



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 12:27 AM UTC

PDB ID : 1Y6F / pdb_00001y6f
Title : alpha-glucosyltransferase in complex with UDP-glucose and DNA containing an abasic site
Authors : Lariviere, L.; Sommer, N.; Morera, S.
Deposited on : 2004-12-06
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

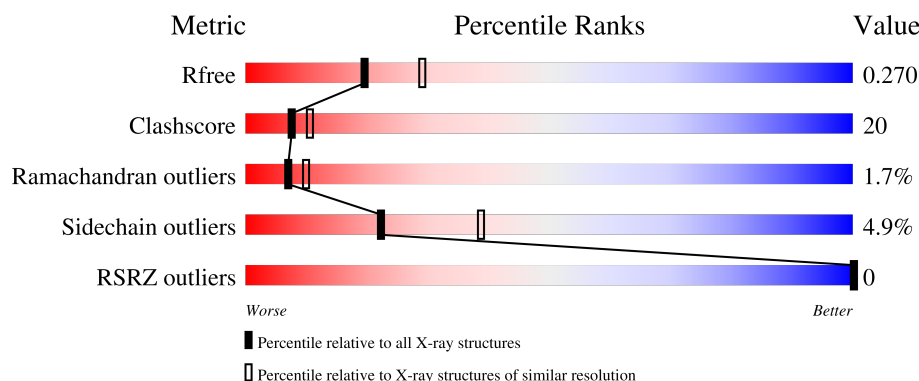
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	C	13	
2	D	13	
3	A	403	
3	B	403	

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	GOL	A	701	-	X	-	-
5	GOL	A	702	-	X	-	-
5	GOL	B	602	-	X	-	-
5	GOL	B	703	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7311 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 DNA chain called 5'-D(*GP*AP*TP*AP*CP*TP*(3DR)P*AP*GP*AP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	13	Total	C	N	O	P	7	0	0
			258	124	49	73	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			261	127	44	78	12			

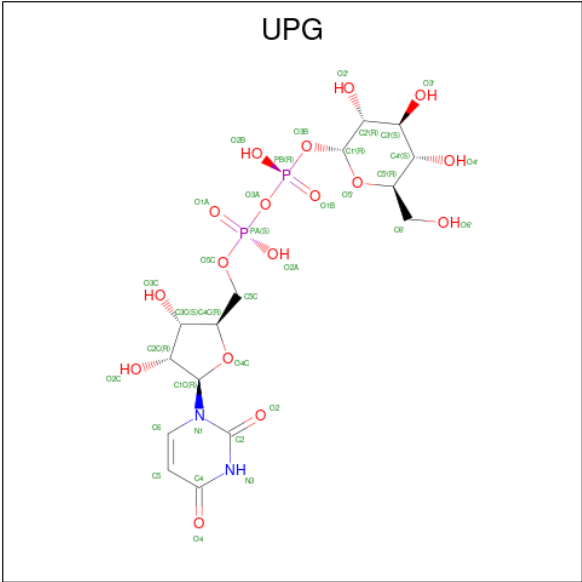
- Molecule 3 is a protein called DNA alpha-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	394	Total	C	N	O	S	0	0	0
			3236	2064	549	605	18			
3	B	394	Total	C	N	O	S	0	0	0
			3233	2062	549	605	17			

There are 6 discrepancies between the modelled and reference sequences:

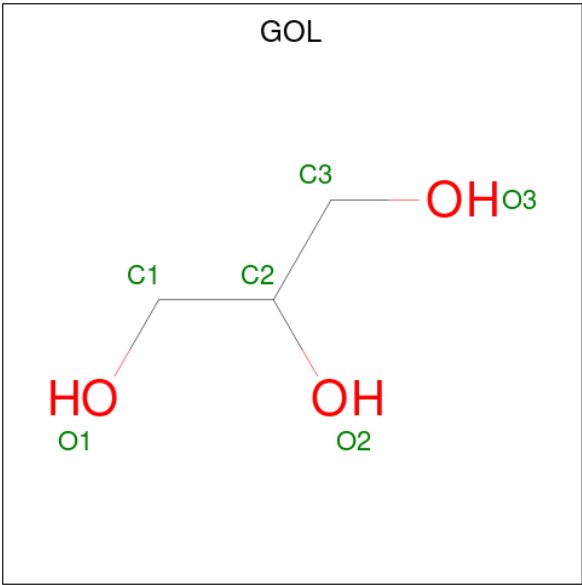
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	MET	-	cloning artifact	UNP P04519
A	999	GLY	-	cloning artifact	UNP P04519
A	1000	SER	-	cloning artifact	UNP P04519
B	998	MET	-	cloning artifact	UNP P04519
B	999	GLY	-	cloning artifact	UNP P04519
B	1000	SER	-	cloning artifact	UNP P04519

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



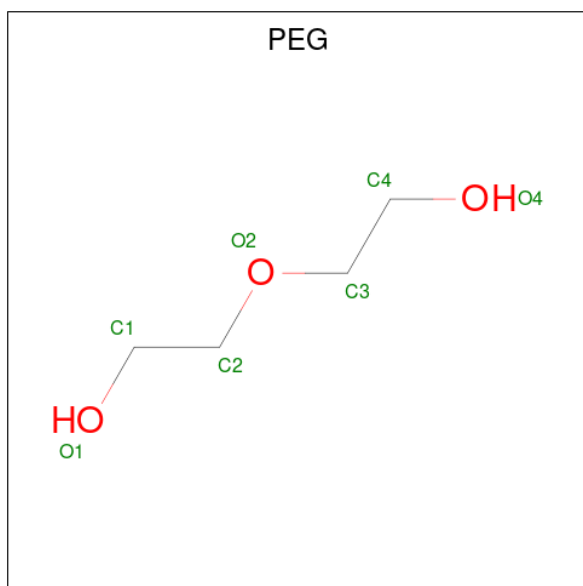
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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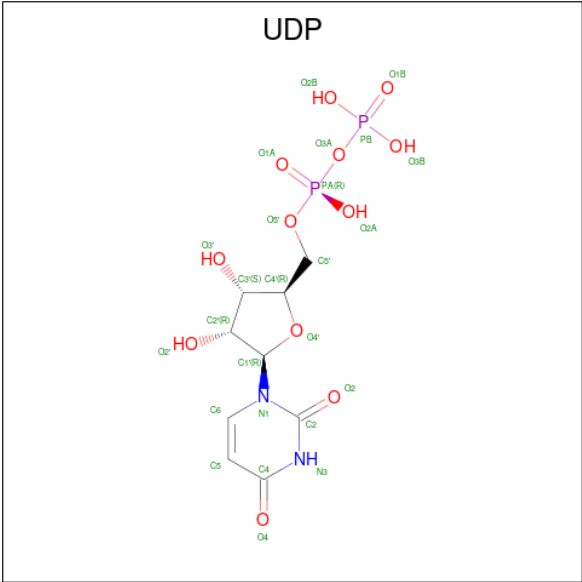
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 8 is water.

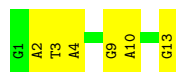
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	3	Total	O	0	0
			3	3		
8	D	11	Total	O	0	0
			11	11		
8	A	115	Total	O	0	0
			115	115		
8	B	95	Total	O	0	0
			95	95		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

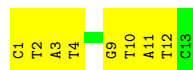
- Molecule 1: 5'-D(*GP*AP*TP*AP*CP*TP*(3DR)P*AP*GP*AP*TP*AP*G)-3'

Chain C: 



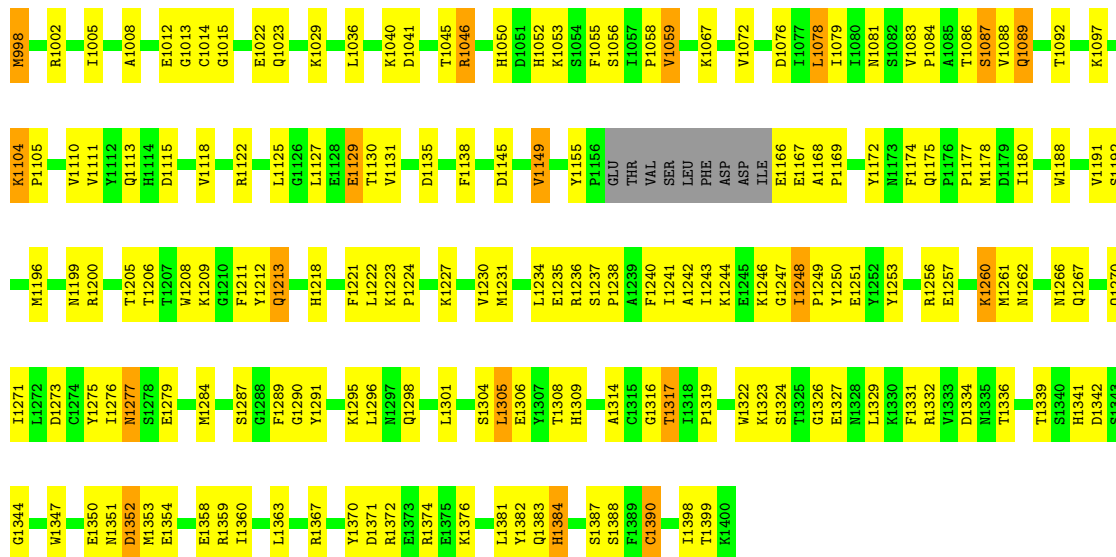
- Molecule 2: 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*GP*TP*AP*TP*C)-3'

Chain D: 



- Molecule 3: DNA alpha-glucosyltransferase

Chain A: 



- Molecule 3: DNA alpha-glucosyltransferase

Chain B: 

W1347	G1254	GLU	Y1088	MET
R1359	M1255	E1167	Q1089	G999
L1363	E1256	Q1175	E1090	S1000
R1367	R1257	P1176	A1091	M1001
D1371	M1262	P1177	T1092	I1002
R1374	L1263	M1178	I1093	I1003
Y1378	A1264	D1179	M1094	M1007
L1381	P1265	I1180	N1095	A1008
Y1382	Q1270	R1184	Y1096	R1009
H1384	I1271	S1185	K1097	G1010
Q1385	L1272	T1186	K1098	E1012
D1386	D1273	Y1187	L1099	G1013
S1387	C1274	W1188	L1100	C1014
C1390	I1276	V1191	I1103	E1022
F1391	M1280	I1194	K1104	Q1023
K1392	Y1291	N1199	R1108	E1029
E1393	Q1292	R1200	Y1112	K1034
Q1394	L1293	W1201	Q1113	V1034
K1400	S1294	I1202	H1114	T1035
	K1295	G1203	D1115	L1036
	L1296	R1204	V1118	V1037
	M1297	W1208	L1119	Y1038
	Q1298	F1211	S1120	A1039
	Q1302	Y1212	R1122	D1041
	R1303	Q1213	R1123	F1044
	S1304	M1214	N1124	T1045
	L1305	H1218	L1125	H1052
	E1306	L1222	E1129	S1056
	Y1307	K1223	R1133	I1057
	T1308	P1224	A1134	P1058
	H1309	A1225	D1135	L1061
	G1313	G1226	D1142	A1062
	A1314	K1227	D1145	Y1065
	W1322	M1231	F1146	Y1065
	K1323	E1232	M1147	L1069
	S1324	G1233	K1148	V1072
	T1325	L1234	V1149	N1073
	G1326	E1235	M1151	D1076
	E1327	R1236	K1152	I1077
	K1330	S1237	E1153	L1078
	F1331	P1238	E1157	N1081
	R1332	A1239	T1158	S1082
	V1333	F1240	VAL	V1083
	D1334	I1243	SER	P1084
	M1335	K1246	LEU	A1085
	T1336	Y1250	PHE	T1086
	T1339		ASP	S1087
	S1340		ILE	
	H1341			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.36Å 123.96Å 86.63Å 90.00° 101.83° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 99.4 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.274 0.197 , 0.270	Depositor DCC
R_{free} test set	1888 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7311	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: 3DR, PEG, UPG, UDP, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.30	0/277	0.67	0/424
2	D	0.30	0/291	0.74	0/447
3	A	0.47	0/3312	0.99	19/4466 (0.4%)
3	B	0.46	0/3309	0.99	19/4463 (0.4%)
All	All	0.46	0/7189	0.97	38/9800 (0.4%)

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1305	LEU	N-CA-C	-8.76	97.89	110.59
3	B	1304	SER	N-CA-C	8.53	122.52	108.96
3	A	1304	SER	N-CA-C	8.38	121.65	108.67
3	A	1305	LEU	N-CA-C	-7.69	99.44	110.59
3	B	1271	ILE	N-CA-C	7.44	118.58	108.17

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	C	258	0	146	7	0
2	D	261	0	150	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3236	0	3175	137	0
3	B	3233	0	3168	125	0
4	A	36	0	22	4	0
5	A	12	0	6	0	0
5	B	12	0	6	0	0
6	A	7	0	10	0	0
6	B	7	0	10	2	0
7	B	25	0	11	1	0
8	A	115	0	0	2	0
8	B	95	0	0	3	0
8	C	3	0	0	1	0
8	D	11	0	0	1	0
All	All	7311	0	6704	278	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 20.

The worst 5 of 278 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)
3:B:1306:GLU:H	3:B:1309:HIS:HD2	0.96	0.95
2:D:1:DC:H2'	2:D:2:DT:H71	1.50	0.93
3:B:1306:GLU:H	3:B:1309:HIS:CD2	1.87	0.93
3:A:1306:GLU:H	3:A:1309:HIS:HD2	1.18	0.91
3:A:1113:GLN:HE21	3:A:1115:ASP:H	1.18	0.88

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	
3	A	390/403 (97%)	346 (89%)	37 (10%)	7 (2%)	6	9
3	B	390/403 (97%)	354 (91%)	30 (8%)	6 (2%)	8	12
All	All	780/806 (97%)	700 (90%)	67 (9%)	13 (2%)	7	10

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1087	SER
3	A	1089	GLN
3	A	1352	ASP
3	B	1090	GLU
3	B	1157	GLU

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	
3	A	359/368 (98%)	343 (96%)	16 (4%)	24	42
3	B	358/368 (97%)	339 (95%)	19 (5%)	20	36
All	All	717/736 (97%)	682 (95%)	35 (5%)	22	39

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	1255	ASN
3	B	1292	GLN
3	B	1296	LEU
3	A	1308	THR
3	A	1213	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	1095	ASN

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Mol	Chain	Res	Type
3	B	1218	HIS
3	B	1394	GLN
3	B	1113	GLN
3	B	1175	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	3DR	C	7	1	8,11,12	0.29	0	7,14,17	0.81	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
1	3DR	C	7	1	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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
5	GOL	A	701	-	5,5,5	4.55	5 (100%)	5,5,5	2.24	2 (40%)
5	GOL	B	602	-	5,5,5	4.50	5 (100%)	5,5,5	2.20	2 (40%)
4	UPG	A	501	-	37,38,38	1.05	2 (5%)	55,58,58	0.86	2 (3%)
6	PEG	B	801	-	6,6,6	0.68	0	5,5,5	0.34	0
7	UDP	B	601	-	25,26,26	0.93	1 (4%)	38,40,40	0.66	1 (2%)
6	PEG	A	802	-	6,6,6	0.72	0	5,5,5	0.35	0
5	GOL	B	703	-	5,5,5	4.45	5 (100%)	5,5,5	2.21	2 (40%)
5	GOL	A	702	-	5,5,5	4.47	5 (100%)	5,5,5	2.25	2 (40%)

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
5	GOL	A	701	-	-	1/4/4/4	-
5	GOL	B	602	-	-	2/4/4/4	-
4	UPG	A	501	-	-	9/23/59/59	0/3/3/3
6	PEG	B	801	-	-	3/4/4/4	-
7	UDP	B	601	-	-	2/16/32/32	0/2/2/2
6	PEG	A	802	-	-	2/4/4/4	-
5	GOL	B	703	-	-	4/4/4/4	-
5	GOL	A	702	-	-	3/4/4/4	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	GOL	C3-C2	-5.66	1.30	1.51
5	A	701	GOL	C1-C2	-5.65	1.30	1.51
5	B	602	GOL	C1-C2	-5.64	1.30	1.51
5	B	703	GOL	C1-C2	-5.55	1.30	1.51
5	A	702	GOL	C3-C2	-5.52	1.30	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	UPG	O3B-C1'-C2'	3.82	115.37	108.38
5	A	702	GOL	O1-C1-C2	3.57	126.43	110.38
5	B	602	GOL	O1-C1-C2	3.50	126.14	110.38
5	A	701	GOL	O1-C1-C2	3.50	126.12	110.38
5	A	701	GOL	O3-C3-C2	3.48	126.03	110.38

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	UPG	C2'-C1'-O3B-PB
4	A	501	UPG	O5'-C1'-O3B-PB
5	A	702	GOL	C1-C2-C3-O3
5	B	703	GOL	O1-C1-C2-C3
5	B	703	GOL	C1-C2-C3-O3

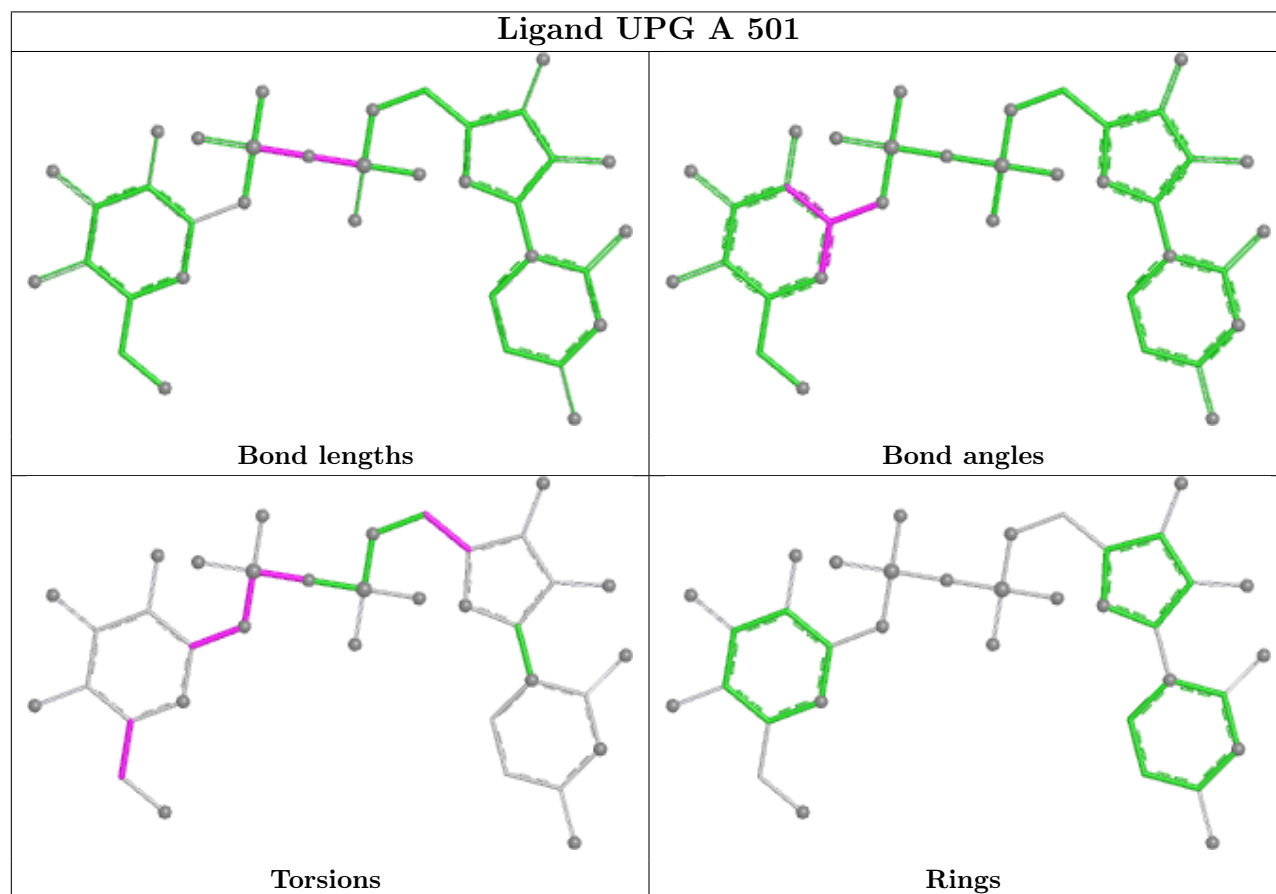
There are no ring outliers.

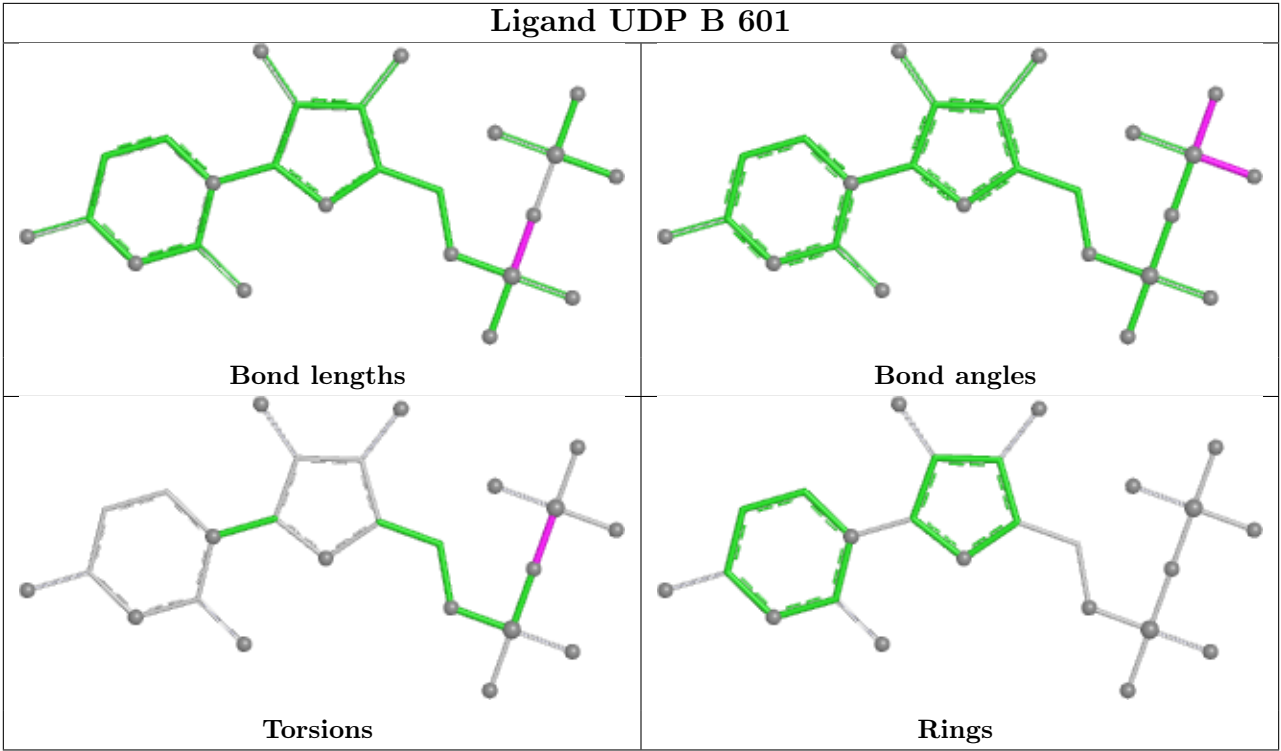
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	UPG	4	0
6	B	801	PEG	2	0
7	B	601	UDP	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	7:3DR	O3'	8:DA	P	3.54

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	C	12/13 (92%)	-0.20	0 100 100	55, 73, 78, 82	0
2	D	13/13 (100%)	-0.12	0 100 100	61, 70, 80, 83	0
3	A	394/403 (97%)	-0.45	0 100 100	24, 50, 76, 94	0
3	B	394/403 (97%)	-0.51	0 100 100	26, 49, 74, 99	0
All	All	813/832 (97%)	-0.47	0 100 100	24, 50, 76, 99	0

There are no RSRZ outliers to report.

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

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
1	3DR	C	7	11/12	0.79	0.09	82,91,97,98	7

6.3 Carbohydrates

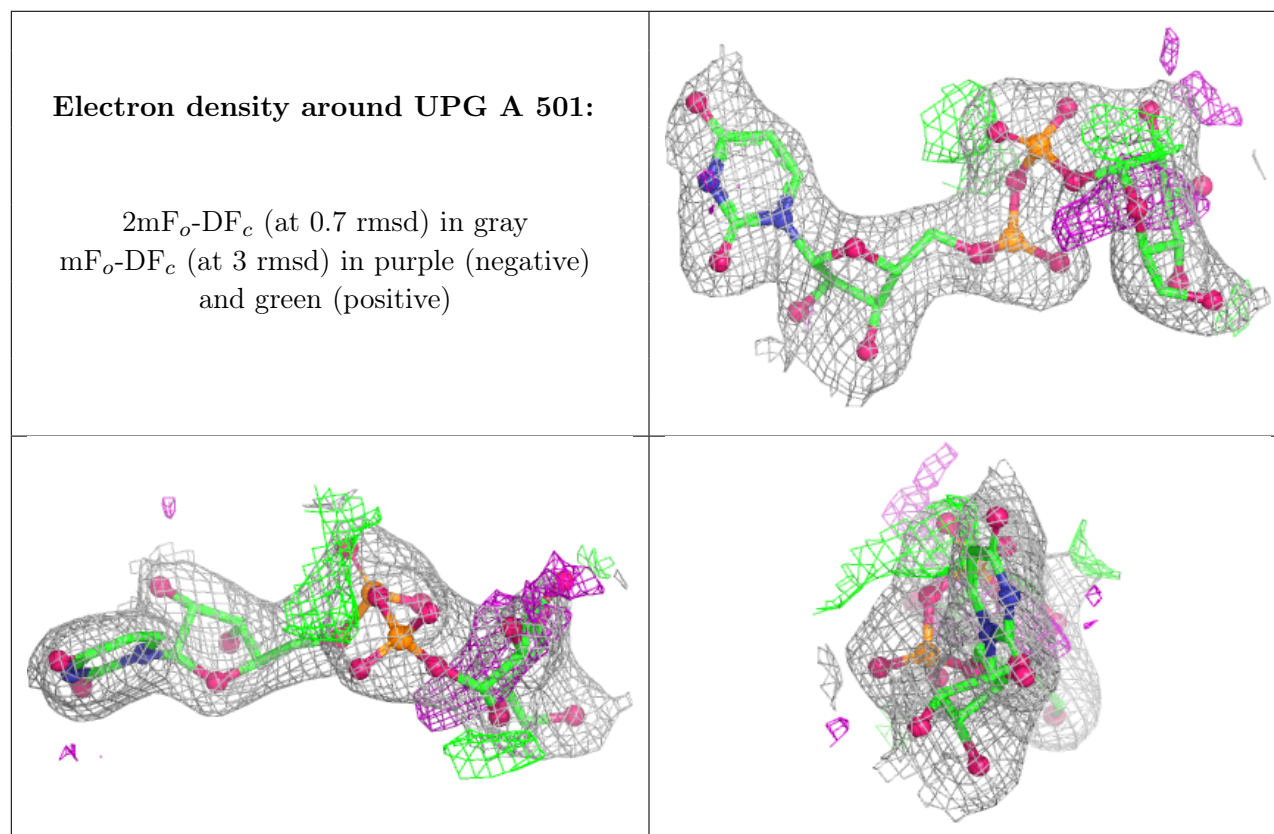
There are no oligosaccharides in this entry.

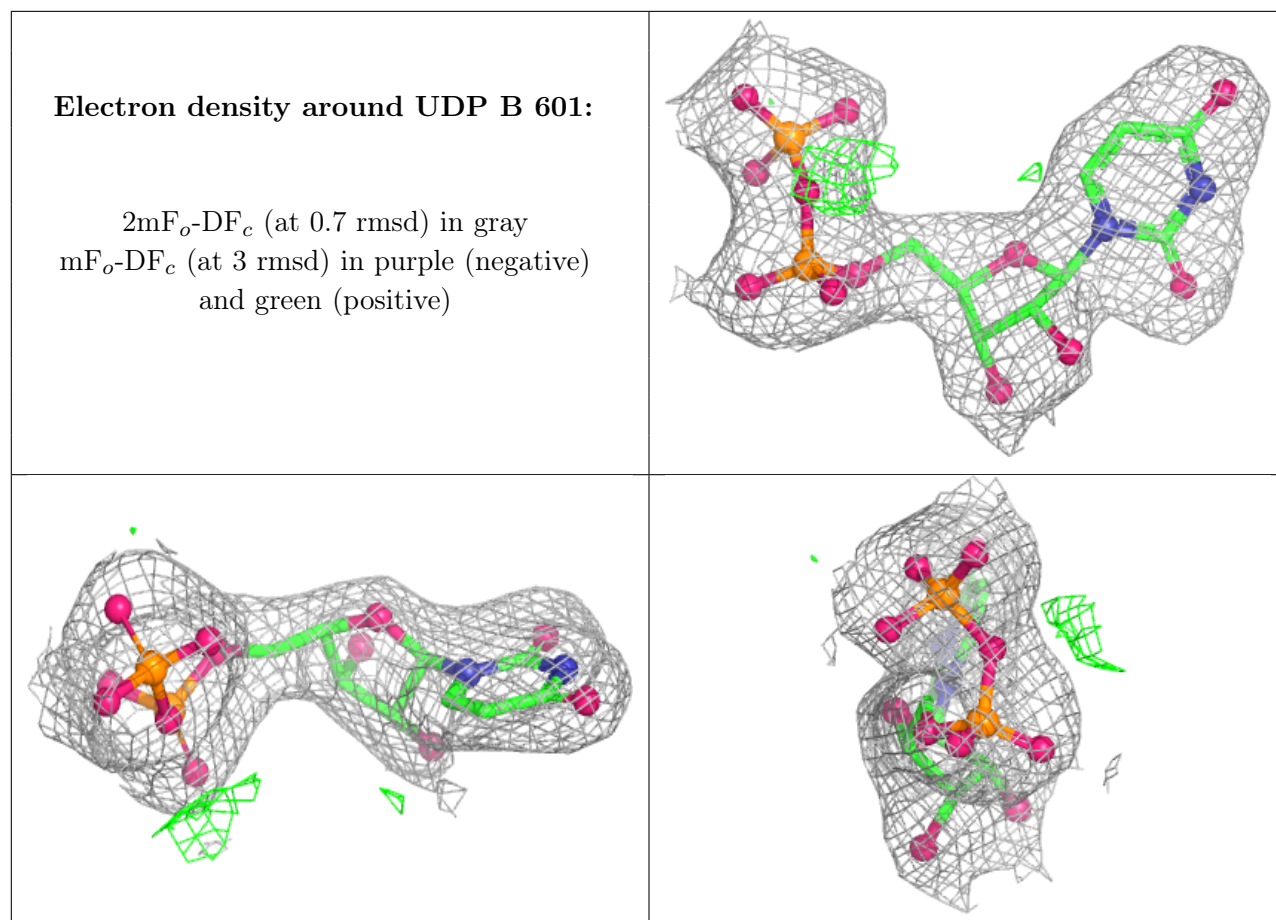
6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
5	GOL	A	702	6/6	0.65	0.11	80,96,98,98	0
6	PEG	A	802	7/7	0.88	0.10	82,84,85,85	0
5	GOL	B	703	6/6	0.90	0.08	54,68,72,73	0
5	GOL	A	701	6/6	0.91	0.08	44,66,69,78	0
5	GOL	B	602	6/6	0.91	0.09	40,50,53,53	0
6	PEG	B	801	7/7	0.92	0.08	45,60,78,82	0
4	UPG	A	501	36/36	0.95	0.08	21,48,77,79	0
7	UDP	B	601	25/25	0.98	0.04	30,43,53,56	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.