



wwPDB X-ray Structure Validation Summary Report ⓘ

May 19, 2020 – 07:21 pm BST

PDB ID : 2VS5
Title : THE BINDING OF UDP-GALACTOSE BY AN ACTIVE SITE MUTANT
OF alpha-1,3 GALACTOSYLTRANSFERASE (alpha3GT)
Authors : Tumbale, P.; Jamaluddin, H.; Thiyagarajan, N.; Brew, K.; Acharya, K.R.
Deposited on : 2008-04-18
Resolution : 1.82 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

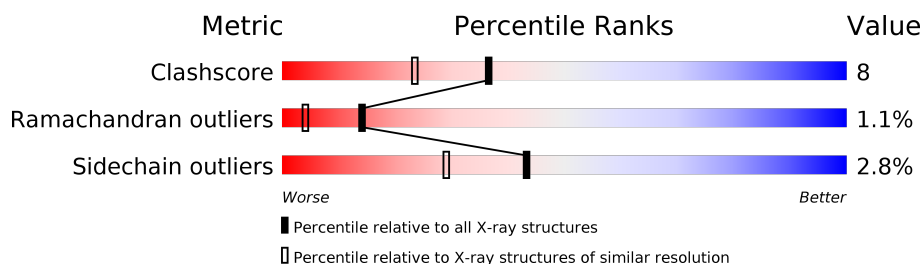
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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))
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5446 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 N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2333	1523	387	411	12			
1	B	278	Total	C	N	O	S	0	0	1
			2307	1511	380	404	12			

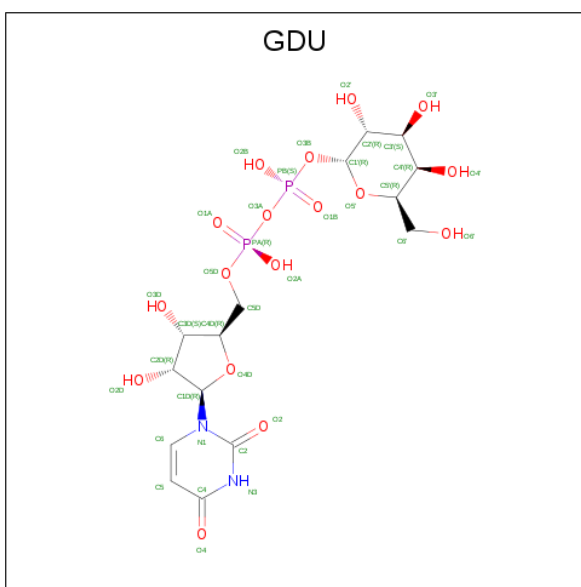
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	GLN	GLU	engineered mutation	UNP P14769
B	317	GLN	GLU	engineered mutation	UNP P14769

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

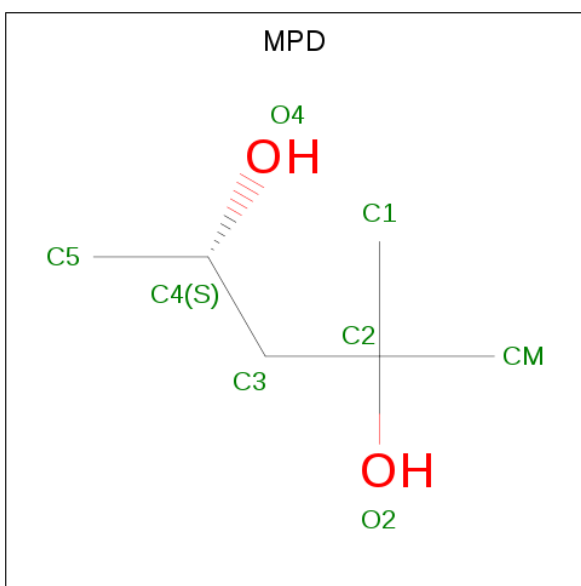
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		

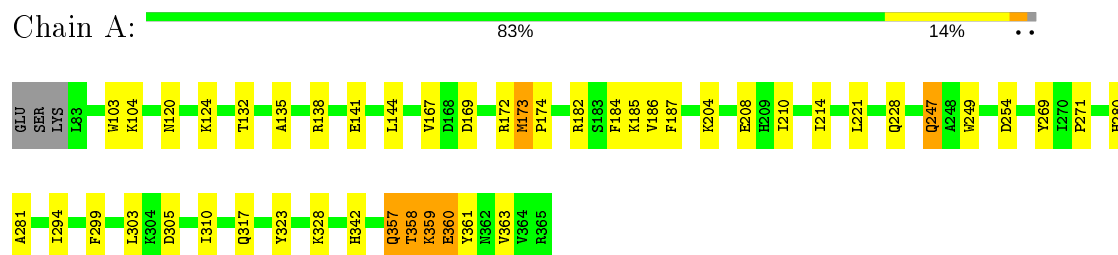
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total 354	O 354	0	0
5	B	369	Total 369	O 369	0	0

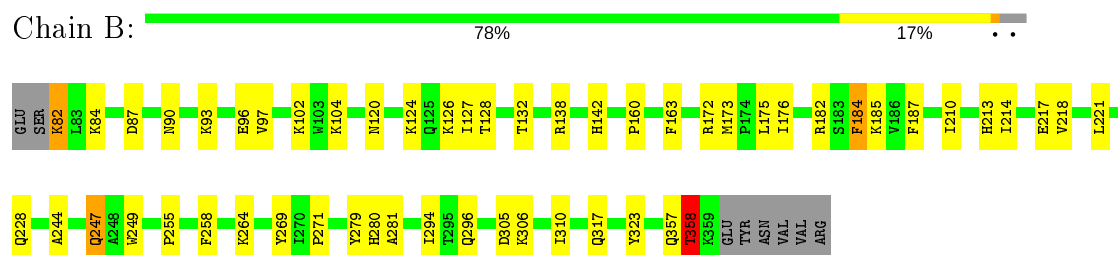
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERASE



- Molecule 1: N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.03Å 91.37Å 94.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.57 – 1.82 24.57 – 1.82	Depositor EDS
% Data completeness (in resolution range)	75.9 (24.57-1.82) 92.6 (24.57-1.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.236 , 0.242 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5446	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.87% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MN, GDU

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	0.36	0/2405	0.61	0/3255
1	B	0.38	0/2379	0.61	0/3224
All	All	0.37	0/4784	0.61	0/6479

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2333	0	2274	34	0
1	B	2307	0	2268	39	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	22	0	0
3	B	36	0	22	0	0
4	B	8	0	13	1	0
5	A	354	0	0	6	0
5	B	369	0	0	12	0
All	All	5446	0	4599	74	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.

The worst 5 of 74 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:254:ASP:HB3	5:A:2231:HOH:O	1.58	1.00
1:B:102:LYS:HE3	5:B:2024:HOH:O	1.72	0.89
1:A:281:ALA:H	1:A:317:GLN:HE21	1.18	0.87
1:B:281:ALA:H	1:B:317:GLN:HE21	1.34	0.76
4:B:1362:MPD:HM1	5:B:2167:HOH:O	1.91	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/286 (98%)	264 (94%)	12 (4%)	5 (2%)	8	1
1	B	276/286 (96%)	261 (95%)	14 (5%)	1 (0%)	34	21
All	All	557/572 (97%)	525 (94%)	26 (5%)	6 (1%)	14	4

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLU
1	A	358	THR
1	A	359	LYS
1	A	361	TYR
1	A	363	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	248 / 257 (96%)	243 (98%)	5 (2%)	55	43
1	B	248 / 257 (96%)	239 (96%)	9 (4%)	35	19
All	All	496 / 514 (96%)	482 (97%)	14 (3%)	43	29

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	173	MET
1	B	182	ARG
1	B	296	GLN
1	B	82	LYS
1	B	247	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	327	ASN
1	B	296	GLN
1	A	313	GLN
1	B	247	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	MPD	B	1362	-	7,7,7	1.61	2 (28%)	9,10,10	2.02	3 (33%)
3	GDU	B	1361	2	31,38,38	3.17	10 (32%)	41,58,58	2.18	5 (12%)
3	GDU	A	1368	2	31,38,38	3.21	9 (29%)	41,58,58	2.15	5 (12%)

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
4	MPD	B	1362	-	-	1/5/5/5	-
3	GDU	B	1361	2	-	5/21/59/59	0/3/3/3
3	GDU	A	1368	2	-	6/21/59/59	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1368	GDU	C6-N1	-14.31	1.18	1.35
3	B	1361	GDU	C6-N1	-14.04	1.18	1.35
3	B	1361	GDU	C6-C5	5.77	1.50	1.38
3	A	1368	GDU	C6-C5	5.76	1.50	1.38
3	A	1368	GDU	C4-N3	3.64	1.39	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1361	GDU	C6-N1-C2	-8.74	107.32	121.20
3	A	1368	GDU	C6-N1-C2	-8.52	107.67	121.20
3	B	1361	GDU	C5-C4-N3	-7.51	106.78	123.31
3	A	1368	GDU	C5-C4-N3	-7.45	106.92	123.31
3	A	1368	GDU	C5-C6-N1	4.70	131.17	120.68

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1368	GDU	O4D-C1D-N1-C6
3	A	1368	GDU	C1'-O3B-PB-O3A
3	B	1361	GDU	C1'-O3B-PB-O3A
3	B	1361	GDU	C4D-C5D-O5D-PA
3	A	1368	GDU	C4D-C5D-O5D-PA

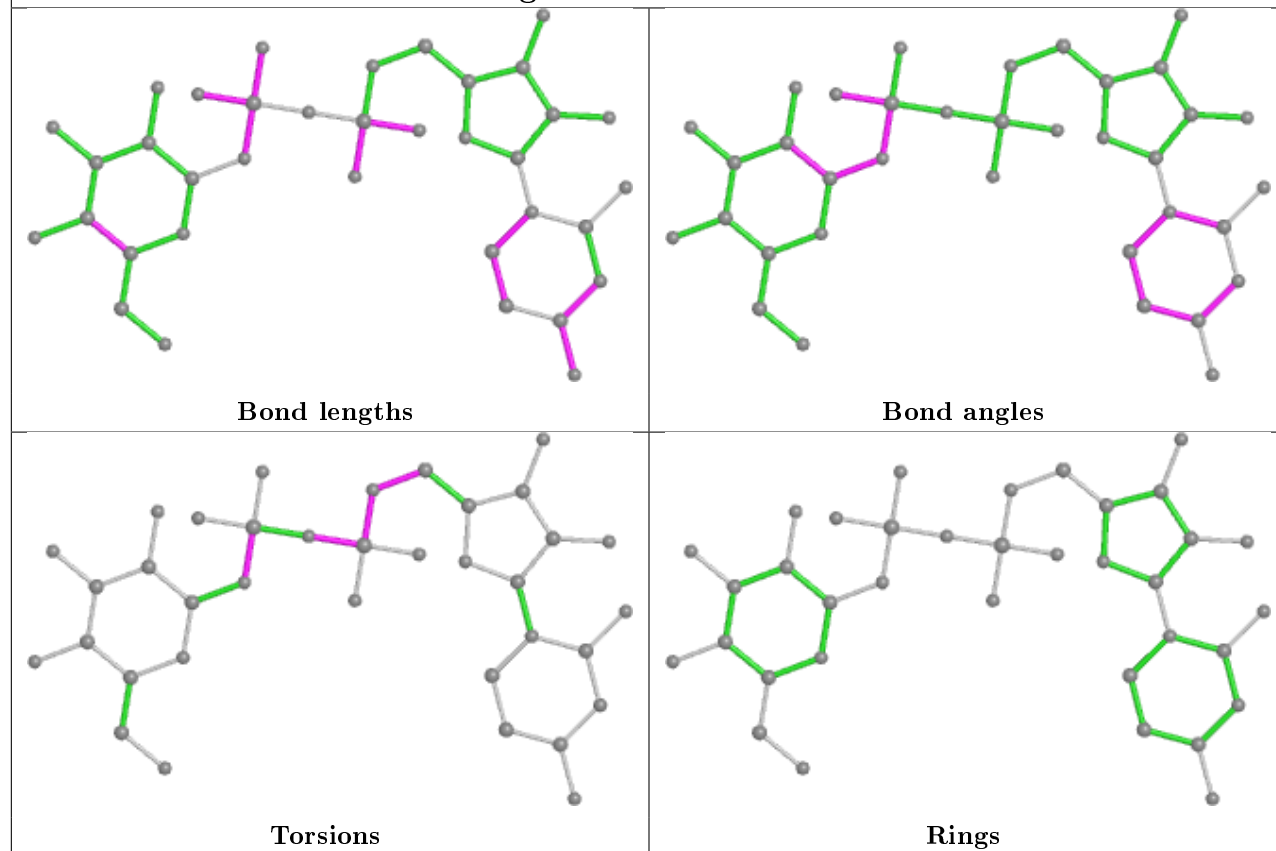
There are no ring outliers.

1 monomer is involved in 1 short contact:

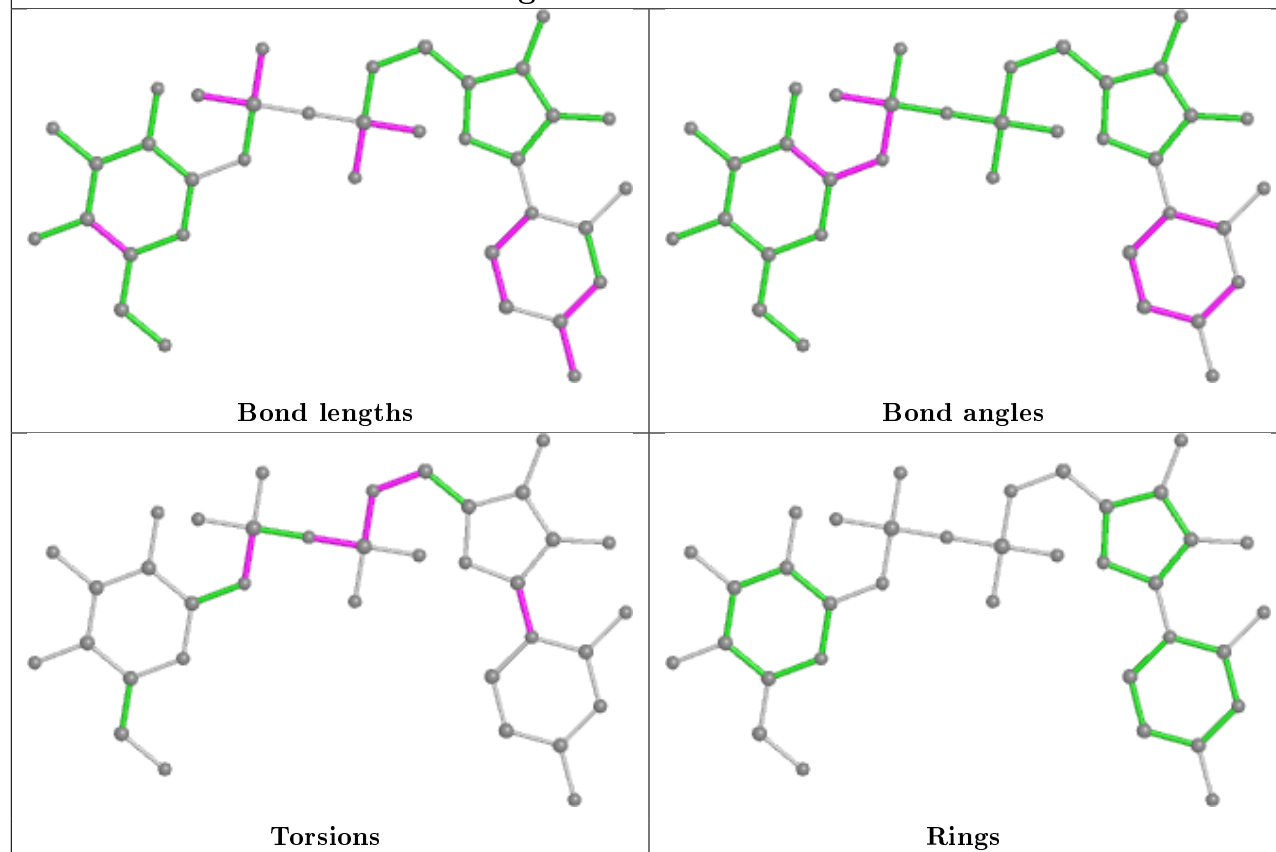
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1362	MPD	1	0

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.

Ligand GDU B 1361



Ligand GDU A 1368



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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

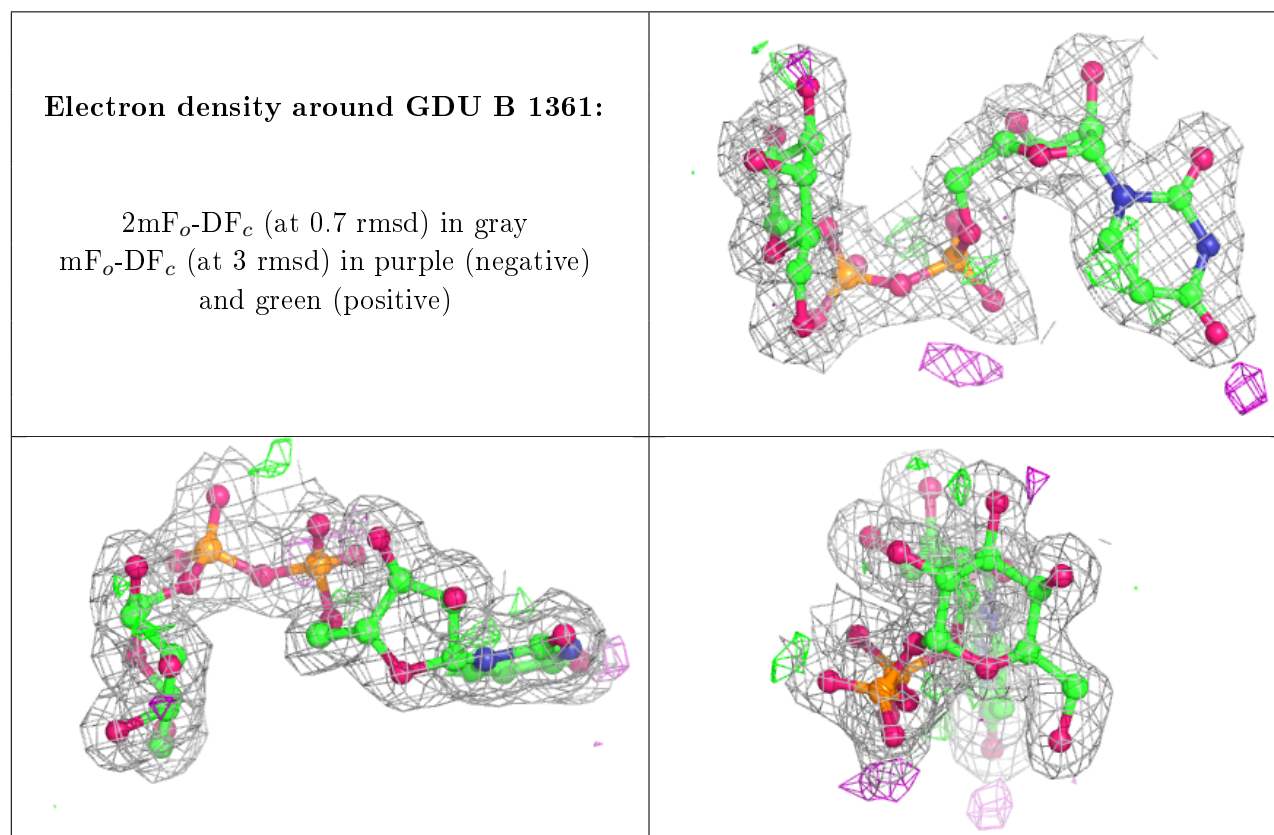
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

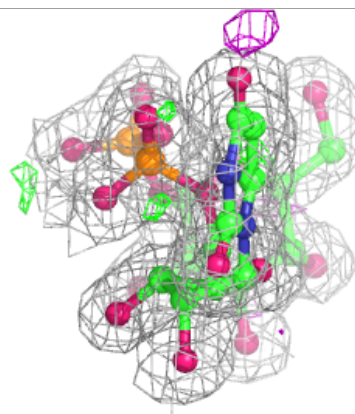
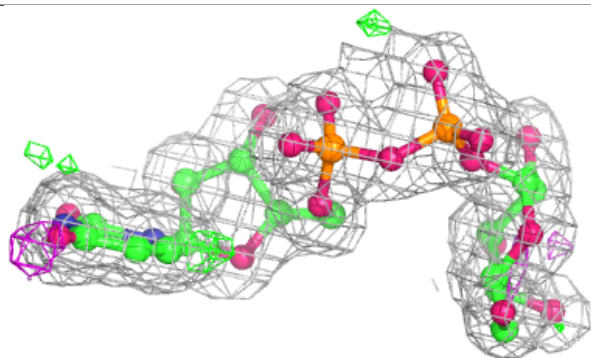
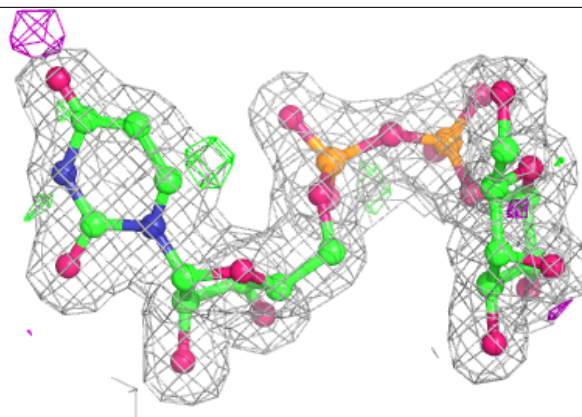
Unable to reproduce the depositors R factor - this section is therefore empty.

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 GDU A 1368:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.