



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:27 PM UTC

PDB ID : 3GUE / pdb_00003gue
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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)

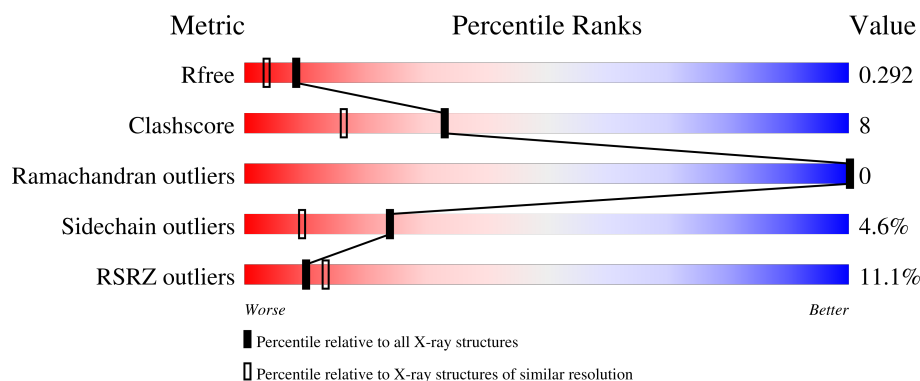
1 Overall quality at a glance

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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	484	5% 79% 16% • •
1	B	484	17% 73% 20% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.

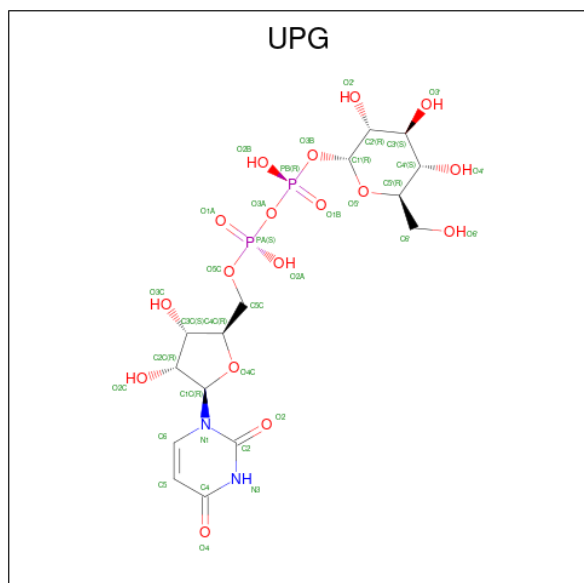
- Molecule 1 is a protein called UTP-glucose-1-phosphate uridylyltransferase 2.

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:

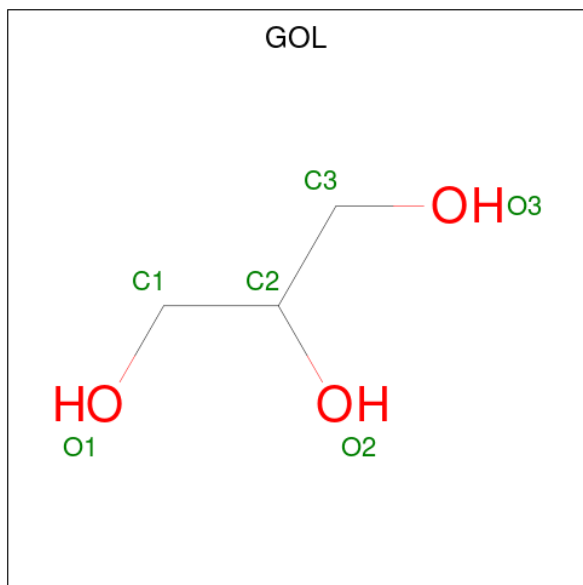
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q388T4
A	52	SER	PHE	conflict	UNP Q388T4
A	471	SER	ASN	conflict	UNP Q388T4
B	0	GLY	-	expression tag	UNP Q388T4
B	52	SER	PHE	conflict	UNP Q388T4
B	471	SER	ASN	conflict	UNP Q388T4

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



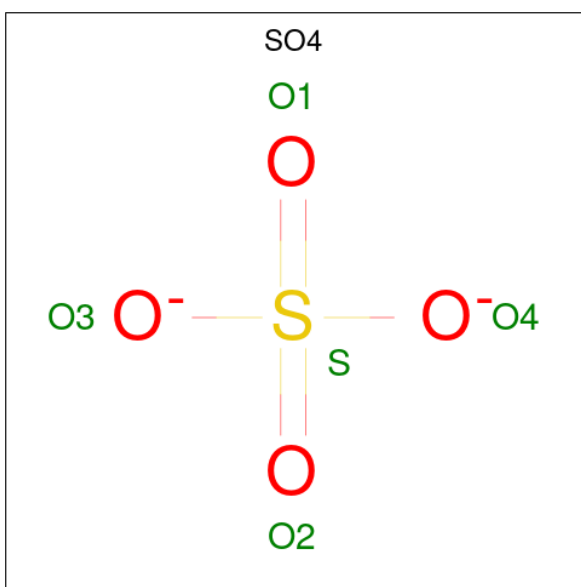
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



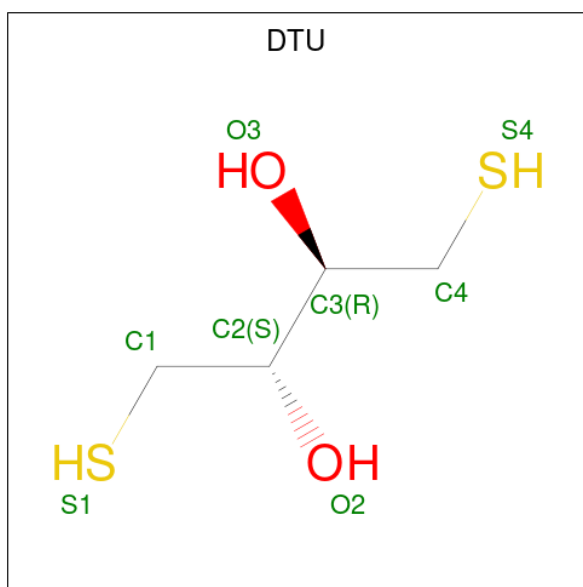
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



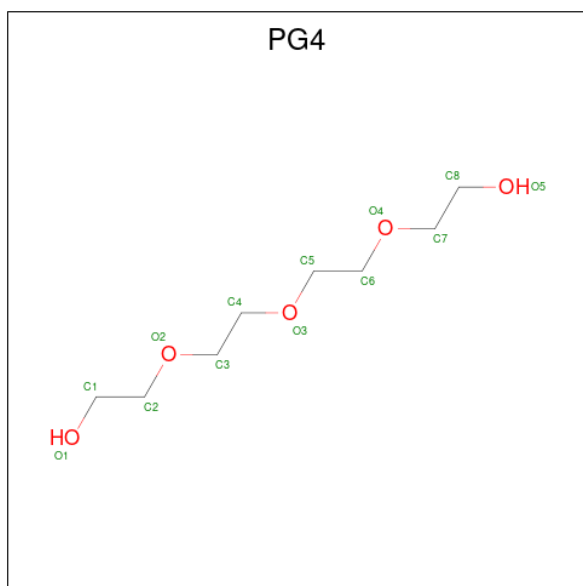
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (CCD ID: DTU) (formula: $C_4H_{10}O_2S_2$).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

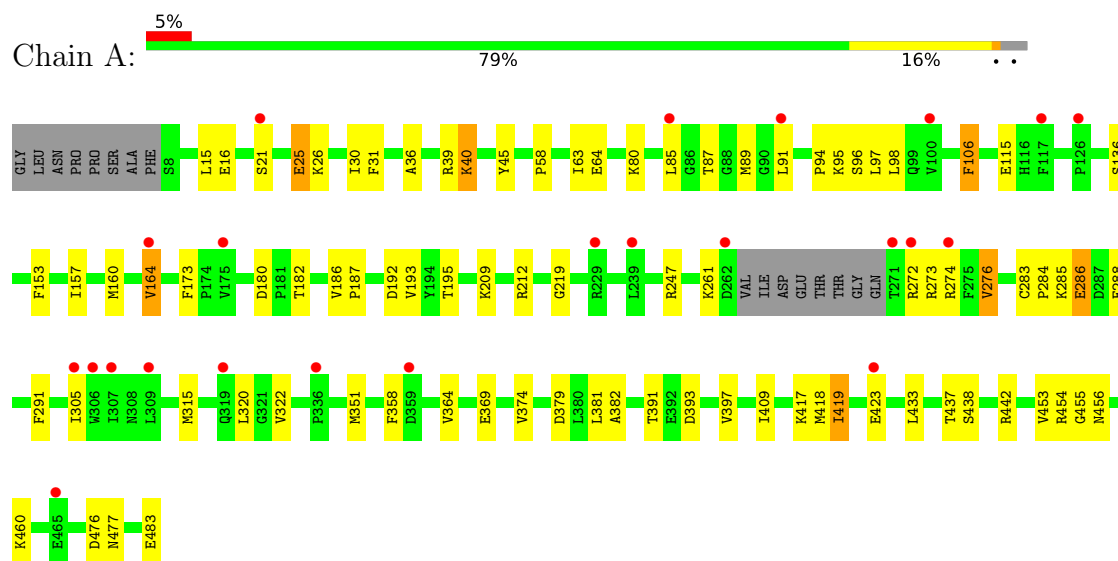
- Molecule 7 is water.

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

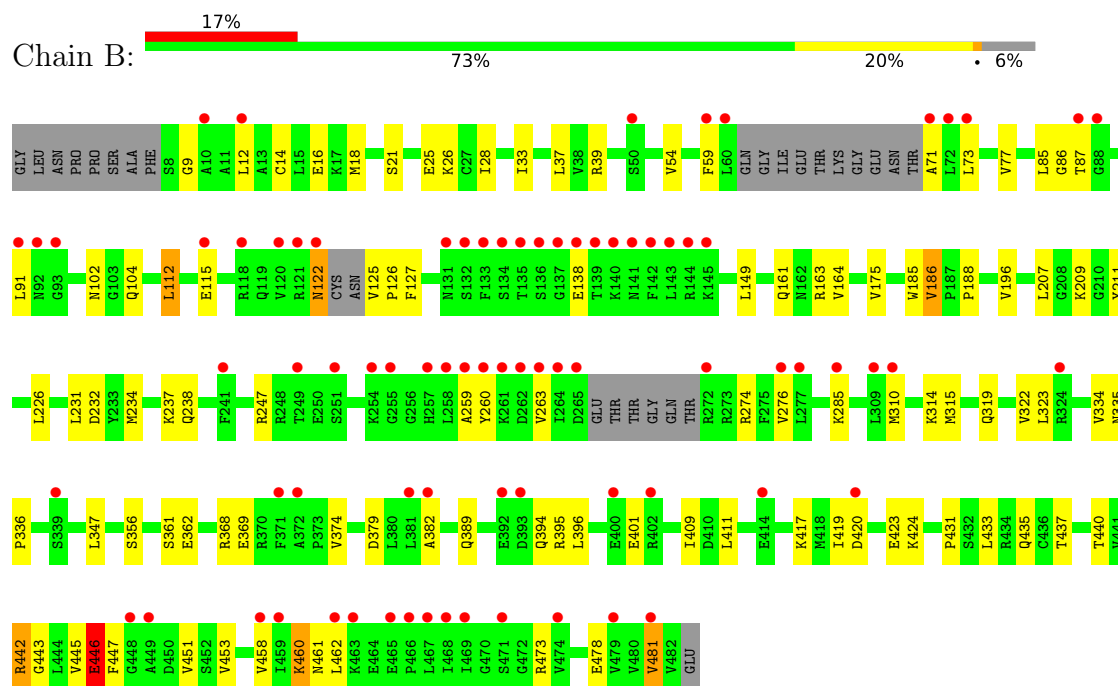
3 Residue-property plots [i](#)

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: UTP-glucose-1-phosphate uridylyltransferase 2



- Molecule 1: UTP-glucose-1-phosphate uridylyltransferase 2



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 25.00 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-1.92) 98.9 (25.00-1.92)	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)	0.38 , 42.6	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	0.89	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: DTU, SO4, GOL, UPG, PG4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.82	1/3770 (0.0%)	1.02	8/5087 (0.2%)
1	B	0.99	9/3645 (0.2%)	1.03	6/4924 (0.1%)
All	All	0.91	10/7415 (0.1%)	1.03	14/10011 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	ARG	NE-CZ	20.39	1.55	1.33
1	B	460	LYS	CE-NZ	12.92	1.88	1.49
1	B	462	LEU	C-N	7.55	1.43	1.33
1	B	462	LEU	CB-CG	7.32	1.68	1.53
1	B	442	ARG	CD-NE	7.07	1.56	1.46
1	B	460	LYS	C-O	-6.09	1.17	1.24
1	B	481	VAL	CB-CG2	5.72	1.71	1.52
1	A	322	VAL	CA-CB	5.60	1.59	1.53
1	B	446	GLU	CD-OE2	5.60	1.35	1.25
1	B	481	VAL	CB-CG1	5.08	1.69	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	442	ARG	CD-NE-CZ	-12.04	107.55	124.40
1	B	122	ASN	CA-CB-CG	-6.93	105.67	112.60
1	A	164	VAL	CA-C-N	-6.50	113.25	120.14
1	A	164	VAL	C-N-CA	-6.50	113.25	120.14
1	A	272	ARG	N-CA-C	6.05	118.10	110.24
1	B	25	GLU	N-CA-C	5.99	117.89	111.36
1	A	193	VAL	N-CA-C	5.57	116.97	110.62
1	A	106	PHE	N-CA-C	-5.38	105.41	111.28
1	A	173	PHE	CA-C-N	-5.38	114.22	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	PHE	C-N-CA	-5.38	114.22	119.76
1	B	9	GLY	N-CA-C	5.18	118.51	112.50
1	A	322	VAL	N-CA-C	5.05	113.64	106.53
1	B	186	VAL	CA-C-N	-5.02	116.00	119.66
1	B	186	VAL	C-N-CA	-5.02	116.00	119.66

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	3695	0	3718	55	0
1	B	3569	0	3559	60	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	115	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 8.

All (115) 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:CE	1:B:460:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ARG:HH21	3:A:485:GOL:H32	1.42	0.83
1:B:18:MET:HE3	1:B:28:ILE:HG23	1.63	0.81
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
1:B:431:PRO:HB3	1:B:451:VAL:HG23	1.81	0.60
1:B:149:LEU:HD23	6:B:490:PG4:H82	1.84	0.60
1:B:310:MET:O	1:B:314:LYS:HG3	2.01	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:391:THR:OG1	1:A:393:ASP:OD1	2.21	0.56
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:91:LEU:HB3	4:A:487:SO4:O3	2.06	0.55
1:A:192:ASP:OD1	5:A:489:DTU:S4	2.61	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:315:MET:HE1	1:A:358:PHE:CD1	2.44	0.53
1:B:369:GLU:HG3	1:B:395:ARG:HH22	1.73	0.53
1:B:12:LEU:O	1:B:16:GLU:HG3	2.09	0.53
1:B:77:VAL:HG13	1:B:126:PRO:HB2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:PHE:CD1	1:B:451:VAL:HG21	2.46	0.51
1:A:305:ILE:CG1	1:A:351:MET:HE3	2.42	0.50
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:283:CYS:SG	1:A:291:PHE:HB2	2.53	0.49
1:B:14:CYS:O	1:B:18:MET:HG3	2.13	0.49
1:B:188:PRO:HB2	3:B:489:GOL:H2	1.94	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
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:71:ALA:N	7:B:853:HOH:O	2.46	0.47
1:B:259:ALA:HB3	1:B:276:VAL:CG1	2.45	0.47
1:A:261:LYS:HB2	1:A:276:VAL:HG11	1.96	0.47
1:A:417:LYS:HG2	1:A:418:MET:HE3	1.94	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: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: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:286:GLU:H	1:A:286:GLU:CD	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:LEU:CD1	1:B:186:VAL:HG23	2.49	0.42
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:A:305:ILE:HG12	1:A:351:MET:HE3	2.00	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:A:15:LEU:C	1:A:15:LEU:HD23	2.46	0.41
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:237:LYS:NZ	1:B:362:GLU:OE2	2.30	0.41
1:B:433:LEU:HD23	1:B:453:VAL:HB	2.03	0.41
1:B:401:GLU:OE2	1:B:435:GLN:OE1	2.38	0.41
1:B:440:THR:HB	1:B:458:VAL:HG22	2.02	0.41
1:A:136:SER:CB	1:A:160:MET:HE1	2.51	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:B:87:THR:HB	1:B:336:PRO:HB3	2.03	0.40
1:B:315:MET:HE3	1:B:323:LEU:HD11	2.02	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:A:261:LYS:HB2	1:A:276:VAL:CG1	2.51	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 ⓘ

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	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 ⓘ

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%)	396 (97%)	14 (3%)	32	16
1	B	393/423 (93%)	369 (94%)	24 (6%)	17	5
All	All	803/846 (95%)	765 (95%)	38 (5%)	24	9

All (38) 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	115	GLU
1	A	186	VAL
1	A	209	LYS
1	A	273	ARG
1	A	274	ARG
1	A	276	VAL
1	A	286	GLU
1	A	320	LEU
1	A	419	ILE
1	A	483	GLU
1	B	21[A]	SER

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Mol	Chain	Res	Type
1	B	21[B]	SER
1	B	33	ILE
1	B	37	LEU
1	B	73	LEU
1	B	102	ASN
1	B	112	LEU
1	B	115	GLU
1	B	138	GLU
1	B	164	VAL
1	B	209	LYS
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	437	THR
1	B	445	VAL
1	B	446	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	415	HIS
1	A	435	GLN
1	A	456	ASN
1	B	104	GLN
1	B	235	HIS
1	B	319	GLN
1	B	389	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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$
2	UPG	B	492	-	37,38,38	1.32	5 (13%)	55,58,58	1.39	4 (7%)
3	GOL	B	491	-	5,5,5	0.23	0	5,5,5	0.40	0
3	GOL	A	486	-	5,5,5	0.47	0	5,5,5	0.31	0
3	GOL	A	490	-	5,5,5	0.38	0	5,5,5	0.31	0
3	GOL	B	489	-	5,5,5	0.44	0	5,5,5	0.49	0
4	SO4	B	484	-	4,4,4	0.21	0	6,6,6	0.27	0
4	SO4	A	487	-	4,4,4	0.36	0	6,6,6	0.34	0
5	DTU	A	489	-	7,7,7	0.71	0	4,8,8	1.29	1 (25%)
6	PG4	B	490	-	12,12,12	0.47	0	11,11,11	0.47	0
4	SO4	B	486	-	4,4,4	0.23	0	6,6,6	0.26	0
4	SO4	B	488	-	4,4,4	0.24	0	6,6,6	0.17	0
3	GOL	A	485	-	5,5,5	0.39	0	5,5,5	1.20	1 (20%)
2	UPG	A	484	-	37,38,38	1.37	3 (8%)	55,58,58	1.34	4 (7%)
4	SO4	B	487	-	4,4,4	0.25	0	6,6,6	0.18	0
4	SO4	A	488	-	4,4,4	0.30	0	6,6,6	0.20	0
4	SO4	B	485	-	4,4,4	0.19	0	6,6,6	0.14	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
2	UPG	B	492	-	-	0/23/59/59	0/3/3/3
3	GOL	B	491	-	-	4/4/4/4	-
3	GOL	A	486	-	-	0/4/4/4	-
3	GOL	A	490	-	-	1/4/4/4	-
3	GOL	B	489	-	-	2/4/4/4	-
3	GOL	A	485	-	-	2/4/4/4	-
2	UPG	A	484	-	-	1/23/59/59	0/3/3/3
5	DTU	A	489	-	2/2/2/2	4/8/8/8	-
6	PG4	B	490	-	-	7/10/10/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	484	UPG	PA-O3A	5.14	1.65	1.59
2	A	484	UPG	PB-O3A	3.39	1.63	1.59
2	B	492	UPG	O4C-C1C	3.05	1.49	1.42
2	B	492	UPG	PA-O3A	2.74	1.62	1.59
2	B	492	UPG	C6-C5	2.45	1.40	1.35
2	B	492	UPG	C5-C4	-2.35	1.38	1.43
2	A	484	UPG	C6-N1	2.27	1.43	1.38
2	B	492	UPG	PA-O2A	-2.08	1.45	1.55

All (10) 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	C5-C4-N3	4.28	120.79	114.80
2	B	492	UPG	C4-N3-C2	-3.95	121.71	126.61
2	A	484	UPG	C5-C4-N3	3.60	119.84	114.80
2	B	492	UPG	C2C-C1C-N1	3.29	122.41	113.25
2	B	492	UPG	N3-C2-N1	3.03	118.84	114.89
2	A	484	UPG	C4-N3-C2	-2.68	123.29	126.61
2	A	484	UPG	C2C-C1C-N1	2.55	120.34	113.25
3	A	485	GOL	O1-C1-C2	-2.17	100.60	110.38
5	A	489	DTU	O3-C3-C2	2.15	114.08	109.57

All (2) chirality outliers are listed below:

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

All (21) torsion outliers are listed below:

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

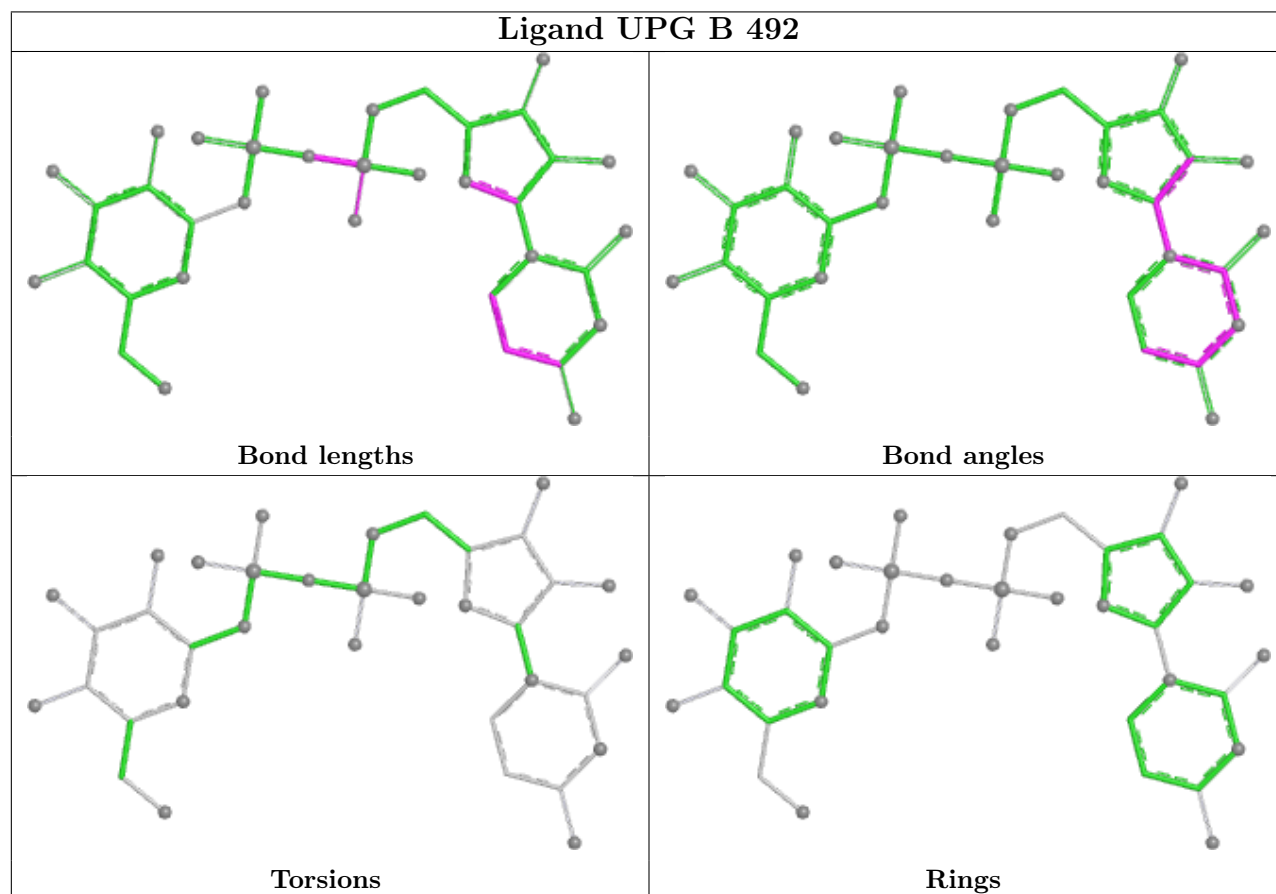
There are no ring outliers.

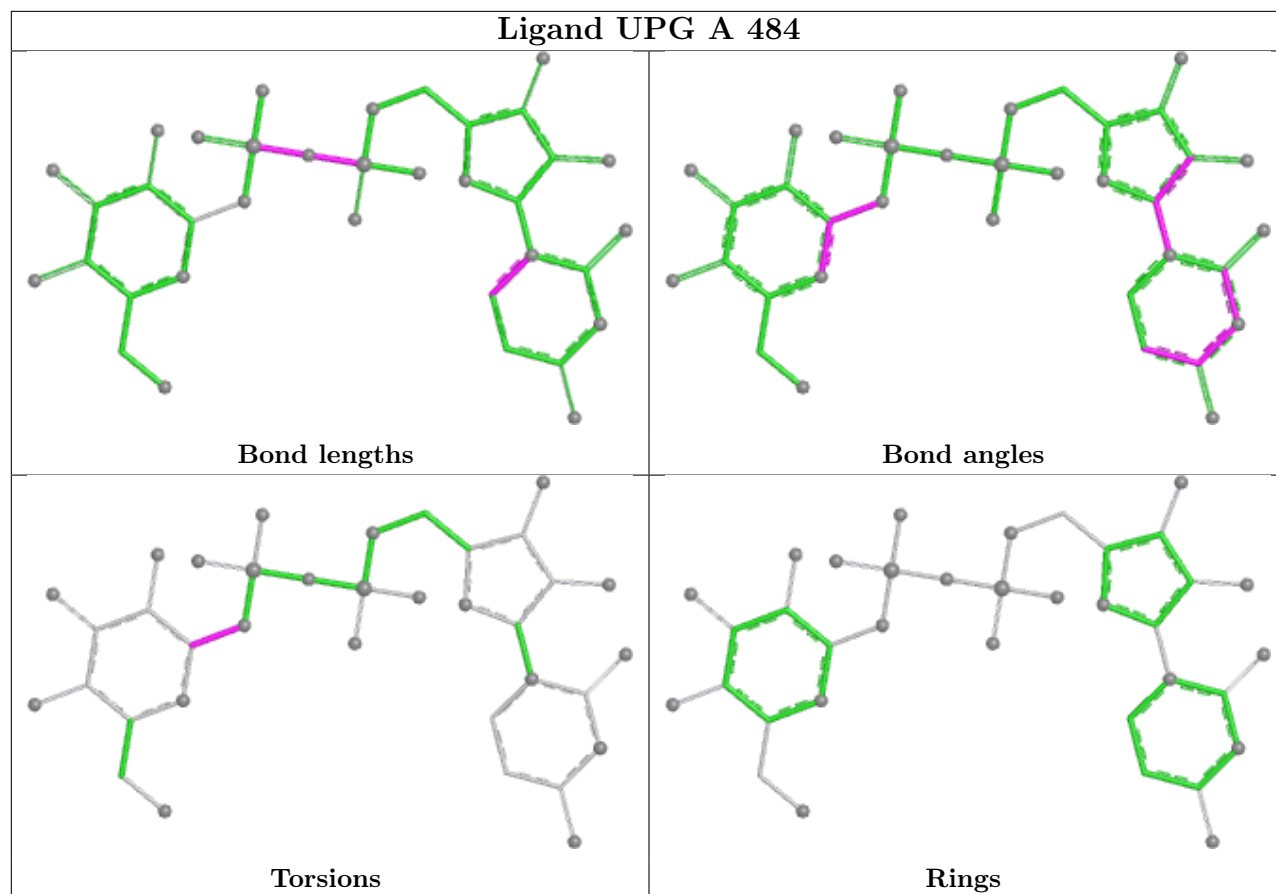
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	491	GOL	1	0
3	B	489	GOL	1	0
4	B	484	SO4	1	0
4	A	487	SO4	1	0
5	A	489	DTU	5	0
6	B	490	PG4	4	0
3	A	485	GOL	2	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%)	0.82	23 (4%) 35 39	16, 27, 32, 39	4 (0%)
1	B	457/484 (94%)	1.24	80 (17%) 4 5	17, 27, 33, 37	4 (0%)
All	All	925/968 (95%)	1.03	103 (11%) 10 13	16, 27, 32, 39	8 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	PHE	8.2
1	B	132	SER	7.1
1	B	264	ILE	6.6
1	B	135	THR	6.5
1	B	134	SER	6.3
1	B	131	ASN	5.6
1	B	142	PHE	5.4
1	B	136	SER	5.1
1	B	139	THR	4.9
1	B	138	GLU	4.8
1	B	71	ALA	4.5
1	B	137	GLY	4.4
1	B	467	LEU	4.2
1	B	481	VAL	4.2
1	B	92	ASN	4.1
1	B	143	LEU	4.1
1	B	265	ASP	3.7
1	A	307	ILE	3.6
1	A	100	VAL	3.5
1	B	263	VAL	3.5
1	B	145	LYS	3.3
1	B	118	ARG	3.3
1	B	462	LEU	3.3
1	B	259	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	144	ARG	3.2
1	B	12	LEU	3.2
1	B	140	LYS	3.2
1	B	459	ILE	3.1
1	B	448	GLY	3.1
1	B	141	ASN	3.1
1	B	262	ASP	3.0
1	B	60	LEU	3.0
1	B	276	VAL	3.0
1	B	121	ARG	3.0
1	A	306	TRP	3.0
1	B	474	VAL	2.9
1	A	117	PHE	2.9
1	B	87	THR	2.9
1	B	261	LYS	2.8
1	A	271	THR	2.8
1	B	458	VAL	2.8
1	B	260	TYR	2.8
1	B	88	GLY	2.7
1	B	91	LEU	2.7
1	A	126	PRO	2.7
1	B	469	ILE	2.7
1	B	414	GLU	2.7
1	A	91	LEU	2.6
1	B	251[A]	SER	2.6
1	B	466	PRO	2.6
1	B	285	LYS	2.6
1	A	272	ARG	2.5
1	B	73	LEU	2.5
1	B	393	ASP	2.5
1	B	50	SER	2.5
1	A	175	VAL	2.5
1	A	465	GLU	2.5
1	A	309	LEU	2.5
1	B	258	LEU	2.5
1	B	115	GLU	2.5
1	A	164	VAL	2.5
1	B	277	LEU	2.4
1	B	392	GLU	2.4
1	A	85	LEU	2.4
1	B	468	ILE	2.4
1	B	10	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	120	VAL	2.4
1	B	255	GLY	2.3
1	B	371	PHE	2.2
1	B	449	ALA	2.2
1	A	21	SER	2.2
1	B	122	ASN	2.2
1	B	249	THR	2.2
1	B	381	LEU	2.2
1	A	359	ASP	2.2
1	B	372	ALA	2.2
1	A	274	ARG	2.2
1	B	272	ARG	2.2
1	B	339	SER	2.2
1	B	471	SER	2.2
1	B	310	MET	2.2
1	B	324	ARG	2.2
1	B	400	GLU	2.1
1	B	420	ASP	2.1
1	B	72	LEU	2.1
1	B	463	LYS	2.1
1	B	257	HIS	2.1
1	B	465	GLU	2.1
1	B	382	ALA	2.1
1	B	479	VAL	2.1
1	B	59	PHE	2.1
1	B	241	PHE	2.1
1	A	262	ASP	2.1
1	B	254	LYS	2.1
1	A	239	LEU	2.1
1	B	309	LEU	2.1
1	A	305	ILE	2.0
1	B	93	GLY	2.0
1	A	319	GLN	2.0
1	A	229	ARG	2.0
1	B	402	ARG	2.0
1	A	423	GLU	2.0
1	A	336	PRO	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

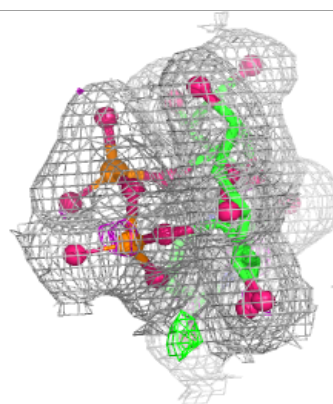
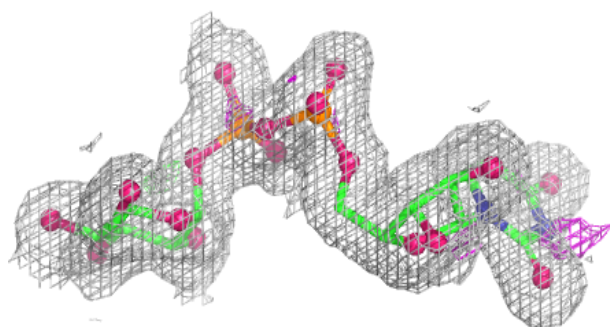
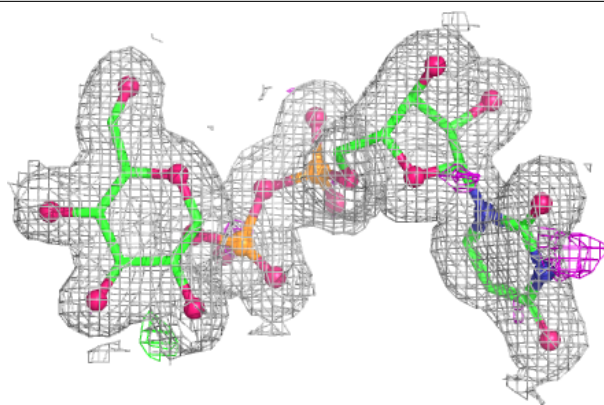
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	488	5/5	0.70	0.17	54,54,55,55	5
6	PG4	B	490	13/13	0.72	0.18	47,47,52,53	0
4	SO4	B	486	5/5	0.74	0.16	58,59,59,60	0
4	SO4	A	487	5/5	0.80	0.15	52,54,56,57	0
4	SO4	B	484	5/5	0.83	0.15	32,32,33,33	5
4	SO4	B	485	5/5	0.86	0.14	57,57,58,59	0
3	GOL	B	491	6/6	0.87	0.14	35,41,41,43	0
4	SO4	B	487	5/5	0.87	0.13	52,54,55,55	0
3	GOL	A	490	6/6	0.88	0.13	27,32,33,34	0
5	DTU	A	489	8/8	0.89	0.13	30,33,38,40	0
3	GOL	B	489	6/6	0.89	0.13	29,30,30,31	0
3	GOL	A	485	6/6	0.93	0.11	18,28,30,31	0
3	GOL	A	486	6/6	0.95	0.08	23,27,28,30	0
4	SO4	A	488	5/5	0.96	0.09	36,37,38,39	5
2	UPG	A	484	36/36	0.96	0.07	15,20,23,23	0
2	UPG	B	492	36/36	0.97	0.06	16,21,24,27	0

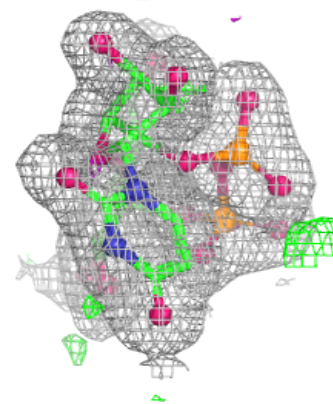
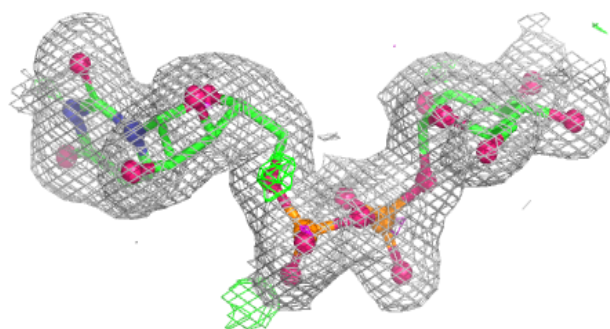
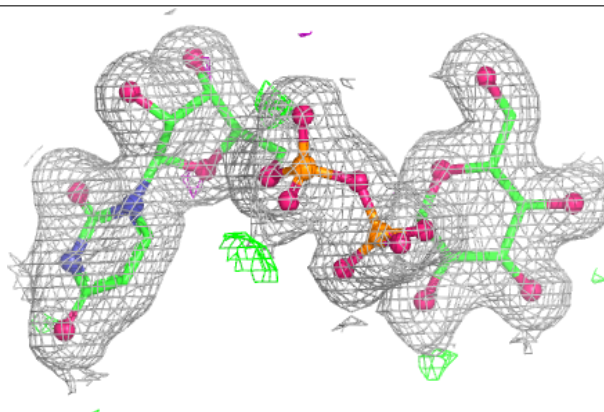
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.