



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:36 pm BST

PDB ID : 3GUE
Title : Crystal Structure of UDP-glucose phosphorylase from Trypanosoma Brucei, (Tb10.389.0330)
Authors : Wernimont, A.K.; Marino, K.; Lin, Y.H.; Mackenzie, F.; Kozieradzki, I.; Cos-sar, D.; Zhao, Y.; Schapira, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Ferguson, M.A.J.; Hui, R.; Amani, M.; Struc-tural Genomics Consortium (SGC)
Deposited on : 2009-03-29
Resolution : 1.92 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

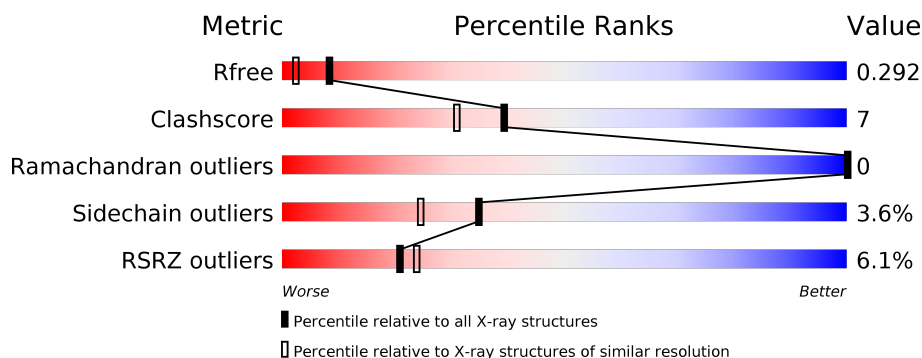
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	484	<div> <div>3%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	B	484	<div> <div>8%</div> <div>75%</div> <div>18%</div> <div>• 6%</div> </div>

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
5	DTU	A	489	X	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8155 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.

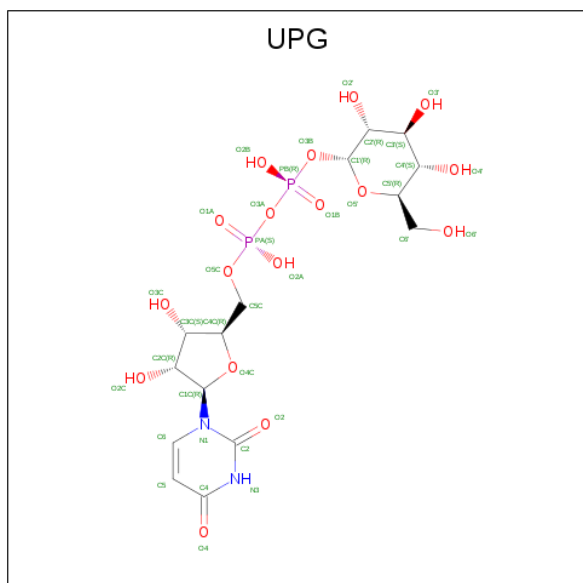
- Molecule 1 is a protein called UTP-glucose-1-phosphate uridylyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	3	0
			3695	2339	639	693	24			
1	B	457	Total	C	N	O	S	0	4	0
			3569	2271	606	669	23			

There are 6 discrepancies between the modelled and reference sequences:

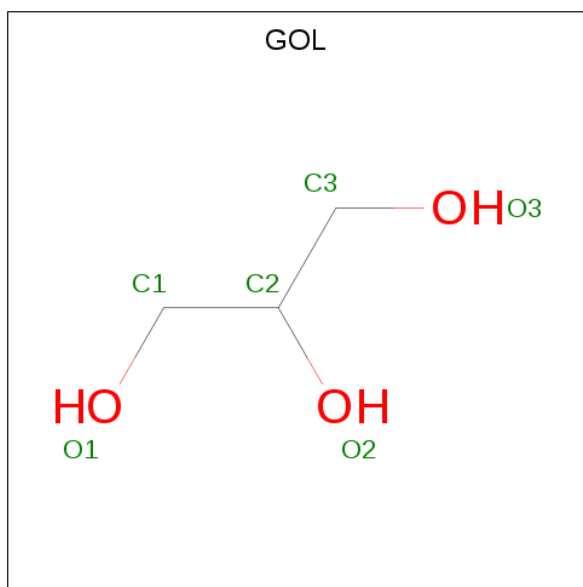
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q388T4
A	52	SER	PHE	CONFLICT	UNP Q388T4
A	471	SER	ASN	CONFLICT	UNP Q388T4
B	0	GLY	-	EXPRESSION TAG	UNP Q388T4
B	52	SER	PHE	CONFLICT	UNP Q388T4
B	471	SER	ASN	CONFLICT	UNP Q388T4

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



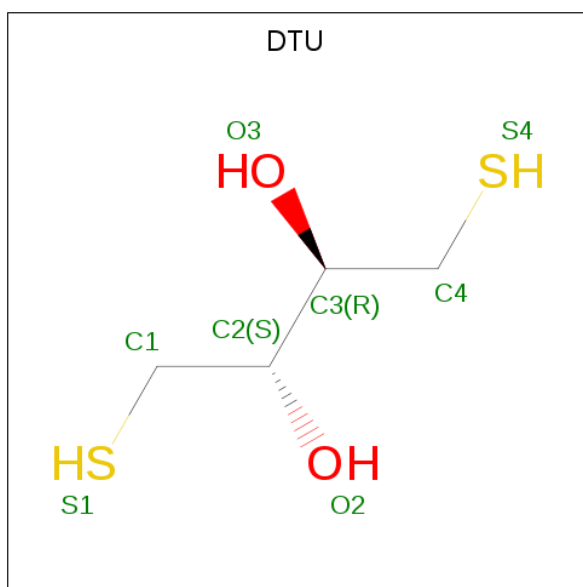
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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



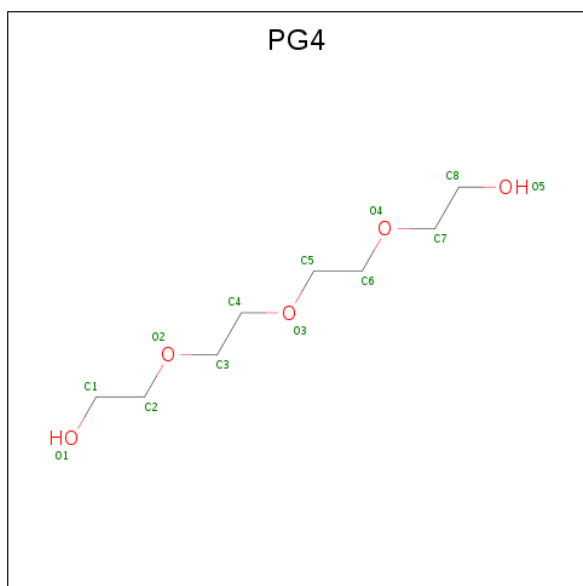
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (2R,3S)-1,4-DIMERCAPTObUTANE-2,3-DIOL (three-letter code: DTU) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	390	Total 390	O 390	0	0
7	B	343	Total 343	O 343	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.70Å 77.48Å 112.21Å 90.00° 117.88° 90.00°	Depositor
Resolution (Å)	25.00 – 1.92 24.80 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-1.92) 98.7 (24.80-1.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.294 0.239 , 0.292	Depositor DCC
R_{free} test set	4791 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8155	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.61% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG4, SO4, DTU, UPG

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	0.66	0/3770	0.71	0/5087
1	B	0.85	11/3645 (0.3%)	0.75	5/4924 (0.1%)
All	All	0.76	11/7415 (0.1%)	0.73	5/10011 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	ARG	NE-CZ	17.25	1.55	1.33
1	B	460	LYS	CE-NZ	15.62	1.88	1.49
1	B	446	GLU	CD-OE2	9.40	1.35	1.25
1	B	481	VAL	CB-CG2	8.85	1.71	1.52
1	B	481	VAL	CB-CG1	7.83	1.69	1.52
1	B	446	GLU	CD-OE1	6.87	1.33	1.25
1	B	479	VAL	CB-CG2	5.92	1.65	1.52
1	B	460	LYS	CD-CE	5.77	1.65	1.51
1	B	122	ASN	CB-CG	5.74	1.64	1.51
1	B	442	ARG	CD-NE	5.70	1.56	1.46
1	B	462	LEU	CB-CG	5.36	1.68	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	442	ARG	CD-NE-CZ	-11.47	107.55	123.60
1	B	460	LYS	CD-CE-NZ	-6.17	97.50	111.70
1	B	462	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	B	458	VAL	CG1-CB-CG2	-5.45	102.18	110.90
1	B	85	LEU	CA-CB-CG	5.32	127.53	115.30

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	3695	0	3718	51	0
1	B	3569	0	3559	59	0
2	A	36	0	22	0	0
2	B	36	0	22	0	0
3	A	18	0	24	2	0
3	B	12	0	16	2	0
4	A	10	0	0	1	0
4	B	25	0	0	1	0
5	A	8	0	10	5	0
6	B	13	0	18	4	0
7	A	390	0	0	6	0
7	B	343	0	0	7	0
All	All	8155	0	7389	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (110) 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:460:LYS:NZ	1:B:460:LYS:CE	1.88	1.34
1:B:127:PHE:H	6:B:490:PG4:H51	1.28	0.97
1:A:195:THR:HG21	5:A:489:DTU:S4	2.17	0.85
1:A:212:ARG:HH21	3:A:485:GOL:H32	1.42	0.83
1:B:59:PHE:HZ	1:B:247:ARG:HH21	1.37	0.72
1:B:39:ARG:NH1	7:B:621:HOH:O	2.22	0.72
1:B:263:VAL:HG21	1:B:274:ARG:HE	1.55	0.72
1:A:438:SER:HB3	1:A:456:ASN:HD22	1.54	0.71
1:A:16:GLU:OE2	7:A:1028:HOH:O	2.07	0.70
1:B:86:GLY:HA3	1:B:91:LEU:HD12	1.76	0.68
1:A:442:ARG:HB2	1:A:460:LYS:HG2	1.78	0.65
1:B:127:PHE:H	6:B:490:PG4:C5	2.07	0.65
1:B:442:ARG:HB2	4:B:484:SO4:O3	1.98	0.64
1:A:89:MET:SD	1:A:95:LYS:HE2	2.38	0.64
1:A:195:THR:CG2	5:A:489:DTU:S4	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:PRO:HB3	1:B:451:VAL:HG23	1.81	0.60
1:B:310:MET:O	1:B:314:LYS:HG3	2.01	0.60
1:B:149:LEU:HD23	6:B:490:PG4:H82	1.84	0.60
1:B:104:GLN:HG2	7:B:827:HOH:O	2.02	0.60
1:B:127:PHE:N	6:B:490:PG4:H51	2.08	0.58
1:A:437:THR:OG1	1:A:456:ASN:ND2	2.36	0.58
1:B:238:GLN:NE2	7:B:568:HOH:O	2.35	0.58
1:B:460:LYS:NZ	1:B:460:LYS:CD	2.66	0.58
1:B:409:ILE:HG22	1:B:411:LEU:CD1	2.34	0.58
1:A:419:ILE:O	1:A:423:GLU:HG3	2.04	0.56
1:A:438:SER:CB	1:A:456:ASN:HD22	2.19	0.56
1:B:409:ILE:CG2	1:B:411:LEU:CD1	2.83	0.56
1:A:247:ARG:NH1	7:A:846:HOH:O	2.35	0.56
1:B:319:GLN:NE2	7:B:690:HOH:O	2.38	0.56
1:A:192:ASP:OD1	5:A:489:DTU:S4	2.61	0.55
1:A:91:LEU:HB3	4:A:487:SO4:O3	2.06	0.55
1:A:369[A]:GLU:HG2	7:A:693:HOH:O	2.05	0.55
1:B:175:VAL:HG11	1:B:334:VAL:HG23	1.87	0.55
1:A:391:THR:OG1	1:A:393:ASP:OD1	2.21	0.54
1:B:369:GLU:HG3	1:B:395:ARG:HH22	1.73	0.53
1:B:77:VAL:HG13	1:B:126:PRO:HB2	1.89	0.53
1:B:12:LEU:O	1:B:16:GLU:HG3	2.09	0.53
1:B:26:LYS:HD2	1:B:322:VAL:HG23	1.92	0.52
1:B:473:ARG:NH2	1:B:478:GLU:OE2	2.43	0.51
1:B:54:VAL:HG22	1:B:260:TYR:CE2	2.44	0.51
1:A:80:LYS:HD2	1:A:219:GLY:HA2	1.93	0.51
1:A:438:SER:HB3	1:A:456:ASN:ND2	2.24	0.51
1:B:447:PHE:CD1	1:B:451:VAL:HG21	2.46	0.51
1:A:45:TYR:HB3	1:A:284:PRO:HG3	1.94	0.49
1:A:63:ILE:HD11	1:A:364:VAL:HG11	1.92	0.49
1:B:85:LEU:HB2	1:B:87:THR:HG23	1.94	0.49
1:B:382:ALA:HB2	1:B:409:ILE:HD12	1.94	0.49
1:A:315:MET:HE1	1:A:358:PHE:CD1	2.48	0.49
1:A:283:CYS:SG	1:A:291:PHE:HB2	2.53	0.49
1:B:188:PRO:HB2	3:B:489:GOL:H2	1.94	0.49
1:B:14:CYS:O	1:B:18:MET:HG3	2.13	0.49
1:A:153:PHE:HA	1:A:157:ILE:HB	1.95	0.48
1:A:433:LEU:HD23	1:A:453:VAL:HB	1.95	0.48
1:B:389:GLN:HB2	7:B:538:HOH:O	2.13	0.48
1:B:417:LYS:HA	3:B:491:GOL:H31	1.96	0.48
1:A:381:LEU:HD23	1:A:409:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LEU:HB3	1:B:394:GLN:HG3	1.96	0.48
1:A:64:GLU:OE1	7:A:937:HOH:O	2.20	0.47
1:B:259:ALA:HB3	1:B:276:VAL:CG1	2.45	0.47
1:B:71:ALA:N	7:B:853:HOH:O	2.46	0.47
1:A:261:LYS:HB2	1:A:276:VAL:HG11	1.96	0.47
1:B:122:ASN:HB2	7:B:783:HOH:O	2.15	0.47
1:A:31:PHE:HB2	5:A:489:DTU:H1C1	1.96	0.47
1:A:36:ALA:O	1:A:40:LYS:HG2	2.15	0.46
1:A:261:LYS:HB3	1:A:261:LYS:HE2	1.72	0.46
1:B:18:MET:CE	1:B:28:ILE:HG23	2.46	0.46
1:B:424:LYS:O	1:B:446:GLU:HB3	2.15	0.46
1:A:180:ASP:OD1	1:A:182:THR:HB	2.16	0.46
1:A:315:MET:HE1	1:A:358:PHE:HA	1.98	0.45
1:B:431:PRO:HB3	1:B:451:VAL:CG2	2.44	0.45
1:B:374:VAL:HA	1:B:379:ASP:CB	2.46	0.45
1:A:438:SER:CB	1:A:456:ASN:ND2	2.79	0.45
1:B:460:LYS:O	1:B:481:VAL:HA	2.17	0.45
1:B:85:LEU:HD11	1:B:186:VAL:HG23	1.99	0.45
1:B:175:VAL:HG11	1:B:334:VAL:CG2	2.47	0.45
1:A:96:SER:HA	1:A:106:PHE:HB2	1.98	0.44
1:A:26:LYS:O	1:A:30:ILE:HG13	2.17	0.44
1:B:374:VAL:HA	1:B:379:ASP:HB3	1.99	0.44
1:B:419:ILE:O	1:B:423:GLU:HG2	2.17	0.44
1:A:369[A]:GLU:OE1	1:A:397:VAL:HB	2.17	0.44
1:A:85:LEU:HB2	1:A:87:THR:HG23	2.00	0.44
1:A:95:LYS:O	1:A:98:LEU:HB2	2.18	0.44
1:B:443:GLY:HA3	1:B:461:ASN:O	2.18	0.44
1:A:288:GLU:HA	1:A:288:GLU:OE1	2.18	0.44
1:A:382:ALA:HB2	1:A:409:ILE:HD12	1.99	0.43
1:A:454:ARG:HB2	1:A:476:ASP:HA	2.00	0.43
1:A:164:VAL:HG11	5:A:489:DTU:H1C1	2.01	0.43
1:A:85:LEU:HD11	1:A:187:PRO:HD2	2.00	0.43
1:B:125:VAL:HA	1:B:126:PRO:HD2	1.84	0.42
1:B:163:ARG:HG2	1:B:185:TRP:CE3	2.54	0.42
1:B:85:LEU:CD1	1:B:186:VAL:HG23	2.49	0.42
1:A:25:GLU:HG2	1:A:26:LYS:N	2.33	0.42
1:B:409:ILE:HG22	1:B:411:LEU:HD13	2.01	0.42
1:B:207:LEU:HD23	1:B:211:TYR:O	2.20	0.42
1:A:374:VAL:HA	1:A:379:ASP:HB3	2.02	0.41
1:B:335:ASN:HA	1:B:336:PRO:HD2	1.91	0.41
1:B:18:MET:HE1	1:B:28:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLY:HA3	1:A:477:ASN:ND2	2.34	0.41
1:A:212:ARG:NH2	3:A:485:GOL:H32	2.23	0.41
1:B:433:LEU:HD23	1:B:453:VAL:HB	2.03	0.41
1:B:440:THR:HB	1:B:458:VAL:HG22	2.02	0.41
1:B:401:GLU:OE2	1:B:435:GLN:OE1	2.38	0.41
1:B:389:GLN:O	1:B:396:LEU:HA	2.21	0.41
1:A:285:LYS:NZ	7:A:926:HOH:O	2.54	0.40
1:A:286:GLU:H	1:A:286:GLU:CD	2.23	0.40
1:B:87:THR:HB	1:B:336:PRO:HB3	2.03	0.40
1:A:261:LYS:HB2	1:A:276:VAL:CG1	2.51	0.40
1:A:58:PRO:HG2	7:A:616:HOH:O	2.21	0.40
1:A:94:PRO:HG2	1:A:97:LEU:HD12	2.03	0.40
1:B:161:GLN:HA	1:B:196:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	467/484 (96%)	455 (97%)	12 (3%)	0	100	100
1	B	453/484 (94%)	437 (96%)	16 (4%)	0	100	100
All	All	920/968 (95%)	892 (97%)	28 (3%)	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	
1	A	410/423 (97%)	400 (98%)	10 (2%)	49	41
1	B	393/423 (93%)	373 (95%)	20 (5%)	24	13
All	All	803/846 (95%)	773 (96%)	30 (4%)	35	23

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

Mol	Chain	Res	Type
1	A	21	SER
1	A	25	GLU
1	A	39	ARG
1	A	40	LYS
1	A	209	LYS
1	A	272	ARG
1	A	274	ARG
1	A	276	VAL
1	A	320	LEU
1	A	483	GLU
1	B	21[A]	SER
1	B	21[B]	SER
1	B	37	LEU
1	B	73	LEU
1	B	102	ASN
1	B	112	LEU
1	B	138	GLU
1	B	164	VAL
1	B	226	LEU
1	B	231	LEU
1	B	232	ASP
1	B	234	MET
1	B	285	LYS
1	B	347	LEU
1	B	356	SER
1	B	361	SER
1	B	368	ARG
1	B	420	ASP
1	B	445	VAL
1	B	446	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	HIS
1	A	456	ASN
1	B	319	GLN
1	B	456	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	SO4	B	487	-	4,4,4	0.15	0	6,6,6	0.20	0
3	GOL	A	490	-	5,5,5	0.37	0	5,5,5	0.29	0
2	UPG	A	484	-	31,38,38	1.46	3 (9%)	41,58,58	1.21	1 (2%)
2	UPG	B	492	-	31,38,38	1.78	4 (12%)	41,58,58	1.09	2 (4%)
3	GOL	B	489	-	5,5,5	0.44	0	5,5,5	0.45	0
5	DTU	A	489	-	7,7,7	0.71	0	4,8,8	1.27	1 (25%)
6	PG4	B	490	-	12,12,12	0.47	0	11,11,11	0.47	0
4	SO4	B	485	-	4,4,4	0.08	0	6,6,6	0.15	0
4	SO4	A	487	-	4,4,4	0.26	0	6,6,6	0.32	0
4	SO4	B	486	-	4,4,4	0.15	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	488	-	4,4,4	0.19	0	6,6,6	0.23	0
3	GOL	A	485	-	5,5,5	0.39	0	5,5,5	1.11	1 (20%)
4	SO4	B	484	-	4,4,4	0.13	0	6,6,6	0.25	0
3	GOL	A	486	-	5,5,5	0.47	0	5,5,5	0.31	0
3	GOL	B	491	-	5,5,5	0.22	0	5,5,5	0.38	0
4	SO4	B	488	-	4,4,4	0.13	0	6,6,6	0.15	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	GOL	A	490	-	-	1/4/4/4	-
2	UPG	A	484	-	-	3/21/59/59	0/3/3/3
2	UPG	B	492	-	-	2/21/59/59	0/3/3/3
3	GOL	B	489	-	-	2/4/4/4	-
5	DTU	A	489	-	2/2/2/2	4/8/8/8	-
6	PG4	B	490	-	-	7/10/10/10	-
3	GOL	A	485	-	-	2/4/4/4	-
3	GOL	A	486	-	-	0/4/4/4	-
3	GOL	B	491	-	-	4/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	484	UPG	C6-N1	6.21	1.43	1.35
2	B	492	UPG	O4C-C1C	5.72	1.49	1.41
2	B	492	UPG	C6-N1	4.60	1.41	1.35
2	B	492	UPG	C4-N3	3.26	1.38	1.33
2	A	484	UPG	C4-N3	2.80	1.37	1.33
2	A	484	UPG	O4C-C1C	2.31	1.44	1.41
2	B	492	UPG	PA-O2A	-2.04	1.45	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	484	UPG	O5'-C1'-O3B	-4.66	105.27	111.36
2	B	492	UPG	PB-O3A-PA	-2.52	124.19	132.83
2	B	492	UPG	O4C-C1C-C2C	-2.21	103.70	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	489	DTU	O3-C3-C2	2.12	114.08	109.72
3	A	485	GOL	O1-C1-C2	-2.00	100.60	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	489	DTU	C2
5	A	489	DTU	C3

All (25) torsion outliers are listed below:

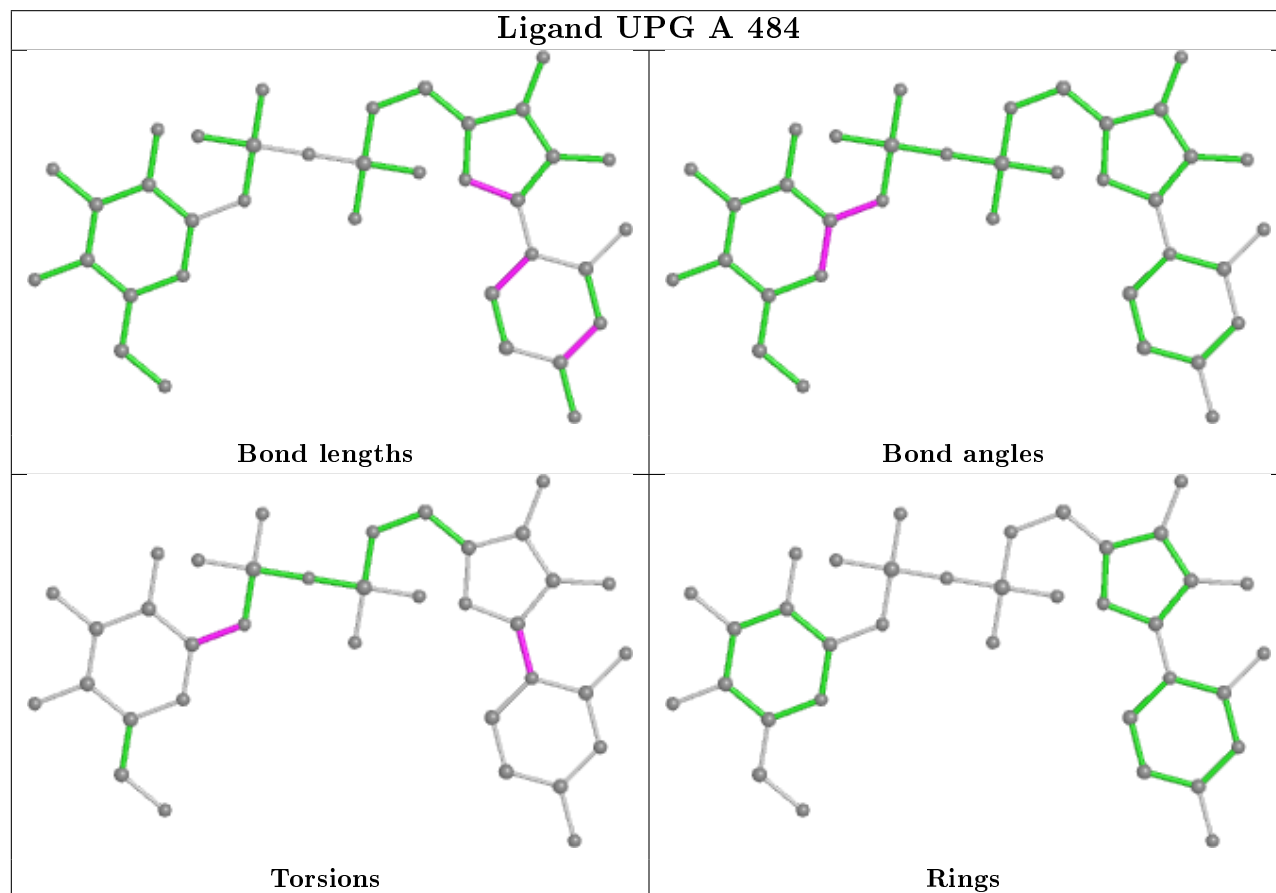
Mol	Chain	Res	Type	Atoms
2	A	484	UPG	C2C-C1C-N1-C6
2	A	484	UPG	O4C-C1C-N1-C6
2	B	492	UPG	C2C-C1C-N1-C6
2	B	492	UPG	O4C-C1C-N1-C6
5	A	489	DTU	C1-C2-C3-O3
5	A	489	DTU	C2-C3-C4-S4
3	A	485	GOL	O1-C1-C2-C3
3	B	491	GOL	O1-C1-C2-C3
6	B	490	PG4	O4-C7-C8-O5
6	B	490	PG4	O3-C5-C6-O4
3	B	489	GOL	C1-C2-C3-O3
3	B	491	GOL	C1-C2-C3-O3
3	B	491	GOL	O1-C1-C2-O2
6	B	490	PG4	O2-C3-C4-O3
5	A	489	DTU	O2-C2-C3-O3
3	A	485	GOL	O1-C1-C2-O2
6	B	490	PG4	O1-C1-C2-O2
6	B	490	PG4	C8-C7-O4-C6
5	A	489	DTU	O3-C3-C4-S4
6	B	490	PG4	C3-C4-O3-C5
2	A	484	UPG	O5'-C1'-O3B-PB
3	B	491	GOL	O2-C2-C3-O3
3	A	490	GOL	O1-C1-C2-C3
3	B	489	GOL	O2-C2-C3-O3
6	B	490	PG4	C1-C2-O2-C3

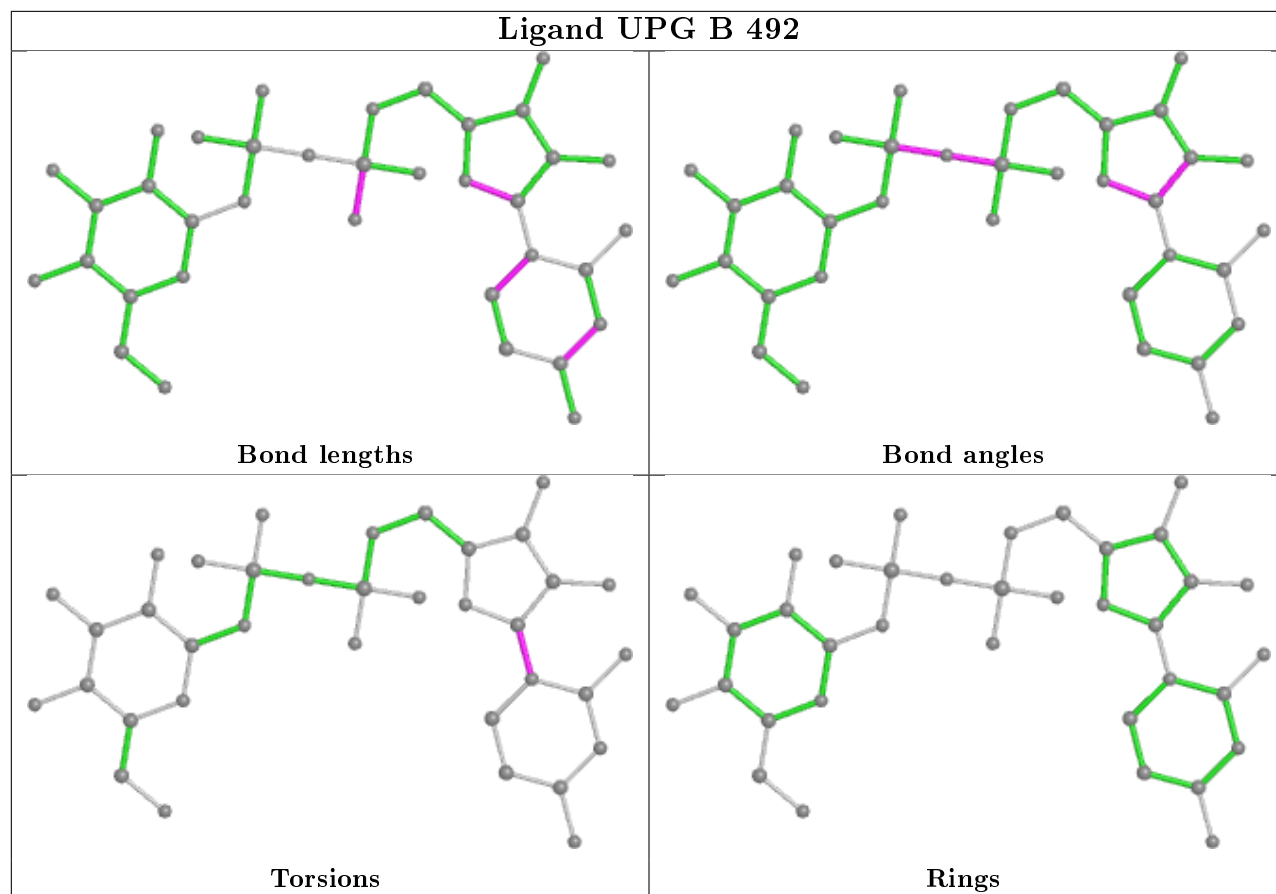
There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	489	GOL	1	0
5	A	489	DTU	5	0
6	B	490	PG4	4	0
4	A	487	SO4	1	0
3	A	485	GOL	2	0
4	B	484	SO4	1	0
3	B	491	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	468/484 (96%)	0.33	15 (3%)	47 50	20, 27, 32, 39	1 (0%)
1	B	457/484 (94%)	0.63	41 (8%)	9 11	18, 27, 33, 37	0
All	All	925/968 (95%)	0.47	56 (6%)	21 24	18, 27, 32, 39	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	ILE	8.2
1	B	475	LEU	5.1
1	B	469	ILE	4.5
1	B	462	LEU	4.5
1	B	467	LEU	4.1
1	B	265	ASP	4.0
1	B	118	ARG	4.0
1	A	272	ARG	3.8
1	B	339	SER	3.8
1	B	459	ILE	3.6
1	B	466	PRO	3.6
1	A	271	THR	3.5
1	B	285	LYS	3.5
1	B	480	VAL	3.4
1	B	414	GLU	3.2
1	B	88	GLY	3.0
1	B	263	VAL	3.0
1	B	448	GLY	3.0
1	B	449	ALA	2.9
1	B	474	VAL	2.8
1	B	167	ILE	2.7
1	B	381	LEU	2.7
1	A	307	ILE	2.7
1	B	400	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	121	ARG	2.7
1	B	481	VAL	2.6
1	A	179	ALA	2.6
1	B	468	ILE	2.6
1	B	340	GLN	2.6
1	B	392	GLU	2.5
1	B	92	ASN	2.5
1	B	87	THR	2.5
1	A	471	SER	2.4
1	B	216	ILE	2.4
1	B	276	VAL	2.4
1	A	229	ARG	2.4
1	B	347	LEU	2.3
1	A	124	ASN	2.3
1	B	479	VAL	2.3
1	B	442	ARG	2.3
1	A	305	ILE	2.2
1	A	285	LYS	2.2
1	B	433	LEU	2.2
1	B	465	GLU	2.2
1	A	102	ASN	2.2
1	B	115	GLU	2.2
1	A	450	ASP	2.1
1	B	420	ASP	2.1
1	A	215	PHE	2.1
1	B	439	LEU	2.1
1	B	382	ALA	2.1
1	B	349	VAL	2.1
1	A	92	ASN	2.1
1	A	468	ILE	2.1
1	B	73	LEU	2.0
1	A	403[A]	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

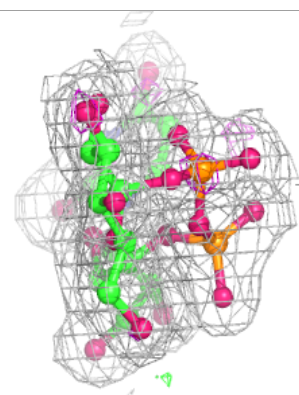
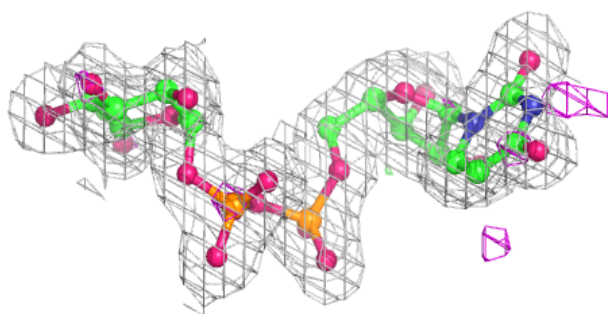
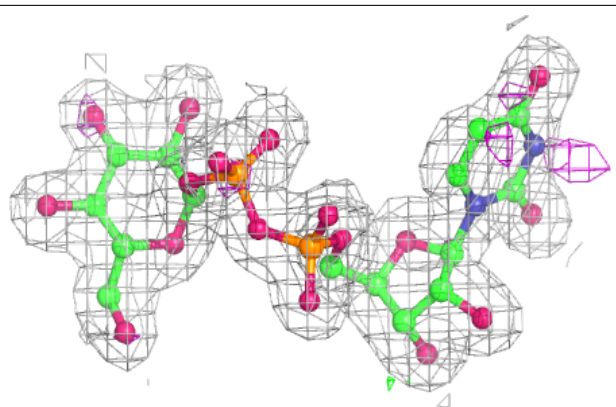
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PG4	B	490	13/13	0.82	0.18	47,47,52,53	0
5	DTU	A	489	8/8	0.88	0.14	30,33,38,40	0
4	SO4	A	487	5/5	0.88	0.19	52,54,56,57	0
4	SO4	B	484	5/5	0.89	0.19	32,32,33,33	5
4	SO4	B	486	5/5	0.90	0.43	58,59,59,60	0
3	GOL	B	491	6/6	0.91	0.14	35,41,41,43	0
4	SO4	B	488	5/5	0.91	0.34	54,54,55,55	5
4	SO4	B	485	5/5	0.93	0.13	57,57,58,59	0
3	GOL	A	490	6/6	0.94	0.09	27,32,33,34	0
3	GOL	A	486	6/6	0.95	0.08	23,27,28,30	0
3	GOL	A	485	6/6	0.95	0.11	18,28,30,31	0
3	GOL	B	489	6/6	0.95	0.11	29,30,30,31	0
2	UPG	A	484	36/36	0.97	0.07	15,20,23,23	0
4	SO4	B	487	5/5	0.97	0.31	52,54,55,55	0
4	SO4	A	488	5/5	0.98	0.14	36,37,38,39	5
2	UPG	B	492	36/36	0.98	0.07	16,21,24,27	0

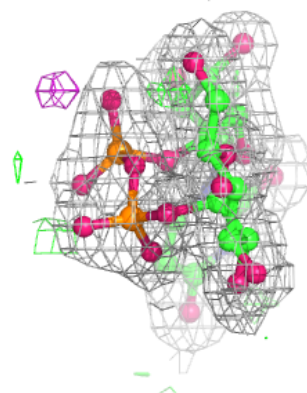
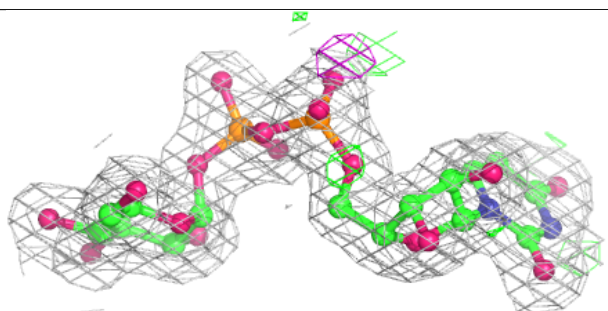
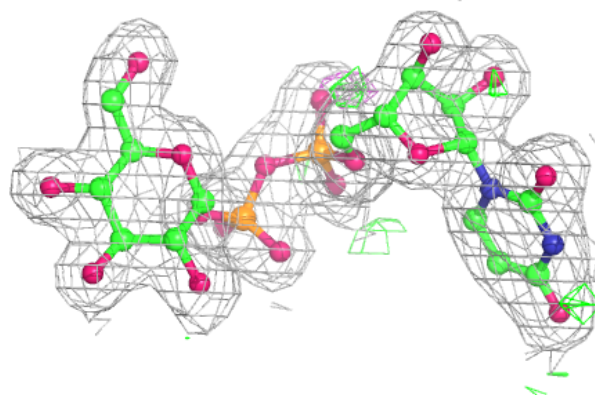
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UPG A 484:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around UPG B 492:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.