Full wwPDB EM Validation Report

Mar 9, 2025 – 12:08 AM JST

PDB ID	:	9IJ1
EMDB ID	:	EMD-60612
Title	:	Cryo-EM Structure of MILI-piRNA-target (22-nt, bilobed)
Authors	:	Li, Z.Q.; Xu, Q.K.; Wu, J.P.; Shen, E.Z.
Deposited on	:	2024-06-21
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

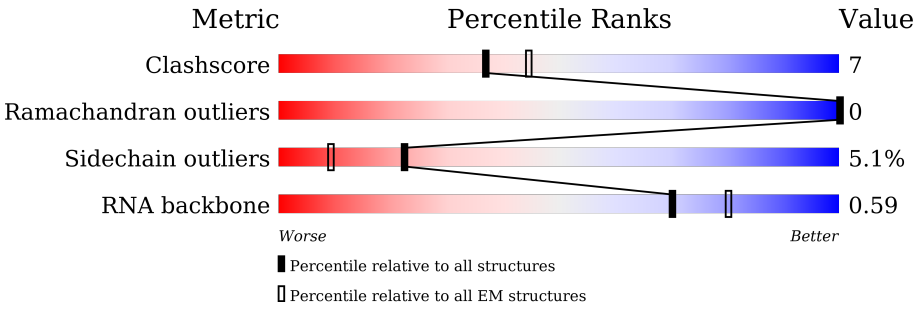
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	971	60% 17% • 22%
2	B	26	42% 38% 12% 8%
3	C	21	48% 19% 29% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7056 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Piwi-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	755	6062	3882	1051	1085	44	0	0

- Molecule 2 is a RNA chain called RNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	26	550	247	95	182	26	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(P*CP*AP*AP*GP*UP*UP*UP*CP*CP*AP*UP*GP*UP*UP*GP*AP*UP*GP*GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	21	443	199	75	148	21	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0

3 Residue-property plots (i)

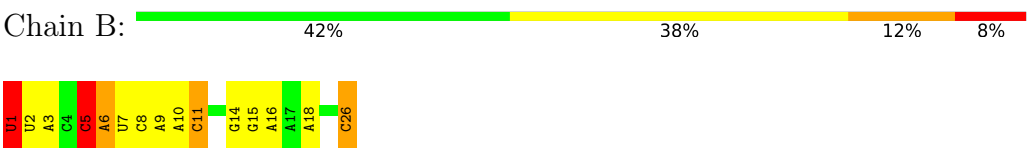
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Piwi-like protein 2

Chain A:

• Molecule 2: RNA (26-MER)

Chain B:



• Molecule 3: RNA (5'-R(P*CP*AP*AP*GP*UP*UP*UP*CP*CP*AP*UP*GP*UP*UP*GP*AP*UP*GP*GP*UP*A)-3')

Chain C:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122269	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMC

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 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	0.29	0/6199	0.68	7/8395 (0.1%)
2	B	0.61	1/590 (0.2%)	1.21	6/914 (0.7%)
3	C	0.37	0/494	1.13	4/765 (0.5%)
All	All	0.33	1/7283 (0.0%)	0.78	17/10074 (0.2%)

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 outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.64	1.48	1.61

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	11	C	C5-C6-N1	7.46	124.73	121.00
1	A	613	MET	CA-CB-CG	7.17	125.50	113.30
1	A	512	MET	CG-SD-CE	6.48	110.56	100.20
1	A	786	LEU	CA-CB-CG	6.47	130.18	115.30
1	A	657	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	228	LEU	CA-CB-CG	6.10	129.32	115.30
2	B	1	U	P-O3'-C3'	6.01	126.91	119.70
2	B	11	C	C6-N1-C2	-5.94	117.92	120.30
2	B	1	U	OP2-P-O3'	5.83	118.04	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	7	U	N3-C2-O2	-5.62	118.27	122.20
3	C	7	U	N1-C2-O2	5.51	126.66	122.80
1	A	622	MET	CA-CB-CG	5.17	122.09	113.30
3	C	17	U	C5-C4-O4	-5.15	122.81	125.90
3	C	8	C	C2-N1-C1'	5.14	124.45	118.80
2	B	5	C	O4'-C1'-N1	5.13	112.30	108.20
1	A	355	LEU	CA-CB-CG	5.05	126.91	115.30
2	B	6	A	N7-C8-N9	5.05	116.32	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	498	MET	Peptide

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6062	0	6156	91	0
2	B	550	0	282	9	0
3	C	443	0	224	9	0
4	A	1	0	0	0	0
All	All	7056	0	6662	101	0

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 (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:CYS:O	1:A:411:LEU:HB2	1.63	0.98
1:A:227:ASN:HB2	1:A:559:HIS:HB3	1.71	0.72
1:A:655:GLN:HA	1:A:658:LEU:HG	1.76	0.68
1:A:719:MET:SD	1:A:719:MET:N	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:GLN:HE22	3:C:18:G:H21	1.44	0.65
1:A:311:GLU:HG2	1:A:313:CYS:H	1.63	0.64
1:A:622:MET:O	1:A:625:LYS:HB2	1.97	0.64
1:A:665:GLN:HE22	1:A:692:VAL:HG23	1.63	0.62
1:A:224:LEU:HB2	1:A:561:ILE:HB	1.82	0.61
1:A:320:PHE:HA	1:A:323:VAL:HG22	1.81	0.61
1:A:851:GLN:HB2	1:A:903:HIS:HB3	1.83	0.60
1:A:652:ARG:O	1:A:656:SER:HB3	2.01	0.60
1:A:929:TYR:HB3	1:A:932:TRP:HE1	1.65	0.59
1:A:326:ARG:NH1	3:C:9:C:OP2	2.34	0.59
1:A:292:GLN:NE2	1:A:297:ASP:OD1	2.35	0.59
1:A:946:HIS:HE1	3:C:13:U:H5'	1.67	0.59
1:A:868:THR:HG21	1:A:899:GLY:H	1.68	0.58
1:A:812:ARG:NH1	1:A:813:ASP:O	2.39	0.56
1:A:326:ARG:NH2	1:A:339:ARG:O	2.38	0.56
1:A:880:THR:HB	1:A:886:ASP:HB2	1.88	0.55
1:A:741:GLY:HA3	1:A:941:PRO:HB2	1.89	0.54
1:A:820:LEU:O	1:A:824:ALA:N	2.39	0.54
1:A:709:ARG:NH1	1:A:713:GLN:OE1	2.41	0.53
1:A:255:ARG:HB3	1:A:272:PHE:HE2	1.73	0.53
1:A:516:THR:HA	1:A:519:ILE:HB	1.90	0.53
1:A:545:ASN:HA	1:A:548:THR:HG22	1.91	0.53
1:A:499:THR:HG23	2:B:9:A:H4'	1.90	0.52
2:B:14:G:H2'	2:B:15:G:H8	1.75	0.51
1:A:363:ALA:HB1	1:A:374:LEU:HD11	1.93	0.51
1:A:366:ARG:NH2	1:A:879:ILE:O	2.44	0.51
1:A:472:HIS:HD2	1:A:489:ILE:HD12	1.76	0.51
1:A:292:GLN:NE2	1:A:293:ARG:O	2.44	0.50
1:A:947:LYS:NZ	2:B:1:U:OP3	2.42	0.50
1:A:755:VAL:HG13	1:A:773:VAL:HG13	1.93	0.50
1:A:662:GLY:HA2	1:A:665:GLN:HG2	1.94	0.50
1:A:342:TYR:HA	1:A:360:GLY:HA3	1.94	0.50
1:A:666:MET:HG3	1:A:719:MET:HG2	1.93	0.49
1:A:272:PHE:HB3	1:A:327:ARG:HH21	1.76	0.49
2:B:5:C:H2'	2:B:6:A:H8	1.79	0.47
1:A:683:LYS:HE3	1:A:696:VAL:HG23	1.96	0.47
1:A:273:ASP:OD2	3:C:7:U:O2'	2.26	0.47
1:A:466:ASP:OD1	1:A:466:ASP:N	2.41	0.47
1:A:608:TYR:HE2	1:A:639:TRP:HD1	1.62	0.47
1:A:286:VAL:HG22	1:A:305:GLN:HB3	1.96	0.47
1:A:860:LEU:HD11	1:A:869:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:U:H2'	2:B:8:C:C6	2.50	0.47
1:A:250:GLU:OE1	1:A:457:ASN:ND2	2.47	0.47
1:A:581:SER:OG	1:A:583:ASP:OD1	2.33	0.47
1:A:251:CYS:HB2	1:A:458:TYR:HD1	1.78	0.47
1:A:248:SER:O	1:A:456:LYS:NZ	2.45	0.46
1:A:273:ASP:HB2	3:C:7:U:H4'	1.98	0.46
1:A:370:GLY:HA3	1:A:878:THR:HG22	1.98	0.46
1:A:815:VAL:HB	1:A:819:GLN:HB3	1.97	0.46
1:A:293:ARG:HB2	1:A:300:ILE:HD11	1.97	0.45
1:A:365:ILE:HG13	1:A:374:LEU:HD13	1.98	0.45
1:A:860:LEU:O	1:A:866:PHE:HA	2.17	0.45
1:A:929:TYR:HD2	1:A:936:ILE:HG21	1.81	0.45
1:A:243:VAL:HG22	1:A:304:ILE:HG22	1.98	0.45
2:B:9:A:H2'	2:B:10:A:C8	2.51	0.45
1:A:524:LYS:HD2	1:A:524:LYS:HA	1.76	0.45
1:A:477:ARG:HG2	1:A:486:LYS:HG3	1.98	0.45
2:B:10:A:H2'	2:B:11:C:C6	2.52	0.44
1:A:687:CYS:HB3	1:A:956:LEU:HD13	1.99	0.44
1:A:651:ILE:HG23	1:A:685:LEU:HD22	1.99	0.44
1:A:763:ASN:ND2	1:A:768:LYS:H	2.16	0.44
1:A:874:VAL:HG22	1:A:889:LEU:HD11	2.00	0.43
1:A:588:LYS:HD2	1:A:588:LYS:HA	1.78	0.43
1:A:888:TYR:HD2	1:A:901:PRO:HG2	1.82	0.43
1:A:436:PRO:HB3	1:A:450:PHE:HB3	2.00	0.43
1:A:951:LEU:HD12	1:A:955:ILE:HD12	2.01	0.43
1:A:222:GLN:HB2	1:A:563:GLY:HA3	2.01	0.43
1:A:254:MET:SD	1:A:254:MET:N	2.92	0.43
1:A:342:TYR:HD1	1:A:360:GLY:HA3	1.82	0.43
1:A:769:TRP:HB2	1:A:970:PHE:HZ	1.84	0.43
3:C:1:C:H2'	3:C:2:A:H8	1.84	0.43
1:A:602:HIS:O	1:A:635:SER:OG	2.34	0.42
3:C:17:U:H2'	3:C:18:G:C8	2.54	0.42
1:A:667:VAL:HB	1:A:694:SER:HA	2.02	0.42
1:A:759:VAL:HG11	1:A:944:TYR:HD2	1.84	0.42
1:A:853:LYS:HD3	1:A:853:LYS:HA	1.79	0.42
2:B:15:G:H2'	2:B:16:A:H8	1.84	0.42
1:A:886:ASP:OD2	1:A:903:HIS:NE2	2.51	0.42
1:A:380:HIS:CE1	1:A:521:LEU:HD11	2.54	0.42
1:A:630:ILE:HD13	1:A:630:ILE:HA	1.86	0.41
1:A:648:GLU:OE1	1:A:652:ARG:NH1	2.53	0.41
1:A:574:ARG:HE	1:A:593:ASP:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:LYS:HD2	1:A:625:LYS:HA	1.74	0.41
1:A:426:ARG:O	1:A:472:HIS:ND1	2.53	0.41
3:C:11:U:H2'	3:C:12:G:C8	2.55	0.41
1:A:739:VAL:HG13	1:A:809:VAL:HB	2.02	0.41
1:A:227:ASN:HB3	1:A:373:PHE:CE1	2.56	0.41
1:A:228:LEU:HD13	1:A:530:LEU:HD21	2.02	0.41
1:A:665:GLN:NE2	1:A:692:VAL:HG23	2.32	0.41
1:A:260:LYS:HA	1:A:260:LYS:HD3	1.86	0.41
1:A:537:ILE:HD13	1:A:537:ILE:HA	1.91	0.41
1:A:565:LEU:HD23	1:A:565:LEU:HA	1.97	0.41
1:A:606:LEU:HD23	1:A:639:TRP:CD1	2.56	0.41
1:A:795:LYS:HA	1:A:795:LYS:HD3	1.73	0.41
1:A:769:TRP:HB2	1:A:970:PHE:CZ	2.56	0.40
3:C:1:C:H2'	3:C:2:A:C8	2.56	0.40
1:A:415:ILE:HD13	2:B:10:A:H4'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 EM 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	751/971 (77%)	694 (92%)	57 (8%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 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 EM 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	683/863 (79%)	648 (95%)	35 (5%)	20 53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	CYS
1	A	258	MET
1	A	316	LEU
1	A	367	ARG
1	A	381	LYS
1	A	385	ASN
1	A	396	TYR
1	A	420	TYR
1	A	422	ASN
1	A	450	PHE
1	A	458	TYR
1	A	504	LYS
1	A	510	ARG
1	A	524	LYS
1	A	560	LYS
1	A	578	PHE
1	A	585	ASN
1	A	586	TRP
1	A	601	MET
1	A	603	PHE
1	A	645	ASP
1	A	655	GLN
1	A	679	TYR
1	A	686	CYS
1	A	709	ARG
1	A	752	MET
1	A	785	SER
1	A	816	SER
1	A	817	ASP
1	A	886	ASP
1	A	906	CYS
1	A	931	ASN
1	A	950	PHE
1	A	969	PHE
1	A	970	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
1	A	896	GLN
1	A	931	ASN
1	A	946	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	26/26 (100%)	5 (19%)	1 (3%)
3	C	20/21 (95%)	7 (35%)	1 (5%)
All	All	46/47 (97%)	12 (26%)	2 (4%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	3	A
2	B	5	C
2	B	18	A
2	B	26	OMC
3	C	8	C
3	C	9	C
3	C	12	G
3	C	13	U
3	C	17	U
3	C	18	G
3	C	21	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	U
3	C	12	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OMC	B	26	2	19,22,23	0.51	0	26,31,34	1.01	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	B	26	2	-	5/9/27/28	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	26	OMC	C1'-N1-C2	2.98	125.07	118.42
2	B	26	OMC	C1'-N1-C6	-2.31	115.81	120.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	26	OMC	O4'-C1'-N1-C2
2	B	26	OMC	O4'-C1'-N1-C6
2	B	26	OMC	C3'-C4'-C5'-O5'
2	B	26	OMC	C4'-C5'-O5'-P
2	B	26	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.