1:A:114:ILE:HG22	1:A:116:PRO:HD3	0.42	1.90	6	1
1:A:83:PHE:HE2	1:A:120:VAL:HG13	0.42	1.70	2	1
1:A:128:PHE:CD1	1:A:157:LEU:HD21	0.41	2.50	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:LEU:C	1:A:207:THR:HG23	0.41	2.35	10	2
1:A:132:LEU:HD13	1:A:133:SER:N	0.41	2.29	9	1
1:A:127:ARG:O	1:A:157:LEU:HD23	0.41	2.15	1	1
1:A:193:ILE:N	1:A:193:ILE:CD1	0.41	2.83	4	1
1:A:48:ALA:HB3	1:A:70:GLU:HB2	0.41	1.92	4	1
1:A:193:ILE:HD13	1:A:212:ILE:O	0.41	2.16	3	1
1:A:85:PHE:CE2	1:A:118:TRP:CD1	0.41	3.09	2	1
1:A:197:LEU:N	1:A:197:LEU:CD1	0.41	2.84	10	1
1:A:199:LEU:HD22	1:A:201:LEU:HD11	0.41	1.93	2	1
1:A:10:ILE:HD12	1:A:36:PHE:CZ	0.41	2.51	8	1
1:A:120:VAL:HG23	1:A:128:PHE:HB3	0.40	1.93	5	1
1:A:269:TYR:CD2	1:A:269:TYR:N	0.40	2.89	9	1
1:A:85:PHE:CD2	1:A:117:ASP:O	0.40	2.74	9	1
1:A:10:ILE:HG23	1:A:36:PHE:CE2	0.40	2.51	3	1
1:A:228:GLY:HA2	1:A:246:ALA:HB2	0.40	1.92	9	1
1:A:91:PHE:CD1	1:A:111:ARG:O	0.40	2.75	5	1
1:A:73:VAL:HG12	1:A:75:TYR:CD1	0.40	2.51	5	1
1:A:154:GLU:OE1	1:A:172:TYR:CD1	0.40	2.75	8	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	176/271 (65%)	163±2 (93±1%)	10±3 (6±1%)	3±2 (2±1%)	13	57
All	All	1760/2710 (65%)	1631 (93%)	101 (6%)	28 (2%)	13	57

All 14 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	236	GLN	6
1	A	78	LEU	4
1	A	237	ASN	4
1	A	5	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	32	PRO	1
1	A	6	TRP	1
1	A	246	ALA	1
1	A	82	ASP	1
1	A	79	GLU	1
1	A	125	ASP	1
1	A	80	ASN	1
1	A	238	GLY	1
1	A	137	PHE	1
1	A	203	ASN	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	150/228 (66%)	112±7 (75±5%)	38±7 (25±5%)	2 24
All	All	1500/2280 (66%)	1123 (75%)	377 (25%)	2 24

All 128 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	123	THR	9
1	A	229	LEU	9
1	A	197	LEU	7
1	A	67	ASP	7
1	A	68	ARG	6
1	A	33	SER	6
1	A	271	PHE	6
1	A	236	GLN	6
1	A	8	PHE	6
1	A	29	LEU	6
1	A	121	LYS	5
1	A	7	HIS	5
1	A	199	LEU	5
1	A	171	TYR	5
1	A	205	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	A	201	LEU	5
1	A	188	PHE	5
1	A	167	LEU	5
1	A	47	LEU	5
1	A	51	GLN	5
1	A	194	ARG	5
1	A	161	PHE	5
1	A	119	ASP	5
1	A	209	TYR	5
1	A	168	ARG	4
1	A	175	ARG	4
1	A	160	THR	4
1	A	157	LEU	4
1	A	110	GLN	4
1	A	231	TYR	4
1	A	84	SER	4
1	A	173	LEU	4
1	A	154	GLU	4
1	A	126	LEU	4
1	A	133	SER	4
1	A	13	MET	4
1	A	124	ASP	4
1	A	230	PHE	4
1	A	243	LEU	4
1	A	112	TRP	4
1	A	240	SER	4
1	A	237	ASN	4
1	A	70	GLU	4
1	A	211	ARG	4
1	A	37	ASN	3
1	A	136	LYS	3
1	A	31	GLU	3
1	A	172	TYR	3
1	A	93	ASN	3
1	A	131	TRP	3
1	A	71	LEU	3
1	A	245	TYR	3
1	A	80	ASN	3
1	A	137	PHE	3
1	A	118	TRP	3
1	A	190	THR	3
1	A	9	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	242	SER	3
1	A	78	LEU	3
1	A	74	HIS	3
1	A	149	THR	3
1	A	233	TYR	3
1	A	82	ASP	3
1	A	87	LEU	3
1	A	6	TRP	3
1	A	235	PHE	3
1	A	15	GLU	3
1	A	94	TYR	2
1	A	109	MET	2
1	A	85	PHE	2
1	A	155	THR	2
1	A	88	THR	2
1	A	170	ASN	2
1	A	50	TYR	2
1	A	189	SER	2
1	A	92	ARG	2
1	A	35	TYR	2
1	A	132	LEU	2
1	A	111	ARG	2
1	A	204	HIS	2
1	A	81	ASP	2
1	A	239	LEU	2
1	A	49	TYR	2
1	A	113	LYS	2
1	A	150	ARG	2
1	A	128	PHE	2
1	A	164	THR	2
1	A	174	GLU	2
1	A	270	SER	2
1	A	163	GLU	2
1	A	72	GLU	2
1	A	135	TYR	2
1	A	5	ASP	2
1	A	200	THR	2
1	A	207	THR	2
1	A	77	PHE	2
1	A	45	ILE	1
1	A	244	GLU	1
1	A	203	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	40	ASN	1
1	A	91	PHE	1
1	A	134	MET	1
1	A	152	GLU	1
1	A	117	ASP	1
1	A	192	GLU	1
1	A	76	GLN	1
1	A	44	ARG	1
1	A	79	GLU	1
1	A	125	ASP	1
1	A	66	PHE	1
1	A	127	ARG	1
1	A	212	ILE	1
1	A	269	TYR	1
1	A	122	LEU	1
1	A	159	TYR	1
1	A	162	ASN	1
1	A	75	TYR	1
1	A	129	ASN	1
1	A	36	PHE	1
1	A	158	GLN	1
1	A	177	PHE	1
1	A	14	TYR	1
1	A	210	THR	1
1	A	153	THR	1
1	A	234	ASP	1
1	A	193	ILE	1
1	A	196	TYR	1
1	A	43	TRP	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 38% for the well-defined parts and 36% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *chemshift7.NMRSTAR*

7.1.1 Bookkeeping

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	1199
Number of shifts mapped to atoms	1199
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	253	0.49 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	219	-0.21 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	253	0.76 ± 0.08	Should be applied
^{15}N	233	-0.62 ± 0.26	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 38%, i.e. 843 atoms were assigned a chemical shift out of a possible 2241. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	680/873 (78%)	166/348 (48%)	348/354 (98%)	166/171 (97%)
Sidechain	157/1021 (15%)	0/599 (0%)	157/371 (42%)	0/51 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	6/347 (2%)	3/181 (2%)	0/155 (0%)	3/11 (27%)
Overall	843/2241 (38%)	169/1128 (15%)	505/880 (57%)	169/233 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 1199 atoms were assigned a chemical shift out of a possible 3352. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	972/1339 (73%)	233/534 (44%)	506/542 (93%)	233/263 (89%)
Sidechain	219/1523 (14%)	0/892 (0%)	219/552 (40%)	0/79 (0%)
Aromatic	8/490 (2%)	4/254 (2%)	0/214 (0%)	4/22 (18%)
Overall	1199/3352 (36%)	237/1680 (14%)	725/1308 (55%)	237/364 (65%)

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 A: