Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 04:43 PM EDT

PDB ID	:	1CVO
Title	:	THE SOLUTION STRUCTURE OF CARDIOTOXIN V FROM NAJA NAJA ATRA
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Deposited on	:	1993-04-28

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

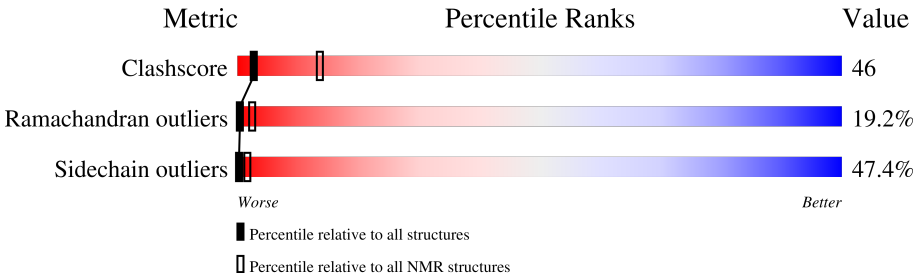
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	62	8% 13% 58% 21%

2 Ensemble composition and analysis (i)

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 990 atoms, of which 504 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CARDIOTOXIN V.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	62	990	312	504	84	82	8	0

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: CARDIOTOXIN V

Chain A: 8% 13% 58% 21%

L1 K2 C3 H4 N5 T6 Q7 L8 P9 F10 I11 Y12 K13 T14 C15 P16 E17 G18 K19 N20 L21 C22 F23 K24 A25 T26 L27 K28 K29 F30 P31 L32 K33 F34 P35 V36 K37 R38 G39 C40 A41 D42 N43 C44 P45 K46 N47 S48 A49 L50 L51 K52 Y53 V54 C55 C56 S57 T58 D59 K60

C61 N62

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: CARDIOTOXIN V

Chain A: 10% 23% 35% 32%

L1 K2 C3 H4 N5 T6 Q7 L8 P9 F10 I11 Y12 K13 P16 E17 G18 K19 N20 L21 C22 F23 K24 A25 T26 L27 K28 K29 F30 P31 L32 K33 F34 P35 V36 K37 R38 G39 C40 A41 D42 N43 C44 P45 K46 N47 S48 A49 L50 L51 K52 Y53 V54 C55 C56 S57 T58 D59 K60 C61

N62

4.2.2 Score per residue for model 2

• Molecule 1: CARDIOTOXIN V

Chain A: 6% 27% 37% 29%

L1 K2 C3 H4 N5 T6 Q7 L8 P9 F10 I11 Y12 K13 T14 C15 P16 E17 G18 K19 N20 L21 C22 F23 K24 A25 T26 L27 K28 K29 F30 P31 L32 K33 F34 P35 V36 K37 R38 G39 C40 A41 D42 N43 C44 P45 K46 N47 S48 A49 L50 L51 K52 Y53 V54 C55 C56 S57 T58 D59 K60

C61
N62

5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 2 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
DSPACE	refinement	

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	1.22±0.00	2±0/497 (0.3± 0.1%)	1.79±0.02	12±1/667 (1.8± 0.1%)
All	All	1.22	3/994 (0.3%)	1.79	24/1334 (1.8%)

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	45.0±5.0
All	All	0	90

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	35	PRO	N-CD	6.20	1.56	1.47	1	1
1	A	9	PRO	N-CD	5.49	1.55	1.47	1	1
1	A	17	GLU	CB-CG	-5.26	1.42	1.52	2	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	23	PHE	CB-CG-CD2	-9.87	113.89	120.80	1	2
1	A	12	TYR	CB-CG-CD1	-8.68	115.79	121.00	2	2
1	A	23	PHE	N-CA-CB	7.99	124.98	110.60	2	1
1	A	53	TYR	CG-CD1-CE1	-7.38	115.40	121.30	1	1
1	A	9	PRO	CA-N-CD	-6.83	101.94	111.50	1	2
1	A	38	ARG	NE-CZ-NH2	-6.71	116.94	120.30	2	1
1	A	58	THR	O-C-N	-6.64	112.07	122.70	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	10	PHE	CB-CG-CD2	-6.55	116.21	120.80	2	1
1	A	10	PHE	CB-CG-CD1	-6.50	116.25	120.80	1	1
1	A	34	PHE	CB-CG-CD2	-6.48	116.27	120.80	1	1
1	A	35	PRO	CA-N-CD	-6.36	102.59	111.50	1	1
1	A	12	TYR	CB-CG-CD2	-6.31	117.21	121.00	2	2
1	A	23	PHE	CA-C-N	-6.02	103.95	117.20	1	2
1	A	30	PHE	CB-CG-CD2	-5.72	116.80	120.80	1	1
1	A	30	PHE	CB-CG-CD1	-5.23	117.14	120.80	2	1
1	A	55	CYS	O-C-N	-5.07	114.59	122.70	2	1
1	A	31	PRO	O-C-N	-5.04	114.63	122.70	1	1
1	A	9	PRO	CB-CA-C	5.03	124.59	112.00	2	1
1	A	38	ARG	NE-CZ-NH1	5.03	122.81	120.30	2	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	3	CYS	Mainchain	2
1	A	4	HIS	Mainchain,Sidechain	2
1	A	6	THR	Mainchain	2
1	A	7	GLN	Mainchain,Sidechain	2
1	A	8	LEU	Peptide	2
1	A	12	TYR	Mainchain,Sidechain	2
1	A	13	LYS	Mainchain	2
1	A	16	PRO	Mainchain	2
1	A	20	ASN	Mainchain,Sidechain	2
1	A	22	CYS	Mainchain	2
1	A	23	PHE	Mainchain,Sidechain	2
1	A	25	ALA	Mainchain	2
1	A	26	THR	Mainchain	2
1	A	29	LYS	Mainchain	2
1	A	30	PHE	Sidechain,Mainchain	2
1	A	31	PRO	Mainchain	2
1	A	32	LEU	Mainchain	2
1	A	34	PHE	Sidechain,Mainchain	2
1	A	37	LYS	Mainchain	2
1	A	43	ASN	Sidechain,Mainchain	2
1	A	49	ALA	Mainchain	2
1	A	51	LEU	Mainchain	2
1	A	53	TYR	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	55	CYS	Mainchain	2
1	A	56	CYS	Mainchain	2
1	A	59	ASP	Sidechain	2
1	A	62	ASN	Sidechain	2
1	A	1	LEU	Mainchain	1
1	A	9	PRO	Mainchain	1
1	A	11	ILE	Mainchain	1
1	A	17	GLU	Mainchain	1
1	A	21	LEU	Mainchain	1
1	A	42	ASP	Sidechain	1
1	A	46	LYS	Mainchain	1
1	A	47	ASN	Mainchain,Sidechain	1
1	A	52	LYS	Mainchain	1
1	A	10	PHE	Mainchain,Sidechain	1
1	A	14	THR	Mainchain	1
1	A	15	CYS	Peptide	1
1	A	19	LYS	Mainchain	1
1	A	24	LYS	Mainchain	1
1	A	33	LYS	Mainchain	1
1	A	35	PRO	Mainchain	1
1	A	36	VAL	Mainchain	1
1	A	38	ARG	Mainchain	1
1	A	39	GLY	Mainchain	1
1	A	40	CYS	Mainchain	1
1	A	41	ALA	Mainchain	1
1	A	54	VAL	Mainchain	1
1	A	57	SER	Mainchain	1
1	A	58	THR	Mainchain	1
1	A	61	CYS	Mainchain	1

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	486	504	503	46±6
All	All	972	1008	1006	91

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ALA:HB2	1:A:53:TYR:CD2	0.73	2.19	2	2
1:A:36:VAL:HG21	1:A:51:LEU:HD11	0.72	1.58	1	1
1:A:25:ALA:HB1	1:A:51:LEU:CD2	0.70	2.14	2	1
1:A:26:THR:HG23	1:A:36:VAL:HB	0.68	1.66	2	1
1:A:25:ALA:HB2	1:A:53:TYR:CG	0.66	2.24	2	2
1:A:34:PHE:N	1:A:35:PRO:CD	0.66	2.59	2	1
1:A:36:VAL:CG1	1:A:37:LYS:N	0.66	2.58	1	1
1:A:32:LEU:HD12	1:A:32:LEU:C	0.65	2.10	2	1
1:A:6:THR:O	1:A:8:LEU:N	0.65	2.30	1	2
1:A:48:SER:OG	1:A:49:ALA:N	0.64	2.29	1	1
1:A:32:LEU:HD22	1:A:32:LEU:C	0.62	2.15	1	1
1:A:36:VAL:HG12	1:A:37:LYS:N	0.62	2.10	1	1
1:A:25:ALA:HB1	1:A:51:LEU:HD21	0.62	1.70	2	1
1:A:29:LYS:CD	1:A:34:PHE:H	0.61	2.09	2	1
1:A:26:THR:HA	1:A:36:VAL:N	0.58	2.12	1	1
1:A:22:CYS:N	1:A:41:ALA:HB3	0.58	2.13	1	1
1:A:16:PRO:HD2	1:A:19:LYS:CB	0.57	2.29	1	1
1:A:45:PRO:HB2	1:A:53:TYR:CG	0.57	2.34	2	1
1:A:22:CYS:HA	1:A:40:CYS:HA	0.54	1.80	1	1
1:A:26:THR:CB	1:A:35:PRO:HA	0.54	2.32	1	1
1:A:16:PRO:HD2	1:A:19:LYS:HB2	0.54	1.79	1	1
1:A:45:PRO:HG2	1:A:53:TYR:CD2	0.53	2.38	2	1
1:A:30:PHE:CD2	1:A:32:LEU:HD12	0.53	2.38	1	1
1:A:58:THR:HG23	1:A:61:CYS:SG	0.53	2.44	1	1
1:A:32:LEU:C	1:A:32:LEU:CD2	0.52	2.77	1	1
1:A:1:LEU:HD21	1:A:59:ASP:N	0.52	2.19	2	1
1:A:51:LEU:HD23	1:A:53:TYR:HD1	0.51	1.65	1	1
1:A:12:TYR:CD2	1:A:12:TYR:N	0.51	2.79	2	2
1:A:36:VAL:CG2	1:A:37:LYS:N	0.51	2.74	2	1
1:A:9:PRO:C	1:A:11:ILE:N	0.51	2.64	1	1
1:A:51:LEU:HD23	1:A:53:TYR:CD1	0.51	2.41	1	1
1:A:7:GLN:NE2	1:A:38:ARG:HD3	0.50	2.21	1	1
1:A:38:ARG:N	1:A:38:ARG:HD2	0.50	2.22	2	1
1:A:10:PHE:O	1:A:11:ILE:C	0.50	2.50	2	1
1:A:23:PHE:C	1:A:62:ASN:HB2	0.50	2.27	2	1
1:A:59:ASP:O	1:A:60:LYS:HG2	0.49	2.07	1	1
1:A:32:LEU:HD22	1:A:33:LYS:N	0.49	2.21	1	1
1:A:10:PHE:CD1	1:A:10:PHE:C	0.49	2.86	1	1
1:A:1:LEU:C	1:A:1:LEU:HD13	0.49	2.28	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ARG:N	1:A:38:ARG:CD	0.48	2.75	2	1
1:A:26:THR:CA	1:A:36:VAL:HB	0.48	2.38	1	1
1:A:33:LYS:HB3	1:A:35:PRO:HD3	0.48	1.84	2	1
1:A:47:ASN:OD1	1:A:53:TYR:HB2	0.48	2.08	2	1
1:A:46:LYS:O	1:A:47:ASN:C	0.48	2.52	2	1
1:A:58:THR:OG1	1:A:59:ASP:N	0.47	2.47	1	1
1:A:25:ALA:CB	1:A:53:TYR:CD1	0.46	2.98	2	1
1:A:33:LYS:HB3	1:A:35:PRO:CD	0.46	2.40	2	1
1:A:32:LEU:O	1:A:33:LYS:CB	0.46	2.64	1	1
1:A:10:PHE:CD1	1:A:10:PHE:N	0.46	2.80	2	1
1:A:49:ALA:O	1:A:50:LEU:HB2	0.45	2.10	2	1
1:A:21:LEU:HD23	1:A:55:CYS:SG	0.45	2.52	2	1
1:A:25:ALA:O	1:A:36:VAL:N	0.44	2.49	1	1
1:A:26:THR:O	1:A:51:LEU:HG	0.44	2.12	2	1
1:A:26:THR:HG22	1:A:35:PRO:HA	0.44	1.89	1	1
1:A:7:GLN:NE2	1:A:38:ARG:NE	0.44	2.66	2	1
1:A:39:GLY:O	1:A:62:ASN:ND2	0.44	2.51	1	1
1:A:17:GLU:CD	1:A:17:GLU:N	0.43	2.72	1	1
1:A:3:CYS:O	1:A:12:TYR:HB2	0.43	2.13	1	1
1:A:51:LEU:CD2	1:A:53:TYR:CD1	0.43	3.02	1	1
1:A:1:LEU:CD2	1:A:59:ASP:CG	0.43	2.87	1	1
1:A:27:LEU:O	1:A:29:LYS:N	0.43	2.52	2	1
1:A:23:PHE:N	1:A:23:PHE:CD1	0.43	2.86	1	1
1:A:23:PHE:CD1	1:A:40:CYS:O	0.43	2.72	1	1
1:A:26:THR:HG22	1:A:35:PRO:HB3	0.43	1.91	1	1
1:A:7:GLN:NE2	1:A:38:ARG:CD	0.42	2.82	1	1
1:A:26:THR:HA	1:A:35:PRO:C	0.42	2.35	1	1
1:A:26:THR:CG2	1:A:35:PRO:HA	0.42	2.45	1	1
1:A:10:PHE:CE1	1:A:12:TYR:CE2	0.42	3.07	1	1
1:A:26:THR:HB	1:A:35:PRO:HA	0.42	1.92	1	1
1:A:30:PHE:O	1:A:32:LEU:N	0.42	2.52	1	2
1:A:19:LYS:HG2	1:A:40:CYS:HB2	0.42	1.91	2	1
1:A:26:THR:HG22	1:A:35:PRO:CA	0.42	2.45	1	1
1:A:17:GLU:N	1:A:17:GLU:OE1	0.42	2.53	1	1
1:A:21:LEU:HG	1:A:56:CYS:O	0.42	2.15	2	1
1:A:44:CYS:O	1:A:45:PRO:O	0.41	2.37	1	1
1:A:1:LEU:HD13	1:A:2:LYS:N	0.41	2.30	2	1
1:A:26:THR:HG22	1:A:35:PRO:CB	0.41	2.44	1	1
1:A:32:LEU:C	1:A:32:LEU:CD1	0.41	2.85	2	1
1:A:1:LEU:HD21	1:A:59:ASP:CA	0.41	2.46	2	1
1:A:51:LEU:HG	1:A:52:LYS:H	0.41	1.76	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LYS:HD2	1:A:34:PHE:H	0.41	1.74	2	1
1:A:45:PRO:CB	1:A:53:TYR:CD2	0.41	3.03	2	1
1:A:16:PRO:HD3	1:A:40:CYS:SG	0.41	2.56	2	1
1:A:23:PHE:CD1	1:A:23:PHE:O	0.40	2.75	1	1
1:A:26:THR:HA	1:A:36:VAL:HB	0.40	1.93	1	1
1:A:29:LYS:HD3	1:A:34:PHE:H	0.40	1.76	2	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	60/62 (97%)	34±2 (58±4%)	14±0 (23±0%)	12±2 (19±4%)	0 2
All	All	120/124 (97%)	69 (58%)	28 (23%)	23 (19%)	0 2

All 15 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	9	PRO	2
1	A	11	ILE	2
1	A	16	PRO	2
1	A	31	PRO	2
1	A	32	LEU	2
1	A	42	ASP	2
1	A	44	CYS	2
1	A	45	PRO	2
1	A	3	CYS	1
1	A	10	PHE	1
1	A	33	LYS	1
1	A	34	PHE	1
1	A	35	PRO	1
1	A	47	ASN	1
1	A	7	GLN	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	57/57 (100%)	30±2 (53±4%)	27±2 (47±4%)	0 1
All	All	114/114 (100%)	60 (53%)	54 (47%)	0 1

All 40 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	2	LYS	2
1	A	11	ILE	2
1	A	12	TYR	2
1	A	17	GLU	2
1	A	23	PHE	2
1	A	28	LYS	2
1	A	32	LEU	2
1	A	38	ARG	2
1	A	47	ASN	2
1	A	51	LEU	2
1	A	57	SER	2
1	A	58	THR	2
1	A	59	ASP	2
1	A	60	LYS	2
1	A	4	HIS	1
1	A	5	ASN	1
1	A	10	PHE	1
1	A	13	LYS	1
1	A	20	ASN	1
1	A	27	LEU	1
1	A	30	PHE	1
1	A	34	PHE	1
1	A	36	VAL	1
1	A	44	CYS	1
1	A	48	SER	1
1	A	52	LYS	1
1	A	55	CYS	1
1	A	56	CYS	1
1	A	62	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	7	GLN	1
1	A	15	CYS	1
1	A	21	LEU	1
1	A	24	LYS	1
1	A	26	THR	1
1	A	29	LYS	1
1	A	33	LYS	1
1	A	40	CYS	1
1	A	45	PRO	1
1	A	46	LYS	1
1	A	61	CYS	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