



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 05:30 AM EDT

PDB ID : 8F4O / pdb_00008f4o
Title : Apo structure of the TPP riboswitch aptamer domain
Authors : Lee, H.-K.; Wang, Y.-X.; Stagno, J.R.
Deposited on : 2022-11-11
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

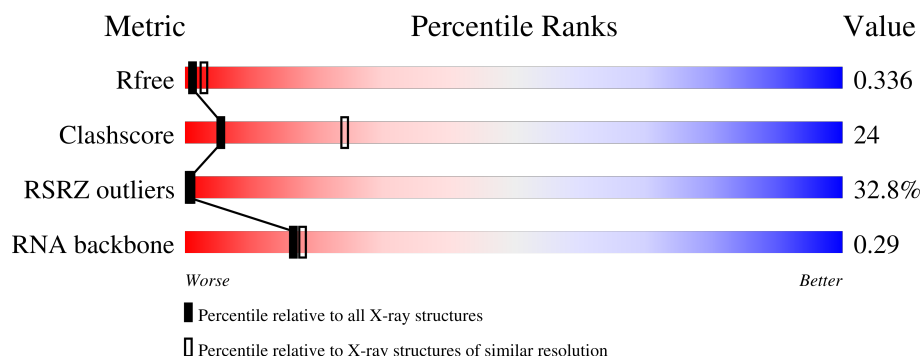
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	83	
1	B	83	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5387 atoms, of which 2151 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

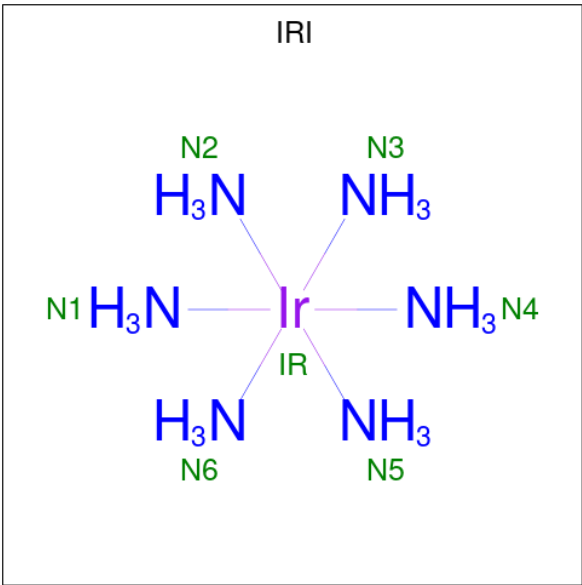
- Molecule 1 is a RNA chain called TPP riboswitch aptamer domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	72	Total	C	H	N	O	P	11	1	0
			2323	689	779	280	503	72			
1	B	65	Total	C	H	N	O	P	0	1	0
			2135	633	714	264	458	66			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	G	-	insertion	GB 1845826323
A	89	G	-	insertion	GB 1845826323
A	90	C	-	insertion	GB 1845826323
A	91	A	-	insertion	GB 1845826323
B	9	G	-	insertion	GB 1845826323
B	89	G	-	insertion	GB 1845826323
B	90	C	-	insertion	GB 1845826323
B	91	A	-	insertion	GB 1845826323

- Molecule 2 is IRIDIUM HEXAMMINE ION (CCD ID: IRI) (formula: H₁₈IrN₆).



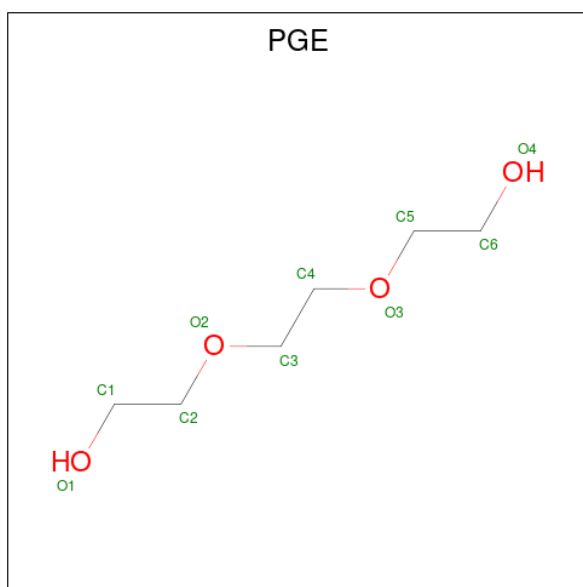
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	H	Ir	N	0	1
			75	54	3	18		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	1
			50	36	2	12		
2	A	1	Total	H	Ir	N	0	1
			50	36	2	12		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	1
			50	36	2	12		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		

Continued on next page...

Continued from previous page...

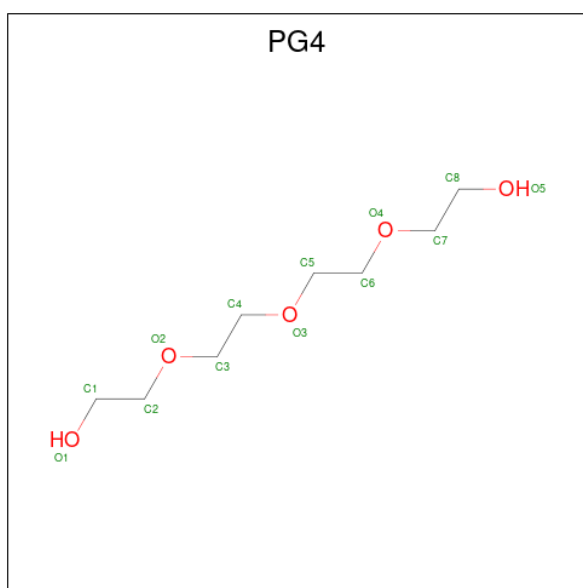
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	A	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	1
			50	36	2	12		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		
2	B	1	Total	H	Ir	N	0	0
			25	18	1	6		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

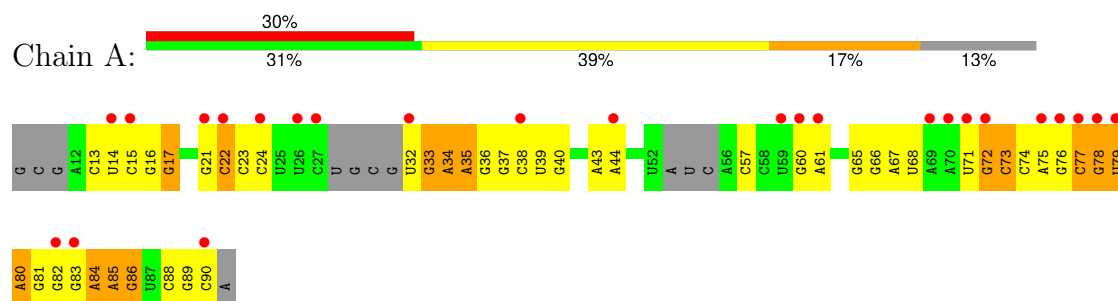


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			31	8	18	5		

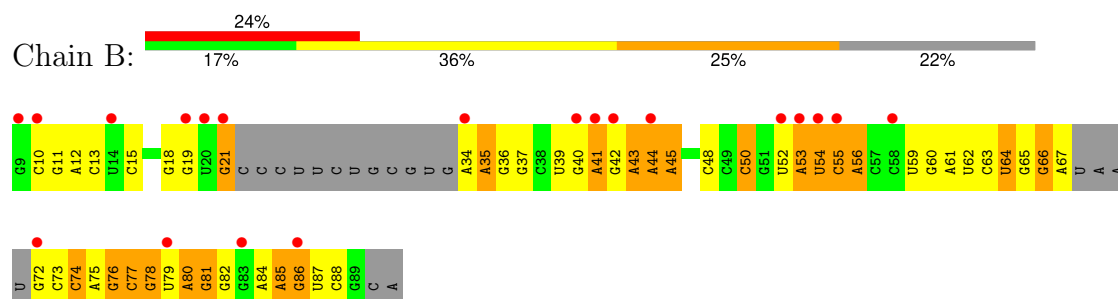
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: TPP riboswitch aptamer domain



• Molecule 1: TPP riboswitch aptamer domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.26Å 139.26Å 97.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.58 – 3.10 45.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.58-3.10) 99.8 (45.58-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487+SVN	Depositor
R, R_{free}	0.282 , 0.317 0.296 , 0.336	Depositor DCC
R_{free} test set	544 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	135.3	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 285.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5387	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, IRI, PG4

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	0.20	0/1725	0.44	0/2684
1	B	0.19	0/1589	0.45	0/2473
All	All	0.20	0/3314	0.45	0/5157

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	1544	779	784	59	0
1	B	1421	714	717	55	0
2	A	154	396	0	24	0
2	B	84	216	0	15	0
3	A	10	14	14	0	0
3	B	10	14	14	0	0
4	B	13	18	18	0	0
All	All	3236	2151	1547	113	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 24.

All (113) 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:78:G:O2'	1:A:79:U:OP1	1.76	1.03
1:B:21:G:O6	2:B:104:IRI:N6	2.03	0.92
1:A:37:G:O6	2:A:113:IRI:N3	2.02	0.91
1:A:21[A]:G:O2'	2:A:115:IRI:N2	2.13	0.81
1:A:32:U:O2'	1:A:33:G:OP2	1.97	0.81
1:B:40:G:H22	1:B:43:A:H5'	1.46	0.80
1:A:79:U:O4	2:B:102[B]:IRI:N3	2.17	0.77
1:A:83:G:O6	2:A:112[A]:IRI:N3	2.18	0.77
1:B:42:G:O6	2:B:106:IRI:N2	2.20	0.75
1:A:65:G:N7	2:A:114:IRI:N4	2.34	0.75
1:B:75:A:OP2	2:B:102[B]:IRI:N1	2.20	0.74
1:A:39:U:OP2	2:A:104[B]:IRI:N2	2.20	0.73
1:A:43:A:OP2	2:A:107:IRI:N4	2.21	0.72
1:A:72:G:O2'	1:A:73:C:OP1	2.10	0.70
1:A:75:A:OP2	2:A:103[B]:IRI:N5	2.25	0.70
1:A:36:G:N7	2:A:113:IRI:N2	2.40	0.69
1:A:82:G:O6	2:A:112[A]:IRI:N6	2.25	0.69
1:B:37:G:O6	2:B:104:IRI:N6	2.26	0.69
1:B:75:A:N7	2:B:102[B]:IRI:N2	2.45	0.65
1:B:35:A:H2'	1:B:36:G:H8	1.62	0.65
1:A:66:G:O6	2:A:114:IRI:N3	2.31	0.63
2:A:117:IRI:N5	1:B:77:C:OP2	2.32	0.63
1:A:83:G:O6	2:A:112[A]:IRI:N4	2.32	0.63
1:B:66:G:O6	2:B:110:IRI:N2	2.33	0.62
1:B:62:U:O4	2:B:109:IRI:N3	2.32	0.62
1:B:40:G:H22	1:B:43:A:C5'	2.13	0.61
1:B:36:G:H3'	1:B:37:G:H8	1.65	0.61
1:A:78:G:HO2'	1:A:79:U:P	2.18	0.59
1:B:85:A:H1'	1:B:86:G:C8	2.38	0.58
2:A:112[B]:IRI:N4	1:B:64:U:OP1	2.36	0.58
1:A:24:C:H42	1:A:35:A:H61	1.51	0.58
1:B:86:G:N7	2:B:107:IRI:N2	2.52	0.58
1:A:77:C:H2'	1:A:77:C:O2	2.03	0.57
1:B:41:A:N3	1:B:48:C:O2'	2.35	0.57
1:B:74:C:H3'	2:B:102[B]:IRI:N1	2.20	0.56
1:A:40:G:N1	1:A:43:A:OP2	2.35	0.56
1:A:21[B]:G:O2'	1:A:22:C:P	2.64	0.56
1:A:24:C:H42	1:A:35:A:N6	2.04	0.56
1:A:21[A]:G:OP2	2:A:109:IRI:N4	2.39	0.55
1:B:75:A:OP2	2:B:102[A]:IRI:N5	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:G:H2'	1:A:90:C:C6	2.43	0.53
1:B:77:C:H5'	1:B:78:G:OP2	2.09	0.53
1:A:75:A:N7	2:A:103[B]:IRI:N3	2.56	0.52
1:B:59:U:H2'	1:B:60:G:O4'	2.10	0.52
1:A:79:U:H3'	1:A:79:U:OP2	2.10	0.52
1:A:72:G:O2'	1:A:73:C:P	2.67	0.52
1:A:24:C:N4	1:A:35:A:H61	2.08	0.52
1:B:53:A:C2	1:B:84:A:N7	2.79	0.51
1:A:15:C:H2'	1:A:16:G:O4'	2.10	0.51
1:A:72:G:HO2'	1:A:73:C:P	2.33	0.51
1:A:85:A:O2'	1:A:86:G:OP2	2.26	0.50
1:B:67:A:N3	1:B:72:G:O6	2.45	0.50
1:B:65:G:N7	2:B:110:IRI:N5	2.59	0.49
1:B:65:G:H2'	1:B:66:G:O4'	2.11	0.49
1:A:21[B]:G:HO2'	1:A:22:C:P	2.35	0.49
1:B:18:G:H2'	1:B:19:G:C8	2.48	0.49
1:A:40:G:O6	2:A:107:IRI:N4	2.46	0.49
1:A:21[A]:G:O6	2:A:113:IRI:N3	2.46	0.48
1:B:60:G:H2'	1:B:61:A:C8	2.47	0.48
1:A:78:G:C2'	1:A:79:U:OP1	2.61	0.48
1:A:79:U:H2'	1:A:80:A:OP2	2.14	0.48
1:B:50:C:H1'	1:B:56:A:H1'	1.96	0.48
1:A:33:G:H3'	1:A:34:A:H8	1.78	0.48
1:B:35:A:O2'	1:B:36:G:H5'	2.13	0.47
1:B:50:C:O2'	1:B:84:A:N1	2.48	0.46
1:A:44:A:H5''	2:A:106:IRI:N5	2.30	0.46
1:B:72:G:H2'	1:B:73:C:O4'	2.15	0.46
1:B:73:C:H2'	1:B:74:C:O4'	2.15	0.46
1:A:75:A:H2'	1:A:76:G:O4'	2.17	0.46
1:A:66:G:H2'	1:A:67:A:O4'	2.16	0.45
1:B:34:A:H2'	1:B:35:A:C4	2.51	0.45
1:A:39:U:P	2:A:104[B]:IRI:N3	2.89	0.45
1:A:71:U:H2'	1:A:72:G:OP2	2.16	0.45
1:B:75:A:C8	2:B:102[B]:IRI:N1	2.84	0.45
1:A:79:U:C2'	1:A:80:A:OP2	2.64	0.45
1:B:66:G:H2'	1:B:67:A:O4'	2.16	0.45
1:B:34:A:O3'	1:B:35:A:O4'	2.35	0.44
1:B:11:G:H2'	1:B:12:A:C8	2.53	0.44
1:B:86:G:C5	2:B:107:IRI:N2	2.85	0.44
1:A:13:C:H2'	1:A:14:U:C6	2.52	0.43
1:B:54:U:H2'	1:B:55:C:H5''	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:A:O2'	1:B:81:G:H5''	2.18	0.43
1:B:53:A:H5''	1:B:54:U:OP1	2.19	0.43
1:A:44:A:C5'	2:A:106:IRI:N5	2.81	0.43
1:B:73:C:C3'	1:B:74:C:H5''	2.48	0.43
1:A:39:U:OP1	2:A:104[B]:IRI:N3	2.52	0.43
1:B:74:C:H5''	1:B:74:C:H6	1.83	0.43
1:A:88:C:O2'	1:A:89:G:H5'	2.19	0.43
2:A:103[A]:IRI:N4	1:B:79:U:O4	2.52	0.43
1:A:60:G:H2'	1:A:61:A:C8	2.54	0.42
1:A:71:U:C2'	1:A:72:G:OP2	2.66	0.42
1:A:34:A:H2'	1:A:35:A:C8	2.55	0.42
1:A:17:G:H1'	1:A:84:A:N3	2.34	0.42
1:A:44:A:OP1	2:A:106:IRI:N4	2.53	0.42
1:B:66:G:C2	1:B:67:A:H1'	2.54	0.42
1:A:72:G:OP1	1:A:72:G:H2'	2.19	0.42
1:B:80:A:C4	1:B:81:G:C8	3.07	0.42
1:B:10:C:H2'	1:B:11:G:C8	2.56	0.41
1:B:11:G:H2'	1:B:12:A:H8	1.85	0.41
1:A:80:A:C8	1:B:63:C:H2'	2.55	0.41
1:A:32:U:HO2'	1:A:33:G:P	2.32	0.41
1:B:53:A:H2	1:B:84:A:H62	1.67	0.41
1:A:57:C:OP1	2:A:116:IRI:N5	2.54	0.41
1:B:76:G:H5''	1:B:77:C:OP2	2.20	0.41
1:A:15:C:C2	1:A:85:A:C2	3.08	0.41
1:A:85:A:O2'	1:A:86:G:P	2.78	0.41
1:B:44:A:C3'	1:B:45:A:H5'	2.50	0.41
1:B:52[B]:U:H1'	1:B:53:A:OP2	2.21	0.41
1:B:86:G:C6	2:B:107:IRI:N2	2.89	0.41
1:B:53:A:H2	1:B:84:A:N7	2.17	0.41
1:B:74:C:H2'	1:B:75:A:O4'	2.21	0.40
1:A:37:G:C6	1:A:38:C:C4	3.08	0.40
1:A:74:C:H2'	1:A:75:A:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	68/83 (81%)	17 (25%)	2 (2%)
1	B	61/83 (73%)	27 (44%)	1 (1%)
All	All	129/166 (77%)	44 (34%)	3 (2%)

All (44) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	17	G
1	A	22	C
1	A	23	C
1	A	33	G
1	A	34	A
1	A	35	A
1	A	68	U
1	A	72	G
1	A	73	C
1	A	77	C
1	A	78	G
1	A	79	U
1	A	80	A
1	A	81	G
1	A	84	A
1	A	85	A
1	A	86	G
1	B	13	C
1	B	15	C
1	B	21	G
1	B	35	A
1	B	39	U
1	B	41	A
1	B	43	A
1	B	44	A
1	B	45	A
1	B	50	C
1	B	53	A
1	B	54	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	55	C
1	B	56	A
1	B	64	U
1	B	66	G
1	B	74	C
1	B	76	G
1	B	77	C
1	B	78	G
1	B	80	A
1	B	81	G
1	B	82	G
1	B	85	A
1	B	86	G
1	B	87	U
1	B	88	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	78	G
1	A	80	A
1	B	80	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

37 ligands are 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	IRI	A	104[A]	-	0,6,6	-	-	-		
2	IRI	A	103[B]	-	0,6,6	-	-	-		
2	IRI	A	102	-	0,6,6	-	-	-		
2	IRI	B	102[B]	-	0,6,6	-	-	-		
2	IRI	B	109	-	0,6,6	-	-	-		
2	IRI	A	101[B]	-	0,6,6	-	-	-		
2	IRI	B	103	-	0,6,6	-	-	-		
2	IRI	A	103[A]	-	0,6,6	-	-	-		
2	IRI	B	102[A]	-	0,6,6	-	-	-		
2	IRI	A	107	-	0,6,6	-	-	-		
2	IRI	A	105	-	0,6,6	-	-	-		
2	IRI	A	115	-	0,6,6	-	-	-		
2	IRI	A	101[A]	-	0,6,6	-	-	-		
3	PGE	B	112	-	9,9,9	0.30	0	8,8,8	0.41	0
2	IRI	A	101[C]	-	0,6,6	-	-	-		
2	IRI	B	101	-	0,6,6	-	-	-		
2	IRI	B	107	-	0,6,6	-	-	-		
2	IRI	A	113	-	0,6,6	-	-	-		
2	IRI	B	105	-	0,6,6	-	-	-		
2	IRI	A	116	-	0,6,6	-	-	-		
2	IRI	B	106	-	0,6,6	-	-	-		
2	IRI	A	112[B]	-	0,6,6	-	-	-		
2	IRI	B	108	-	0,6,6	-	-	-		
2	IRI	A	111	-	0,6,6	-	-	-		
2	IRI	B	110	-	0,6,6	-	-	-		
2	IRI	A	112[A]	-	0,6,6	-	-	-		
2	IRI	B	111	-	0,6,6	-	-	-		
2	IRI	A	110	-	0,6,6	-	-	-		
2	IRI	A	108	-	0,6,6	-	-	-		
2	IRI	A	104[B]	-	0,6,6	-	-	-		
4	PG4	B	113	-	12,12,12	0.16	0	11,11,11	0.59	0
3	PGE	A	118	-	9,9,9	0.34	0	8,8,8	0.34	0
2	IRI	A	106	-	0,6,6	-	-	-		
2	IRI	B	104	-	0,6,6	-	-	-		
2	IRI	A	114	-	0,6,6	-	-	-		
2	IRI	A	109	-	0,6,6	-	-	-		
2	IRI	A	117	-	0,6,6	-	-	-		

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
4	PG4	B	113	-	-	5/10/10/10	-
3	PGE	B	112	-	-	2/7/7/7	-
3	PGE	A	118	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	113	PG4	C1-C2-O2-C3
3	B	112	PGE	O2-C3-C4-O3
4	B	113	PG4	O3-C5-C6-O4
4	B	113	PG4	O2-C3-C4-O3
3	A	118	PGE	O2-C3-C4-O3
3	B	112	PGE	C6-C5-O3-C4
3	A	118	PGE	C6-C5-O3-C4
4	B	113	PG4	O4-C7-C8-O5
4	B	113	PG4	C8-C7-O4-C6

There are no ring outliers.

20 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	103[B]	IRI	2	0
2	B	102[B]	IRI	5	0
2	B	109	IRI	1	0
2	A	103[A]	IRI	1	0
2	B	102[A]	IRI	1	0
2	A	107	IRI	2	0
2	A	115	IRI	1	0
2	B	107	IRI	3	0
2	A	113	IRI	3	0
2	A	116	IRI	1	0
2	B	106	IRI	1	0
2	A	112[B]	IRI	1	0
2	B	110	IRI	2	0
2	A	112[A]	IRI	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	104[B]	IRI	3	0
2	A	106	IRI	3	0
2	B	104	IRI	2	0
2	A	114	IRI	2	0
2	A	109	IRI	1	0
2	A	117	IRI	1	0

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	72/83 (86%)	2.04	25 (34%)	1 0	62, 131, 241, 274	13 (18%)
1	B	65/83 (78%)	1.76	20 (30%)	1 1	64, 131, 228, 245	16 (24%)
All	All	137/166 (82%)	1.91	45 (32%)	1 0	62, 131, 241, 274	29 (21%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52[A]	U	7.4
1	A	60	G	7.2
1	A	72	G	7.1
1	B	55	C	7.0
1	A	70	A	6.6
1	A	59	U	6.5
1	A	32	U	5.6
1	A	76	G	5.5
1	A	61	A	5.4
1	B	10	C	5.2
1	A	21[A]	G	5.0
1	A	77	C	5.0
1	B	19	G	4.9
1	A	78	G	4.1
1	B	53	A	4.1
1	A	75	A	4.0
1	B	54	U	3.7
1	A	22	C	3.7
1	A	14	U	3.6
1	A	71	U	3.6
1	B	20	U	3.6
1	B	44	A	3.5
1	B	9	G	3.4
1	A	90	C	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	14	U	3.0
1	A	27	C	2.9
1	A	82	G	2.8
1	A	38	C	2.7
1	A	79	U	2.7
1	B	42	G	2.6
1	B	41	A	2.6
1	A	69	A	2.6
1	B	40	G	2.5
1	B	21	G	2.5
1	A	44	A	2.5
1	B	86	G	2.5
1	B	58	C	2.4
1	B	34	A	2.4
1	A	24	C	2.4
1	B	79	U	2.4
1	A	15	C	2.3
1	A	26	U	2.3
1	A	83	G	2.2
1	B	72	G	2.1
1	B	83	G	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	B	113	13/13	0.50	0.21	147,200,237,240	0
3	PGE	A	118	10/10	0.68	0.17	125,175,195,210	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IRI	A	109	7/7	0.68	0.19	128,189,231,231	25
3	PGE	B	112	10/10	0.70	0.17	99,132,159,166	0
2	IRI	B	101	7/7	0.76	0.18	105,136,163,177	25
2	IRI	A	108	7/7	0.78	0.19	184,224,251,251	25
2	IRI	B	108	7/7	0.80	0.19	188,232,256,256	25
2	IRI	A	102	7/7	0.80	0.20	132,171,209,209	25
2	IRI	A	110	7/7	0.82	0.16	118,173,188,188	25
2	IRI	A	106	7/7	0.82	0.32	95,119,146,146	25
2	IRI	B	109	7/7	0.84	0.21	106,137,166,166	25
2	IRI	A	117	7/7	0.84	0.14	144,212,235,308	0
2	IRI	B	106	7/7	0.86	0.30	134,163,187,187	25
2	IRI	A	101[B]	7/7	0.87	0.28	117,141,157,157	25
2	IRI	A	101[C]	7/7	0.87	0.28	93,125,147,147	25
2	IRI	A	101[A]	7/7	0.87	0.28	116,149,173,173	25
2	IRI	A	111	7/7	0.90	0.14	143,180,204,204	0
2	IRI	B	103	7/7	0.90	0.18	127,156,197,197	25
2	IRI	B	107	7/7	0.92	0.12	153,198,229,229	25
2	IRI	B	105	7/7	0.92	0.12	120,170,227,227	25
2	IRI	A	104[B]	7/7	0.93	0.22	89,129,159,159	25
2	IRI	A	105	7/7	0.93	0.15	166,211,258,258	25
2	IRI	A	104[A]	7/7	0.93	0.22	101,124,144,159	25
2	IRI	B	110	7/7	0.94	0.10	152,186,224,224	0
2	IRI	A	116	7/7	0.94	0.12	87,121,145,147	25
2	IRI	A	103[A]	7/7	0.94	0.18	108,135,165,165	25
2	IRI	A	103[B]	7/7	0.94	0.18	102,129,171,171	25
2	IRI	A	112[B]	7/7	0.96	0.17	103,151,174,174	25
2	IRI	A	115	7/7	0.96	0.13	112,143,167,167	0
2	IRI	A	112[A]	7/7	0.96	0.17	107,151,179,179	25
2	IRI	B	104	7/7	0.97	0.11	133,179,212,212	25
2	IRI	A	107	7/7	0.98	0.07	83,121,160,160	25
2	IRI	A	113	7/7	0.98	0.14	101,129,163,163	0
2	IRI	A	114	7/7	0.98	0.14	73,124,162,162	0
2	IRI	B	102[A]	7/7	0.99	0.06	107,142,173,173	25
2	IRI	B	102[B]	7/7	0.99	0.06	116,153,168,168	25
2	IRI	B	111	7/7	0.99	0.10	108,134,169,169	0

6.5 Other polymers

There are no such residues in this entry.