Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 06:00 PM EST

PDB ID	:	2E60
Title	:	Solution structure of the surp1 domain in splicing factor, arginine/serine-rich 8
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Deposited on	:	2006-12-25

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:

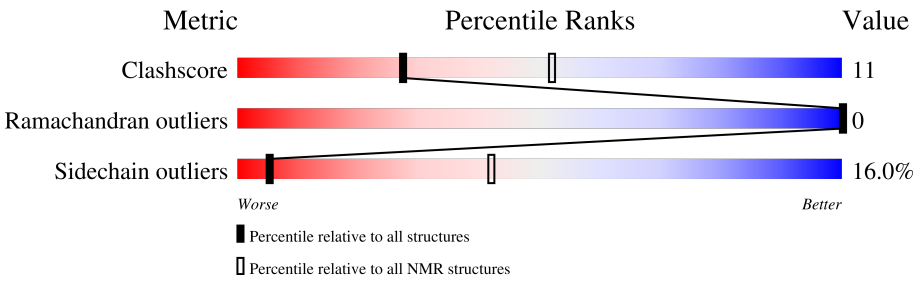
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	101	46% 19% • 35%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:19-A:84 (66)	0.13	11

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 and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1582 atoms, of which 793 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Splicing factor, arginine/serine-rich 8.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1582	500	793	138	147	4	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q8IV81
A	2	SER	-	cloning artifact	UNP Q8IV81
A	3	SER	-	cloning artifact	UNP Q8IV81
A	4	GLY	-	cloning artifact	UNP Q8IV81
A	5	SER	-	cloning artifact	UNP Q8IV81
A	6	SER	-	cloning artifact	UNP Q8IV81
A	7	GLY	-	cloning artifact	UNP Q8IV81

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: Splicing factor, arginine/serine-rich 8

Chain A: 46% 19% • 35%

G1 S2 S3 G4 S5 S6 G7 V8 A9 P10 L11 G12 L13 S14 V15 P16 S17 D18 P23 M27 I31 T34 A35 S36 F37 V38 Q44 F45 E46 L49 K50 N56 L62 Y67 L68 N69 P70 Y71 Y72 K73 F74 I75 Q76 T85 V86 L87 A88 E89 N90 K91

S92 D93 E94 K95 K96 K97 S98 G99 V100 S101

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: Splicing factor, arginine/serine-rich 8

Chain A: 42% 23% • 35%

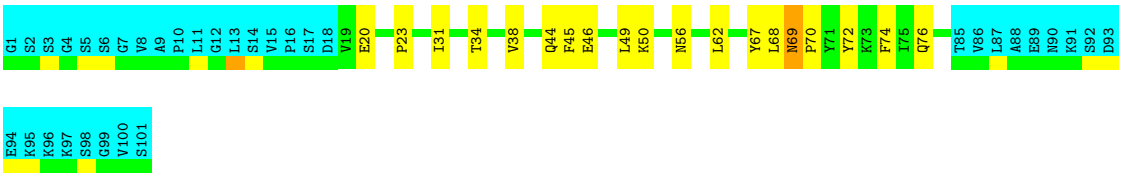
G1 S2 S3 G4 S5 S6 G7 V8 A9 P10 L11 G12 L13 S14 V15 P16 S17 D18 P23 K26 I31 E32 R33 T34 A35 S36 F37 V38 C39 R40 Q44 F45 E46 L49 K50 R55 N56 S57 L62 R63 Y67 L68 N69 P70 Y71 Y72 K73 F74 I75 Q76 T85

V86 L87 A88 E89 N90 K91 S92 D93 E94 K95 K96 K97 S98 G99 V100 S101

4.2.2 Score per residue for model 2

• Molecule 1: Splicing factor, arginine/serine-rich 8

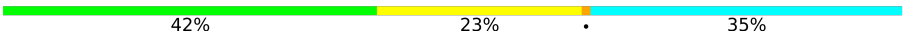
Chain A: 47% 18% • 35%



4.2.3 Score per residue for model 3

- Molecule 1: Splicing factor, arginine/serine-rich 8

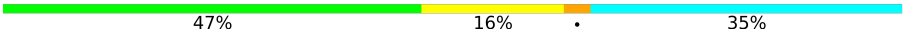
Chain A:

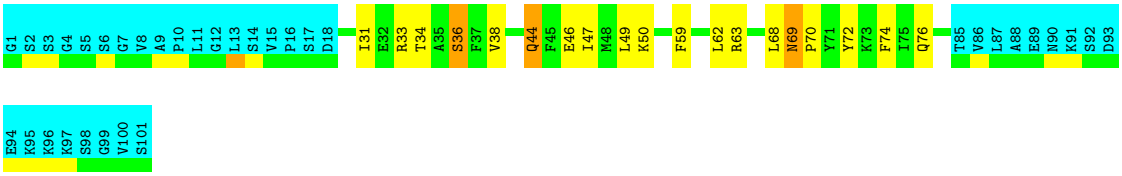


4.2.4 Score per residue for model 4

- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A:

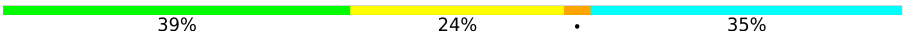


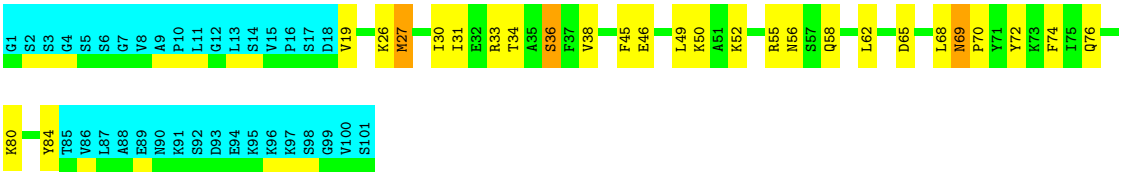


4.2.5 Score per residue for model 5

- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A:





4.2.6 Score per residue for model 6

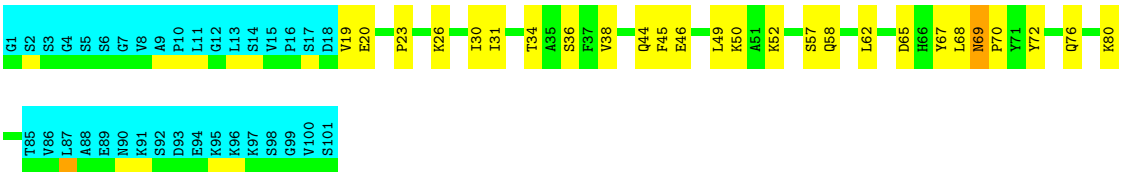
- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A: 45% 19% • 35%

4.2.7 Score per residue for model 7

- Molecule 1: Splicing factor, arginine/serine-rich 8

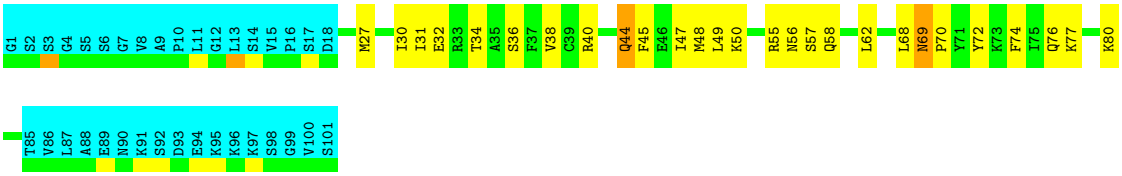
Chain A: 40% 25% • 35%



4.2.8 Score per residue for model 8

- Molecule 1: Splicing factor, arginine/serine-rich 8

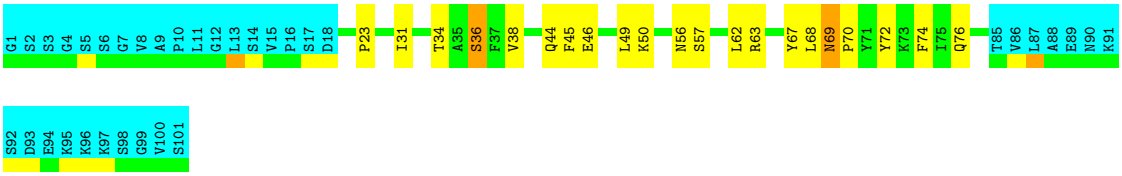
Chain A: 39% 25% • 35%



4.2.9 Score per residue for model 9

- Molecule 1: Splicing factor, arginine/serine-rich 8

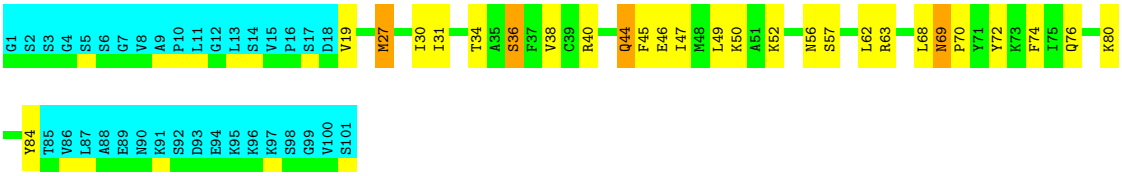
Chain A: 45% 19% • 35%



4.2.10 Score per residue for model 10

- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A: 39% 23% • 35%



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A: 46% 19% • 35%

4.2.12 Score per residue for model 12

- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A: 40% 25% • 35%

4.2.13 Score per residue for model 13

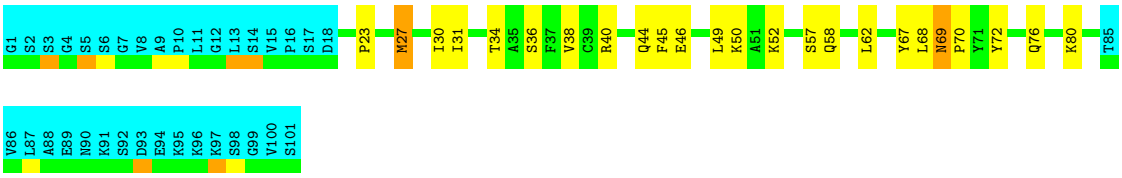
- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A: 44% 21% • 35%

4.2.14 Score per residue for model 14

• Molecule 1: Splicing factor, arginine/serine-rich 8

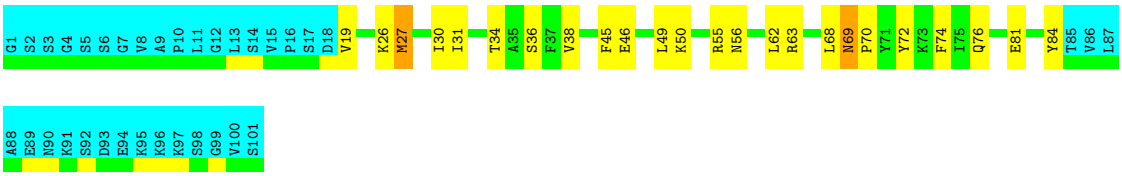
Chain A: 42% 22% • 35%



4.2.15 Score per residue for model 15

• Molecule 1: Splicing factor, arginine/serine-rich 8

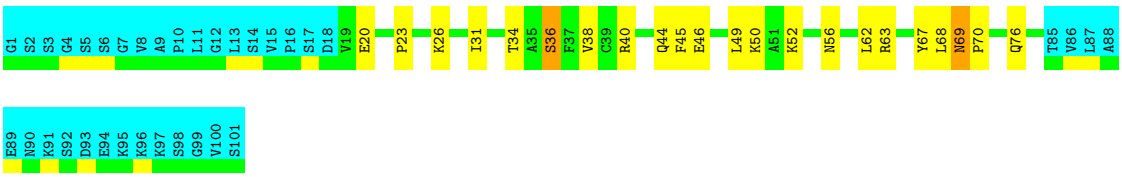
Chain A: 42% 22% • 35%



4.2.16 Score per residue for model 16

• Molecule 1: Splicing factor, arginine/serine-rich 8

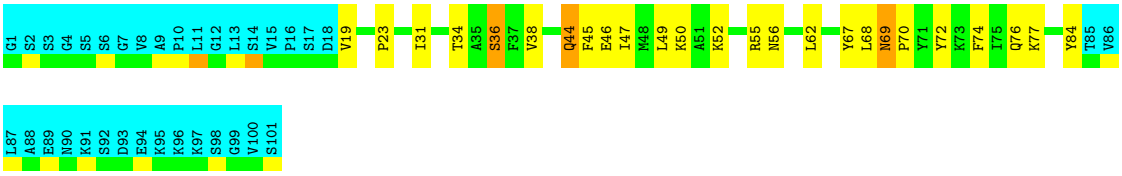
Chain A: 44% 20% • 35%



4.2.17 Score per residue for model 17

• Molecule 1: Splicing factor, arginine/serine-rich 8

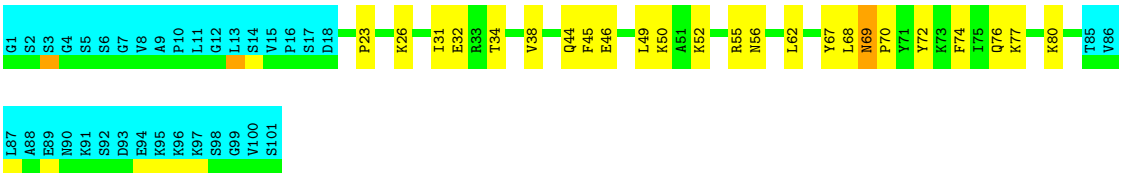
Chain A: 41% 22% • 35%



4.2.18 Score per residue for model 18

- Molecule 1: Splicing factor, arginine/serine-rich 8

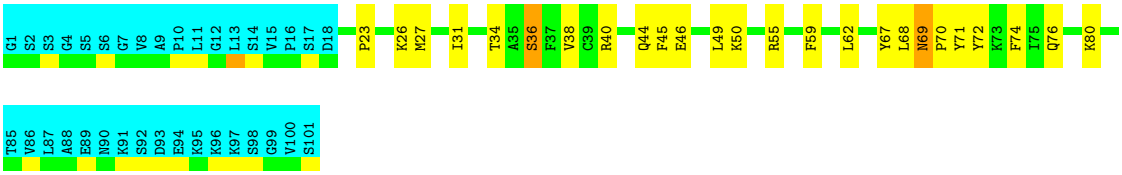
Chain A: 42% 23% • 35%



4.2.19 Score per residue for model 19

- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A: 41% 23% • 35%



4.2.20 Score per residue for model 20

- Molecule 1: Splicing factor, arginine/serine-rich 8

Chain A: 41% 24% • 35%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations,structures with the lowest energy,target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	554	555	555	12±2
All	All	11080	11100	11100	240

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:HD11	1:A:68:LEU:HD13	0.81	1.50	7	20
1:A:45:PHE:CD2	1:A:49:LEU:HD11	0.67	2.24	14	17
1:A:23:PRO:HD3	1:A:67:TYR:OH	0.66	1.90	16	12
1:A:38:VAL:HG21	1:A:72:TYR:OH	0.62	1.94	20	19
1:A:50:LYS:HG2	1:A:62:LEU:HD13	0.61	1.70	14	18
1:A:50:LYS:CG	1:A:62:LEU:HD13	0.60	2.25	7	20
1:A:30:ILE:HD13	1:A:58:GLN:HB3	0.60	1.73	8	4
1:A:34:THR:O	1:A:38:VAL:HG23	0.60	1.96	20	20
1:A:27:MET:HA	1:A:30:ILE:HD12	0.60	1.73	20	6
1:A:50:LYS:HG3	1:A:62:LEU:HD13	0.59	1.75	16	5
1:A:50:LYS:HD2	1:A:62:LEU:HD22	0.58	1.76	8	5
1:A:69:ASN:N	1:A:70:PRO:HD2	0.55	2.17	9	20
1:A:44:GLN:HA	1:A:47:ILE:HD12	0.53	1.79	8	5
1:A:19:VAL:HG22	1:A:70:PRO:HB2	0.53	1.80	10	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:HD11	1:A:68:LEU:CD1	0.51	2.34	19	10
1:A:46:GLU:HA	1:A:49:LEU:HD12	0.50	1.83	4	18
1:A:59:PHE:O	1:A:62:LEU:HD12	0.49	2.07	19	1
1:A:31:ILE:CD1	1:A:68:LEU:HD13	0.49	2.32	7	10
1:A:59:PHE:HB3	1:A:62:LEU:HD12	0.46	1.88	11	2
1:A:69:ASN:N	1:A:70:PRO:CD	0.44	2.80	9	20
1:A:45:PHE:CE2	1:A:49:LEU:HD11	0.41	2.51	20	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	66/101 (65%)	61±1 (92±1%)	5±1 (8±1%)	0±0 (0±0%)	100	100
All	All	1320/2020 (65%)	1218 (92%)	102 (8%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	57/85 (67%)	48±2 (84±4%)	9±2 (16±4%)	5	42
All	All	1140/1700 (67%)	958 (84%)	182 (16%)	5	42

All 22 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	69	ASN	20

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Mol	Chain	Res	Type	Models (Total)
1	A	76	GLN	20
1	A	36	SER	18
1	A	44	GLN	17
1	A	56	ASN	16
1	A	55	ARG	10
1	A	27	MET	10
1	A	63	ARG	9
1	A	80	LYS	9
1	A	26	LYS	8
1	A	57	SER	8
1	A	52	LYS	8
1	A	40	ARG	6
1	A	20	GLU	5
1	A	32	GLU	4
1	A	77	LYS	4
1	A	83	ARG	2
1	A	33	ARG	2
1	A	58	GLN	2
1	A	65	ASP	2
1	A	48	MET	1
1	A	81	GLU	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