



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:38 PM BST

PDB ID : 6K8D
Title : UDP-glucose pyrophosphorylase with UPG from Acinetobacter Baumannii
Authors : Lee, J.H.; Kang, L.W.
Deposited on : 2019-06-11
Resolution : 2.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

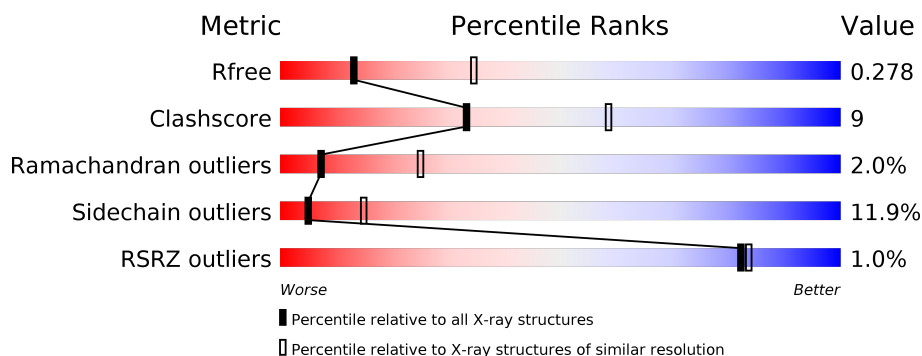
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	290	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 78%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 78% 17% 6% </div> </div>
1	B	290	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 77%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 77% 19% . </div> </div>
1	C	290	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 22%, green 74%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 74% 22% . </div> </div>
1	D	290	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 26%, green 71%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 71% 26% .. </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8837 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.

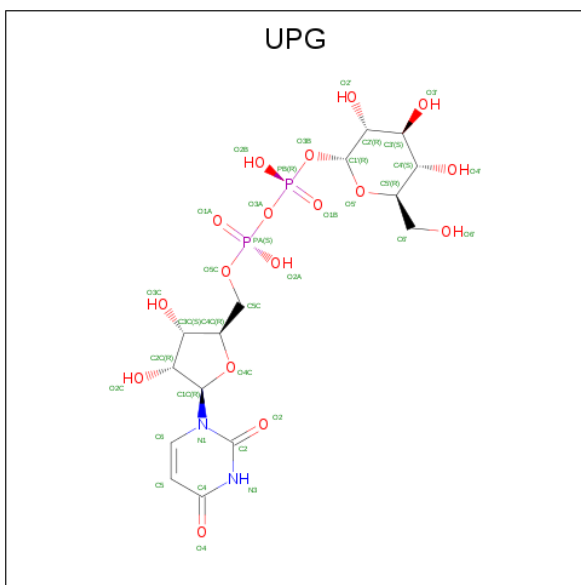
- Molecule 1 is a protein called UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2168	1379	363	415	11			
1	B	290	Total	C	N	O	S	0	0	0
			2163	1377	362	413	11			
1	C	290	Total	C	N	O	S	0	0	0
			2157	1371	361	414	11			
1	D	288	Total	C	N	O	S	0	0	0
			2154	1371	362	410	11			

There are 4 discrepancies between the modelled and reference sequences:

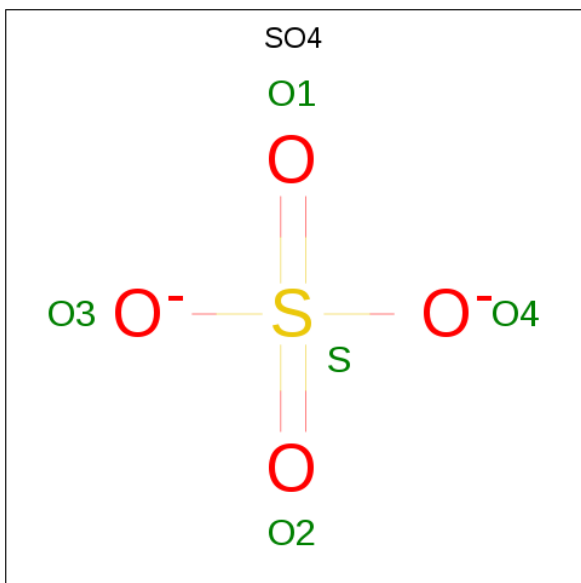
Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LEU	GLN	engineered mutation	UNP X2KZJ9
B	286	LEU	GLN	engineered mutation	UNP X2KZJ9
C	286	LEU	GLN	engineered mutation	UNP X2KZJ9
D	286	LEU	GLN	engineered mutation	UNP X2KZJ9

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by author).



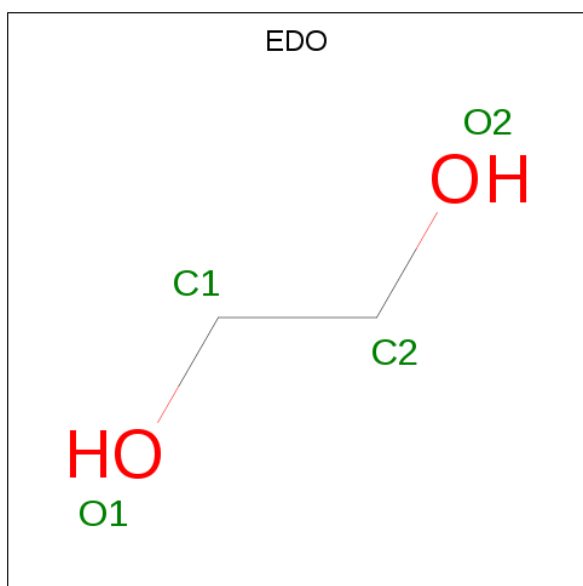
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 15	N 2	O 17	P 2	0	0
2	B	1	Total 36	C 15	N 2	O 17	P 2	0	0
2	C	1	Total 36	C 15	N 2	O 17	P 2	0	0
2	D	1	Total 36	C 15	N 2	O 17	P 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

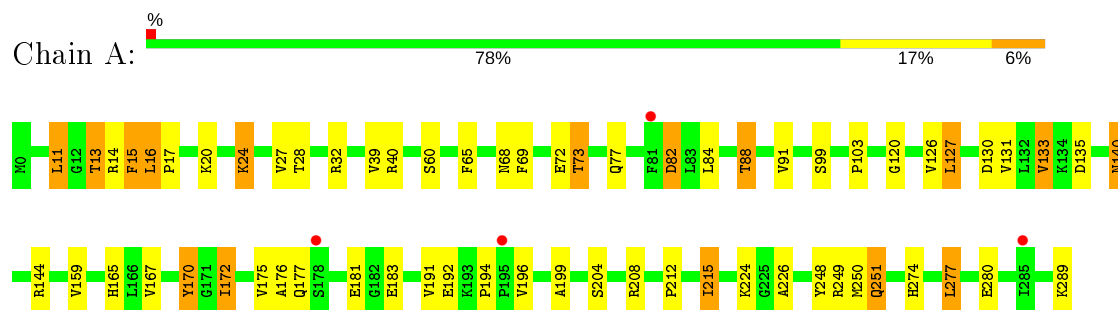
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	D	2	Total	O	0	0
			2	2		

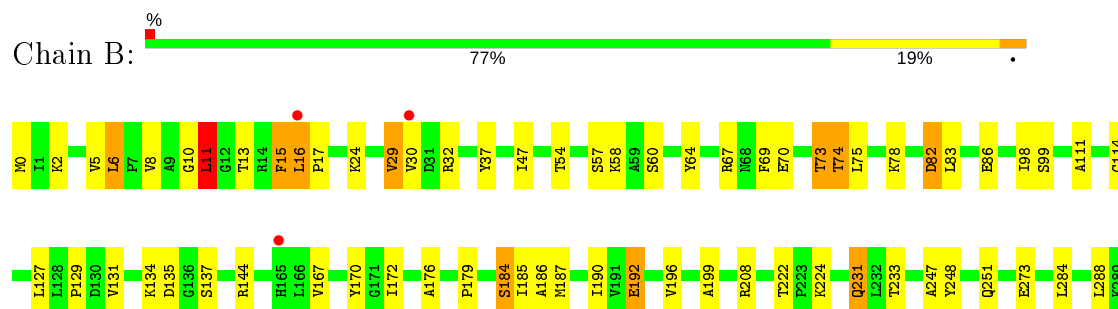
3 Residue-property plots [i](#)

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.

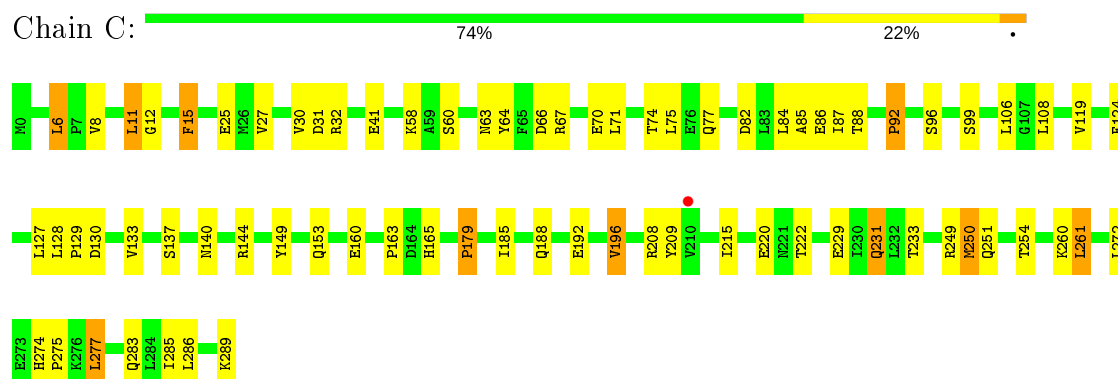
- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase



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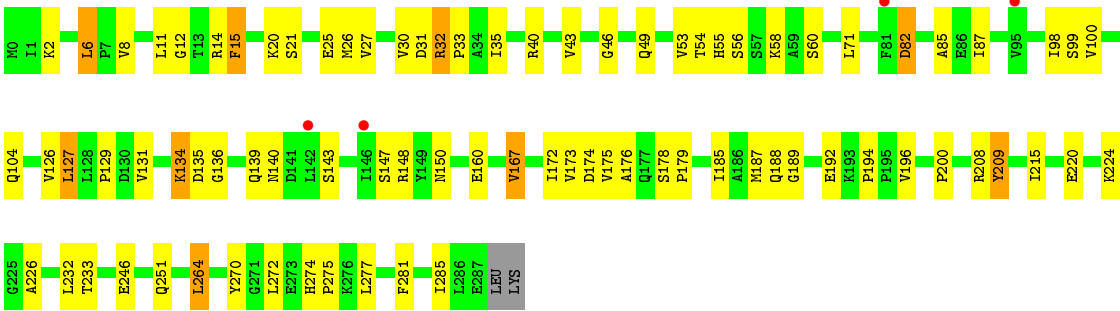


- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.53Å 114.38Å 114.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.47 – 2.94 40.44 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.8 (40.47-2.94) 96.9 (40.44-2.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.218 , 0.280 0.216 , 0.278	Depositor DCC
R_{free} test set	1479 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 20.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.450 for -h,l,k 0.038 for -k,-h,l 0.036 for l,-k,h 0.033 for l,h,k 0.033 for k,l,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8837	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, UPG, EDO, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/2204	0.80	0/2996
1	B	0.69	0/2199	0.81	0/2988
1	C	0.69	0/2192	0.84	0/2975
1	D	0.70	0/2188	0.83	0/2967
All	All	0.69	0/8783	0.82	0/11926

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	PHE	Peptide
1	A	77	GLN	Peptide
1	B	15	PHE	Peptide

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	2168	0	2164	41	0
1	B	2163	0	2157	39	0
1	C	2157	0	2122	41	0
1	D	2154	0	2140	46	0
2	A	36	0	22	1	0
2	B	36	0	22	0	0
2	C	36	0	22	2	0
2	D	36	0	22	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	1	0
3	D	10	0	0	0	0
4	A	4	0	6	0	0
5	B	6	0	8	1	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	8837	0	8685	150	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 9.

All (150) 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:A:69:PHE:O	1:A:73:THR:HG23	1.77	0.83
1:B:192:GLU:HG3	1:B:231:GLN:HG2	1.60	0.83
1:B:192:GLU:HG2	1:B:233:THR:OG1	1.89	0.72
1:C:31:ASP:OD1	1:C:32:ARG:HD2	1.90	0.72
1:B:70:GLU:O	1:B:74:THR:HG23	1.91	0.71
1:A:84:LEU:O	1:A:88:THR:OG1	2.06	0.70
1:D:82:ASP:O	1:D:85:ALA:HB3	1.94	0.68
1:A:274:HIS:ND1	1:A:277:LEU:HD12	2.09	0.67
1:C:66:ASP:OD1	1:C:67:ARG:N	2.27	0.67
1:C:6:LEU:HD23	1:C:6:LEU:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:HD23	1:D:127:LEU:N	2.10	0.66
1:A:140:ASN:C	1:A:140:ASN:HD22	1.99	0.66
1:A:192:GLU:O	1:A:194:PRO:HD3	1.97	0.64
1:C:192:GLU:HG3	1:C:231:GLN:HG2	1.79	0.64
1:C:67:ARG:HD3	1:D:104:GLN:HE21	1.64	0.62
1:D:192:GLU:HG2	1:D:233:THR:OG1	1.99	0.62
1:B:167:VAL:HG11	1:B:199:ALA:HB2	1.81	0.62
1:A:16:LEU:HD13	1:C:87:ILE:HG23	1.80	0.61
1:D:6:LEU:N	1:D:6:LEU:HD23	2.16	0.61
1:B:64:TYR:O	1:D:20:LYS:NZ	2.33	0.61
1:C:128:LEU:HD13	2:C:301:UPG:H5C2	1.84	0.60
1:C:12:GLY:O	1:C:15:PHE:N	2.34	0.60
1:D:274:HIS:ND1	1:D:277:LEU:HB2	2.17	0.59
1:C:25:GLU:OE1	1:C:58:LYS:NZ	2.35	0.59
1:C:41:GLU:OE1	1:C:208:ARG:NE	2.36	0.58
1:D:8:VAL:HG12	1:D:129:PRO:HG3	1.84	0.58
1:A:167:VAL:HG11	1:A:199:ALA:HB2	1.86	0.58
1:A:16:LEU:HD13	1:C:87:ILE:CG2	2.34	0.58
1:A:181:GLU:HA	1:A:249:ARG:HG2	1.85	0.58
1:C:67:ARG:CD	1:D:104:GLN:HE21	2.17	0.58
1:B:69:PHE:O	1:B:73:THR:HG23	2.04	0.57
1:A:165:HIS:HA	1:A:196:VAL:HG22	1.85	0.57
1:C:60:SER:HA	1:C:63:ASN:HD22	1.70	0.57
1:A:16:LEU:HD21	1:C:71:LEU:HD21	1.86	0.57
1:C:82:ASP:O	1:C:85:ALA:HB3	2.06	0.56
1:B:184:SER:HB3	1:B:248:TYR:HA	1.88	0.56
1:C:179:PRO:HB3	1:C:185:ILE:HB	1.88	0.56
1:D:174:ASP:HB3	1:D:200:PRO:CB	2.37	0.55
1:D:167:VAL:HG22	1:D:172:ILE:HG12	1.88	0.55
1:D:173:VAL:CG2	1:D:187:MET:SD	2.95	0.55
1:D:6:LEU:HD22	1:D:127:LEU:HB2	1.88	0.55
1:A:126:VAL:C	1:A:127:LEU:HD23	2.27	0.55
1:C:133:VAL:HG13	1:C:250:MET:CE	2.37	0.55
1:A:159:VAL:HA	1:A:204:SER:O	2.07	0.54
1:D:174:ASP:OD1	1:D:189:GLY:N	2.41	0.54
1:C:274:HIS:ND1	1:C:277:LEU:HB2	2.23	0.54
1:D:31:ASP:OD1	1:D:32:ARG:HD2	2.08	0.54
1:B:54:THR:OG1	1:B:58:LYS:HB2	2.08	0.53
1:C:137:SER:OG	1:C:144:ARG:NH2	2.42	0.53
1:B:111:ALA:O	1:B:114:CYS:HB2	2.09	0.53
1:B:144:ARG:NH2	5:B:304:GOL:H2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HD23	1:B:6:LEU:N	2.25	0.52
1:B:16:LEU:HD13	1:D:87:ILE:CG2	2.39	0.52
1:B:75:LEU:O	1:B:78:LYS:O	2.27	0.52
1:A:192:GLU:C	1:A:194:PRO:HD3	2.30	0.51
1:A:16:LEU:CD1	1:C:87:ILE:HG23	2.41	0.51
1:C:6:LEU:HD22	1:C:127:LEU:HB2	1.93	0.51
1:A:192:GLU:OE2	2:A:301:UPG:O2'	2.28	0.51
1:B:8:VAL:HG12	1:B:129:PRO:HG3	1.92	0.51
1:D:8:VAL:O	1:D:58:LYS:HE3	2.12	0.50
1:C:108:LEU:HD12	1:C:108:LEU:O	2.12	0.50
1:D:175:VAL:HG11	1:D:178:SER:HA	1.93	0.50
1:A:274:HIS:CE1	1:A:277:LEU:HD12	2.46	0.49
1:B:5:VAL:C	1:B:6:LEU:HD23	2.32	0.49
1:D:8:VAL:O	1:D:58:LYS:CE	2.60	0.49
1:D:127:LEU:CD2	1:D:127:LEU:N	2.73	0.49
1:B:30:VAL:HG13	1:D:264:LEU:HD11	1.93	0.49
1:D:209:TYR:CE2	1:D:232:LEU:HD23	2.46	0.49
1:D:134:LYS:HG3	1:D:270:TYR:CZ	2.47	0.49
1:A:17:PRO:HB3	1:C:86:GLU:HG3	1.94	0.49
1:A:16:LEU:CD1	1:C:87:ILE:CG2	2.91	0.49
1:B:10:GLY:C	1:B:11:LEU:O	2.50	0.49
1:B:16:LEU:HD13	1:D:87:ILE:HG23	1.94	0.49
1:B:83:LEU:O	1:B:86:GLU:N	2.46	0.49
1:C:70:GLU:O	1:C:74:THR:HG22	2.12	0.49
1:A:16:LEU:O	1:A:16:LEU:HD22	2.12	0.49
1:C:8:VAL:HG12	1:C:129:PRO:HG3	1.96	0.48
1:D:179:PRO:HB3	1:D:185:ILE:HB	1.96	0.48
1:A:165:HIS:HA	1:A:196:VAL:CG2	2.43	0.48
1:C:119:VAL:HG11	1:C:124:PHE:CD1	2.48	0.48
1:B:134:LYS:HE3	1:B:273:GLU:HG3	1.95	0.48
1:D:131:VAL:O	1:D:208:ARG:NH2	2.46	0.48
1:A:144:ARG:NH1	1:A:251:GLN:HG2	2.28	0.48
1:B:83:LEU:H	1:B:83:LEU:HD22	1.79	0.48
1:B:13:THR:O	1:B:16:LEU:HB2	2.14	0.47
1:A:144:ARG:HD2	1:A:248:TYR:OH	2.14	0.47
1:A:167:VAL:HG13	1:A:172:ILE:HD13	1.96	0.47
1:A:24:LYS:O	1:A:27:VAL:HG22	2.14	0.47
1:D:147:SER:HA	1:D:150:ASN:HB2	1.97	0.47
1:C:149:TYR:O	1:C:153:GLN:N	2.46	0.47
1:D:12:GLY:O	1:D:15:PHE:N	2.40	0.47
1:D:148:ARG:NH2	1:D:246:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PRO:HB2	1:B:67:ARG:HD3	1.96	0.46
1:D:274:HIS:CE1	1:D:277:LEU:HD12	2.50	0.46
1:B:11:LEU:HD13	1:B:11:LEU:N	2.31	0.46
1:C:163:PRO:O	1:C:165:HIS:O	2.34	0.46
1:B:16:LEU:N	1:B:17:PRO:CD	2.79	0.46
1:A:20:LYS:NZ	1:C:64:TYR:O	2.41	0.46
1:C:11:LEU:O	3:C:302:SO4:O3	2.34	0.45
1:A:280:GLU:HG2	1:C:261:LEU:HD21	1.97	0.45
1:B:16:LEU:HD21	1:D:71:LEU:HD21	1.98	0.45
1:C:192:GLU:HG3	1:C:231:GLN:CG	2.44	0.45
1:D:126:VAL:C	1:D:127:LEU:HD23	2.36	0.45
1:A:140:ASN:C	1:A:140:ASN:ND2	2.70	0.45
1:B:187:MET:SD	1:B:247:ALA:HB2	2.57	0.45
1:D:49:GLN:HE21	1:D:98:ILE:HG13	1.82	0.45
1:C:106:LEU:O	1:C:229:GLU:HA	2.17	0.44
1:D:173:VAL:HG21	1:D:187:MET:SD	2.57	0.44
1:B:184:SER:HB3	1:B:248:TYR:CA	2.47	0.44
1:D:8:VAL:CG1	1:D:129:PRO:HG3	2.46	0.44
1:D:139:GLN:OE1	1:D:143:SER:CB	2.65	0.44
1:A:131:VAL:O	1:A:208:ARG:NH2	2.51	0.44
1:B:192:GLU:CG	1:B:231:GLN:HG2	2.39	0.44
1:A:212:PRO:O	1:A:215:ILE:HG22	2.18	0.44
1:B:131:VAL:O	1:B:208:ARG:NH2	2.50	0.44
1:B:98:ILE:N	1:B:98:ILE:HD13	2.33	0.43
1:D:26:MET:HA	1:D:33:PRO:HB3	2.00	0.43
1:B:179:PRO:HG3	1:B:185:ILE:HB	2.01	0.43
1:C:272:LEU:HD11	1:C:285:ILE:CD1	2.48	0.43
1:A:280:GLU:CG	1:C:261:LEU:HD21	2.49	0.43
1:A:11:LEU:N	1:A:11:LEU:CD1	2.81	0.43
1:C:133:VAL:HG13	1:C:250:MET:HE3	1.99	0.43
1:D:281:PHE:O	1:D:285:ILE:HG13	2.19	0.42
1:C:71:LEU:HA	1:C:71:LEU:HD12	1.89	0.42
1:D:167:VAL:HG22	1:D:172:ILE:CG1	2.48	0.42
1:A:250:MET:HB2	1:A:250:MET:HE2	1.90	0.42
1:B:170:TYR:O	1:B:192:GLU:O	2.36	0.42
1:D:172:ILE:HD13	1:D:194:PRO:CG	2.48	0.42
1:A:13:THR:HG22	1:C:75:LEU:HD21	2.02	0.42
1:A:159:VAL:HG22	1:A:248:TYR:O	2.19	0.42
1:B:167:VAL:HG13	1:B:172:ILE:HD13	2.02	0.42
1:C:6:LEU:N	1:C:6:LEU:CD2	2.80	0.42
1:D:43:VAL:O	1:D:46:GLY:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:HG22	1:B:186:ALA:O	2.20	0.42
1:A:13:THR:O	1:A:14:ARG:C	2.57	0.42
1:D:136:GLY:HA3	1:D:251:GLN:HE22	1.85	0.41
1:B:29:VAL:HB	1:B:37:TYR:HE2	1.86	0.41
1:A:170:TYR:CD1	1:A:170:TYR:N	2.88	0.41
1:A:39:VAL:HG21	1:A:65:PHE:CZ	2.55	0.41
1:B:2:LYS:O	1:B:47:ILE:HA	2.20	0.41
1:D:55:HIS:HB3	1:D:58:LYS:HD3	2.03	0.41
1:D:167:VAL:HG22	1:D:172:ILE:CD1	2.50	0.41
1:A:133:VAL:HG12	1:A:133:VAL:O	2.20	0.41
2:C:301:UPG:O1A	2:C:301:UPG:H3C	2.20	0.41
1:A:68:ASN:O	1:A:72:GLU:HG3	2.21	0.41
1:B:6:LEU:HD22	1:B:127:LEU:HB2	2.02	0.41
1:B:8:VAL:CG1	1:B:129:PRO:HG3	2.51	0.41
1:C:11:LEU:CD1	1:C:11:LEU:N	2.85	0.40
1:D:25:GLU:HB3	1:D:35:ILE:HB	2.02	0.40
1:D:53:VAL:HA	1:D:100:VAL:O	2.22	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	288/290 (99%)	252 (88%)	29 (10%)	7 (2%)	6	21
1	B	288/290 (99%)	254 (88%)	28 (10%)	6 (2%)	7	24
1	C	288/290 (99%)	247 (86%)	36 (12%)	5 (2%)	9	29
1	D	286/290 (99%)	239 (84%)	42 (15%)	5 (2%)	9	29
All	All	1150/1160 (99%)	992 (86%)	135 (12%)	23 (2%)	7	25

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	82	ASP
1	A	176	ALA
1	B	11	LEU
1	B	29	VAL
1	B	82	ASP
1	B	176	ALA
1	A	120	GLY
1	B	196	VAL
1	D	56	SER
1	A	226	ALA
1	C	77	GLN
1	C	196	VAL
1	C	275	PRO
1	D	226	ALA
1	B	224	LYS
1	D	176	ALA
1	C	92	PRO
1	D	30	VAL
1	A	215	ILE
1	D	275	PRO
1	C	30	VAL
1	A	133	VAL

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	229/246 (93%)	202 (88%)	27 (12%)	5	15
1	B	228/246 (93%)	205 (90%)	23 (10%)	7	22
1	C	226/246 (92%)	195 (86%)	31 (14%)	3	10
1	D	227/246 (92%)	200 (88%)	27 (12%)	5	15
All	All	910/984 (92%)	802 (88%)	108 (12%)	5	15

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	15	PHE
1	A	16	LEU
1	A	24	LYS
1	A	28	THR
1	A	32	ARG
1	A	40	ARG
1	A	60	SER
1	A	73	THR
1	A	82	ASP
1	A	88	THR
1	A	91	VAL
1	A	99	SER
1	A	127	LEU
1	A	130	ASP
1	A	135	ASP
1	A	140	ASN
1	A	170	TYR
1	A	172	ILE
1	A	175	VAL
1	A	177	GLN
1	A	183	GLU
1	A	191	VAL
1	A	224	LYS
1	A	251	GLN
1	A	277	LEU
1	A	289	LYS
1	B	0	MET
1	B	6	LEU
1	B	11	LEU
1	B	15	PHE
1	B	16	LEU
1	B	24	LYS
1	B	32	ARG
1	B	57	SER
1	B	60	SER
1	B	73	THR
1	B	74	THR
1	B	82	ASP
1	B	99	SER
1	B	135	ASP
1	B	137	SER
1	B	184	SER

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Mol	Chain	Res	Type
1	B	190	ILE
1	B	192	GLU
1	B	222	THR
1	B	231	GLN
1	B	251	GLN
1	B	284	LEU
1	B	288	LEU
1	C	6	LEU
1	C	11	LEU
1	C	15	PHE
1	C	27	VAL
1	C	84	LEU
1	C	88	THR
1	C	92	PRO
1	C	96	SER
1	C	99	SER
1	C	130	ASP
1	C	140	ASN
1	C	160	GLU
1	C	179	PRO
1	C	188	GLN
1	C	196	VAL
1	C	209	TYR
1	C	215	ILE
1	C	220	GLU
1	C	222	THR
1	C	231	GLN
1	C	233	THR
1	C	249	ARG
1	C	250	MET
1	C	251	GLN
1	C	254	THR
1	C	260	LYS
1	C	261	LEU
1	C	277	LEU
1	C	283	GLN
1	C	286	LEU
1	C	289	LYS
1	D	2	LYS
1	D	6	LEU
1	D	11	LEU
1	D	14	ARG

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Mol	Chain	Res	Type
1	D	15	PHE
1	D	21	SER
1	D	27	VAL
1	D	32	ARG
1	D	40	ARG
1	D	54	THR
1	D	60	SER
1	D	82	ASP
1	D	99	SER
1	D	127	LEU
1	D	134	LYS
1	D	135	ASP
1	D	140	ASN
1	D	160	GLU
1	D	167	VAL
1	D	188	GLN
1	D	196	VAL
1	D	209	TYR
1	D	215	ILE
1	D	220	GLU
1	D	224	LYS
1	D	264	LEU
1	D	272	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	140	ASN
1	B	180	ASN
1	B	283	GLN
1	C	188	GLN
1	C	228	ASN
1	C	251	GLN
1	C	253	GLN
1	D	49	GLN
1	D	104	GLN
1	D	153	GLN
1	D	221	ASN
1	D	253	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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$
3	SO4	A	302	-	4,4,4	0.33	0	6,6,6	0.11	0
2	UPG	B	301	-	31,38,38	0.80	1 (3%)	41,58,58	1.06	2 (4%)
3	SO4	B	303	-	4,4,4	0.34	0	6,6,6	0.09	0
2	UPG	C	301	-	31,38,38	0.81	1 (3%)	41,58,58	1.23	3 (7%)
4	EDO	A	304	-	3,3,3	0.11	0	2,2,2	0.13	0
3	SO4	C	302	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	D	303	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	D	302	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	B	302	-	4,4,4	0.35	0	6,6,6	0.09	0
5	GOL	B	304	-	5,5,5	0.12	0	5,5,5	0.32	0
3	SO4	A	303	-	4,4,4	0.36	0	6,6,6	0.07	0
2	UPG	A	301	-	31,38,38	0.84	1 (3%)	41,58,58	1.11	2 (4%)
2	UPG	D	301	-	31,38,38	0.78	1 (3%)	41,58,58	1.25	6 (14%)

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	301	-	-	6/21/59/59	0/3/3/3
2	UPG	C	301	-	-	2/21/59/59	0/3/3/3
4	EDO	A	304	-	-	1/1/1/1	-
5	GOL	B	304	-	-	2/4/4/4	-
2	UPG	A	301	-	-	4/21/59/59	0/3/3/3
2	UPG	D	301	-	-	5/21/59/59	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	UPG	C4-N3	3.18	1.38	1.33
2	C	301	UPG	C4-N3	3.12	1.38	1.33
2	B	301	UPG	C4-N3	3.06	1.38	1.33
2	D	301	UPG	C4-N3	3.05	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	UPG	C5-C4-N3	-4.13	114.23	123.31
2	D	301	UPG	C5-C4-N3	-4.07	114.35	123.31
2	C	301	UPG	C5-C4-N3	-4.07	114.35	123.31
2	B	301	UPG	C5-C4-N3	-3.98	114.55	123.31
2	C	301	UPG	O5'-C1'-O3B	-3.80	106.40	111.36
2	C	301	UPG	PB-O3A-PA	-3.50	120.80	132.83
2	D	301	UPG	C1'-O5'-C5'	3.41	120.38	113.69
2	A	301	UPG	O5'-C1'-O3B	-2.59	107.98	111.36
2	D	301	UPG	PB-O3A-PA	-2.49	124.28	132.83
2	B	301	UPG	PB-O3A-PA	-2.48	124.31	132.83
2	D	301	UPG	O2A-PA-O1A	2.30	123.61	112.24
2	D	301	UPG	O2B-PB-O1B	2.12	122.72	112.24
2	D	301	UPG	O3A-PB-O3B	-2.10	98.25	102.48

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	UPG	C2C-C1C-N1-C6
2	B	301	UPG	O4C-C1C-N1-C6
2	B	301	UPG	O4C-C4C-C5C-O5C

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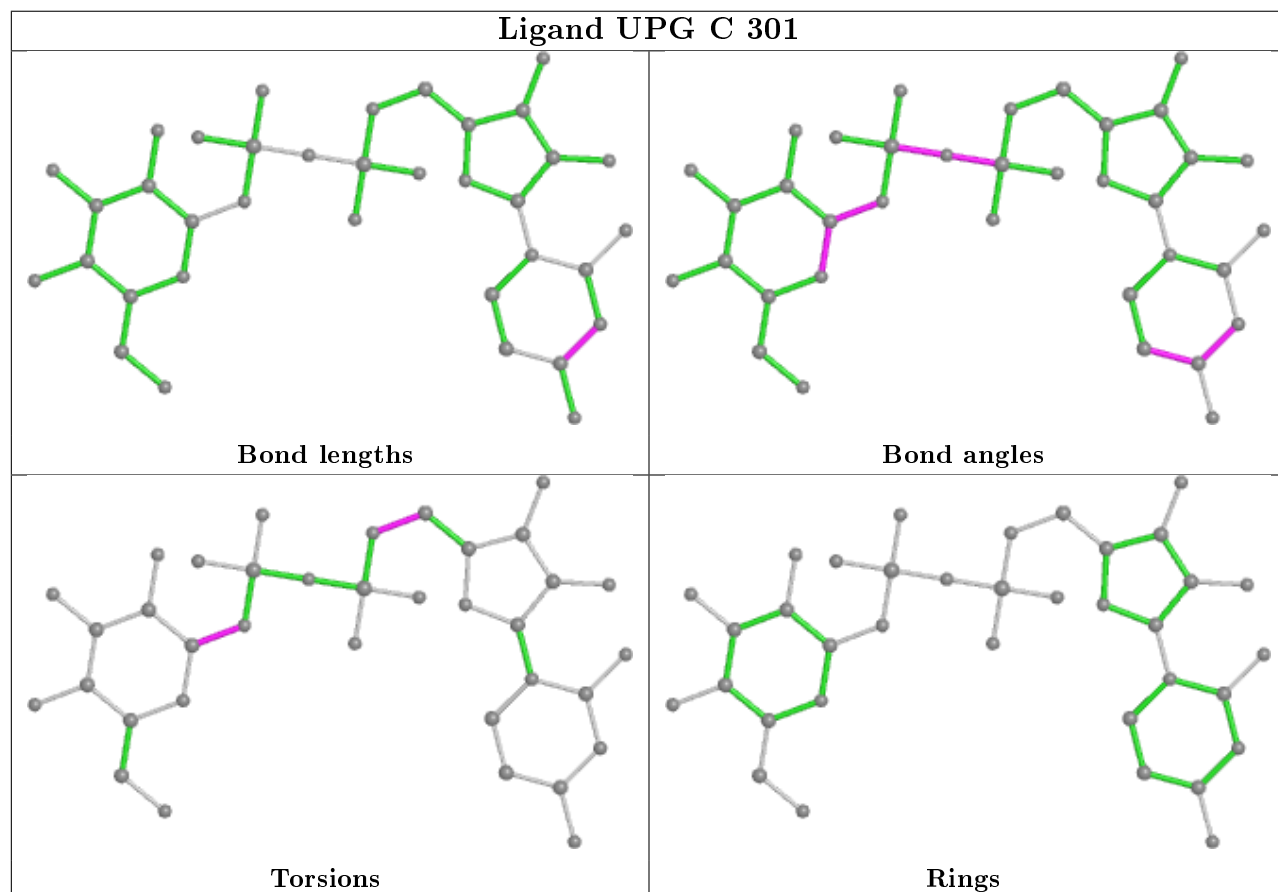
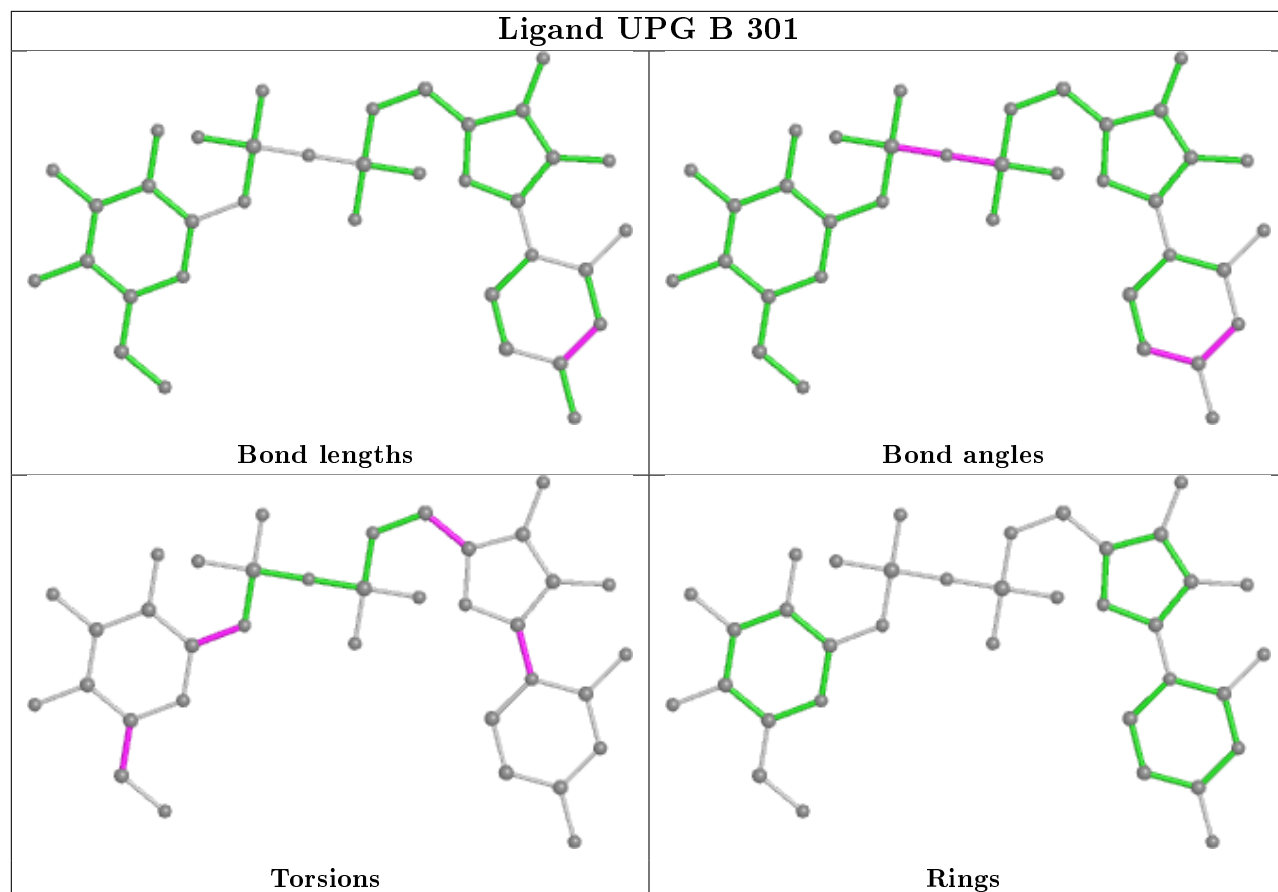
Mol	Chain	Res	Type	Atoms
2	A	301	UPG	C3C-C4C-C5C-O5C
2	A	301	UPG	O4C-C4C-C5C-O5C
2	A	301	UPG	C5C-O5C-PA-O1A
2	D	301	UPG	O5'-C1'-O3B-PB
2	D	301	UPG	C4'-C5'-C6'-O6'
2	D	301	UPG	O5'-C5'-C6'-O6'
2	B	301	UPG	C2'-C1'-O3B-PB
2	D	301	UPG	C2'-C1'-O3B-PB
2	B	301	UPG	O5'-C5'-C6'-O6'
2	C	301	UPG	C4C-C5C-O5C-PA
2	A	301	UPG	C5C-O5C-PA-O3A
4	A	304	EDO	O1-C1-C2-O2
2	C	301	UPG	O5'-C1'-O3B-PB
2	B	301	UPG	C4'-C5'-C6'-O6'
5	B	304	GOL	O1-C1-C2-C3
2	D	301	UPG	C1'-O3B-PB-O3A
5	B	304	GOL	O1-C1-C2-O2

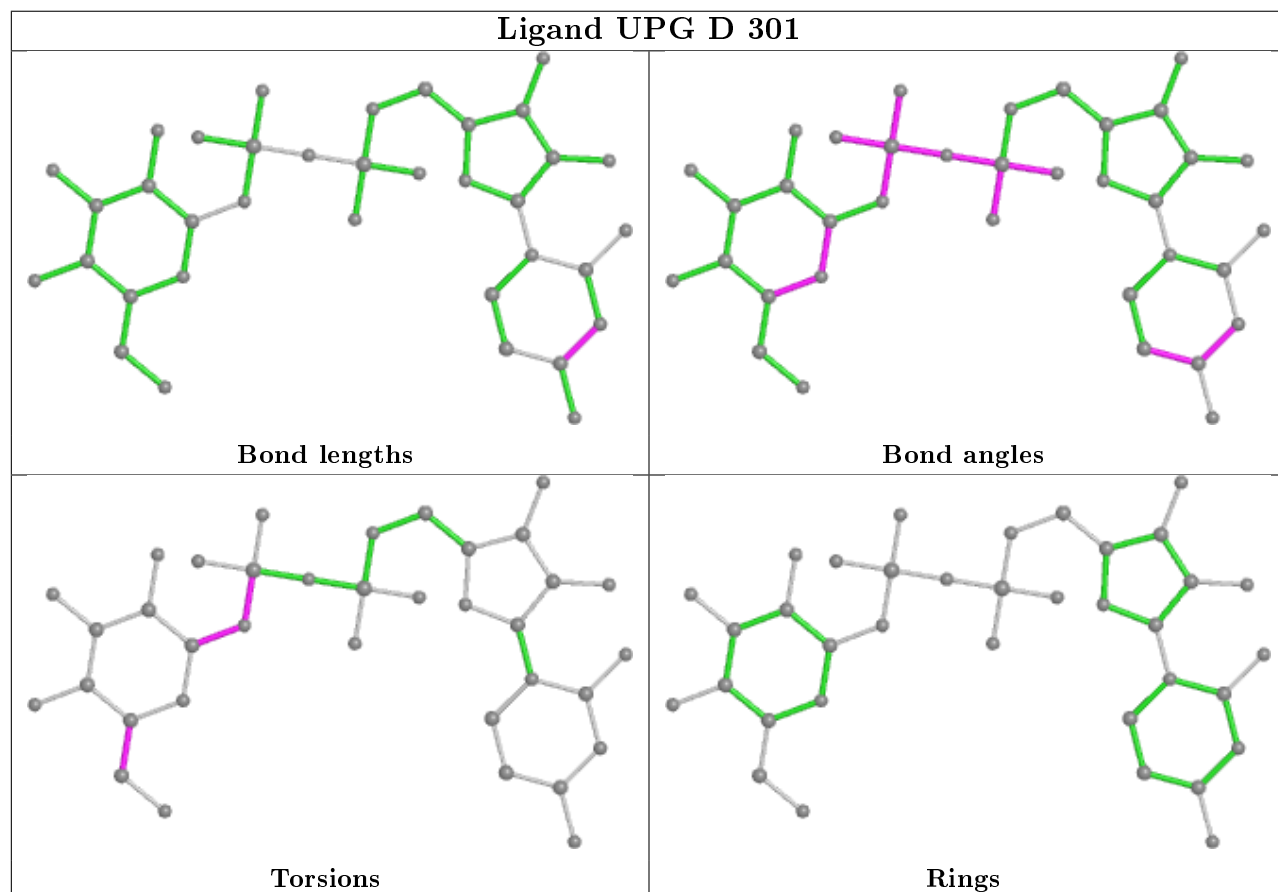
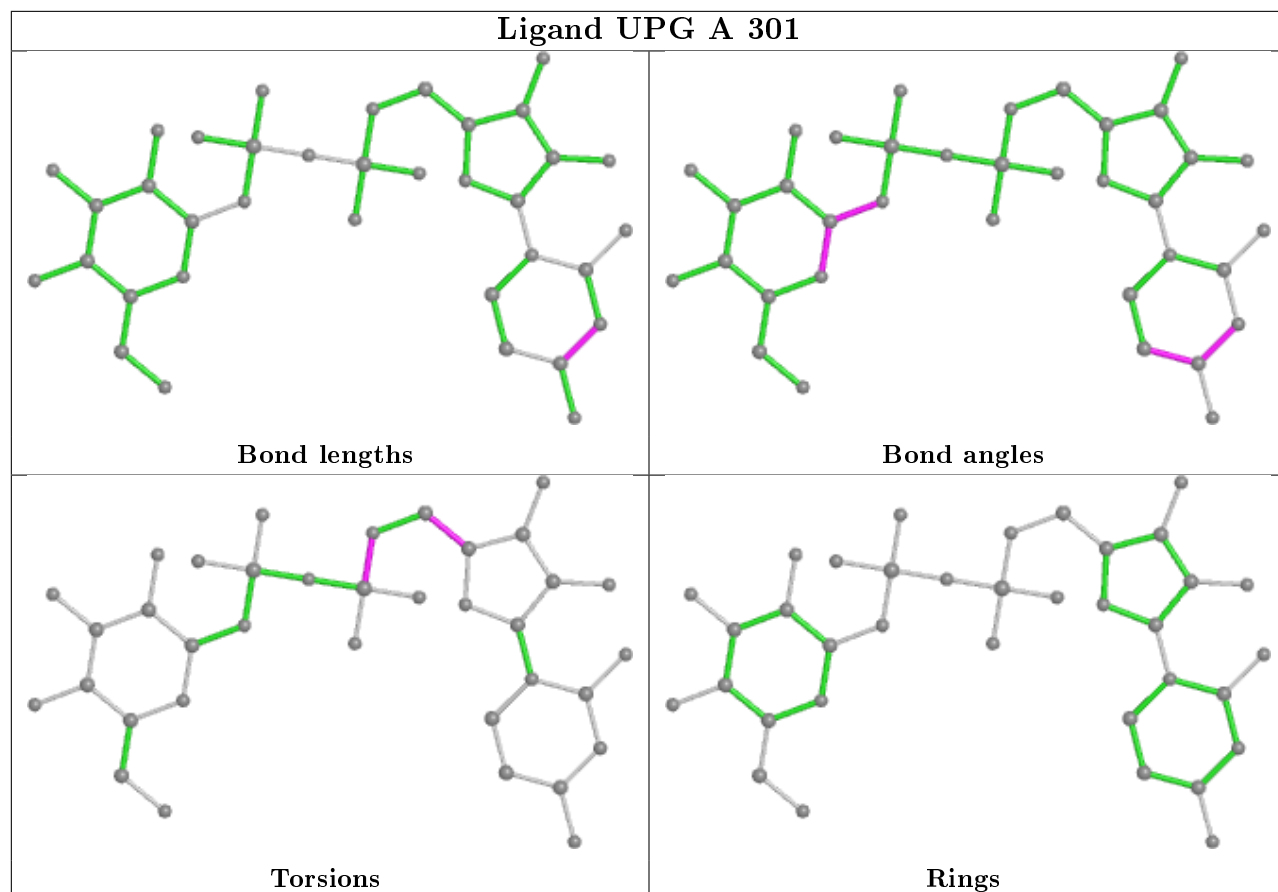
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	UPG	2	0
3	C	302	SO4	1	0
5	B	304	GOL	1	0
2	A	301	UPG	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	290/290 (100%)	0.12	4 (1%) 75 77	39, 68, 103, 133	0
1	B	290/290 (100%)	0.08	3 (1%) 82 83	40, 69, 104, 131	0
1	C	290/290 (100%)	0.12	1 (0%) 94 94	45, 76, 103, 142	0
1	D	288/290 (99%)	0.15	4 (1%) 75 77	43, 76, 101, 129	0
All	All	1158/1160 (99%)	0.12	12 (1%) 82 83	39, 73, 103, 142	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	HIS	4.2
1	B	16	LEU	3.6
1	C	210	VAL	3.3
1	A	195	PRO	3.2
1	A	81	PHE	3.2
1	D	146	ILE	3.2
1	D	142	LEU	2.6
1	A	178	SER	2.6
1	B	30	VAL	2.6
1	D	81	PHE	2.6
1	A	285	ILE	2.3
1	D	95	VAL	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 monosaccharides in this entry.

6.4 Ligands

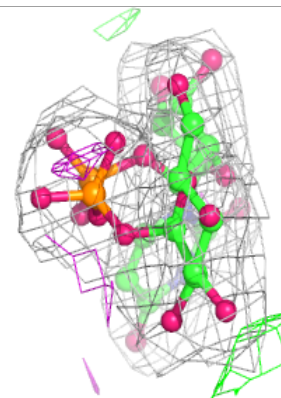
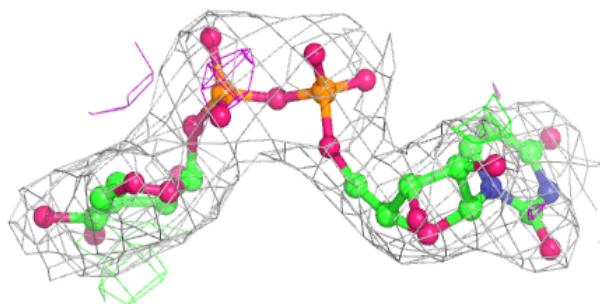
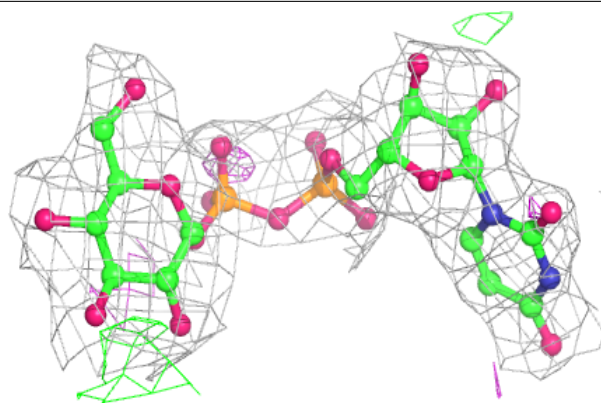
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	302	5/5	0.83	0.12	115,119,129,132	0
4	EDO	A	304	4/4	0.84	0.20	82,83,89,91	0
3	SO4	B	303	5/5	0.84	0.15	111,113,130,135	0
3	SO4	A	303	5/5	0.84	0.14	127,132,136,138	0
5	GOL	B	304	6/6	0.86	0.16	87,92,96,96	0
3	SO4	A	302	5/5	0.89	0.17	114,121,130,131	0
3	SO4	D	303	5/5	0.91	0.13	143,144,150,150	0
3	SO4	D	302	5/5	0.94	0.10	115,123,126,132	0
2	UPG	B	301	36/36	0.95	0.17	52,62,68,73	0
2	UPG	C	301	36/36	0.95	0.16	48,58,67,74	0
2	UPG	D	301	36/36	0.95	0.14	47,57,69,71	0
2	UPG	A	301	36/36	0.96	0.17	46,60,71,75	0
3	SO4	B	302	5/5	0.96	0.10	99,99,110,112	0

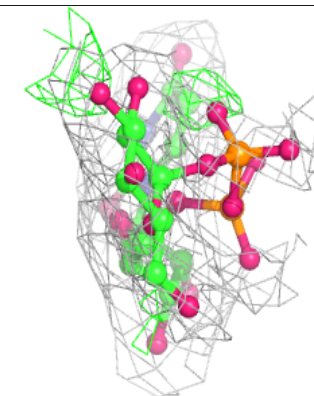
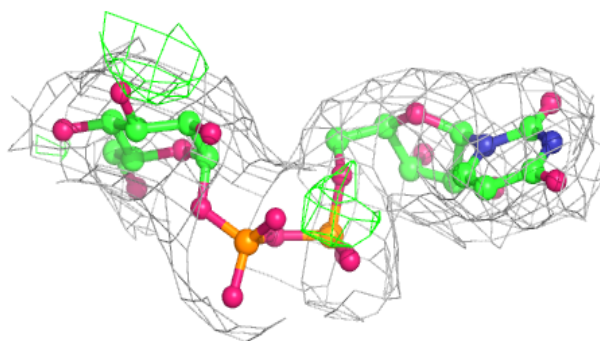
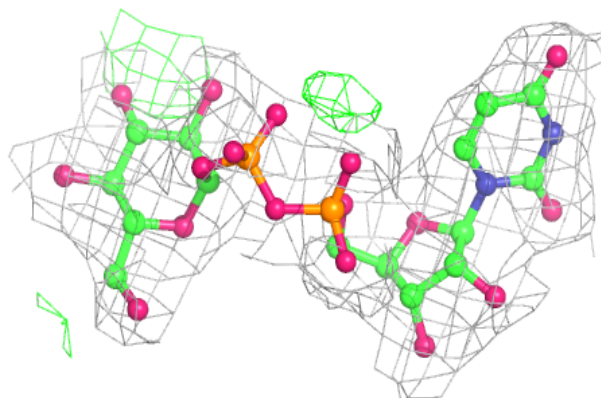
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UPG B 301:

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

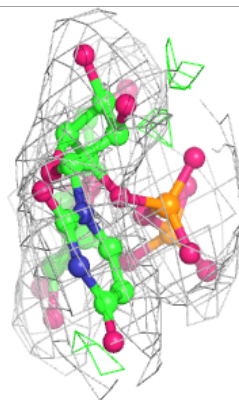
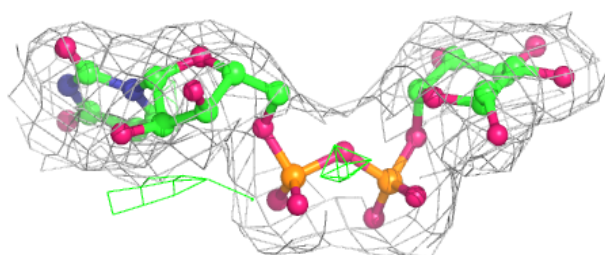
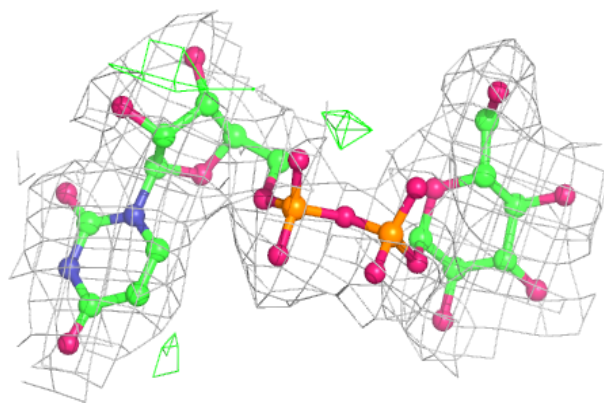
**Electron density around UPG C 301:**

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

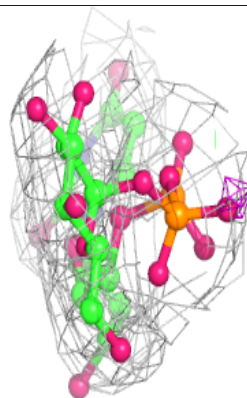
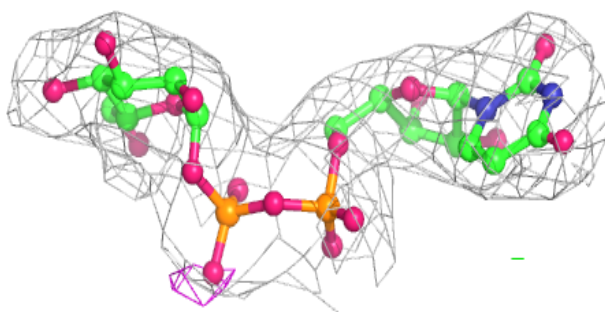
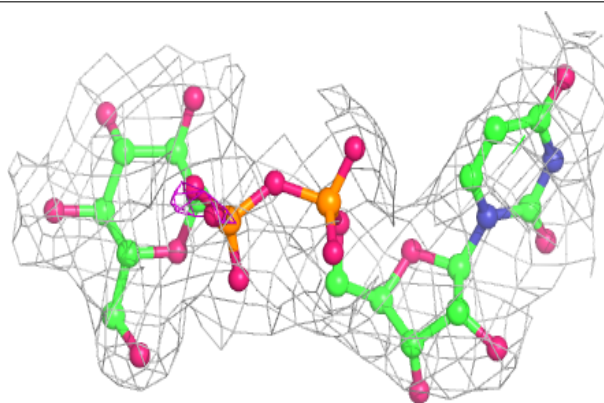


Electron density around UPG D 301:

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

**Electron density around UPG A 301:**

$2mF_o-DF_c$ (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.