Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:21 AM EDT

PDB ID	:	4K6O
Title	:	X-ray structure uridine phosphorylase from Vibrio cholerae in complex with 6-methyluracil at 1.17 A resolution
Authors	:	Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.
Deposited on	:	2013-04-16
Resolution	:	1.17 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 (i) 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 (i)) were used in the production of this report:

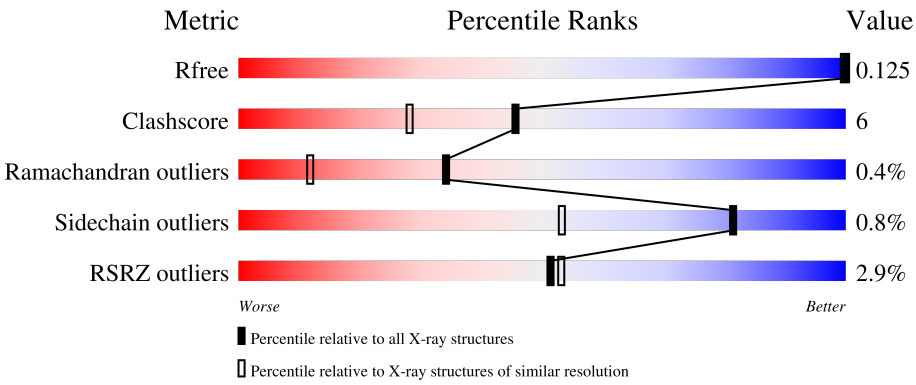
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.17 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	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

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 <=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	253	3% 90% 9%
1	B	253	4% 87% 10% • •
1	C	253	3% 88% 9% •
1	D	253	4% 90% 9%
1	E	253	% 91% 8% •

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Mol	Chain	Length	Quality of chain
1	F	253	% 88% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EOH	A	308	-	-	X	-
7	EOH	C	311	-	-	X	-
7	EOH	D	307	-	-	X	-
7	EOH	E	307	-	-	X	-
7	EOH	F	308	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 28389 atoms, of which 13201 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.

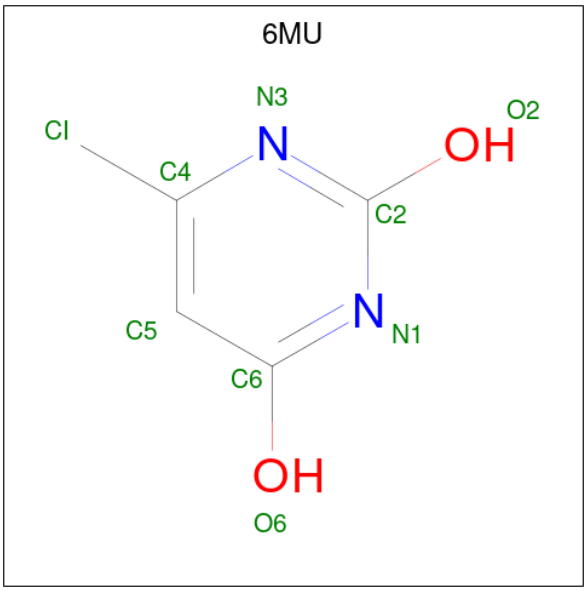
- Molecule 1 is a protein called Uridine phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	252	4363	1342	2227	375	401	18	0	46	0
1	B	248	4197	1296	2147	355	381	18	0	39	0
1	C	247	4117	1273	2106	339	379	20	0	33	0
1	D	252	4260	1316	2173	357	396	18	0	40	0
1	E	251	4290	1322	2201	359	390	18	0	39	0
1	F	252	4255	1314	2189	350	384	18	0	36	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	3	3	3	0	0
2	B	2	2	2	0	0
2	C	3	3	3	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	2	2	2	0	0

- Molecule 3 is 6-methylpyrimidine-2,4-diol (three-letter code: 6MU) (formula: $C_5H_6N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	15	5	6	2	2	0	0
3	B	1	15	5	6	2	2	0	0
3	C	1	15	5	6	2	2	0	0
3	D	1	15	5	6	2	2	0	0
3	E	1	15	5	6	2	2	0	0
3	F	1	15	5	6	2	2	0	0

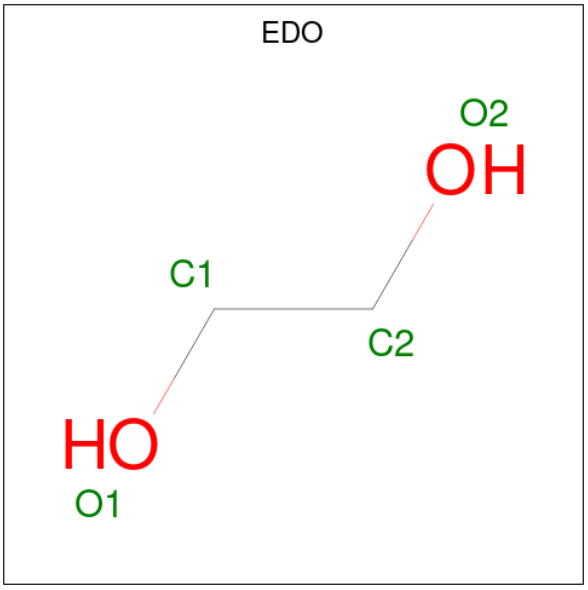
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0
4	B	3	3	3	0	0
4	C	3	3	3	0	0
4	D	3	3	3	0	0
4	E	2	2	2	0	0
4	F	3	3	3	0	0

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

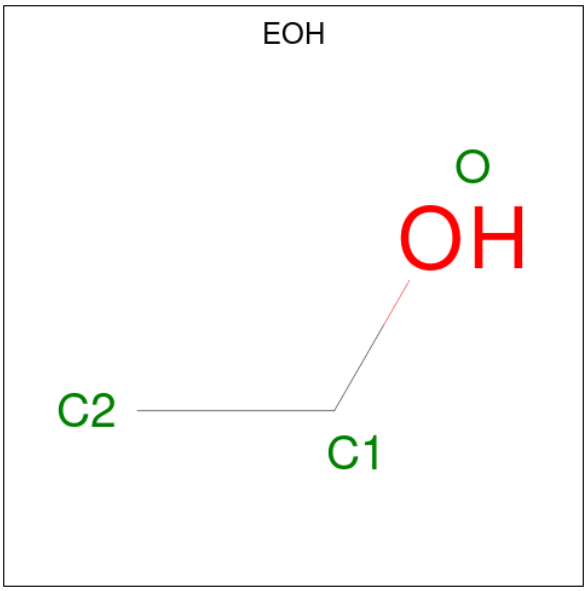
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



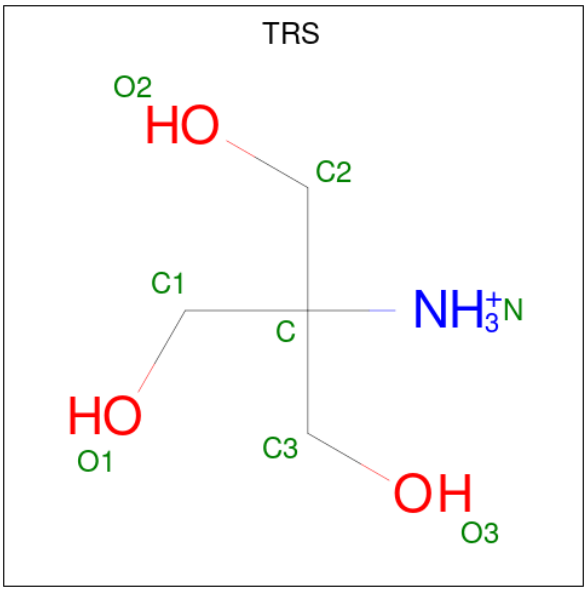
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 10 2 6 2	0	0
6	B	1	Total C H O 10 2 6 2	0	0
6	D	1	Total C H O 10 2 6 2	0	0
6	F	1	Total C H O 10 2 6 2	0	0

- Molecule 7 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



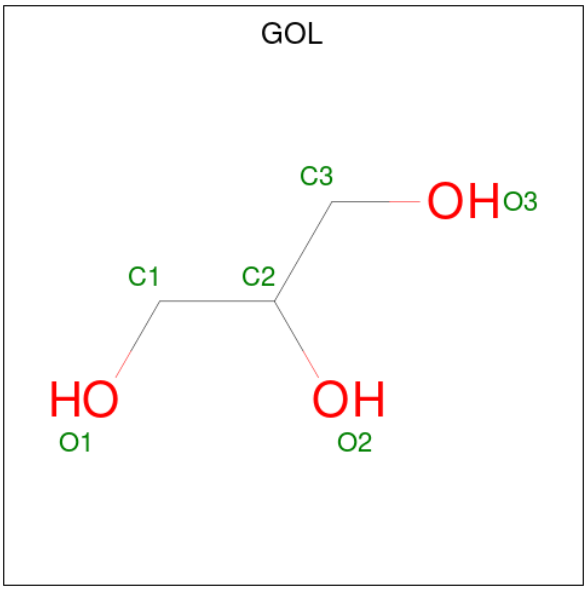
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	9	2	6	1	0	0
7	B	1	9	2	6	1	0	0
7	C	1	9	2	6	1	0	0
7	C	1	9	2	6	1	0	0
7	D	1	9	2	6	1	0	0
7	E	1	9	2	6	1	0	0
7	F	1	9	2	6	1	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	B	1	20	4	12	1	3	0	0
			Total	C	H	N	O		
8	C	1	20	4	12	1	3	0	0
			Total	C	H	N	O		
8	E	1	20	4	12	1	3	0	0
			Total	C	H	N	O		
8	E	1	20	4	12	1	3	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	C	1	14	3	8	3	0	0

- Molecule 10 is water.

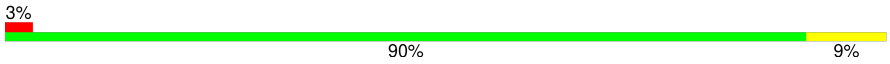
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	434	444	444	0	10
10	B	365	382	382	0	17
10	C	390	405	405	0	14
10	D	424	447	447	0	22
10	E	437	452	452	0	15
10	F	432	458	458	0	25

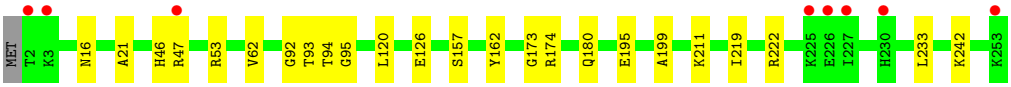
3 Residue-property plots (i)

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: Uridine phosphorylase

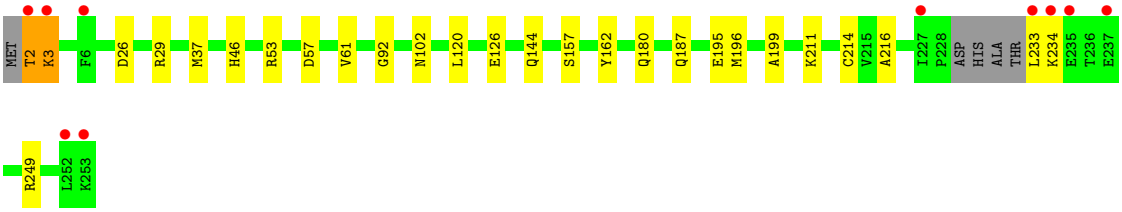
Chain A:





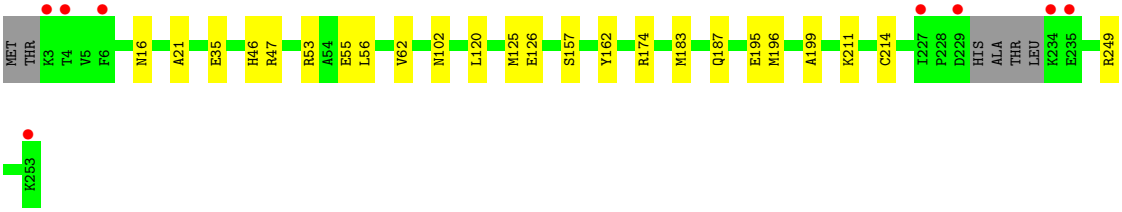
• Molecule 1: Uridine phosphorylase

Chain B:



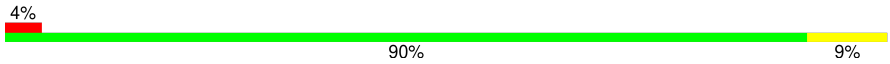
• Molecule 1: Uridine phosphorylase

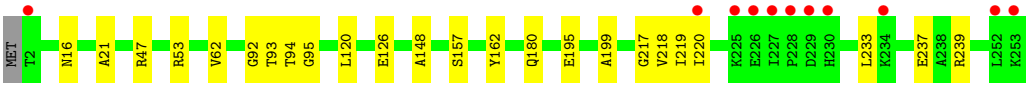
Chain C:



• Molecule 1: Uridine phosphorylase

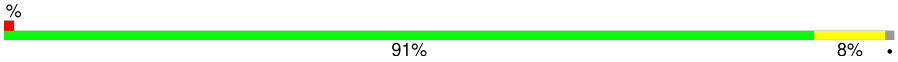
Chain D:

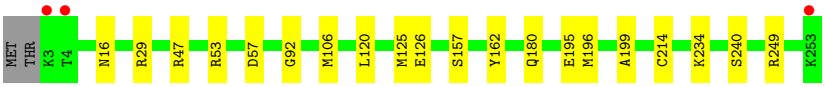




• Molecule 1: Uridine phosphorylase

Chain E:





- Molecule 1: Uridine phosphorylase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.01Å 97.10Å 93.02Å 90.00° 119.99° 90.00°	Depositor
Resolution (Å)	40.28 – 1.17 80.55 – 1.17	Depositor EDS
% Data completeness (in resolution range)	94.1 (40.28-1.17) 94.1 (80.55-1.17)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 1.17Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.108 , 0.128 0.106 , 0.125	Depositor DCC
R_{free} test set	22537 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	7.9	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.107 for -h-l,k,h 0.107 for l,k,-h-l 0.014 for h,-k,-h-l 0.015 for -h-l,-k,l 0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	28389	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TRS, CL, EDO, MG, NA, 6MU, EOH, GOL

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	0.31	0/2283	0.56	0/3085
1	B	0.31	0/2207	0.58	0/2977
1	C	0.34	0/2137	0.60	0/2885
1	D	0.32	0/2230	0.57	0/3012
1	E	0.32	0/2236	0.58	0/3018
1	F	0.33	0/2216	0.58	0/2995
All	All	0.32	0/13309	0.58	0/17972

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	2136	2227	2138	26	0
1	B	2050	2147	2058	22	0
1	C	2011	2106	2071	20	0
1	D	2087	2173	2106	26	0
1	E	2089	2201	2141	15	0
1	F	2066	2189	2148	25	0
2	A	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	1	0
2	C	3	0	0	1	0
2	D	1	0	0	1	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
3	A	9	6	5	2	0
3	B	9	6	4	0	0
3	C	9	6	4	0	0
3	D	9	6	5	1	0
3	E	9	6	4	0	0
3	F	9	6	4	2	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	A	4	6	6	0	0
6	B	4	6	6	1	0
6	D	4	6	6	1	0
6	F	4	6	6	0	0
7	A	3	6	6	4	0
7	B	3	6	6	1	0
7	C	6	12	12	5	0
7	D	3	6	6	4	0
7	E	3	6	6	4	0
7	F	3	6	6	4	0
8	B	8	12	12	1	0
8	C	8	12	12	1	0
8	E	16	24	24	6	0
9	C	6	8	8	2	0
10	A	444	0	0	25	0
10	B	382	0	0	17	0
10	C	405	0	0	13	0
10	D	447	0	0	23	0
10	E	452	0	0	10	0
10	F	458	0	0	19	0
All	All	15188	13201	12810	163	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 6.

All (163) 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:180[A]:GLN:NE2	10:B:474:HOH:O	1.85	1.09
1:F:214[B]:CYS:SG	10:F:712:HOH:O	2.14	1.03
1:A:95[A]:GLY:O	10:A:770:HOH:O	1.79	1.00
1:A:93[B]:THR:HG23	10:A:831:HOH:O	1.62	0.97
1:E:214[B]:CYS:SG	10:E:579:HOH:O	2.23	0.97
2:B:301:CL:CL	10:B:733:HOH:O	2.19	0.97
1:F:53[B]:ARG:NH2	10:F:779:HOH:O	1.98	0.95
1:D:93[A]:THR:HG23	10:D:819:HOH:O	1.66	0.95
1:A:211:LYS:NZ	10:A:633:HOH:O	2.02	0.93
1:D:180[A]:GLN:NE2	10:D:457:HOH:O	2.02	0.91
1:A:126[A]:GLU:OE1	10:A:834:HOH:O	1.88	0.90
1:C:126[B]:GLU:OE1	10:C:494:HOH:O	1.89	0.90
1:B:126[B]:GLU:OE2	10:B:504:HOH:O	1.89	0.90
1:D:95[B]:GLY:O	10:D:820:HOH:O	1.90	0.89
1:E:126[B]:GLU:OE1	10:E:554:HOH:O	1.90	0.88
1:A:180[B]:GLN:OE1	10:A:440:HOH:O	1.92	0.87
3:A:303:6MU:O6	10:A:562:HOH:O	1.92	0.87
1:D:53[B]:ARG:NH2	10:D:625:HOH:O	2.07	0.86
1:A:95[A]:GLY:N	10:A:512:HOH:O	2.06	0.84
10:B:765[B]:HOH:O	1:C:125[B]:MET:SD	2.35	0.84
1:D:126[B]:GLU:OE1	10:D:598:HOH:O	1.96	0.84
2:D:301:CL:CL	10:D:559:HOH:O	2.33	0.83
1:A:174[A]:ARG:NH2	10:A:703[A]:HOH:O	2.12	0.81
1:C:211[A]:LYS:NZ	10:C:605:HOH:O	2.13	0.81
1:C:35[B]:GLU:OE2	10:C:787:HOH:O	1.99	0.79
1:C:187[B]:GLN:OE1	10:C:491:HOH:O	1.98	0.79
1:C:174[B]:ARG:NH1	10:C:555:HOH:O	2.13	0.79
1:E:180[A]:GLN:NE2	10:E:718:HOH:O	2.16	0.77
9:C:312:GOL:H2	10:D:821:HOH:O	1.84	0.77
8:E:305:TRS:H32	3:F:303:6MU:N3	2.00	0.77
1:E:106[B]:MET:SD	10:E:456:HOH:O	2.43	0.76
1:C:187[B]:GLN:NE2	10:C:689:HOH:O	2.19	0.76
1:D:53[A]:ARG:NH1	10:D:658[A]:HOH:O	2.19	0.75
1:C:16[B]:ASN:OD1	10:C:736:HOH:O	2.05	0.75
1:D:92[A]:GLY:O	10:D:819:HOH:O	2.04	0.75
1:A:93[B]:THR:CG2	10:A:831:HOH:O	2.25	0.74
1:E:214[B]:CYS:SG	10:E:571:HOH:O	2.43	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106[B]:MET:SD	10:F:461:HOH:O	2.45	0.74
10:E:437:HOH:O	7:F:308:EOH:H23	1.89	0.73
1:F:126[B]:GLU:OE2	10:F:787:HOH:O	2.06	0.73
1:A:92[B]:GLY:O	10:A:831:HOH:O	2.06	0.73
7:C:311:EOH:H12	1:D:120:LEU:HD22	1.71	0.72
2:A:309:CL:CL	10:F:440[A]:HOH:O	2.45	0.72
2:C:303:CL:CL	10:C:446:HOH:O	2.45	0.71
1:D:237[B]:GLU:OE1	10:D:816:HOH:O	2.07	0.71
7:D:307:EOH:H22	10:D:562:HOH:O	1.91	0.71
1:B:92[A]:GLY:O	10:B:552:HOH:O	2.10	0.70
1:E:92[B]:GLY:O	10:E:445[B]:HOH:O	2.10	0.69
2:A:302:CL:CL	10:A:491:HOH:O	2.46	0.69
7:F:308:EOH:H22	10:F:622:HOH:O	1.92	0.69
1:A:120:LEU:HD22	7:B:310:EOH:H11	1.75	0.69
1:F:183[B]:MET:HE1	1:F:222:ARG:NH2	2.08	0.68
1:C:120:LEU:HD22	7:D:307:EOH:H12	1.76	0.68
1:F:180[B]:GLN:OE1	10:F:545:HOH:O	2.11	0.67
1:D:92[A]:GLY:C	10:D:819:HOH:O	2.33	0.67
3:D:302:6MU:O6	10:D:810:HOH:O	2.12	0.67
1:D:237[B]:GLU:OE2	10:D:780:HOH:O	2.14	0.66
3:A:303:6MU:C6	10:A:512:HOH:O	2.43	0.66
1:D:93[A]:THR:CG2	10:D:819:HOH:O	2.33	0.66
1:C:214[B]:CYS:SG	10:C:756:HOH:O	2.52	0.66
1:F:235[A]:GLU:OE1	10:F:565:HOH:O	2.11	0.66
7:E:307:EOH:H12	1:F:120:LEU:HD22	1.78	0.65
1:B:187[A]:GLN:NE2	10:B:658:HOH:O	2.30	0.64
1:E:29:ARG:NH2	1:E:240[A]:SER:OG	2.31	0.64
1:A:92[B]:GLY:C	10:A:831:HOH:O	2.36	0.63
10:D:595:HOH:O	7:E:307:EOH:H22	1.98	0.63
1:A:94[A]:THR:HA	10:A:530:HOH:O	1.98	0.63
1:B:46[B]:HIS:ND1	10:B:645[B]:HOH:O	2.31	0.61
10:B:631:HOH:O	7:C:311:EOH:H22	2.00	0.61
1:E:120:LEU:HD22	7:F:308:EOH:H12	1.81	0.61
1:B:214[B]:CYS:SG	10:B:583:HOH:O	2.56	0.60
7:A:308:EOH:H12	1:B:120:LEU:HD22	1.82	0.60
1:C:55[B]:GLU:OE1	10:C:585:HOH:O	2.12	0.60
1:B:3:LYS:NZ	10:B:736:HOH:O	2.34	0.59
1:D:16:ASN:HB2	1:D:53[A]:ARG:HD2	1.84	0.58
1:B:144:GLN:NE2	10:B:468:HOH:O	2.36	0.58
10:C:427:HOH:O	7:D:307:EOH:H23	2.02	0.58
1:A:95[A]:GLY:CA	10:A:512:HOH:O	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53[B]:ARG:HG2	10:B:588:HOH:O	2.05	0.56
10:C:428:HOH:O	7:D:307:EOH:H21	2.06	0.56
1:A:242[A]:LYS:NZ	10:A:779:HOH:O	2.38	0.55
1:B:53[B]:ARG:NH2	10:B:542:HOH:O	2.36	0.55
1:A:16:ASN:HB2	1:A:53[A]:ARG:HD2	1.90	0.54
8:E:305:TRS:C3	3:F:303:6MU:N3	2.70	0.54
1:F:2:THR:N	10:F:768[B]:HOH:O	2.40	0.54
7:A:308:EOH:H22	10:A:584:HOH:O	2.08	0.54
7:C:311:EOH:H21	10:D:427:HOH:O	2.08	0.54
1:F:26:ASP:HB3	1:F:29[B]:ARG:HG2	1.90	0.54
1:C:102:ASN:OD1	7:C:310:EOH:H23	2.07	0.53
1:D:148:ALA:HB2	1:D:239[B]:ARG:HD3	1.91	0.53
10:E:428:HOH:O	7:F:308:EOH:H21	2.07	0.53
8:E:305:TRS:H31	10:F:831:HOH:O	2.08	0.53
1:C:196:MET:HB2	8:C:309:TRS:H21	1.90	0.52
8:E:305:TRS:H21	10:F:831:HOH:O	2.08	0.52
1:B:26:ASP:HB3	1:B:29:ARG:HG2	1.91	0.52
6:D:306:EDO:H12	1:E:125:MET:HB3	1.92	0.51
1:F:104:GLY:O	1:F:239:ARG:NH1	2.44	0.51
7:C:311:EOH:H23	10:D:418:HOH:O	2.09	0.51
1:D:94[A]:THR:O	1:D:218:VAL:HA	2.11	0.51
8:E:305:TRS:C3	10:F:831:HOH:O	2.60	0.50
1:F:16[A]:ASN:HB2	1:F:53[A]:ARG:HD2	1.92	0.50
1:F:37:MET:SD	1:F:61[B]:VAL:HG21	2.51	0.50
1:B:102:ASN:HA	6:B:309:EDO:H22	1.93	0.50
1:B:37:MET:SD	1:B:61[B]:VAL:HG21	2.53	0.49
7:E:307:EOH:H21	10:F:430:HOH:O	2.12	0.49
1:B:196:MET:HB2	8:B:308:TRS:H21	1.94	0.49
1:D:94[A]:THR:N	1:D:217:GLY:O	2.45	0.49
1:E:16[A]:ASN:HB2	1:E:53:ARG:HD2	1.95	0.49
1:E:196:MET:HB2	8:E:306:TRS:H21	1.95	0.49
1:D:239[B]:ARG:NH2	10:D:723:HOH:O	2.43	0.48
1:C:56:LEU:HD11	1:C:249[B]:ARG:HE	1.79	0.48
1:F:184[A]:LYS:HE2	10:F:829:HOH:O	2.13	0.48
7:E:307:EOH:H23	10:F:423:HOH:O	2.14	0.48
1:D:219[A]:ILE:HB	1:D:233:LEU:HD22	1.97	0.47
1:D:47[A]:ARG:CZ	10:D:672:HOH:O	2.62	0.47
1:D:47[A]:ARG:NH2	10:D:672:HOH:O	2.47	0.47
1:E:47[B]:ARG:NH1	10:E:657:HOH:O	2.48	0.47
1:A:21:ALA:CB	1:A:62[B]:VAL:HG13	2.45	0.47
1:F:53[B]:ARG:NH1	10:F:551:HOH:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183[B]:MET:HE1	1:F:222:ARG:CZ	2.45	0.47
1:B:92[B]:GLY:O	1:B:216:ALA:CB	2.63	0.47
1:A:46[A]:HIS:NE2	10:A:631:HOH:O	2.34	0.46
1:C:47[B]:ARG:HH22	9:C:312:GOL:H11	1.80	0.46
1:B:211[B]:LYS:NZ	10:B:529:HOH:O	2.28	0.46
1:C:183[A]:MET:HE2	10:C:747:HOH:O	2.16	0.46
7:A:308:EOH:C2	10:A:584:HOH:O	2.64	0.46
1:F:246[B]:GLU:CD	10:F:778:HOH:O	2.53	0.46
1:C:16[A]:ASN:HB2	1:C:53:ARG:HD2	1.97	0.45
1:A:21:ALA:HB2	1:A:62[B]:VAL:HG13	1.98	0.45
1:B:26:ASP:HB3	1:B:29:ARG:CG	2.46	0.45
1:A:173[A]:GLY:O	10:A:613:HOH:O	2.17	0.44
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.98	0.44
1:D:157:SER:HB3	1:D:199:ALA:HB2	1.99	0.44
1:A:95[A]:GLY:C	10:A:770:HOH:O	2.42	0.44
1:D:180[A]:GLN:NE2	10:D:499:HOH:O	2.48	0.44
1:E:157:SER:HB3	1:E:199:ALA:HB2	2.00	0.44
1:B:57:ASP:OD2	1:B:249:ARG:HG3	2.18	0.43
1:C:157:SER:HB3	1:C:199:ALA:HB2	2.00	0.43
1:F:57:ASP:OD2	1:F:249:ARG:HG3	2.19	0.43
1:A:157:SER:HB3	1:A:199:ALA:HB2	2.01	0.43
1:F:21:ALA:HA	1:F:62[A]:VAL:O	2.17	0.43
1:F:235[B]:GLU:HG3	10:F:572:HOH:O	2.18	0.43
7:A:308:EOH:H21	10:B:435:HOH:O	2.19	0.43
1:A:242[A]:LYS:HD2	10:A:771:HOH:O	2.19	0.42
1:E:234[A]:LYS:NZ	10:E:769:HOH:O	2.51	0.42
1:C:21:ALA:HA	1:C:62[A]:VAL:O	2.18	0.42
1:D:21:ALA:HB2	1:D:62[B]:VAL:HG13	2.01	0.42
1:D:21:ALA:CB	1:D:62[B]:VAL:HG13	2.49	0.42
1:A:95[A]:GLY:HA3	10:A:512:HOH:O	2.18	0.42
1:A:219[B]:ILE:HB	1:A:233:LEU:HD22	2.02	0.42
1:D:95[B]:GLY:C	10:D:820:HOH:O	2.49	0.42
1:F:2:THR:HG23	1:F:2:THR:O	2.20	0.42
1:C:46:HIS:CD2	1:C:47[B]:ARG:HG3	2.56	0.41
1:F:135:VAL:O	1:F:139[B]:MET:HG2	2.19	0.41
1:B:2:THR:HB	10:B:574:HOH:O	2.19	0.41
1:B:53[B]:ARG:NH2	10:B:674:HOH:O	2.52	0.41
1:F:157:SER:HB3	1:F:199:ALA:HB2	2.03	0.41
1:E:57:ASP:OD2	1:E:249[A]:ARG:HG3	2.21	0.41
1:F:15[B]:LEU:HG	1:F:62[B]:VAL:CG2	2.51	0.41
1:F:246[B]:GLU:OE2	10:F:778:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222[B]:ARG:HG2	10:A:677:HOH:O	2.21	0.41
1:D:95[A]:GLY:HA2	1:D:220[A]:ILE:O	2.21	0.40
1:A:47[B]:ARG:CZ	10:A:713:HOH:O	2.69	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	
1	A	297/253 (117%)	292 (98%)	4 (1%)	1 (0%)	41	17
1	B	283/253 (112%)	277 (98%)	5 (2%)	1 (0%)	34	12
1	C	276/253 (109%)	271 (98%)	4 (1%)	1 (0%)	34	12
1	D	289/253 (114%)	284 (98%)	4 (1%)	1 (0%)	41	17
1	E	289/253 (114%)	283 (98%)	5 (2%)	1 (0%)	41	17
1	F	288/253 (114%)	284 (99%)	3 (1%)	1 (0%)	41	17
All	All	1722/1518 (113%)	1691 (98%)	25 (2%)	6 (0%)	34	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	TYR
1	E	162	TYR
1	A	162	TYR
1	B	162	TYR
1	C	162	TYR
1	F	162	TYR

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	
1	A	244/203 (120%)	243 (100%)	1 (0%)	91	75
1	B	236/203 (116%)	231 (98%)	5 (2%)	53	15
1	C	230/203 (113%)	229 (100%)	1 (0%)	91	75
1	D	238/203 (117%)	237 (100%)	1 (0%)	91	75
1	E	240/203 (118%)	239 (100%)	1 (0%)	91	75
1	F	238/203 (117%)	237 (100%)	1 (0%)	91	75
All	All	1426/1218 (117%)	1416 (99%)	10 (1%)	81	57

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	B	2	THR
1	B	3	LYS
1	B	195	GLU
1	B	233	LEU
1	B	234	LYS
1	C	195	GLU
1	D	195	GLU
1	E	195	GLU
1	F	195	GLU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 32 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
3	6MU	F	303	-	8,9,9	2.80	6 (75%)	10,12,12	1.33	1 (10%)
8	TRS	E	305	-	7,7,7	0.59	0	9,9,9	0.97	1 (11%)
7	EOH	C	311	-	2,2,2	0.43	0	1,1,1	0.30	0
7	EOH	D	307	-	2,2,2	0.42	0	1,1,1	0.32	0
7	EOH	E	307	-	2,2,2	0.41	0	1,1,1	0.47	0
6	EDO	D	306	-	3,3,3	0.41	0	2,2,2	0.32	0
3	6MU	C	304	-	8,9,9	2.78	6 (75%)	10,12,12	1.22	1 (10%)
8	TRS	C	309	-	7,7,7	0.45	0	9,9,9	0.46	0
6	EDO	A	307	-	3,3,3	0.40	0	2,2,2	0.32	0
7	EOH	F	308	-	2,2,2	0.42	0	1,1,1	0.22	0
8	TRS	B	308	-	7,7,7	0.47	0	9,9,9	0.39	0
6	EDO	B	309	-	3,3,3	0.44	0	2,2,2	0.35	0
7	EOH	A	308	-	2,2,2	0.44	0	1,1,1	0.32	0
3	6MU	D	302	-	8,9,9	2.92	5 (62%)	10,12,12	1.23	1 (10%)
3	6MU	A	303	-	8,9,9	2.97	5 (62%)	10,12,12	1.27	1 (10%)
3	6MU	B	303	-	8,9,9	2.81	6 (75%)	10,12,12	1.26	1 (10%)
6	EDO	F	307	-	3,3,3	0.38	0	2,2,2	0.36	0
9	GOL	C	312	-	5,5,5	0.41	0	5,5,5	0.53	0
3	6MU	E	302	-	8,9,9	2.84	6 (75%)	10,12,12	1.33	1 (10%)
7	EOH	C	310	-	2,2,2	0.20	0	1,1,1	0.70	0
8	TRS	E	306	-	7,7,7	0.37	0	9,9,9	0.47	0
7	EOH	B	310	-	2,2,2	0.42	0	1,1,1	0.24	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	6MU	F	303	-	-	-	0/1/1/1
8	TRS	E	305	-	-	4/9/9/9	-
3	6MU	C	304	-	-	-	0/1/1/1
3	6MU	D	302	-	-	-	0/1/1/1
3	6MU	E	302	-	-	-	0/1/1/1
3	6MU	A	303	-	-	-	0/1/1/1
8	TRS	C	309	-	-	0/9/9/9	-
8	TRS	E	306	-	-	1/9/9/9	-
6	EDO	A	307	-	-	0/1/1/1	-
8	TRS	B	308	-	-	0/9/9/9	-
3	6MU	B	303	-	-	-	0/1/1/1
6	EDO	B	309	-	-	1/1/1/1	-
6	EDO	F	307	-	-	1/1/1/1	-
9	GOL	C	312	-	-	2/4/4/4	-
6	EDO	D	306	-	-	1/1/1/1	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	6MU	C5-C4	4.32	1.46	1.38
3	F	303	6MU	C5-C6	-4.25	1.33	1.41
3	D	302	6MU	C5-C4	4.19	1.46	1.38
3	E	302	6MU	C5-C6	-4.14	1.33	1.41
3	B	303	6MU	C5-C6	-3.97	1.33	1.41
3	C	304	6MU	C5-C6	-3.87	1.33	1.41
3	A	303	6MU	C2-N3	3.68	1.44	1.36
3	D	302	6MU	C5-C6	-3.67	1.34	1.41
3	B	303	6MU	C5-C4	3.65	1.45	1.38
3	C	304	6MU	C5-C4	3.63	1.45	1.38
3	A	303	6MU	C5-C6	-3.60	1.34	1.41
3	D	302	6MU	C2-N3	3.59	1.44	1.36
3	E	302	6MU	C5-C4	3.58	1.45	1.38
3	F	303	6MU	C5-C4	3.58	1.45	1.38
3	A	303	6MU	C6-N1	3.52	1.42	1.34
3	E	302	6MU	C2-N3	3.47	1.43	1.36
3	D	302	6MU	C6-N1	3.44	1.41	1.34
3	F	303	6MU	C2-N3	3.34	1.43	1.36
3	B	303	6MU	C2-N3	3.28	1.43	1.36
3	B	303	6MU	C6-N1	3.13	1.41	1.34
3	E	302	6MU	C6-N1	3.11	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	6MU	C4-N3	-3.09	1.29	1.34
3	C	304	6MU	C6-N1	3.08	1.41	1.34
3	C	304	6MU	C2-N3	3.02	1.42	1.36
3	F	303	6MU	C6-N1	2.99	1.40	1.34
3	C	304	6MU	C4-N3	-2.93	1.29	1.34
3	D	302	6MU	C4-N3	-2.90	1.29	1.34
3	B	303	6MU	C4-N3	-2.74	1.30	1.34
3	E	302	6MU	C4-N3	-2.62	1.30	1.34
3	F	303	6MU	C4-N3	-2.49	1.30	1.34
3	C	304	6MU	C2-N1	-2.42	1.31	1.36
3	E	302	6MU	C2-N1	-2.36	1.31	1.36
3	B	303	6MU	C2-N1	-2.34	1.31	1.36
3	F	303	6MU	C2-N1	-2.27	1.31	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	303	6MU	C2-N1-C6	3.26	119.72	114.21
3	C	304	6MU	C2-N1-C6	3.24	119.67	114.21
3	E	302	6MU	C2-N1-C6	3.16	119.54	114.21
3	B	303	6MU	C2-N1-C6	3.08	119.40	114.21
3	A	303	6MU	C2-N1-C6	2.95	119.18	114.21
3	D	302	6MU	C2-N1-C6	2.69	118.74	114.21
8	E	305	TRS	C3-C-C2	2.31	116.82	110.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	305	TRS	C1-C-C2-O2
8	E	305	TRS	C3-C-C2-O2
8	E	305	TRS	N-C-C2-O2
9	C	312	GOL	C1-C2-C3-O3
9	C	312	GOL	O2-C2-C3-O3
6	B	309	EDO	O1-C1-C2-O2
6	F	307	EDO	O1-C1-C2-O2
8	E	306	TRS	N-C-C1-O1
8	E	305	TRS	C2-C-C1-O1
6	D	306	EDO	O1-C1-C2-O2

There are no ring outliers.

17 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	303	6MU	2	0
8	E	305	TRS	5	0
7	C	311	EOH	4	0
7	D	307	EOH	4	0
7	E	307	EOH	4	0
6	D	306	EDO	1	0
8	C	309	TRS	1	0
7	F	308	EOH	4	0
8	B	308	TRS	1	0
6	B	309	EDO	1	0
7	A	308	EOH	4	0
3	D	302	6MU	1	0
3	A	303	6MU	2	0
9	C	312	GOL	2	0
7	C	310	EOH	1	0
8	E	306	TRS	1	0
7	B	310	EOH	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	252/253 (99%)	-0.13	8 (3%)	47	49	5, 9, 22, 42	0
1	B	248/253 (98%)	-0.17	10 (4%)	38	39	5, 9, 20, 39	0
1	C	247/253 (97%)	-0.21	8 (3%)	47	49	5, 8, 19, 35	0
1	D	252/253 (99%)	-0.09	11 (4%)	34	36	5, 9, 24, 41	0
1	E	251/253 (99%)	-0.29	3 (1%)	79	79	5, 7, 15, 33	0
1	F	252/253 (99%)	-0.30	3 (1%)	79	79	5, 7, 14, 32	0
All	All	1502/1518 (98%)	-0.20	43 (2%)	51	53	5, 8, 20, 42	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	10.6
1	B	233	LEU	8.8
1	F	2	THR	8.3
1	A	2	THR	7.3
1	C	229	ASP	6.4
1	D	228	PRO	5.7
1	D	225	LYS	5.5
1	A	226	GLU	4.9
1	A	227	ILE	4.8
1	D	2	THR	4.5
1	E	253	LYS	4.4
1	D	226	GLU	4.1
1	C	6	PHE	4.1
1	D	227	ILE	4.1
1	B	6[A]	PHE	4.0
1	B	253	LYS	4.0
1	D	253[A]	LYS	3.9
1	C	4	THR	3.5
1	E	3	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	225	LYS	3.4
1	B	234	LYS	3.2
1	C	234	LYS	3.1
1	A	253	LYS	3.1
1	D	220[A]	ILE	2.9
1	B	227	ILE	2.9
1	E	4	THR	2.9
1	C	235	GLU	2.9
1	D	230	HIS	2.8
1	C	227	ILE	2.8
1	B	235	GLU	2.7
1	D	229	ASP	2.5
1	A	3	LYS	2.5
1	D	234	LYS	2.5
1	B	3	LYS	2.4
1	B	252	LEU	2.4
1	D	252[A]	LEU	2.4
1	F	3	LYS	2.2
1	F	4	THR	2.2
1	C	253	LYS	2.2
1	A	230	HIS	2.1
1	C	3	LYS	2.1
1	A	47[A]	ARG	2.0
1	B	237	GLU	2.0

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 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
6	EDO	B	309	4/4	0.69	0.31	19,23,25,27	10
4	MG	D	304	1/1	0.72	0.33	22,22,22,22	1
7	EOH	C	310	3/3	0.75	0.24	20,20,20,20	0
4	MG	F	305	1/1	0.77	0.32	17,17,17,17	1
8	TRS	E	305	8/8	0.78	0.27	20,28,33,34	0
9	GOL	C	312	6/6	0.81	0.28	24,29,35,35	0
6	EDO	F	307	4/4	0.83	0.25	21,25,28,29	10
3	6MU	A	303	9/9	0.85	0.24	9,14,17,19	15
7	EOH	F	308	3/3	0.85	0.18	12,15,18,22	9
7	EOH	A	308	3/3	0.86	0.18	11,13,16,19	9
7	EOH	C	311	3/3	0.86	0.20	13,16,18,21	9
7	EOH	E	307	3/3	0.86	0.24	13,15,17,21	9
8	TRS	B	308	8/8	0.87	0.17	8,13,17,19	20
6	EDO	A	307	4/4	0.87	0.24	26,31,32,33	10
6	EDO	D	306	4/4	0.87	0.23	25,30,30,30	10
3	6MU	D	302	9/9	0.88	0.20	8,12,15,16	15
7	EOH	D	307	3/3	0.89	0.18	16,20,20,24	0
4	MG	C	306	1/1	0.91	0.32	29,29,29,29	1
7	EOH	B	310	3/3	0.92	0.19	15,18,21,21	9
8	TRS	E	306	8/8	0.92	0.19	10,20,24,26	0
8	TRS	C	309	8/8	0.92	0.12	8,13,18,19	20
4	MG	C	305	1/1	0.94	0.39	17,17,17,17	1
4	MG	B	305	1/1	0.95	0.33	13,13,13,13	1
4	MG	D	305	1/1	0.96	0.33	13,13,13,13	1
4	MG	E	308	1/1	0.97	0.26	17,17,17,17	1
4	MG	E	303	1/1	0.97	0.20	20,20,20,20	1
4	MG	F	304	1/1	0.98	0.20	18,18,18,18	1
2	CL	F	302	1/1	0.98	0.06	17,17,17,17	1
3	6MU	F	303	9/9	0.99	0.06	7,8,12,12	0
4	MG	A	305	1/1	0.99	0.25	13,13,13,13	1
4	MG	B	304	1/1	0.99	0.15	16,16,16,16	1
2	CL	B	301	1/1	0.99	0.04	19,19,19,19	1
4	MG	B	306	1/1	0.99	0.06	12,12,12,12	1
2	CL	C	301	1/1	0.99	0.08	15,15,15,15	1
2	CL	C	303	1/1	0.99	0.04	23,23,23,23	0
4	MG	C	307	1/1	0.99	0.23	12,12,12,12	1
2	CL	D	301	1/1	0.99	0.07	13,13,13,13	1
2	CL	A	301	1/1	0.99	0.08	29,29,29,29	0
2	CL	A	302	1/1	0.99	0.06	15,15,15,15	1
3	6MU	B	303	9/9	0.99	0.07	7,8,12,12	0
3	6MU	C	304	9/9	0.99	0.07	6,8,12,12	0
2	CL	A	309	1/1	0.99	0.04	21,21,21,21	0
3	6MU	E	302	9/9	0.99	0.06	7,9,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	D	303	1/1	1.00	0.24	16,16,16,16	1
4	MG	F	306	1/1	1.00	0.07	17,17,17,17	0
5	NA	A	306	1/1	1.00	0.05	7,7,7,7	1
5	NA	B	307	1/1	1.00	0.04	10,10,10,10	0
5	NA	C	308	1/1	1.00	0.06	7,7,7,7	0
5	NA	E	304	1/1	1.00	0.05	7,7,7,7	0
2	CL	C	302	1/1	1.00	0.05	10,10,10,10	0
2	CL	E	301	1/1	1.00	0.07	10,10,10,10	1
4	MG	A	304	1/1	1.00	0.18	15,15,15,15	1
2	CL	F	301	1/1	1.00	0.07	11,11,11,11	1
2	CL	B	302	1/1	1.00	0.03	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.