



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2026 – 10:56 am BST

PDB ID : 7PO6 / pdb_00007po6
Title : Xist (m6A)UCG tetraloop RNA bound to the YTH domain of YTHDC1
Authors : Jones, A.N.; Mourao, A.; Sattler, M.
Deposited on : 2021-09-08
Resolution : 1.77 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

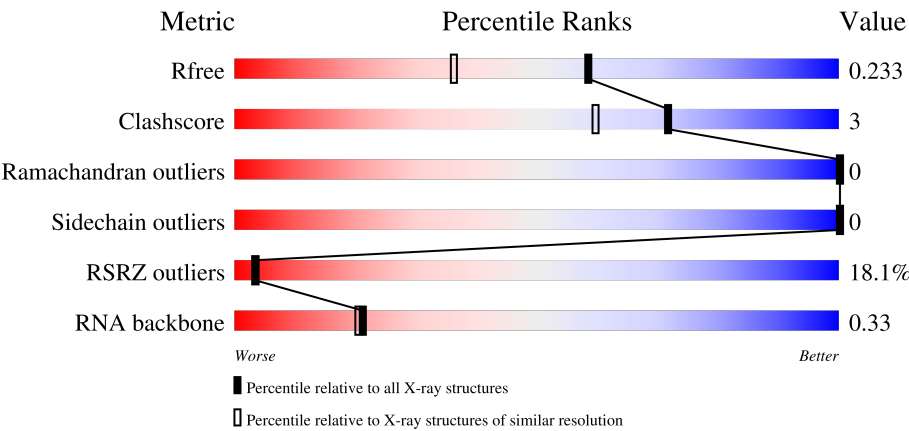
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)
RNA backbone	3983	1032 (2.20-1.36)

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	D	14	14%7% 79%
1	E	14	7%14% 79%
1	F	14	7%14%14% 71%
2	A	169	17% 94%

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Mol	Chain	Length	Quality of chain
2	B	169	14% 91% 7%
2	C	169	22% 91% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8526 atoms, of which 4139 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 RNA (5'-R(*(6MZ)P*UP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	3	Total	C	H	N	O	P	0	0	0
			93	29	33	10	19	2			
1	E	3	Total	C	H	N	O	P	0	0	0
			98	29	35	10	21	3			
1	F	4	Total	C	H	N	O	P	0	0	0
			125	39	43	15	25	3			

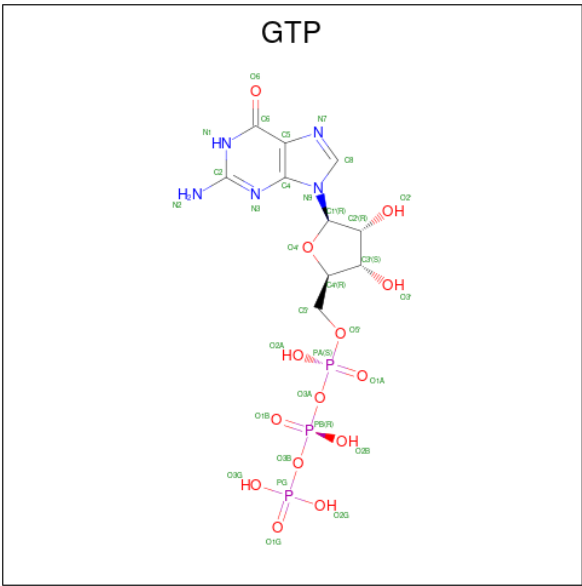
- Molecule 2 is a protein called Isoform 2 of YTH domain-containing protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	166	Total	C	H	N	O	S	0	3	0
			2623	840	1316	232	230	5			
2	A	163	Total	C	H	N	O	S	7	3	0
			2566	824	1286	225	225	6			
2	C	166	Total	C	H	N	O	S	0	3	0
			2646	846	1330	235	229	6			

There are 12 discrepancies between the modelled and reference sequences:

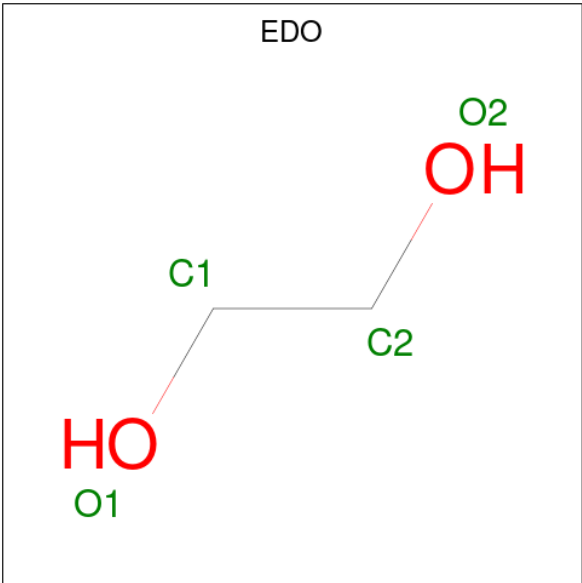
Chain	Residue	Modelled	Actual	Comment	Reference
B	341	GLY	-	expression tag	UNP Q96MU7
B	342	GLY	-	expression tag	UNP Q96MU7
B	343	GLY	-	expression tag	UNP Q96MU7
B	344	GLY	-	expression tag	UNP Q96MU7
A	341	GLY	-	expression tag	UNP Q96MU7
A	342	GLY	-	expression tag	UNP Q96MU7
A	343	GLY	-	expression tag	UNP Q96MU7
A	344	GLY	-	expression tag	UNP Q96MU7
C	341	GLY	-	expression tag	UNP Q96MU7
C	342	GLY	-	expression tag	UNP Q96MU7
C	343	GLY	-	expression tag	UNP Q96MU7
C	344	GLY	-	expression tag	UNP Q96MU7

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



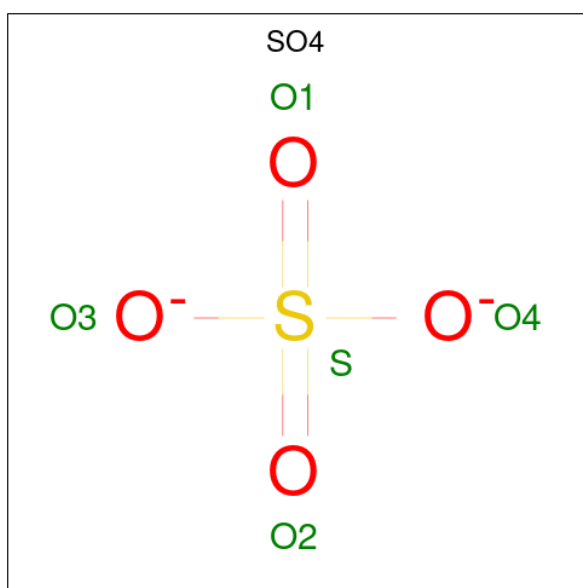
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	B	1	10	2	6	2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O S	0	0
			5	4 1		
5	B	1	Total	O S	0	0
			5	4 1		
5	B	1	Total	O S	0	0
			5	4 1		
5	A	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0

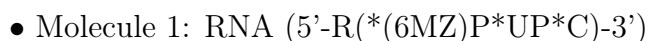
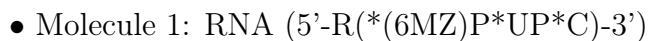
- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

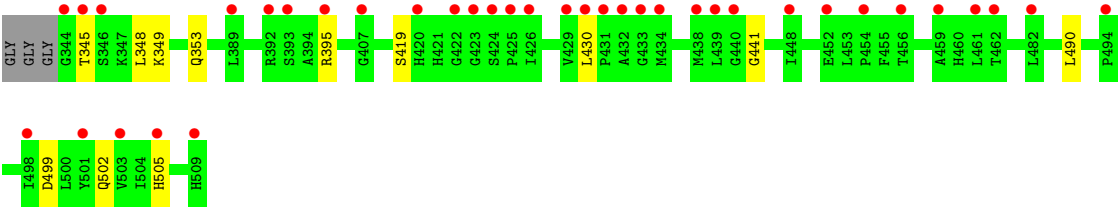
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	5	Total H O 11 6 5	0	0
7	B	70	Total H O 84 14 70	0	0
7	A	64	Total H O 76 12 64	0	0
7	C	45	Total H O 55 10 45	0	0
7	E	5	Total O 5 5	0	0
7	F	3	Total O 3 3	0	0

- Molecule 1: RNA (5'-R*(6MZ)P*UP*C)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.44Å 85.12Å 88.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 1.77 48.34 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.34-1.77) 98.7 (48.34-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.200 , 0.232 0.200 , 0.233	Depositor DCC
R_{free} test set	2899 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8526	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: EDO, GTP, NA, SO4, 6MZ

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	D	0.74	0/43	1.96	1/64 (1.6%)
1	E	0.43	0/43	0.70	0/64
1	F	0.51	0/69	0.73	0/105
2	A	0.50	0/1331	0.63	0/1798
2	B	0.52	0/1357	0.62	0/1833
2	C	0.45	0/1367	0.62	0/1846
All	All	0.49	0/4210	0.65	1/5710 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	U	O5'-P-OP1	-11.04	74.87	108.00

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	D	60	33	35	4	0
1	E	63	35	35	0	0
1	F	82	43	44	0	0
2	A	1280	1286	1261	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1307	1316	1299	8	0
2	C	1316	1330	1297	12	0
3	D	23	12	12	3	0
4	A	8	12	12	0	0
4	B	16	24	24	2	0
4	C	4	6	6	0	0
5	A	5	0	0	1	0
5	B	15	0	0	0	0
5	C	15	0	0	0	0
6	C	1	0	0	0	0
7	A	64	12	0	1	0
7	B	70	14	0	1	0
7	C	45	10	0	0	0
7	D	5	6	0	0	0
7	E	5	0	0	0	0
7	F	3	0	0	0	0
All	All	4387	4139	4025	27	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 3.

All (27) 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:D:5:C:O3'	3:D:101:GTP:PA	2.31	0.88
1:D:5:C:C3'	3:D:101:GTP:PA	2.92	0.57
2:A:382:VAL:HG12	7:A:760:HOH:O	2.03	0.57
2:C:345:THR:HG22	2:C:349:LYS:HD2	1.88	0.54
2:B:389:LEU:HD23	2:B:392:ARG:HH21	1.73	0.53
2:C:348:LEU:HD23	2:C:490:LEU:HD23	1.94	0.50
2:C:499:ASP:OD1	2:C:502:GLN:NE2	2.45	0.49
2:C:499:ASP:HB3	2:C:502:GLN:OE1	2.13	0.49
2:C:419:SER:HB2	2:C:441:GLY:HA3	1.96	0.48
2:B:495:ASP:H	4:B:607:EDO:H21	1.78	0.48
2:C:430:LEU:HD12	2:C:430:LEU:H	1.77	0.48
1:D:5:C:H3'	3:D:101:GTP:PA	2.55	0.47
2:C:505:HIS:O	2:C:505:HIS:ND1	2.47	0.47
2:B:494:PRO:HA	4:B:607:EDO:H21	1.96	0.47
2:C:353:GLN:O	2:C:395:ARG:HD3	2.15	0.46
2:C:499:ASP:CB	2:C:502:GLN:OE1	2.65	0.45
2:A:444:LYS:HE2	5:A:603:SO4:O4	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:U:O2'	1:D:5:C:H5'	2.18	0.44
2:C:430:LEU:HD12	2:C:430:LEU:N	2.33	0.43
2:B:404:ARG:HG2	2:B:405:GLU:HG3	2.00	0.42
2:A:431:PRO:HG2	2:A:434:MET:CE	2.51	0.41
2:C:499:ASP:OD1	2:C:502:GLN:CD	2.64	0.41
2:C:499:ASP:CG	2:C:502:GLN:OE1	2.63	0.41
2:B:427:HIS:HB3	7:B:769:HOH:O	2.20	0.40
2:B:499:ASP:HB3	2:B:502:GLN:HB2	2.04	0.40
2:B:415:LEU:HD11	2:B:443:PHE:CD2	2.56	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 X-ray entries followed by that with respect to entries of similar resolution.

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	
2	A	164/169 (97%)	160 (98%)	4 (2%)	0	100	100
2	B	167/169 (99%)	165 (99%)	2 (1%)	0	100	100
2	C	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
All	All	498/507 (98%)	489 (98%)	9 (2%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	
2	A	140/145 (97%)	140 (100%)	0	100	100
2	B	142/145 (98%)	142 (100%)	0	100	100
2	C	143/145 (99%)	143 (100%)	0	100	100
All	All	425/435 (98%)	425 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	427	HIS
2	B	468	HIS
2	A	420	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	2/14 (14%)	1 (50%)	0
1	E	2/14 (14%)	1 (50%)	0
1	F	3/14 (21%)	1 (33%)	0
All	All	7/42 (16%)	3 (42%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	4	U
1	E	4	U
1	F	4	U

There are no RNA pucker outliers to report.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	6MZ	E	3	1	22,25,26	2.32	4 (18%)	30,36,39	3.38	12 (40%)
1	6MZ	D	3	1	22,22,26	2.47	5 (22%)	30,32,39	3.12	12 (40%)
1	6MZ	F	3	1	21,21,26	4.19	7 (33%)	26,31,39	3.31	15 (57%)

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
1	6MZ	E	3	1	-	1/9/27/28	0/3/3/3
1	6MZ	D	3	1	-	0/8/24/28	0/3/3/3
1	6MZ	F	3	1	-	0/6/22/28	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	3	6MZ	C3'-C4'	-14.12	1.32	1.52
1	D	3	6MZ	C6-N6	10.11	1.45	1.34
1	F	3	6MZ	C6-N6	9.75	1.44	1.34
1	E	3	6MZ	C6-N6	9.33	1.44	1.34
1	F	3	6MZ	O4'-C4'	5.37	1.60	1.44
1	F	3	6MZ	O3'-C3'	2.83	1.49	1.43
1	D	3	6MZ	C5-C6	-2.50	1.35	1.41
1	D	3	6MZ	C5-C4	-2.46	1.34	1.39
1	D	3	6MZ	C6-N1	-2.40	1.31	1.35
1	F	3	6MZ	O4'-C1'	-2.38	1.36	1.42
1	E	3	6MZ	C5-C4	-2.36	1.34	1.39
1	D	3	6MZ	C5-N7	-2.27	1.34	1.39
1	F	3	6MZ	C5-C4	-2.25	1.34	1.39
1	E	3	6MZ	C2-N1	2.22	1.38	1.33
1	E	3	6MZ	C5-N7	-2.14	1.35	1.39
1	F	3	6MZ	C5-C6	-2.07	1.36	1.41

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	6MZ	C4-N9-C1'	-7.44	108.87	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	6MZ	C5-C4-N3	-7.40	117.09	126.75
1	D	3	6MZ	C5-C4-N3	-6.95	117.68	126.75
1	E	3	6MZ	C1'-N9-C8	6.79	142.46	127.14
1	D	3	6MZ	N3-C4-N9	6.71	138.15	127.08
1	F	3	6MZ	C4-C5-C6	6.40	121.77	116.81
1	E	3	6MZ	N3-C4-N9	6.38	137.59	127.08
1	F	3	6MZ	C5-C4-N3	-6.36	118.45	126.75
1	F	3	6MZ	C4-N9-C1'	-6.20	111.83	126.59
1	D	3	6MZ	C4-N9-C1'	-5.90	112.54	126.59
1	F	3	6MZ	N3-C4-N9	5.67	136.43	127.08
1	E	3	6MZ	C4-C5-C6	5.46	121.04	116.81
1	D	3	6MZ	N1-C2-N3	-5.41	120.13	128.60
1	F	3	6MZ	C1'-N9-C8	5.16	138.79	127.14
1	D	3	6MZ	C4-C5-C6	5.14	120.80	116.81
1	E	3	6MZ	N1-C2-N3	-4.97	120.83	128.60
1	D	3	6MZ	C1'-N9-C8	4.96	138.32	127.14
1	E	3	6MZ	C5-C6-N1	4.80	123.31	118.20
1	D	3	6MZ	C6-C5-N7	-4.69	127.32	132.39
1	E	3	6MZ	C2-N3-C4	4.27	121.83	111.75
1	F	3	6MZ	O4'-C1'-N9	-4.04	100.10	108.06
1	E	3	6MZ	N9-C8-N7	-3.95	108.51	113.91
1	F	3	6MZ	C6-C5-N7	-3.87	128.20	132.39
1	D	3	6MZ	C2-N3-C4	3.66	120.41	111.75
1	F	3	6MZ	N1-C2-N3	-3.64	122.92	128.60
1	F	3	6MZ	N9-C8-N7	-3.55	109.06	113.91
1	E	3	6MZ	C6-C5-N7	-3.38	128.73	132.39
1	F	3	6MZ	C4-N9-C8	3.25	109.25	105.73
1	D	3	6MZ	N9-C8-N7	-3.25	109.47	113.91
1	D	3	6MZ	C4-N9-C8	3.06	109.05	105.73
1	F	3	6MZ	C2-N3-C4	2.91	118.63	111.75
1	D	3	6MZ	C5-C6-N1	2.75	121.13	118.20
1	E	3	6MZ	C4-N9-C8	2.70	108.66	105.73
1	E	3	6MZ	C5-N7-C8	2.66	107.28	103.51
1	F	3	6MZ	C5-C6-N1	2.51	120.88	118.20
1	F	3	6MZ	C9-N6-C6	2.49	125.02	122.87
1	F	3	6MZ	C3'-C2'-C1'	2.43	106.04	101.43
1	D	3	6MZ	C9-N6-C6	2.28	124.84	122.87
1	F	3	6MZ	C5-N7-C8	2.11	106.51	103.51

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	3	6MZ	C4'-C5'-O5'-P

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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

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	$\# Z > 2$
4	EDO	B	607	-	3,3,3	0.61	0	2,2,2	0.65	0
5	SO4	B	602	-	4,4,4	0.11	0	6,6,6	0.15	0
5	SO4	C	604	-	4,4,4	0.13	0	6,6,6	0.22	0
4	EDO	A	601	-	3,3,3	0.50	0	2,2,2	0.36	0
5	SO4	C	601	-	4,4,4	0.16	0	6,6,6	0.12	0
5	SO4	C	603	-	4,4,4	0.20	0	6,6,6	0.28	0
5	SO4	B	606	-	4,4,4	0.12	0	6,6,6	0.25	0
4	EDO	A	602	-	3,3,3	0.49	0	2,2,2	0.62	0
4	EDO	B	603	-	3,3,3	0.60	0	2,2,2	0.40	0
4	EDO	C	602	-	3,3,3	0.47	0	2,2,2	0.54	0
5	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.21	0
4	EDO	B	605	-	3,3,3	0.45	0	2,2,2	0.36	0
5	SO4	A	603	-	4,4,4	0.10	0	6,6,6	0.19	0
3	GTP	D	101	-	23,25,34	0.48	0	32,37,54	0.41	0
4	EDO	B	601	-	3,3,3	0.56	0	2,2,2	0.60	0

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	EDO	B	607	-	-	1/1/1/1	-
4	EDO	A	601	-	-	0/1/1/1	-
4	EDO	A	602	-	-	1/1/1/1	-
4	EDO	B	603	-	-	0/1/1/1	-
4	EDO	C	602	-	-	1/1/1/1	-
4	EDO	B	605	-	-	0/1/1/1	-
3	GTP	D	101	-	-	0/7/25/38	0/3/3/3
4	EDO	B	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	EDO	O1-C1-C2-O2
4	C	602	EDO	O1-C1-C2-O2
4	B	607	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	607	EDO	2	0
5	A	603	SO4	1	0
3	D	101	GTP	3	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	D	2/14 (14%)	0.91	0	100 100	66, 66, 66, 87	0
1	E	2/14 (14%)	0.89	0	100 100	83, 83, 83, 91	0
1	F	3/14 (21%)	0.90	1 (33%)	1 1	68, 68, 77, 95	0
2	A	163/169 (96%)	1.12	29 (17%)	4 4	33, 66, 94, 108	1 (0%)
2	B	166/169 (98%)	0.93	24 (14%)	6 6	32, 62, 87, 113	2 (1%)
2	C	166/169 (98%)	1.47	37 (22%)	2 2	38, 74, 100, 132	1 (0%)
All	All	502/549 (91%)	1.17	91 (18%)	3 3	32, 68, 96, 132	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	424	SER	5.5
2	B	343	GLY	5.0
2	B	508	ARG	4.7
2	A	501	TYR	4.6
2	B	427	HIS	4.4
2	B	424	SER	4.2
2	C	509	HIS	4.1
2	C	423	GLY	4.0
2	C	430	LEU	4.0
2	A	499	ASP	3.8
2	A	345	THR	3.7
2	C	431	PRO	3.7
2	B	434	MET	3.6
2	C	344	GLY	3.6
2	A	502	GLN	3.6
2	C	422	GLY	3.4
2	C	425	PRO	3.4
2	B	503	VAL	3.4
2	C	432	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	454	PRO	3.2
2	B	425	PRO	3.2
2	A	506	LYS	3.1
2	C	501	TYR	3.1
2	C	389	LEU	3.0
2	A	420	HIS	3.0
2	C	459	ALA	3.0
2	B	500	LEU	2.9
2	C	433	GLY	2.9
2	A	503	VAL	2.9
2	B	344	GLY	2.8
2	B	430	LEU	2.8
2	C	456	THR	2.8
2	A	429	VAL	2.7
2	B	501	TYR	2.7
2	A	430	LEU	2.7
2	A	440	GLY	2.7
2	A	436	ALA	2.7
2	C	420	HIS	2.7
2	C	345	THR	2.6
2	A	439	LEU	2.6
2	C	503	VAL	2.6
2	B	498	ILE	2.6
2	B	432	ALA	2.6
2	A	437	LYS	2.6
2	A	434	MET	2.6
2	C	438	MET	2.5
2	A	421	HIS	2.5
2	C	392	ARG	2.5
2	C	434	MET	2.5
2	C	461	LEU	2.5
2	B	433	GLY	2.5
2	B	505	HIS	2.5
2	B	423	GLY	2.4
2	A	425	PRO	2.4
2	C	439	LEU	2.4
2	B	345	THR	2.4
2	C	505	HIS	2.4
2	C	395	ARG	2.3
2	B	437	LYS	2.3
2	A	346	SER	2.3
2	A	507	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	482	LEU	2.3
1	F	6	G	2.3
2	A	423	GLY	2.3
2	C	498	ILE	2.3
2	C	429	VAL	2.3
2	B	431	PRO	2.2
2	C	346	SER	2.2
2	A	474	GLY	2.2
2	C	440	GLY	2.2
2	A	350	TYR	2.2
2	A	497	SER	2.1
2	C	462	THR	2.1
2	A	473	ILE	2.1
2	C	448	ILE	2.1
2	C	407	GLY	2.1
2	B	504	ILE	2.1
2	C	452	GLU	2.1
2	B	389	LEU	2.1
2	C	494	PRO	2.1
2	B	420	HIS	2.1
2	C	426	ILE	2.1
2	A	422	GLY	2.0
2	A	382	VAL	2.0
2	C	393	SER	2.0
2	B	506	LYS	2.0
2	A	472	LYS	2.0
2	A	433	GLY	2.0
2	B	393	SER	2.0
2	A	468	HIS	2.0
2	A	505	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å ²)	Q<0.9
1	6MZ	E	3	23/24	0.92	0.12	52,70,117,138	0
1	6MZ	F	3	19/24	0.94	0.10	54,57,75,75	0
1	6MZ	D	3	20/24	0.96	0.09	46,54,67,71	0

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
5	SO4	B	602	5/5	0.69	0.15	93,95,108,122	0
5	SO4	A	603	5/5	0.72	0.14	93,97,129,136	0
5	SO4	C	604	5/5	0.75	0.13	88,88,112,115	0
5	SO4	C	603	5/5	0.77	0.11	80,83,107,109	0
5	SO4	B	604	5/5	0.77	0.11	81,86,109,122	0
3	GTP	D	101	23/32	0.80	0.17	76,116,156,174	0
5	SO4	B	606	5/5	0.81	0.12	77,83,90,98	0
5	SO4	C	601	5/5	0.81	0.10	84,88,115,128	0
6	NA	C	605	1/1	0.82	0.22	78,78,78,78	0
4	EDO	B	607	4/4	0.84	0.20	59,77,93,93	0
4	EDO	B	603	4/4	0.85	0.18	65,80,92,96	0
4	EDO	B	605	4/4	0.89	0.17	60,72,79,79	0
4	EDO	A	602	4/4	0.91	0.14	65,78,84,86	0
4	EDO	C	602	4/4	0.91	0.14	62,74,82,90	0
4	EDO	B	601	4/4	0.98	0.08	51,61,63,66	0
4	EDO	A	601	4/4	0.98	0.09	50,60,64,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.