



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2025 – 12:09 AM JST

PDB ID : 9IJ5  
EMDB ID : EMD-60616  
Title : Cryo-EM Structure of MILI(K853A)-piRNA-target  
Authors : Li, Z.Q.; Xu, Q.K.; Wu, J.P.; Shen, E.Z.  
Deposited on : 2024-06-21  
Resolution : 2.80 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](mailto: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>.

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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

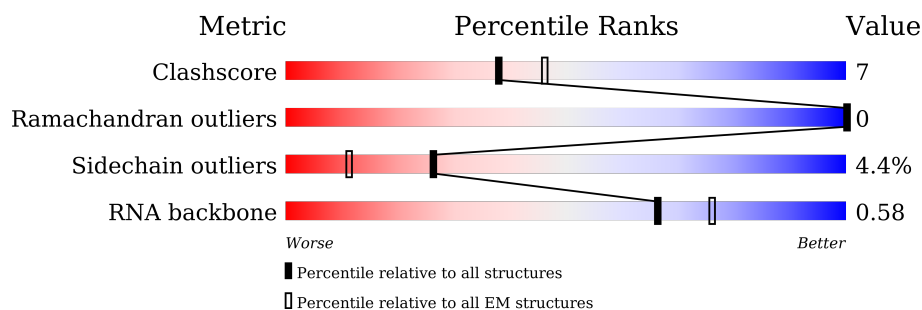
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	971	
2	B	26	
3	C	25	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7139 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
1	A	755	Total	C	N	O	S	0	0
			6057	3883	1048	1082	44		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	ALA	LYS	engineered mutation	UNP Q8CDG1

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

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

- Molecule 3 is a RNA chain called RNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	25	Total	C	N	O	P	0	0
			531	238	93	175	25		

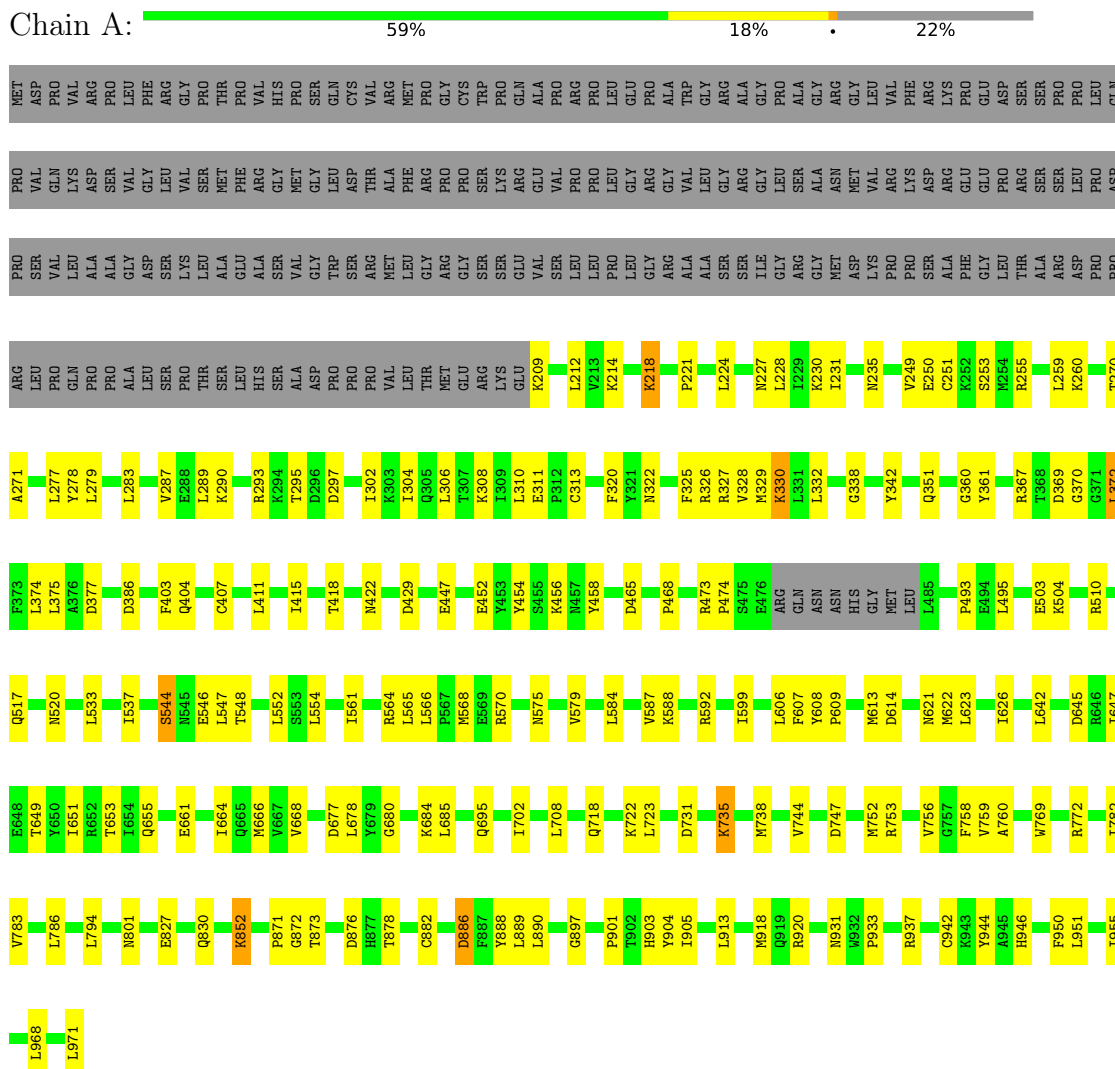
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

### 3 Residue-property plots

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

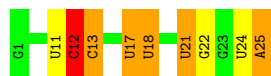


#### • Molecule 2: RNA (26-MER)



- Molecule 3: RNA (25-MER)

Chain C: 64% 12% 20% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93580	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 ( $e^-/\text{\AA}^2$ )	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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.38	0/6194	0.73	10/8391 (0.1%)
2	B	0.75	1/590 (0.2%)	1.23	6/914 (0.7%)
3	C	0.61	0/593	1.27	10/920 (1.1%)
All	All	0.44	1/7377 (0.0%)	0.84	26/10225 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.89	1.48	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	PRO	CA-N-CD	-10.03	97.46	111.50
2	B	11	C	C5-C6-N1	8.14	125.07	121.00
1	A	329	MET	CA-CB-CG	7.48	126.01	113.30
2	B	11	C	C6-N1-C2	-7.09	117.46	120.30
3	C	12	C	C6-N1-C2	-6.49	117.70	120.30
2	B	8	C	C6-N1-C2	-6.36	117.76	120.30
3	C	21	U	N1-C2-O2	6.20	127.14	122.80
3	C	21	U	N3-C2-O2	-6.18	117.88	122.20
3	C	12	C	C5-C6-N1	6.17	124.08	121.00
3	C	13	C	C5-C6-N1	6.05	124.03	121.00
1	A	372	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	794	LEU	CB-CG-CD1	-5.86	101.03	111.00
3	C	13	C	C6-N1-C2	-5.56	118.08	120.30
2	B	24	C	C2-N1-C1'	5.54	124.89	118.80
2	B	8	C	C5-C6-N1	5.48	123.74	121.00
1	A	279	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	290	LYS	CA-CB-CG	5.30	125.05	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	11	U	C2-N1-C1'	5.27	124.03	117.70
3	C	11	U	N1-C2-O2	5.26	126.48	122.80
1	A	613	MET	CA-CB-CG	5.21	122.16	113.30
2	B	24	C	C6-N1-C2	-5.19	118.22	120.30
3	C	18	U	N3-C4-O4	5.14	123.00	119.40
1	A	950	PHE	CB-CG-CD1	5.11	124.38	120.80
1	A	794	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	495	LEU	CB-CG-CD1	5.08	119.63	111.00
3	C	17	U	C5-C4-O4	-5.03	122.88	125.90

There are no chirality outliers.

There are no planarity outliers.

## 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	6057	0	6162	95	0
2	B	550	0	282	4	0
3	C	531	0	268	2	0
4	A	1	0	0	0	0
All	All	7139	0	6712	98	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 (98) 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	1.91	0.70
1:A:599:ILE:HD11	1:A:723:LEU:HB3	1.77	0.66
1:A:782:ILE:HD13	1:A:786:LEU:HD12	1.77	0.65
1:A:326:ARG:O	1:A:330:LYS:HB3	1.97	0.65
1:A:293:ARG:HG3	1:A:295:THR:H	1.61	0.64
1:A:332:LEU:HD11	1:A:537:ILE:HG13	1.82	0.62
1:A:418:THR:O	1:A:422:ASN:HA	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG23	1:A:552:LEU:HD22	1.83	0.60
1:A:886:ASP:OD2	1:A:903:HIS:NE2	2.36	0.59
1:A:322:ASN:ND2	3:C:12:C:O3'	2.34	0.58
1:A:338:GLY:O	1:A:422:ASN:ND2	2.35	0.58
1:A:209:LYS:N	1:A:882:CYS:HG	2.02	0.58
1:A:271:ALA:HB3	1:A:278:TYR:HB2	1.85	0.57
1:A:251:CYS:HG	1:A:253:SER:HG	1.53	0.57
1:A:386:ASP:N	1:A:386:ASP:OD1	2.38	0.57
1:A:230:LYS:HZ1	1:A:374:LEU:HB2	1.71	0.56
1:A:224:LEU:HB2	1:A:561:ILE:HG13	1.86	0.56
1:A:270:THR:OG1	1:A:327:ARG:NH2	2.39	0.56
1:A:588:LYS:NZ	3:C:25:A:O3'	2.38	0.56
1:A:758:PHE:HB3	1:A:772:ARG:O	2.06	0.56
1:A:931:ASN:HB2	1:A:971:LEU:HD22	1.89	0.55
1:A:769:TRP:HB2	1:A:968:LEU:HD21	1.89	0.55
1:A:289:LEU:HB2	1:A:302:ILE:HB	1.89	0.55
1:A:547:LEU:HG	1:A:552:LEU:HB2	1.88	0.54
1:A:680:GLY:HA2	1:A:955:ILE:HG23	1.88	0.54
1:A:218:LYS:O	1:A:564:ARG:NH1	2.40	0.54
1:A:680:GLY:O	1:A:684:LYS:HB2	2.09	0.53
1:A:651:ILE:HG23	1:A:685:LEU:HD22	1.89	0.53
1:A:587:VAL:HG22	1:A:933:PRO:HG2	1.91	0.52
1:A:827:GLU:HA	1:A:830:GLN:HG2	1.92	0.52
1:A:718:GLN:NE2	1:A:931:ASN:OD1	2.42	0.52
1:A:649:THR:O	1:A:653:THR:OG1	2.27	0.51
1:A:702:ILE:HA	1:A:708:LEU:HD11	1.93	0.51
1:A:370:GLY:HA3	1:A:878:THR:HG23	1.93	0.51
1:A:942:CYS:O	1:A:946:HIS:HB2	2.11	0.51
1:A:520:ASN:OD1	1:A:897:GLY:N	2.44	0.51
1:A:666:MET:HE1	1:A:722:LYS:HB2	1.91	0.50
1:A:235:ASN:OD1	1:A:235:ASN:N	2.44	0.50
1:A:259:LEU:HD21	1:A:277:LEU:HD22	1.94	0.50
1:A:454:TYR:HA	1:A:458:TYR:HB2	1.94	0.50
1:A:614:ASP:N	1:A:614:ASP:OD1	2.43	0.50
1:A:367:ARG:HA	1:A:372:LEU:HA	1.94	0.49
1:A:738:MET:HE2	1:A:760:ALA:HB1	1.96	0.48
1:A:327:ARG:NH1	1:A:546:GLU:OE2	2.46	0.48
1:A:592:ARG:HE	1:A:592:ARG:HB2	1.55	0.48
1:A:645:ASP:N	1:A:645:ASP:OD1	2.45	0.48
1:A:227:ASN:HD22	1:A:375:LEU:HD23	1.79	0.47
1:A:951:LEU:HD23	1:A:955:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:ASP:OD1	1:A:876:ASP:N	2.46	0.47
1:A:718:GLN:NE2	1:A:971:LEU:O	2.47	0.47
1:A:668:VAL:HG13	1:A:695:GLN:HB3	1.98	0.46
1:A:465:ASP:OD1	1:A:465:ASP:N	2.44	0.46
1:A:452:GLU:O	1:A:456:LYS:HB3	2.16	0.46
1:A:468:PRO:HD2	1:A:493:PRO:HG2	1.97	0.45
1:A:623:LEU:HD23	1:A:626:ILE:HD11	1.98	0.45
1:A:661:GLU:HG2	1:A:664:ILE:HG13	1.98	0.45
1:A:212:LEU:HB2	1:A:214:LYS:HE2	1.98	0.45
1:A:325:PHE:HA	1:A:328:VAL:HG12	1.98	0.45
1:A:361:TYR:CZ	1:A:533:LEU:HB2	2.52	0.45
1:A:328:VAL:HG11	1:A:547:LEU:HD13	1.98	0.45
1:A:342:TYR:HA	1:A:360:GLY:HA3	1.99	0.45
1:A:537:ILE:HG21	1:A:554:LEU:HD12	2.00	0.44
1:A:260:LYS:HD2	1:A:260:LYS:HA	1.72	0.44
1:A:287:VAL:HB	1:A:304:ILE:HB	1.99	0.44
1:A:570:ARG:HG2	1:A:579:VAL:HG23	2.00	0.44
1:A:759:VAL:HG21	1:A:944:TYR:HB3	2.00	0.44
1:A:888:TYR:HB3	1:A:901:PRO:HB2	2.00	0.44
1:A:622:MET:O	1:A:626:ILE:HG12	2.17	0.43
1:A:872:GLY:CA	1:A:890:LEU:O	2.67	0.43
1:A:889:LEU:HB3	1:A:904:TYR:HE2	1.83	0.43
1:A:735:LYS:HE2	1:A:735:LYS:HB2	1.70	0.43
1:A:872:GLY:N	1:A:890:LEU:O	2.51	0.43
1:A:744:VAL:HG12	1:A:756:VAL:HG22	2.01	0.43
1:A:913:LEU:HD13	1:A:918:MET:HG2	2.00	0.43
1:A:608:TYR:HA	1:A:609:PRO:HD3	1.91	0.43
1:A:415:ILE:HG13	2:B:10:A:H4'	2.01	0.42
1:A:283:LEU:HD13	1:A:287:VAL:HG21	2.00	0.42
1:A:249:VAL:HB	1:A:293:ARG:HH22	1.84	0.42
1:A:544:SER:O	1:A:548:THR:OG1	2.30	0.42
1:A:565:LEU:HA	1:A:873:THR:HA	2.01	0.42
1:A:607:PHE:HB3	1:A:642:LEU:HD11	2.02	0.42
2:B:8:C:H2'	2:B:9:A:C8	2.55	0.42
2:B:17:A:H2'	2:B:18:A:C8	2.54	0.42
1:A:647:ILE:HD13	1:A:678:LEU:HD13	2.02	0.41
1:A:886:ASP:HB2	1:A:905:ILE:HA	2.01	0.41
1:A:473:ARG:HA	1:A:474:PRO:HD3	1.93	0.41
1:A:568:MET:H	1:A:568:MET:HG3	1.64	0.41
1:A:920:ARG:HA	1:A:920:ARG:HD2	1.74	0.41
1:A:228:LEU:HD22	1:A:374:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:HG21	1:A:456:LYS:HA	2.03	0.41
1:A:250:GLU:O	1:A:255:ARG:NH2	2.53	0.41
1:A:783:VAL:HA	1:A:830:GLN:NE2	2.36	0.41
2:B:16:A:H2'	2:B:17:A:C8	2.56	0.41
1:A:566:LEU:HD23	1:A:566:LEU:HA	1.96	0.40
1:A:311:GLU:HG3	1:A:313:CYS:H	1.85	0.40
1:A:308:LYS:HD3	1:A:310:LEU:HD21	2.03	0.40
1:A:852:LYS:HG2	1:A:937:ARG:NH1	2.37	0.40
1:A:584:LEU:HD12	1:A:871:PRO:HB2	2.03	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%)	704 (94%)	47 (6%)	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	683/862 (79%)	653 (96%)	30 (4%)	24	56

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	LYS
1	A	297	ASP
1	A	306	LEU
1	A	320	PHE
1	A	330	LYS
1	A	351	GLN
1	A	369	ASP
1	A	377	ASP
1	A	403	PHE
1	A	404	GLN
1	A	429	ASP
1	A	447	GLU
1	A	503	GLU
1	A	504	LYS
1	A	510	ARG
1	A	517	GLN
1	A	544	SER
1	A	575	ASN
1	A	606	LEU
1	A	621	ASN
1	A	655	GLN
1	A	677	ASP
1	A	731	ASP
1	A	735	LYS
1	A	747	ASP
1	A	752	MET
1	A	753	ARG
1	A	801	ASN
1	A	852	LYS
1	A	886	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	830	GLN

### 5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	25/26 (96%)	7 (28%)	0
3	C	24/25 (96%)	8 (33%)	0
All	All	49/51 (96%)	15 (30%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	3	A
2	B	6	A
2	B	7	U
2	B	10	A
2	B	24	C
2	B	26	OMC
3	C	12	C
3	C	13	C
3	C	17	U
3	C	18	U
3	C	21	U
3	C	22	G
3	C	24	U
3	C	25	A

There are no RNA pucker outliers to report.

## 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	0.53	0	26,31,34	0.82	1 (3%)

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	-	2/9/27/28	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	OMC	C1'-N1-C2	2.19	123.31	118.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	26	OMC	C4'-C5'-O5'-P
2	B	26	OMC	C3'-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.