WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Feb 23, 2022 – 01:05 PM EST

PDB ID	:	1YHP
Title	:	Solution Structure of Ca2+-free DdCAD-1
Authors	:	Lin, Z.; Huang, H.B.; Siu, C.H.; Yang, D.W.
Deposited on	:	2005-01-10

The following versions of software and data (see references ⓘ) were used in the production of this report:

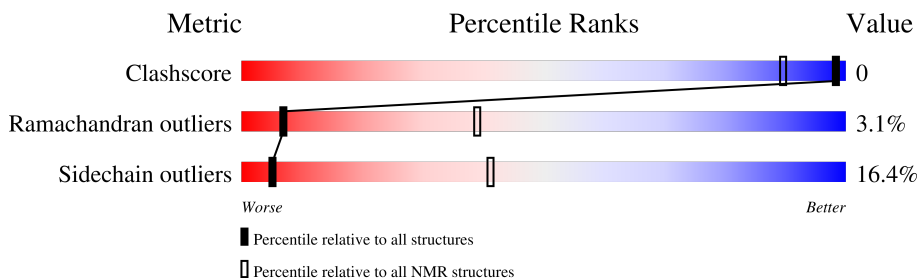|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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	Percentile Ranks	Value
Clashscore		0
Ramachandran outliers		3.1%
Sidechain outliers		16.4%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	212	92% 8%

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 6 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:2-A:213 (212)	0.64	6

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, 6, 7, 8
2	5, 10
Single-model clusters	9

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3036 atoms, of which 1360 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-dependent cell adhesion molecule-1.

Mol	Chain	Residues	Atoms						Trace
1	A	212	Total	C	H	N	O	S	0
			3036	1061	1360	276	332	7	

4 Residue-property plots ⓘ

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: Calcium-dependent cell adhesion molecule-1
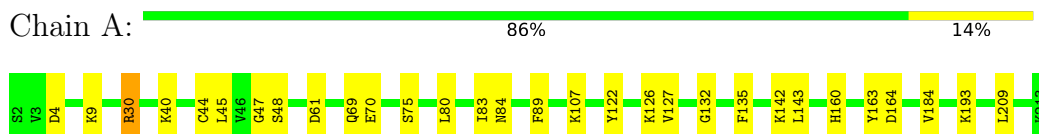
Chain A:
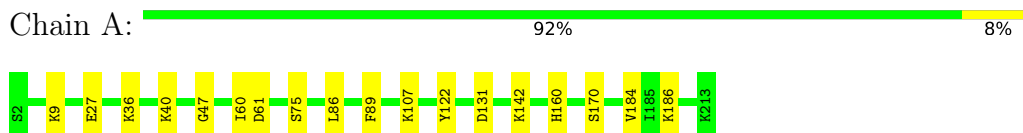
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calcium-dependent cell adhesion molecule-1

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Calcium-dependent cell adhesion molecule-1

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Calcium-dependent cell adhesion molecule-1
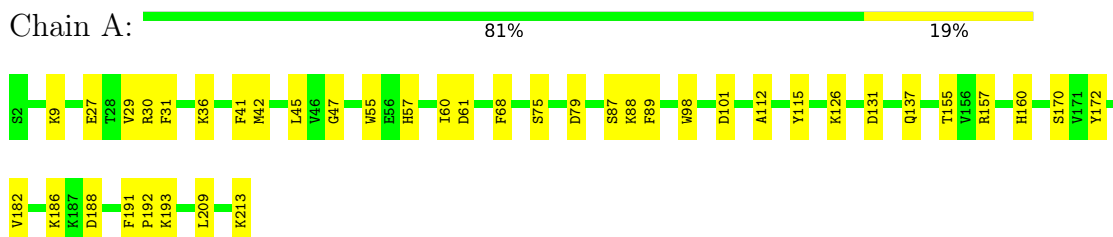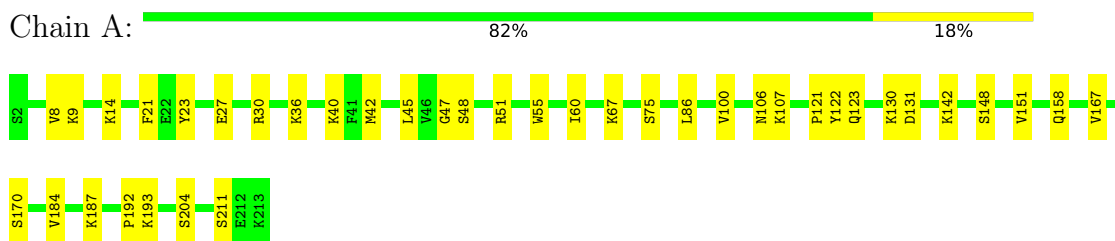

4.2.4 Score per residue for model 4

• Molecule 1: Calcium-dependent cell adhesion molecule-1

4.2.5 Score per residue for model 5

• Molecule 1: Calcium-dependent cell adhesion molecule-1

4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Calcium-dependent cell adhesion molecule-1
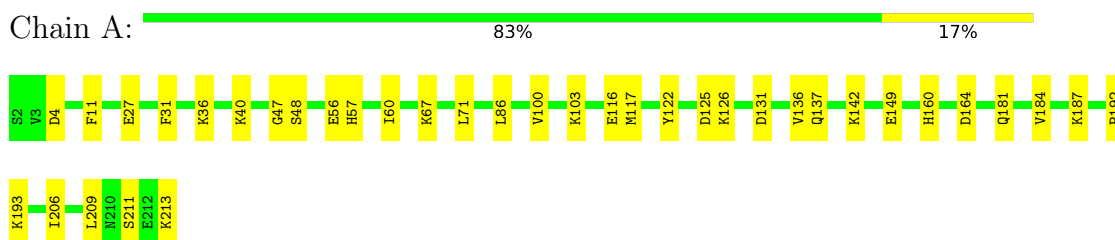
4.2.7 Score per residue for model 7

• Molecule 1: Calcium-dependent cell adhesion molecule-1
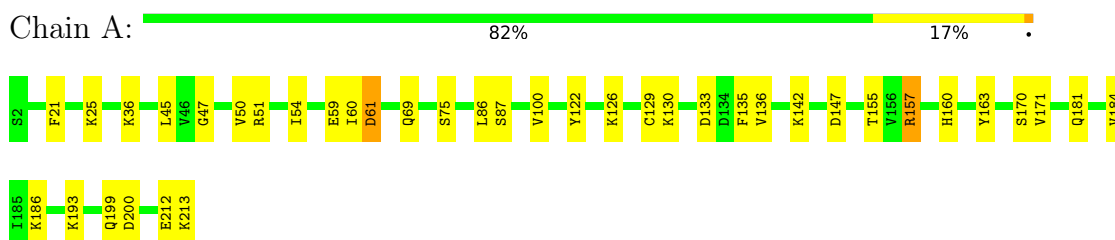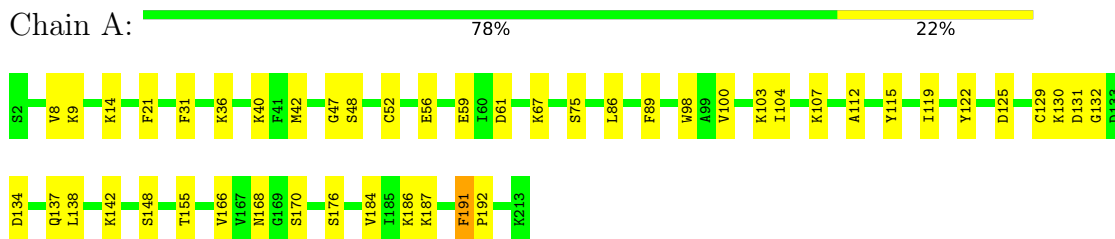
Chain A:
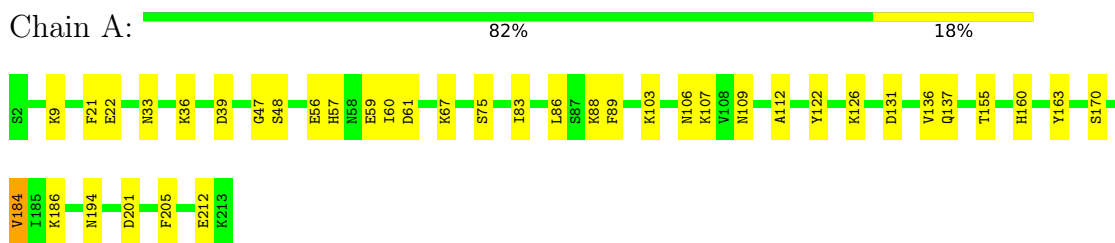
4.2.8 Score per residue for model 8

• Molecule 1: Calcium-dependent cell adhesion molecule-1

Chain A:
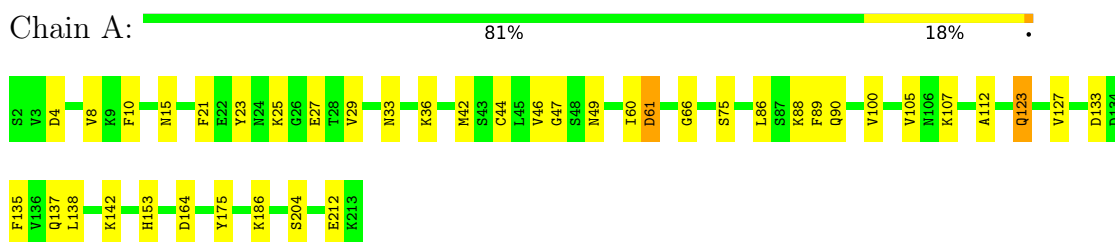
4.2.9 Score per residue for model 9

• Molecule 1: Calcium-dependent cell adhesion molecule-1

Chain A:
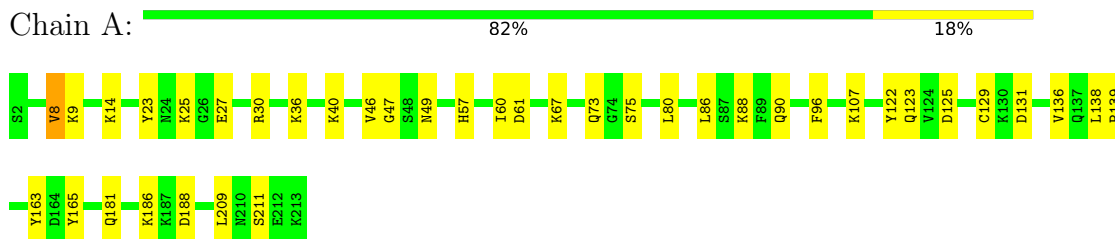
4.2.10 Score per residue for model 10

• Molecule 1: Calcium-dependent cell adhesion molecule-1

Chain A:
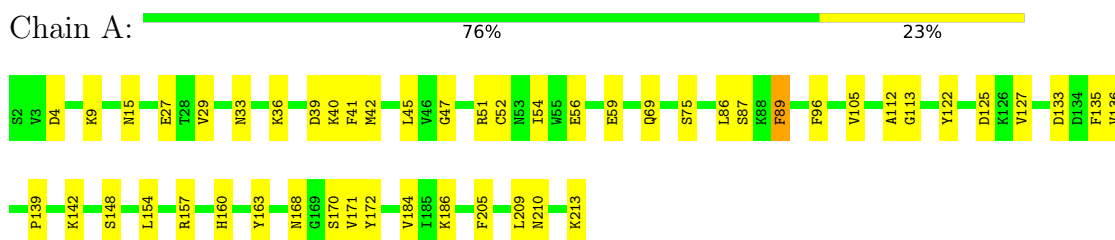
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 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	1.0.5
CYANA	refinement	1.0.5

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	0.71±0.01	0±0/1716 (0.0± 0.0%)	0.98±0.03	1±1/2332 (0.0± 0.0%)
All	All	0.71	0/17160 (0.0%)	0.98	9/23320 (0.0%)

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	0.2±0.4
All	All	0	2

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	115	TYR	CB-CG-CD2	-7.72	116.36	121.00	2	1
1	A	30	ARG	NE-CZ-NH1	7.28	123.94	120.30	9	4
1	A	172	TYR	CB-CG-CD2	-5.53	117.68	121.00	10	1
1	A	157	ARG	NE-CZ-NH1	5.34	122.97	120.30	4	2
1	A	51	ARG	NE-CZ-NH1	5.01	122.81	120.30	3	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	23	TYR	Sidechain	2

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	1676	1360	1613	1±1
All	All	16760	13600	16130	8

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:129:CYS:HA	1:A:136:VAL:HG21	0.53	1.81	4	1
1:A:8:VAL:HG12	1:A:46:VAL:HA	0.47	1.86	9	1
1:A:96:PHE:CD2	1:A:139:PRO:HB2	0.45	2.46	9	1
1:A:184:VAL:HG13	1:A:205:PHE:CE2	0.44	2.47	7	1
1:A:8:VAL:HG23	1:A:23:TYR:CD2	0.44	2.47	8	1
1:A:96:PHE:CD2	1:A:139:PRO:CB	0.41	3.03	10	1
1:A:54:ILE:HD12	1:A:89:PHE:CE2	0.41	2.50	10	1
1:A:191:PHE:CG	1:A:192:PRO:HD2	0.40	2.51	5	1

6.3   Torsion angles ⓘ

6.3.1   Protein backbone ⓘ

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	210/212 (99%)	180±2 (86±1%)	23±2 (11±1%)	7±1 (3±0%)	7	39
All	All	2100/2120 (99%)	1800 (86%)	234 (11%)	66 (3%)	7	39

All 25 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	47	GLY	10
1	A	122	TYR	7
1	A	48	SER	5
1	A	61	ASP	5
1	A	112	ALA	5
1	A	135	PHE	4
1	A	192	PRO	3
1	A	193	LYS	3
1	A	123	GLN	3
1	A	125	ASP	3
1	A	131	ASP	3
1	A	132	GLY	2
1	A	84	ASN	1
1	A	143	LEU	1
1	A	41	PHE	1
1	A	121	PRO	1
1	A	59	GLU	1
1	A	106	ASN	1
1	A	15	ASN	1
1	A	66	GLY	1
1	A	80	LEU	1
1	A	136	VAL	1
1	A	165	TYR	1
1	A	42	MET	1
1	A	113	GLY	1

6.3.2 Protein sidechains ⓘ

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	193/193 (100%)	161±5 (84±2%)	32±5 (16±2%)	5	41
All	All	1930/1930 (100%)	1613 (84%)	317 (16%)	5	41

All 116 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	75	SER	9

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Mol	Chain	Res	Type	Models (Total)
1	A	36	LYS	9
1	A	86	LEU	8
1	A	9	LYS	7
1	A	142	LYS	7
1	A	184	VAL	7
1	A	60	ILE	7
1	A	186	LYS	7
1	A	40	LYS	6
1	A	89	PHE	6
1	A	107	LYS	6
1	A	160	HIS	6
1	A	27	GLU	6
1	A	170	SER	6
1	A	45	LEU	5
1	A	126	LYS	5
1	A	163	TYR	5
1	A	209	LEU	5
1	A	137	GLN	5
1	A	21	PHE	5
1	A	67	LYS	5
1	A	100	VAL	5
1	A	4	ASP	4
1	A	42	MET	4
1	A	57	HIS	4
1	A	88	LYS	4
1	A	155	THR	4
1	A	213	LYS	4
1	A	61	ASP	4
1	A	56	GLU	4
1	A	69	GLN	3
1	A	127	VAL	3
1	A	164	ASP	3
1	A	29	VAL	3
1	A	31	PHE	3
1	A	87	SER	3
1	A	131	ASP	3
1	A	8	VAL	3
1	A	14	LYS	3
1	A	130	LYS	3
1	A	148	SER	3
1	A	187	LYS	3
1	A	211	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	25	LYS	3
1	A	133	ASP	3
1	A	181	GLN	3
1	A	212	GLU	3
1	A	59	GLU	3
1	A	103	LYS	3
1	A	138	LEU	3
1	A	136	VAL	3
1	A	33	ASN	3
1	A	44	CYS	2
1	A	83	ILE	2
1	A	193	LYS	2
1	A	55	TRP	2
1	A	98	TRP	2
1	A	157	ARG	2
1	A	188	ASP	2
1	A	191	PHE	2
1	A	204	SER	2
1	A	51	ARG	2
1	A	171	VAL	2
1	A	52	CYS	2
1	A	129	CYS	2
1	A	168	ASN	2
1	A	39	ASP	2
1	A	49	ASN	2
1	A	90	GLN	2
1	A	105	VAL	2
1	A	30	ARG	1
1	A	70	GLU	1
1	A	80	LEU	1
1	A	68	PHE	1
1	A	79	ASP	1
1	A	101	ASP	1
1	A	172	TYR	1
1	A	182	VAL	1
1	A	106	ASN	1
1	A	122	TYR	1
1	A	151	VAL	1
1	A	158	GLN	1
1	A	167	VAL	1
1	A	50	VAL	1
1	A	54	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	147	ASP	1
1	A	199	GLN	1
1	A	200	ASP	1
1	A	104	ILE	1
1	A	115	TYR	1
1	A	119	ILE	1
1	A	134	ASP	1
1	A	166	VAL	1
1	A	176	SER	1
1	A	11	PHE	1
1	A	71	LEU	1
1	A	116	GLU	1
1	A	117	MET	1
1	A	149	GLU	1
1	A	206	ILE	1
1	A	22	GLU	1
1	A	109	ASN	1
1	A	194	ASN	1
1	A	201	ASP	1
1	A	10	PHE	1
1	A	46	VAL	1
1	A	123	GLN	1
1	A	153	HIS	1
1	A	175	TYR	1
1	A	73	GLN	1
1	A	15	ASN	1
1	A	41	PHE	1
1	A	125	ASP	1
1	A	154	LEU	1
1	A	205	PHE	1
1	A	210	ASN	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 monosaccharides 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 (i)

No chemical shift data were provided