



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2022 – 05:56 PM EST

PDB ID : 2GO9
Title : RRM domains 1 and 2 of Prp24 from *S. cerevisiae*
Authors : Reiter, N.J.; Lee, D.H.; Tonelli, M.; Kwan, S.K.; Brow, D.A.; Butcher, S.E.
Deposited on : 2006-04-12

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 : 2.27
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

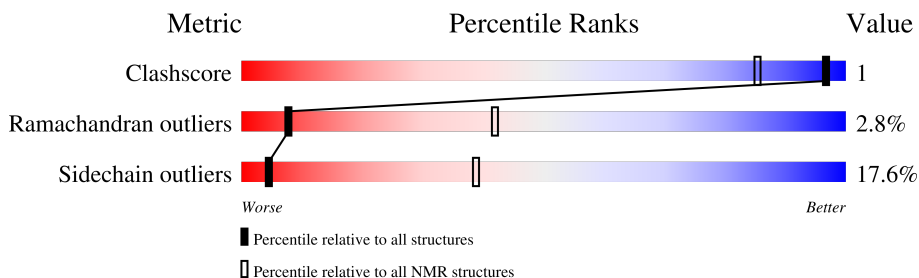
1 Overall quality at a glance

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	161	

2 Ensemble composition and analysis

This entry contains 10 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:3-A:158 (156)	1.18	9

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2656 atoms, of which 1346 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U4/U6 snRNA-associated splicing factor PRP24.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	161	2656	839	1346	231	235	5	0

There is a discrepancy between the modelled and reference sequences:

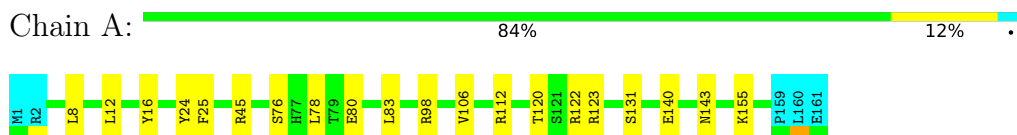
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P49960

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: U4/U6 snRNA-associated splicing factor PRP24

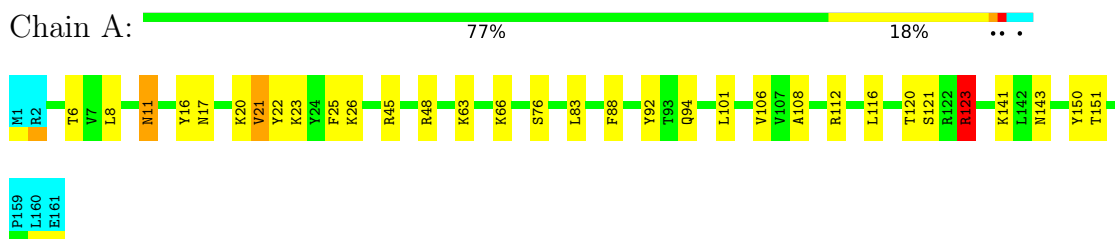


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

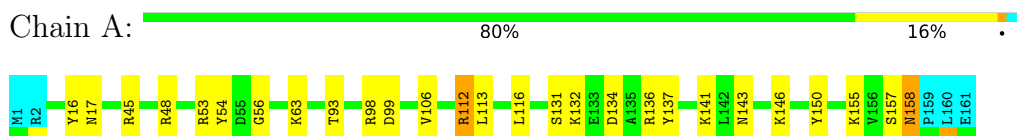
4.2.1 Score per residue for model 1

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



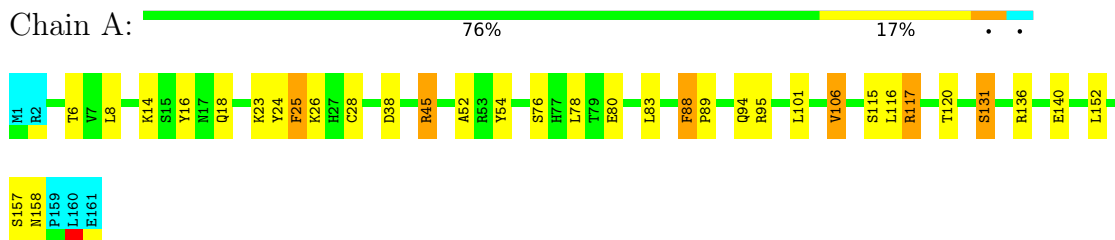
4.2.2 Score per residue for model 2

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



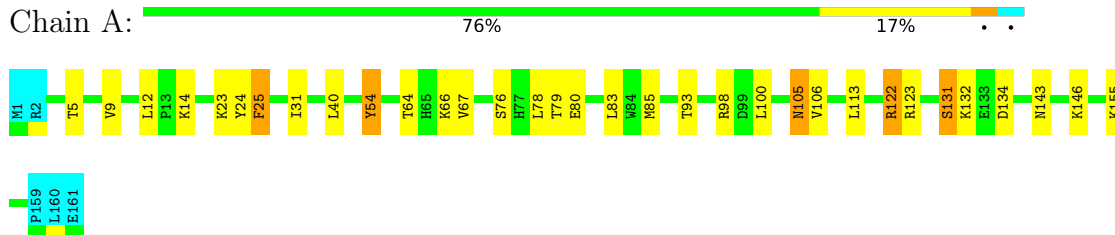
4.2.3 Score per residue for model 3

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



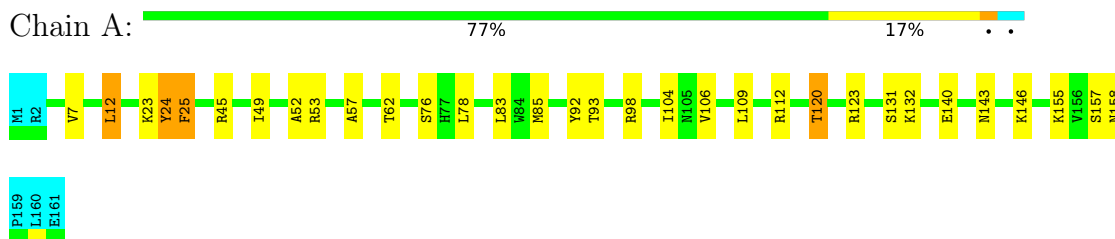
4.2.4 Score per residue for model 4

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



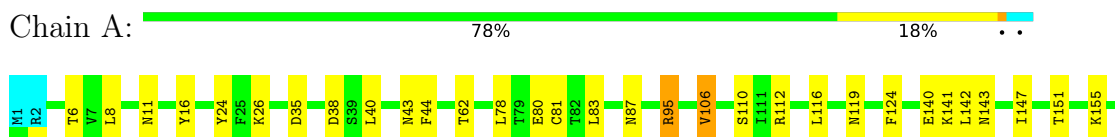
4.2.5 Score per residue for model 5

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



4.2.6 Score per residue for model 6

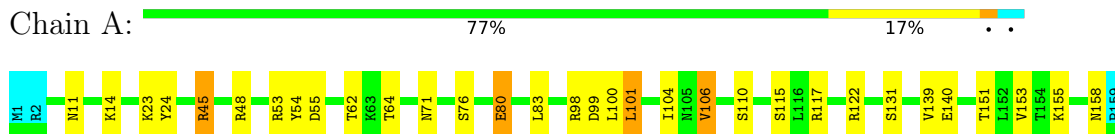
- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24





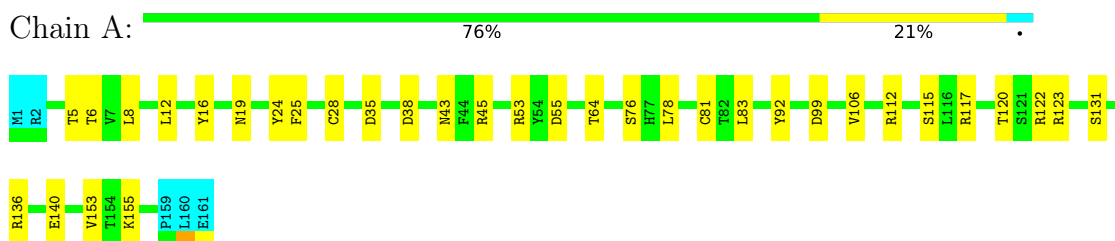
4.2.7 Score per residue for model 7

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



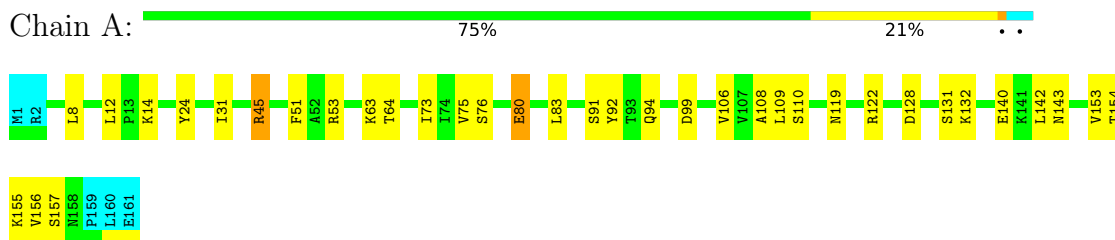
4.2.8 Score per residue for model 8

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



4.2.9 Score per residue for model 9 (medoid)

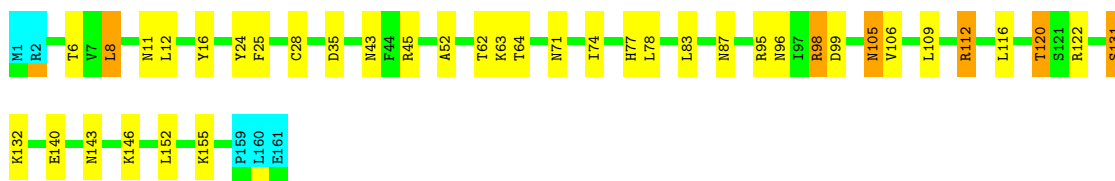
- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24



4.2.10 Score per residue for model 10

- Molecule 1: U4/U6 snRNA-associated splicing factor PRP24





5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	2.1.4
CYANA	structure solution	2.1.4

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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	A	0.63±0.01	0±0/1293 (0.0± 0.0%)	1.04±0.02	1±1/1753 (0.1± 0.1%)
All	All	0.63	0/12930 (0.0%)	1.04	9/17530 (0.1%)

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	A	0.0±0.0	3.0±1.0
All	All	0	30

There are no bond-length outliers.

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	A	45	ARG	NE-CZ-NH2	-6.44	117.08	120.30	7	2
1	A	21	VAL	CA-CB-CG2	6.20	120.20	110.90	1	1
1	A	95	ARG	NE-CZ-NH1	5.60	123.10	120.30	10	1
1	A	123	ARG	NE-CZ-NH2	-5.39	117.60	120.30	1	1
1	A	112	ARG	NE-CZ-NH2	-5.33	117.64	120.30	10	1
1	A	64	THR	CA-CB-CG2	5.23	119.72	112.40	4	1
1	A	98	ARG	NE-CZ-NH2	-5.07	117.77	120.30	7	1
1	A	95	ARG	CD-NE-CZ	5.06	130.69	123.60	3	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	A	45	ARG	Sidechain	4
1	A	54	TYR	Sidechain	4
1	A	136	ARG	Sidechain	3
1	A	112	ARG	Sidechain	2
1	A	24	TYR	Sidechain	2
1	A	98	ARG	Sidechain	2
1	A	16	TYR	Sidechain	2
1	A	53	ARG	Sidechain	2
1	A	22	TYR	Sidechain	1
1	A	92	TYR	Sidechain	1
1	A	123	ARG	Sidechain	1
1	A	137	TYR	Sidechain	1
1	A	117	ARG	Sidechain	1
1	A	122	ARG	Sidechain	1
1	A	95	ARG	Sidechain	1
1	A	108	ALA	Peptide	1
1	A	154	THR	Peptide	1

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	1267	1300	1300	2±1
All	All	12670	13000	13000	18

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:PHE:CG	1:A:89:PRO:HD2	0.53	2.38	3	1
1:A:16:TYR:CD2	1:A:21:VAL:HG12	0.51	2.40	1	1
1:A:101:LEU:HD13	1:A:108:ALA:HB2	0.50	1.84	1	1
1:A:64:THR:HG21	1:A:74:ILE:HA	0.49	1.83	10	1
1:A:88:PHE:CG	1:A:152:LEU:HD21	0.49	2.43	3	1
1:A:31:ILE:HD11	1:A:51:PHE:CE2	0.48	2.44	9	1
1:A:64:THR:HB	1:A:75:VAL:HG22	0.48	1.86	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ARG:HG3	1:A:56:GLY:H	0.47	1.69	2	1
1:A:8:LEU:HD21	1:A:109:LEU:HD21	0.44	1.89	10	1
1:A:101:LEU:HD22	1:A:101:LEU:C	0.43	2.34	7	1
1:A:25:PHE:CE2	1:A:49:ILE:HD13	0.42	2.49	5	1
1:A:9:VAL:HG11	1:A:12:LEU:HD21	0.42	1.91	4	1
1:A:147:ILE:HD12	1:A:147:ILE:N	0.42	2.29	6	1
1:A:106:VAL:HG13	1:A:131:SER:HB2	0.42	1.91	10	1
1:A:7:VAL:CG1	1:A:57:ALA:HB1	0.42	2.45	5	1
1:A:25:PHE:CD1	1:A:26:LYS:N	0.41	2.88	3	1
1:A:25:PHE:CD2	1:A:31:ILE:HD13	0.41	2.50	4	1
1:A:101:LEU:HA	1:A:104:ILE:HG22	0.41	1.93	7	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	156/161 (97%)	135±3 (87±2%)	17±4 (11±3%)	4±2 (3±1%)	8	42
All	All	1560/1610 (97%)	1351 (87%)	166 (11%)	43 (3%)	8	42

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	106	VAL	8
1	A	131	SER	7
1	A	11	ASN	4
1	A	12	LEU	4
1	A	52	ALA	3
1	A	120	THR	3
1	A	80	GLU	3
1	A	122	ARG	3
1	A	105	ASN	2
1	A	81	CYS	2
1	A	116	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	67	VAL	1
1	A	117	ARG	1
1	A	63	LYS	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	142/147 (97%)	117±2 (82±2%)	25±2 (18±2%)	4	39
All	All	1420/1470 (97%)	1170 (82%)	250 (18%)	4	39

All 85 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	83	LEU	9
1	A	155	LYS	8
1	A	76	SER	7
1	A	143	ASN	7
1	A	24	TYR	7
1	A	140	GLU	7
1	A	8	LEU	6
1	A	25	PHE	6
1	A	78	LEU	6
1	A	6	THR	5
1	A	23	LYS	5
1	A	45	ARG	5
1	A	112	ARG	5
1	A	99	ASP	5
1	A	132	LYS	5
1	A	116	LEU	4
1	A	120	THR	4
1	A	123	ARG	4
1	A	146	LYS	4
1	A	157	SER	4
1	A	158	ASN	4
1	A	14	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	80	GLU	4
1	A	106	VAL	4
1	A	62	THR	4
1	A	48	ARG	3
1	A	63	LYS	3
1	A	94	GLN	3
1	A	141	LYS	3
1	A	151	THR	3
1	A	16	TYR	3
1	A	93	THR	3
1	A	98	ARG	3
1	A	28	CYS	3
1	A	38	ASP	3
1	A	115	SER	3
1	A	131	SER	3
1	A	92	TYR	3
1	A	35	ASP	3
1	A	43	ASN	3
1	A	110	SER	3
1	A	153	VAL	3
1	A	17	ASN	2
1	A	26	LYS	2
1	A	66	LYS	2
1	A	88	PHE	2
1	A	150	TYR	2
1	A	113	LEU	2
1	A	134	ASP	2
1	A	101	LEU	2
1	A	117	ARG	2
1	A	5	THR	2
1	A	40	LEU	2
1	A	85	MET	2
1	A	100	LEU	2
1	A	105	ASN	2
1	A	122	ARG	2
1	A	53	ARG	2
1	A	109	LEU	2
1	A	87	ASN	2
1	A	119	ASN	2
1	A	142	LEU	2
1	A	55	ASP	2
1	A	64	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	71	ASN	2
1	A	11	ASN	1
1	A	20	LYS	1
1	A	121	SER	1
1	A	18	GLN	1
1	A	54	TYR	1
1	A	79	THR	1
1	A	12	LEU	1
1	A	104	ILE	1
1	A	44	PHE	1
1	A	95	ARG	1
1	A	124	PHE	1
1	A	139	VAL	1
1	A	19	ASN	1
1	A	73	ILE	1
1	A	91	SER	1
1	A	128	ASP	1
1	A	156	VAL	1
1	A	77	HIS	1
1	A	96	ASN	1
1	A	152	LEU	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

No chemical shift data were provided