



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:47 AM BST

PDB ID : 6WEA
Title : YTH domain of human YTHDC1 with a 10mer Oligo Containing N6mA
Authors : Horton, J.R.; Cheng, X.
Deposited on : 2020-04-01
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

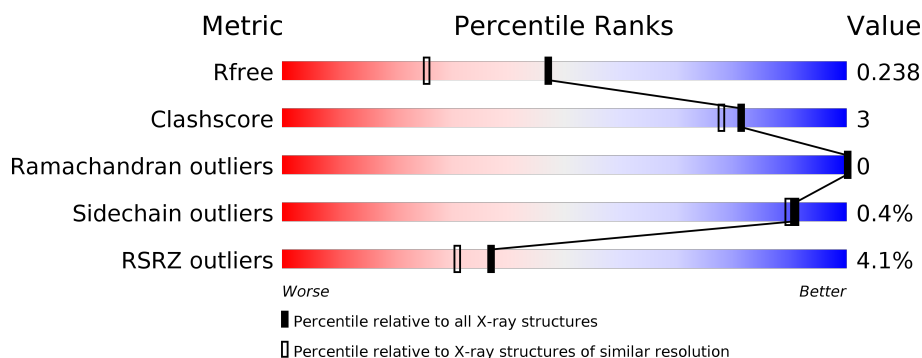
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	166	<div> <div>93%</div> <div>5% •</div> </div>
1	B	166	<div> <div>%</div> <div>94%</div> <div>• •</div> </div>
1	C	166	<div> <div>13%</div> <div>87%</div> <div>11% •</div> </div>
1	D	166	<div> <div>3%</div> <div>92%</div> <div>5% •</div> </div>
2	E	10	<div> <div>90%</div> <div>10%</div> </div>
2	F	10	<div> <div>60%</div> <div>30%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	10	 80%20%
2	H	10	 70%30%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6586 atoms, of which 0 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 protein called YTH domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	1	0
			1292	832	231	223	6			
1	B	163	Total	C	N	O	S	0	3	0
			1299	837	229	227	6			
1	C	163	Total	C	N	O	S	0	4	0
			1285	826	228	225	6			
1	D	162	Total	C	N	O	S	0	3	0
			1294	834	231	223	6			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*CP*GP*GP*(6MA)P*CP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			201	97	36	59	9			
2	F	10	Total	C	N	O	P	0	0	0
			201	97	36	59	9			
2	G	10	Total	C	N	O	P	0	0	0
			201	97	36	59	9			
2	H	10	Total	C	N	O	P	0	0	0
			201	97	36	59	9			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 2 2	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	153	Total O 153 153	0	0
6	B	137	Total O 137 137	0	0
6	C	30	Total O 30 30	0	0
6	D	62	Total O 62 62	0	0
6	E	39	Total O 39 39	0	0
6	F	15	Total O 15 15	0	0
6	G	38	Total O 38 38	0	0
6	H	23	Total O 23 23	0	0

3 Residue-property plots

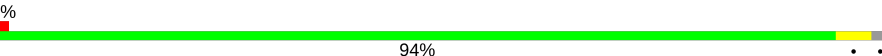
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: YTH domain-containing protein 1

Chain A: 




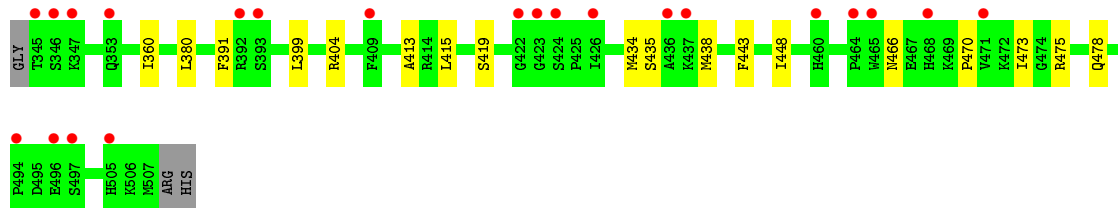
- Molecule 1: YTH domain-containing protein 1

Chain B: 



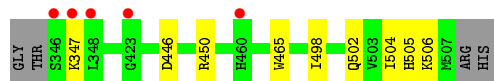
- Molecule 1: YTH domain-containing protein 1

Chain C: 




- Molecule 1: YTH domain-containing protein 1

Chain D: 



- Molecule 2: DNA (5'-D(*CP*GP*CP*GP*GP*(6MA)P*CP*TP*TP*C)-3')

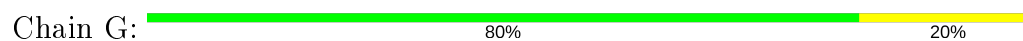
Chain E: 



- Molecule 2: DNA (5'-D(*CP*GP*CP*GP*GP*(6MA)P*CP*TP*TP*C)-3')



- Molecule 2: DNA (5'-D(*CP*GP*CP*GP*GP*(6MA)P*CP*TP*TP*C)-3')



- Molecule 2: DNA (5'-D(*CP*GP*CP*GP*GP*(6MA)P*CP*TP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.94Å 42.64Å 119.87Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	40.59 – 1.80 40.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (40.59-1.80) 95.1 (40.59-1.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.210 , 0.237 0.210 , 0.238	Depositor DCC
R_{free} test set	1997 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6586	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8167e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 6MA, EDO, SO4

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	0.32	0/1328	0.47	0/1794
1	B	0.31	0/1340	0.46	0/1810
1	C	0.26	0/1327	0.43	0/1799
1	D	0.29	0/1333	0.44	0/1800
2	E	0.70	0/198	0.94	0/301
2	F	0.57	0/198	0.97	0/301
2	G	0.61	0/198	0.90	0/301
2	H	0.62	0/198	0.95	0/301
All	All	0.36	0/6120	0.55	0/8407

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 [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	1292	0	1299	7	0
1	B	1299	0	1315	3	0
1	C	1285	0	1261	13	0
1	D	1294	0	1300	5	0
2	E	201	0	116	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	201	0	116	5	0
2	G	201	0	116	1	0
2	H	201	0	116	1	0
3	A	24	0	36	2	0
3	B	12	0	18	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
3	G	4	0	6	1	0
4	A	30	0	0	0	0
4	B	20	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	A	2	0	0	0	0
6	A	153	0	0	2	0
6	B	137	0	0	0	0
6	C	30	0	0	0	0
6	D	62	0	0	1	0
6	E	39	0	0	0	0
6	F	15	0	0	0	0
6	G	38	0	0	0	0
6	H	23	0	0	0	0
All	All	6586	0	5711	31	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 (31) 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:B:450[A]:ARG:NH2	1:B:497:SER:OG	2.25	0.69
1:A:450[B]:ARG:NH2	1:A:497:SER:OG	2.26	0.69
2:G:7:DC:H42	3:G:101:EDO:H22	1.61	0.65
1:A:406:SER:HB2	3:A:610:EDO:H11	1.78	0.63
1:A:345:THR:N	6:A:703:HOH:O	2.31	0.63
1:D:450[B]:ARG:HG3	1:D:498:ILE:HD11	1.85	0.58
1:D:505:HIS:ND1	6:D:701:HOH:O	2.34	0.54
2:F:4:DG:H2''	2:F:5:DG:C8	2.44	0.53
1:C:466:ASN:ND2	1:C:478:GLN:OE1	2.43	0.51
1:C:404:ARG:HG3	2:F:7:DC:H5'	1.93	0.51
1:A:408:LYS:HD2	3:A:610:EDO:H12	1.95	0.48
1:D:446:ASP:OD2	1:D:506:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:DG:H2''	2:H:5:DG:C8	2.49	0.47
1:C:391:PHE:HB2	1:C:415:LEU:HD23	1.96	0.47
1:A:503:VAL:HG23	6:A:721:HOH:O	2.14	0.46
1:A:415:LEU:HD23	1:A:445:ILE:HG22	1.98	0.46
1:C:470:PRO:HG2	1:C:473:ILE:HD12	1.97	0.45
1:C:404:ARG:HH21	2:F:6:6MA:H4'	1.83	0.44
1:C:475:ARG:HG3	2:F:7:DC:O4'	2.18	0.43
1:D:347:LYS:HG3	1:D:504:ILE:HD11	2.01	0.43
1:B:431:PRO:HD2	1:B:434:MET:HE2	2.01	0.43
1:C:380:LEU:HD21	1:C:434:MET:HE3	2.01	0.43
1:D:502:GLN:O	1:D:506:LYS:HD2	2.19	0.42
1:C:419:SER:HB3	1:C:443:PHE:CZ	2.53	0.42
1:B:446:ASP:HB3	1:B:503:VAL:HG22	2.02	0.42
1:C:360:ILE:HG13	1:C:399:LEU:HB3	2.02	0.41
1:C:435:SER:OG	1:C:438:MET:HG3	2.20	0.41
1:C:415:LEU:HD11	1:C:443:PHE:CD2	2.55	0.41
1:C:413:ALA:HA	1:C:448[B]:ILE:HG12	2.02	0.40
1:A:439:LEU:HA	1:A:439:LEU:HD23	1.90	0.40
1:C:404:ARG:NH2	2:F:6:6MA:OP1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
1	A	162/166 (98%)	161 (99%)	1 (1%)	0	100	100
1	B	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
1	C	165/166 (99%)	164 (99%)	1 (1%)	0	100	100
1	D	163/166 (98%)	162 (99%)	1 (1%)	0	100	100
All	All	654/664 (98%)	650 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	
1	A	139/145 (96%)	139 (100%)	0	100	100
1	B	142/145 (98%)	141 (99%)	1 (1%)	84	81
1	C	136/145 (94%)	136 (100%)	0	100	100
1	D	139/145 (96%)	138 (99%)	1 (1%)	84	81
All	All	556/580 (96%)	554 (100%)	2 (0%)	91	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	416	SER
1	D	465	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
2	6MA	H	6	2	18,24,25	3.38	6 (33%)	15,34,37	2.35	5 (33%)
2	6MA	G	6	2	18,24,25	3.28	5 (27%)	15,34,37	2.11	5 (33%)
2	6MA	F	6	2	18,24,25	3.44	5 (27%)	15,34,37	2.16	4 (26%)
2	6MA	E	6	2	18,24,25	3.31	5 (27%)	15,34,37	2.22	4 (26%)

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	6MA	H	6	2	-	1/5/23/24	0/3/3/3
2	6MA	G	6	2	-	1/5/23/24	0/3/3/3
2	6MA	F	6	2	-	1/5/23/24	0/3/3/3
2	6MA	E	6	2	-	1/5/23/24	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	6	6MA	O4'-C1'	7.95	1.60	1.42
2	F	6	6MA	O4'-C1'	7.83	1.59	1.42
2	E	6	6MA	O4'-C1'	7.80	1.59	1.42
2	H	6	6MA	O4'-C1'	7.75	1.59	1.42
2	H	6	6MA	O4'-C4'	-7.20	1.28	1.45
2	F	6	6MA	O4'-C4'	-7.18	1.28	1.45
2	E	6	6MA	O4'-C4'	-6.75	1.29	1.45
2	G	6	6MA	O4'-C4'	-6.62	1.30	1.45
2	E	6	6MA	C6-N6	6.47	1.45	1.35
2	F	6	6MA	C6-N6	6.22	1.45	1.35
2	H	6	6MA	C6-N6	6.19	1.45	1.35
2	G	6	6MA	C6-N6	5.93	1.44	1.35
2	F	6	6MA	C2'-C1'	-5.91	1.35	1.52
2	H	6	6MA	C2'-C1'	-5.63	1.36	1.52
2	E	6	6MA	C2'-C1'	-5.48	1.37	1.52
2	G	6	6MA	C2'-C1'	-5.38	1.37	1.52
2	F	6	6MA	O3'-C3'	-2.98	1.37	1.43
2	H	6	6MA	O3'-C3'	-2.56	1.37	1.43
2	H	6	6MA	O5'-C5'	-2.39	1.38	1.44
2	G	6	6MA	O3'-C3'	-2.16	1.38	1.43
2	E	6	6MA	O3'-C3'	-2.05	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	6MA	C2-N1-C6	5.38	121.20	116.59
2	F	6	6MA	C2-N1-C6	4.99	120.87	116.59
2	H	6	6MA	C2-N1-C6	4.89	120.78	116.59
2	G	6	6MA	C2-N1-C6	4.74	120.66	116.59
2	H	6	6MA	N3-C2-N1	-4.71	121.32	128.68
2	F	6	6MA	N3-C2-N1	-4.62	121.45	128.68
2	G	6	6MA	N3-C2-N1	-4.51	121.63	128.68
2	E	6	6MA	N3-C2-N1	-4.45	121.72	128.68
2	H	6	6MA	C1-N6-C6	-4.03	119.40	122.87
2	F	6	6MA	C1-N6-C6	-3.09	120.21	122.87
2	E	6	6MA	C4-C5-N7	-2.85	106.43	109.40
2	G	6	6MA	C4-C5-N7	-2.82	106.46	109.40
2	H	6	6MA	C4-C5-N7	-2.73	106.55	109.40
2	E	6	6MA	C3'-C2'-C1'	2.46	108.71	102.54
2	F	6	6MA	C4-C5-N7	-2.39	106.91	109.40
2	H	6	6MA	C4'-O4'-C1'	-2.36	103.75	109.45
2	G	6	6MA	C3'-C2'-C1'	2.20	108.06	102.54
2	G	6	6MA	C1-N6-C6	-2.12	121.05	122.87

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	6	6MA	C4'-C5'-O5'-P
2	H	6	6MA	C4'-C5'-O5'-P
2	G	6	6MA	C4'-C5'-O5'-P
2	E	6	6MA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	6	6MA	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	SO4	C	602	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	B	601	-	3,3,3	0.52	0	2,2,2	0.24	0
4	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	A	608	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	D	603	-	3,3,3	0.44	0	2,2,2	0.33	0
4	SO4	A	613	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	D	602	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	B	604	-	4,4,4	0.13	0	6,6,6	0.07	0
3	EDO	A	601	-	3,3,3	0.50	0	2,2,2	0.30	0
4	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.04	0
3	EDO	B	607	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	A	609	-	3,3,3	0.45	0	2,2,2	0.45	0
3	EDO	A	611	-	3,3,3	0.46	0	2,2,2	0.32	0
4	SO4	D	601	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	A	607	-	4,4,4	0.12	0	6,6,6	0.06	0
4	SO4	B	603	-	4,4,4	0.15	0	6,6,6	0.06	0
3	EDO	B	606	-	3,3,3	0.42	0	2,2,2	0.40	0
4	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.04	0
3	EDO	G	101	-	3,3,3	0.44	0	2,2,2	0.44	0
3	EDO	A	605	-	3,3,3	0.46	0	2,2,2	0.34	0
4	SO4	A	606	-	4,4,4	0.15	0	6,6,6	0.05	0
3	EDO	C	601	-	3,3,3	0.45	0	2,2,2	0.36	0
4	SO4	A	602	-	4,4,4	0.15	0	6,6,6	0.07	0
3	EDO	A	610	-	3,3,3	0.48	0	2,2,2	0.28	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
3	EDO	A	611	-	-	0/1/1/1	-
3	EDO	A	608	-	-	1/1/1/1	-
3	EDO	B	601	-	-	0/1/1/1	-
3	EDO	B	606	-	-	1/1/1/1	-
3	EDO	B	607	-	-	1/1/1/1	-
3	EDO	A	609	-	-	0/1/1/1	-
3	EDO	G	101	-	-	1/1/1/1	-
3	EDO	A	605	-	-	0/1/1/1	-
3	EDO	D	603	-	-	0/1/1/1	-
3	EDO	C	601	-	-	0/1/1/1	-
3	EDO	A	601	-	-	0/1/1/1	-
3	EDO	A	610	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	608	EDO	O1-C1-C2-O2
3	B	606	EDO	O1-C1-C2-O2
3	B	607	EDO	O1-C1-C2-O2
3	G	101	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	101	EDO	1	0
3	A	610	EDO	2	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	163/166 (98%)	-0.38	0 100 100	6, 13, 30, 41	0
1	B	163/166 (98%)	-0.16	1 (0%) 89 87	8, 16, 47, 73	0
1	C	163/166 (98%)	0.82	22 (13%) 3 2	25, 42, 59, 74	0
1	D	162/166 (97%)	0.11	5 (3%) 49 43	16, 25, 47, 61	0
2	E	9/10 (90%)	-0.68	0 100 100	11, 13, 22, 26	0
2	F	9/10 (90%)	-0.21	0 100 100	15, 25, 42, 55	0
2	G	9/10 (90%)	-0.63	0 100 100	15, 16, 29, 31	0
2	H	9/10 (90%)	-0.48	0 100 100	22, 24, 28, 39	0
All	All	687/704 (97%)	0.07	28 (4%) 37 31	6, 23, 53, 74	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	345	THR	4.5
1	C	346	SER	4.5
1	D	346	SER	4.2
1	C	465	TRP	4.0
1	C	423	GLY	3.1
1	C	464	PRO	3.0
1	C	496	GLU	3.0
1	B	345	THR	3.0
1	C	494	PRO	2.9
1	D	423	GLY	2.7
1	C	471	VAL	2.7
1	C	422	GLY	2.7
1	C	424	SER	2.7
1	C	437	LYS	2.6
1	D	460	HIS	2.6
1	C	392	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	348	LEU	2.5
1	C	468	HIS	2.5
1	C	497	SER	2.5
1	C	436	ALA	2.4
1	D	347	LYS	2.4
1	C	409	PHE	2.3
1	C	426	ILE	2.3
1	C	460	HIS	2.2
1	C	353	GLN	2.1
1	C	393	SER	2.0
1	C	347	LYS	2.0
1	C	505	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	6MA	H	6	22/23	0.90	0.11	20,22,26,27	0
2	6MA	F	6	22/23	0.94	0.10	33,35,37,37	0
2	6MA	G	6	22/23	0.96	0.09	8,9,15,17	0
2	6MA	E	6	22/23	0.97	0.09	8,10,14,15	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
3	EDO	B	607	4/4	0.67	0.22	41,43,45,47	0
4	SO4	B	602	5/5	0.77	0.23	70,72,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	G	101	4/4	0.78	0.16	41,41,42,42	0
4	SO4	A	603	5/5	0.82	0.20	73,73,75,75	0
3	EDO	A	610	4/4	0.84	0.22	39,41,43,45	0
4	SO4	A	604	5/5	0.85	0.20	71,72,73,73	0
4	SO4	A	613	5/5	0.86	0.17	77,77,78,79	0
4	SO4	B	605	5/5	0.86	0.21	60,62,62,63	0
3	EDO	A	611	4/4	0.86	0.12	44,46,47,49	0
4	SO4	A	606	5/5	0.87	0.17	68,69,70,70	0
4	SO4	B	604	5/5	0.87	0.17	77,77,77,78	0
3	EDO	A	605	4/4	0.88	0.20	29,29,31,34	0
3	EDO	A	609	4/4	0.91	0.21	33,34,36,37	0
4	SO4	D	602	5/5	0.91	0.14	66,66,67,67	0
3	EDO	B	606	4/4	0.91	0.18	38,38,39,39	0
3	EDO	A	608	4/4	0.91	0.21	38,38,38,39	0
3	EDO	C	601	4/4	0.94	0.11	33,34,35,36	0
4	SO4	D	601	5/5	0.95	0.15	41,41,42,43	0
4	SO4	C	602	5/5	0.95	0.17	66,67,67,67	0
3	EDO	D	603	4/4	0.97	0.08	23,24,24,24	0
4	SO4	B	603	5/5	0.98	0.07	35,36,37,37	0
3	EDO	A	601	4/4	0.98	0.10	10,10,10,13	0
3	EDO	B	601	4/4	0.98	0.09	9,11,11,12	0
4	SO4	A	602	5/5	0.98	0.09	33,34,34,37	0
4	SO4	A	607	5/5	0.98	0.14	43,44,45,45	0
5	NA	A	612[A]	1/1	0.99	0.21	5,5,5,5	1
5	NA	A	612[B]	1/1	0.99	0.21	5,5,5,5	1

6.5 Other polymers

There are no such residues in this entry.