



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:33 AM UTC

PDB ID : 1Y6G / pdb_00001y6g
Title : alpha-glucosyltransferase in complex with UDP and a 13_mer DNA containing a HMU base at 2.8 Å resolution
Authors : Lariviere, L.; Sommer, N.; Morera, S.
Deposited on : 2004-12-06
Resolution : 2.80 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

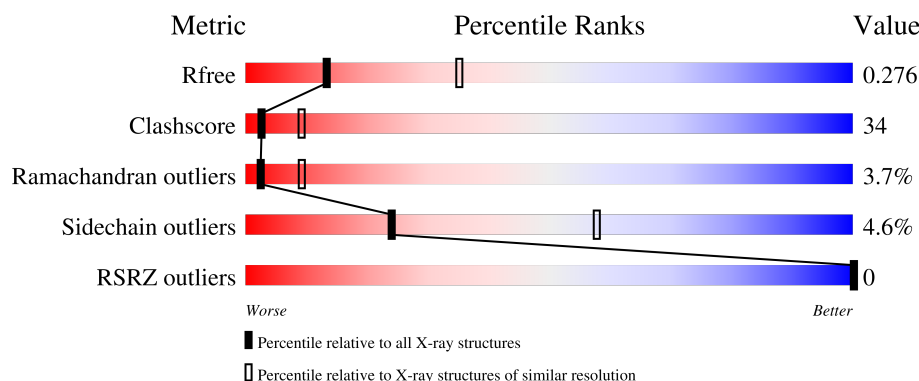
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

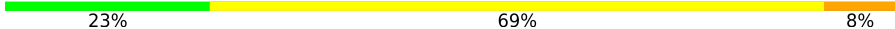
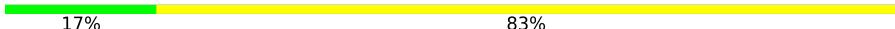
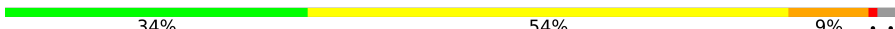
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	 23% 69% 8%
2	D	12	 17% 83%
3	A	403	 34% 54% 9% . .
3	B	403	 50% 41% 6% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7132 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*(5HU)P*AP*GP*AP*T P*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	13	Total	C	N	O	P	0	0	0
			268	129	51	76	12			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*GP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			242	118	41	72	11			

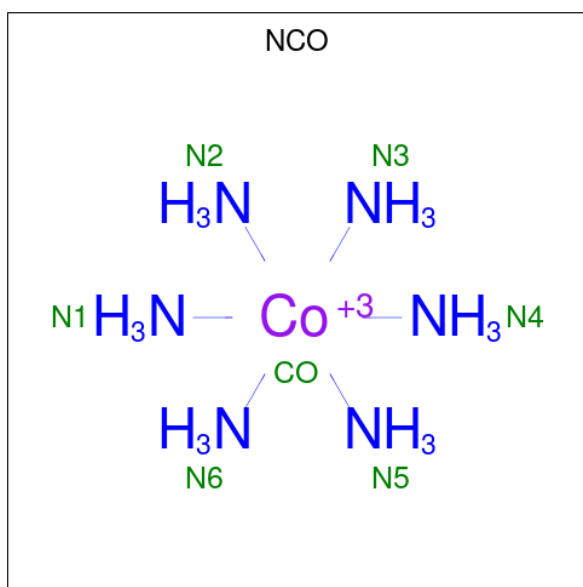
- Molecule 3 is a protein called DNA alpha-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	392	Total	C	N	O	S	0	0	0
			3212	2051	544	599	18			
3	B	393	Total	C	N	O	S	0	0	0
			3227	2059	548	602	18			

There are 6 discrepancies between the modelled and reference sequences:

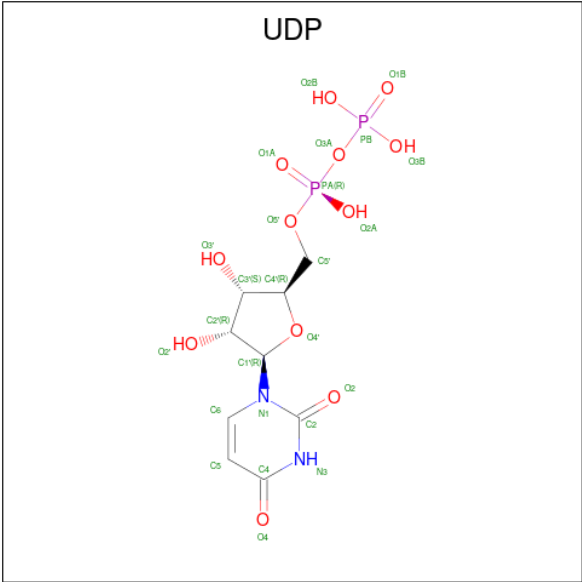
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	MET	-	cloning artifact	UNP P04519
A	999	GLY	-	cloning artifact	UNP P04519
A	1000	SER	-	cloning artifact	UNP P04519
B	998	MET	-	cloning artifact	UNP P04519
B	999	GLY	-	cloning artifact	UNP P04519
B	1000	SER	-	cloning artifact	UNP P04519

- Molecule 4 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: CoH₁₈N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	Co	N	0	0
			7	1	6		
4	A	1	Total	Co	N	0	0
			7	1	6		
4	A	1	Total	Co	N	0	0
			7	1	6		
4	A	1	Total	Co	N	0	0
			7	1	6		
4	B	1	Total	Co	N	0	0
			7	1	6		
4	B	1	Total	Co	N	0	0
			7	1	6		
4	B	1	Total	Co	N	0	0
			7	1	6		

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

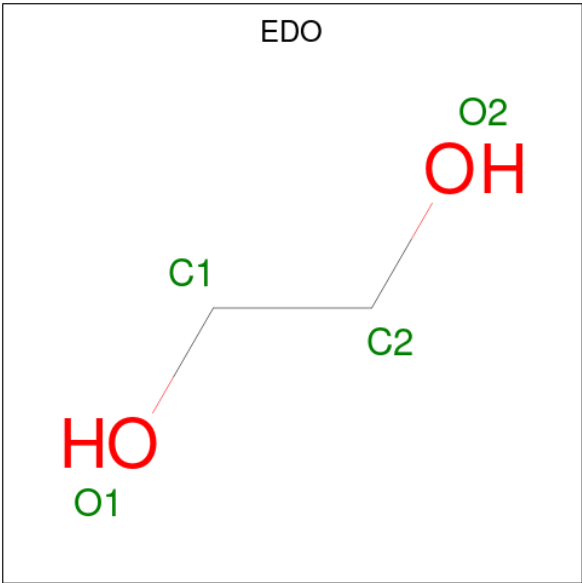


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

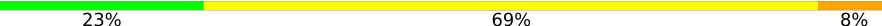
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	O	0	0
			1	1		
8	A	30	Total	O	0	0
			30	30		
8	B	48	Total	O	0	0
			48	48		

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.

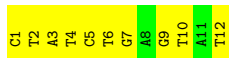
- Molecule 1: 5'-D(*GP*AP*TP*AP*CP*TP*(5HU)P*AP*GP*AP*TP*AP*G)-3'

Chain C: 



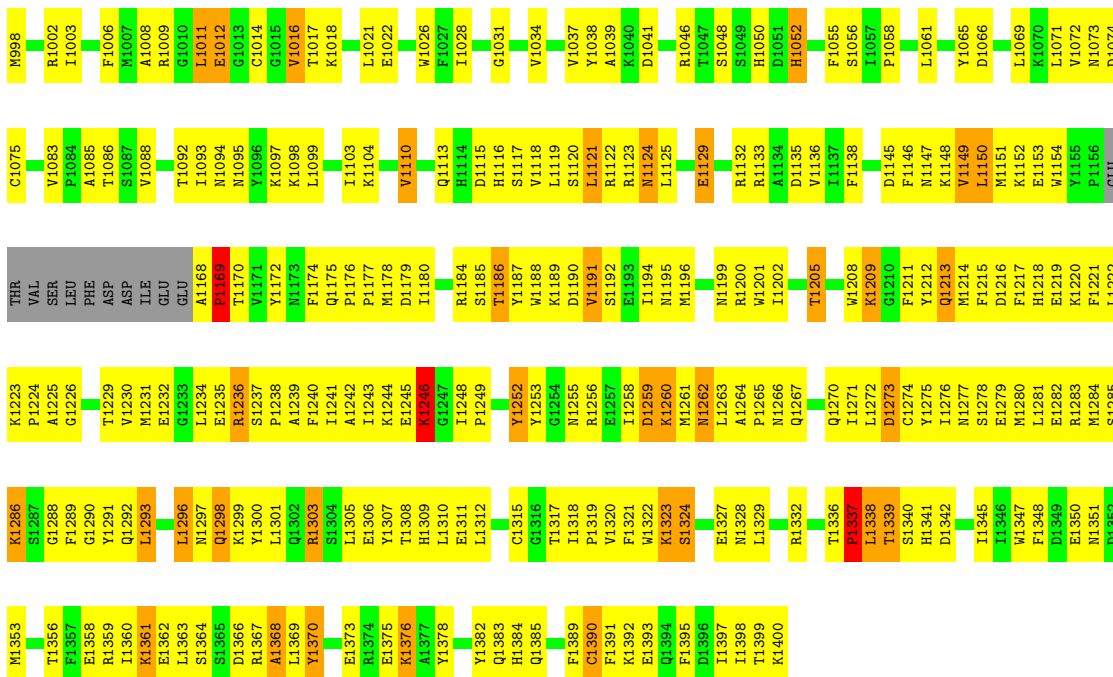
- Molecule 2: 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*GP*TP*AP*T)-3'

Chain D: 



- Molecule 3: DNA alpha-glucosyltransferase

Chain A: 



- Molecule 3: DNA alpha-glucosyltransferase

Chain B:  50% 41% 6%

M998	K1097	T1170	Y1252	W1322
R1002	K1098	V1171	Y1253	K1323
R1009	L1099	F1174	G1254	S1324
E1012	I1103	P1176	N1255	T1325
G1013	K1104	P1177	R1256	G1326
C1014	P1105	I1180	E1257	E1327
T1017	S1106	Y1183	I1258	W1328
K1018	I1107	V1184	M1261	L1329
Q1023	V1111	R1184	N1262	R1332
K1029	Y1112	S1185	A1263	V1333
T1035	Q1113	T1186	P1265	D1334
Y1038	H1114	W1187	N1266	W1335
K1042	D1115	W1188	Q1267	T1336
S1043	V1118	M1195	I1271	T1339
F1044	L1119	M1196	L1272	S1340
T1045	S1120	N1197	D1273	H1341
R1046	L1121	I1198	G1274	D1342
H1052	R1122	N1199	Y1275	S1343
K1053	R1123	R1200	I1276	G1344
S1056	N1124	W1201	I1277	W1347
I1057	L1125	I1202	S1278	E1350
P1058	E1129	G1203	E1279	W1351
V1059	T1130	R1204	M1280	D1352
I1060	W1131	T1205	L1281	M1353
L1061	R1132	T1206	E1282	E1354
A1062	R1133	T1207	R1283	S1355
K1063	A1134	W1208	M1284	T1356
E1064	F1138	K1209	S1287	F1357
Y1065	D1142	Y1212	G1288	E1358
A1068	D1145	Q1213	F1289	R1359
V1072	K1148	H1218	G1290	I1360
N1073	W1149	L1150	Y1291	L1363
D1074	L1151	S1228	Q1292	Y1370
C1075	M1151	T1229	L1293	E1373
D1076	W1154	E1232	N1297	R1374
N1081	Y1155	P1237	Q1298	A1377
S1082	P1156	S1238	L1300	Y1378
V1083	E1157	A1238	S1304	H1384
T1086	THR	F1240	L1305	Q1385
E1090	VAL	I1241	Y1307	D1386
N1094	SER	A1242	T1308	C1390
Y1095	LEU	I1243	H1309	Q1394
Y1096	PHE	I1244	L1310	T1399
	ASP	K1245	L1312	K1400
	ASP	E1246		
	ILE	K1246		
	GLU	Y1250		
	GLU	E1251		
	A1168			
	P1169			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.99Å 120.52Å 86.81Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 99.0 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.287 0.210 , 0.276	Depositor DCC
R_{free} test set	1120 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7132	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: NCO, UDP, 5HU, CL, EDO

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	0.32	0/277	0.68	0/424
2	D	0.31	0/270	0.73	0/415
3	A	0.48	0/3288	0.99	18/4435 (0.4%)
3	B	0.53	0/3303	1.04	22/4454 (0.5%)
All	All	0.49	0/7138	0.99	40/9728 (0.4%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1246	LYS	N-CA-C	-12.43	98.10	113.38
3	B	1304	SER	N-CA-C	9.33	123.13	108.67
3	B	1344	GLY	N-CA-C	-8.16	104.85	113.58
3	B	1309	HIS	N-CA-C	-7.98	101.66	111.40
3	A	1376	LYS	N-CA-C	-7.35	104.45	113.41

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	268	0	149	22	0
2	D	242	0	139	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3212	0	3152	282	0
3	B	3227	0	3169	161	0
4	A	21	0	0	2	0
4	B	21	0	0	1	0
4	D	7	0	0	0	0
5	A	25	0	11	1	0
5	B	25	0	11	2	0
6	B	1	0	0	0	0
7	B	4	0	6	0	0
8	A	30	0	0	1	0
8	B	48	0	0	1	0
8	D	1	0	0	0	0
All	All	7132	0	6637	466	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 34.

The worst 5 of 466 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:C:2:DA:H2''	1:C:3:DT:H5'	1.30	1.06
3:A:1213:GLN:H	3:A:1213:GLN:HE21	1.07	1.02
3:A:1252:TYR:OH	3:A:1273:ASP:HB3	1.59	1.02
1:C:7:5HU:H5A1	3:A:1237:SER:HA	1.43	0.98
3:A:1218:HIS:HA	3:A:1222:LEU:HB2	1.50	0.94

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	388/403 (96%)	308 (79%)	61 (16%)	19 (5%)	1	6
3	B	389/403 (96%)	326 (84%)	53 (14%)	10 (3%)	4	15
All	All	777/806 (96%)	634 (82%)	114 (15%)	29 (4%)	2	9

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1185	SER
3	A	1188	TRP
3	A	1339	THR
3	A	1367	ARG
3	B	1244	LYS

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	356/368 (97%)	334 (94%)	22 (6%)	16	45
3	B	358/368 (97%)	347 (97%)	11 (3%)	35	70
All	All	714/736 (97%)	681 (95%)	33 (5%)	24	58

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	1212	TYR
3	B	1213	GLN
3	B	1277	ASN
3	A	1236	ARG
3	A	1213	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	1218	HIS

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Mol	Chain	Res	Type
3	B	1351	ASN
3	B	1267	GLN
3	B	1328	ASN
3	B	1384	HIS

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	5HU	C	7	1	19,22,23	0.91	2 (10%)	25,31,34	0.86	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	5HU	C	7	1	-	6/9/23/24	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	5HU	C6-C5	2.76	1.42	1.35
1	C	7	5HU	C4-C5	-2.57	1.39	1.45

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	7	5HU	C6-C5-C5A-O5B
1	C	7	5HU	C2'-C1'-N1-C2
1	C	7	5HU	C2'-C1'-N1-C6
1	C	7	5HU	C4-C5-C5A-O5B
1	C	7	5HU	O4'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	7	5HU	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NCO	A	1401	-	6,6,6	1.49	0	-		
4	NCO	B	2020	-	6,6,6	1.61	0	-		
4	NCO	B	2018	-	6,6,6	1.48	0	-		
5	UDP	B	2021	-	25,26,26	0.86	1 (4%)	38,40,40	0.61	1 (2%)
4	NCO	A	1402	-	6,6,6	1.55	0	-		
4	NCO	D	1003	-	6,6,6	1.56	0	-		
7	EDO	B	2022	-	3,3,3	0.66	0	2,2,2	0.07	0
4	NCO	B	2019	-	6,6,6	1.65	0	-		
5	UDP	A	1404	-	25,26,26	0.90	1 (4%)	38,40,40	0.58	1 (2%)
4	NCO	A	1403	-	6,6,6	1.67	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
7	EDO	B	2022	-	-	1/1/1/1	-
5	UDP	A	1404	-	-	5/16/32/32	0/2/2/2
5	UDP	B	2021	-	-	4/16/32/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1404	UDP	PA-O3A	3.27	1.63	1.59
5	B	2021	UDP	PA-O3A	2.85	1.62	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2021	UDP	O2B-PB-O1B	2.28	119.72	110.83
5	A	1404	UDP	O2B-PB-O1B	2.28	119.70	110.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1404	UDP	C5'-O5'-PA-O2A
5	A	1404	UDP	PA-O3A-PB-O2B
5	B	2021	UDP	C5'-O5'-PA-O1A
5	B	2021	UDP	C5'-O5'-PA-O2A
5	A	1404	UDP	PA-O3A-PB-O3B

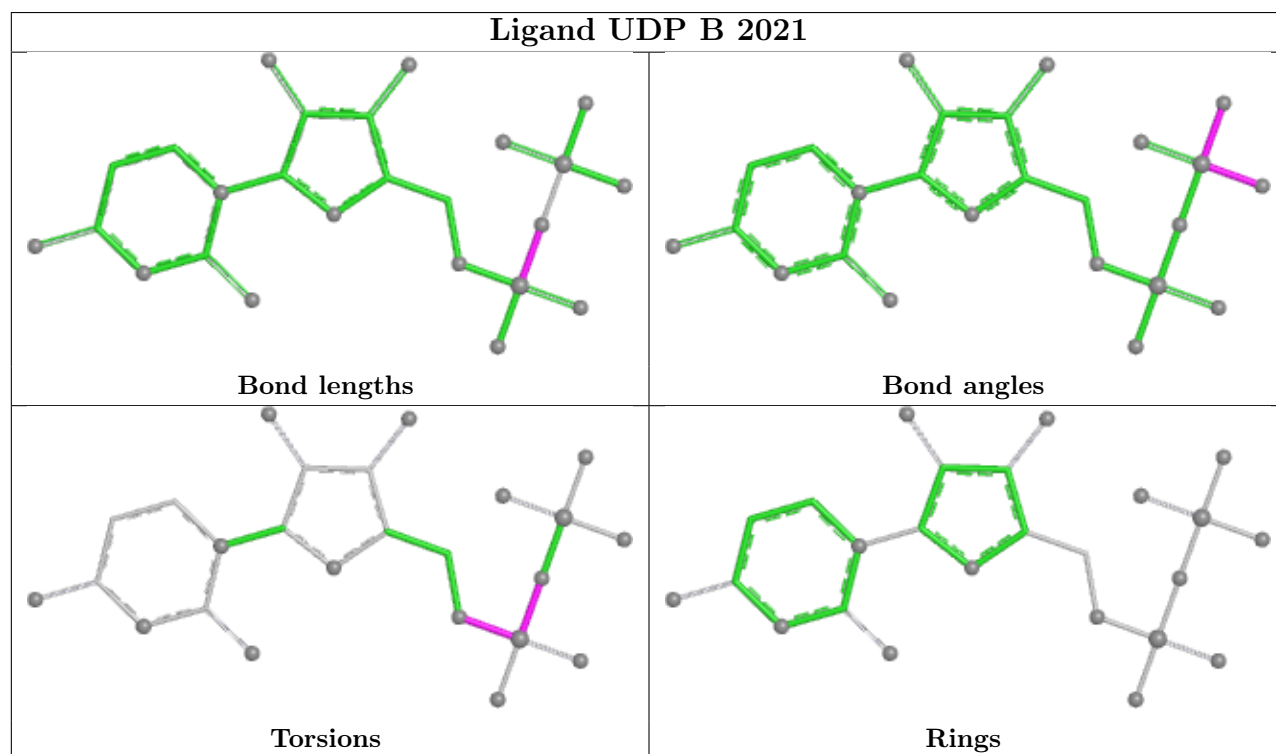
There are no ring outliers.

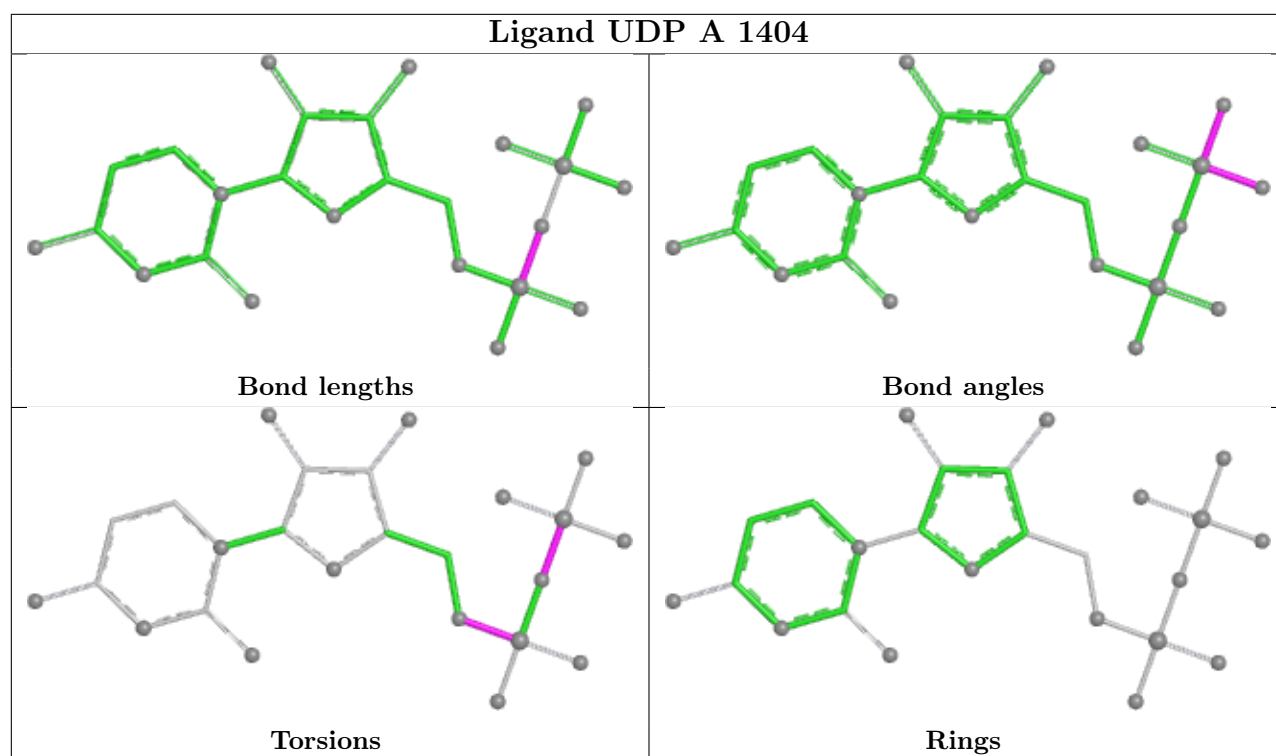
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1401	NCO	1	0
5	B	2021	UDP	2	0
4	B	2019	NCO	1	0
5	A	1404	UDP	1	0
4	A	1403	NCO	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	C	12/13 (92%)	0.21	0 100 100	53, 98, 100, 100	0
2	D	12/12 (100%)	0.13	0 100 100	64, 88, 100, 100	0
3	A	392/403 (97%)	-0.25	0 100 100	32, 62, 89, 96	0
3	B	393/403 (97%)	-0.53	0 100 100	27, 50, 68, 91	0
All	All	809/831 (97%)	-0.37	0 100 100	27, 56, 87, 100	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	5HU	C	7	21/22	0.78	0.11	85,98,99,99	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

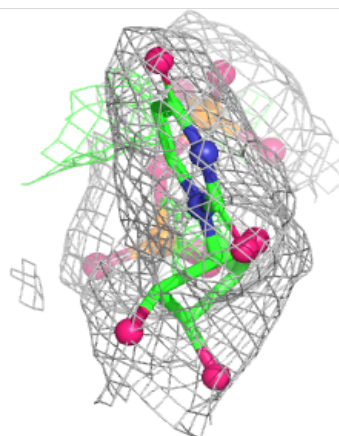
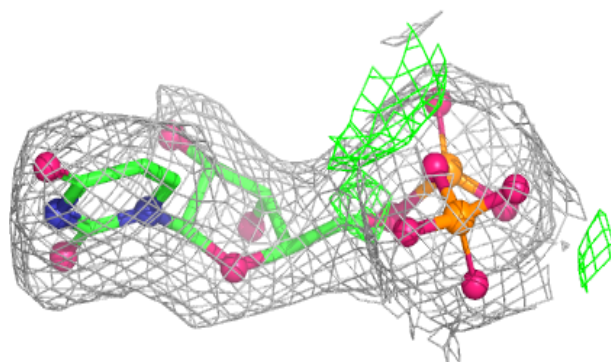
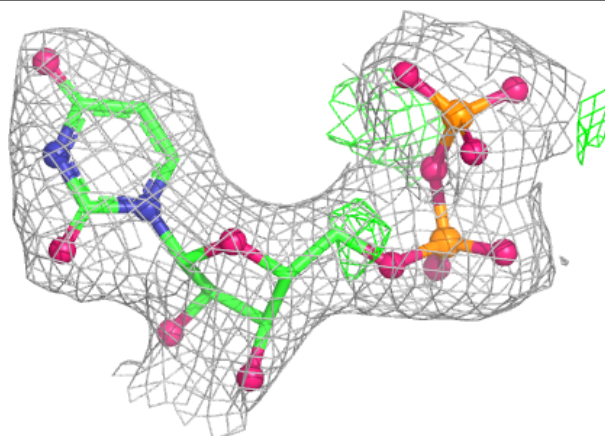
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	NCO	A	1402	7/7	0.77	0.18	99,99,99,99	7
4	NCO	B	2020	7/7	0.77	0.27	99,99,99,99	7
4	NCO	B	2019	7/7	0.78	0.39	98,98,99,99	7
7	EDO	B	2022	4/4	0.79	0.07	64,64,65,65	0
4	NCO	A	1403	7/7	0.80	0.34	99,99,99,99	7
4	NCO	D	1003	7/7	0.90	0.12	92,92,93,93	0
6	CL	B	2017	1/1	0.93	0.08	65,65,65,65	0
4	NCO	A	1401	7/7	0.94	0.09	93,94,94,95	0
4	NCO	B	2018	7/7	0.95	0.09	84,84,85,85	0
5	UDP	A	1404	25/25	0.95	0.07	39,46,55,56	0
5	UDP	B	2021	25/25	0.97	0.07	35,39,42,43	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.

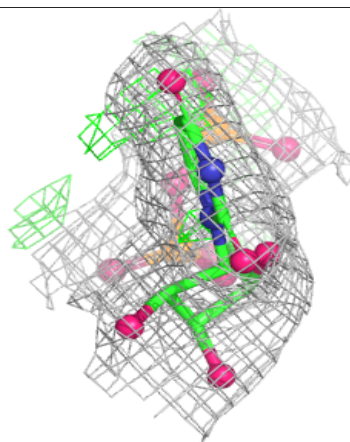
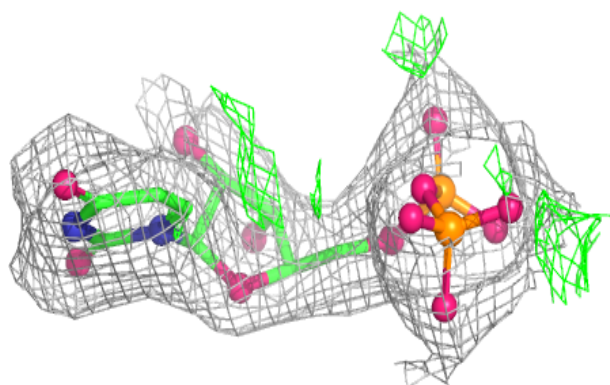
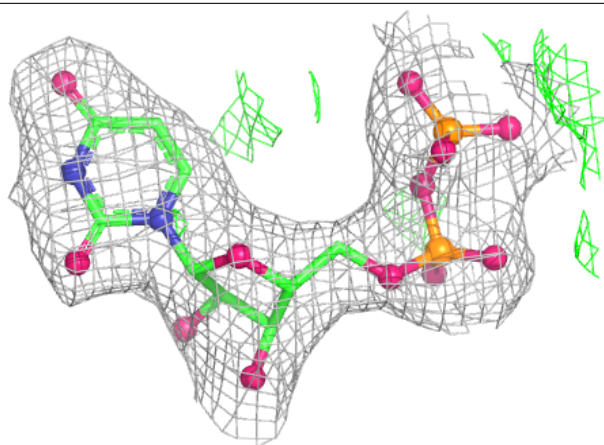
Electron density around UDP A 1404:

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 UDP B 2021:

$2mF_o-DF_c$ (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.