Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 07:25 AM EDT

PDB ID	:	5UW1
Title	:	Activated state yGsy2p in complex with UDP-galactose
Authors	:	Mahalingan, K.K.; Hurley, T.D.
Deposited on	:	2017-02-20
Resolution	:	3.26 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 (i) 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 (i)) were used in the production of this report:

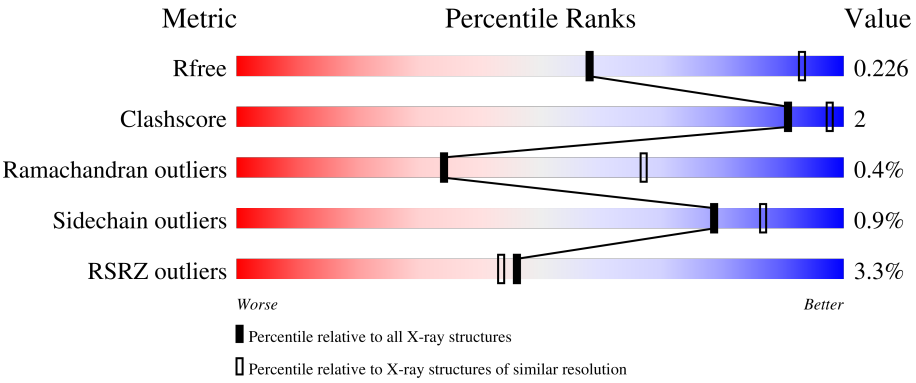
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 <=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	720	2% 82% 6% 11%
1	B	720	2% 82% 6% 11%
1	C	720	2% 84% • 11%
1	D	720	6% 82% 5% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20503 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5039	3223	860	937	19			
1	B	638	Total	C	N	O	S	0	0	0
			5117	3271	884	943	19			
1	C	638	Total	C	N	O	S	0	0	0
			5110	3265	883	943	19			
1	D	630	Total	C	N	O	S	0	0	0
			5029	3211	870	929	19			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	169	GLN	GLU	engineered mutation	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	SER	ALA	conflict	UNP P27472
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	169	GLN	GLU	engineered mutation	UNP P27472
B	535	SER	ALA	conflict	UNP P27472
C	-19	MET	-	initiating methionine	UNP P27472
C	-18	GLY	-	expression tag	UNP P27472
C	-17	SER	-	expression tag	UNP P27472
C	-16	SER	-	expression tag	UNP P27472
C	-15	HIS	-	expression tag	UNP P27472
C	-14	HIS	-	expression tag	UNP P27472
C	-13	HIS	-	expression tag	UNP P27472
C	-12	HIS	-	expression tag	UNP P27472
C	-11	HIS	-	expression tag	UNP P27472
C	-10	HIS	-	expression tag	UNP P27472
C	-9	SER	-	expression tag	UNP P27472
C	-8	SER	-	expression tag	UNP P27472
C	-7	GLY	-	expression tag	UNP P27472
C	-6	LEU	-	expression tag	UNP P27472
C	-5	VAL	-	expression tag	UNP P27472
C	-4	PRO	-	expression tag	UNP P27472
C	-3	ARG	-	expression tag	UNP P27472
C	-2	GLY	-	expression tag	UNP P27472
C	-1	SER	-	expression tag	UNP P27472

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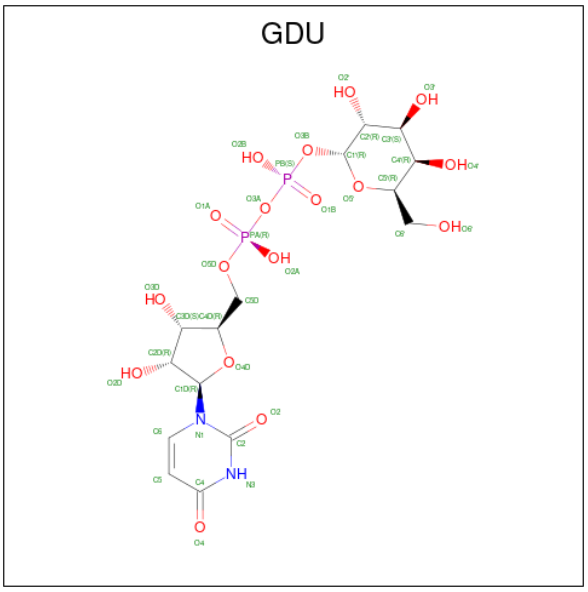
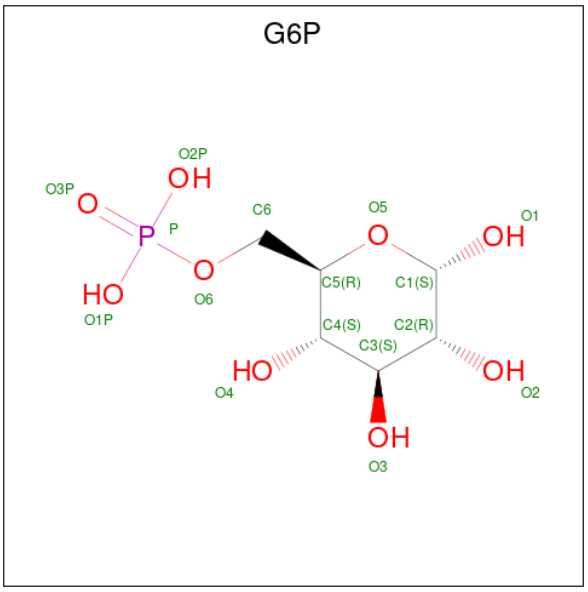
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P27472
C	169	GLN	GLU	engineered mutation	UNP P27472
C	535	SER	ALA	conflict	UNP P27472
D	-19	MET	-	initiating methionine	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression tag	UNP P27472
D	-15	HIS	-	expression tag	UNP P27472
D	-14	HIS	-	expression tag	UNP P27472
D	-13	HIS	-	expression tag	UNP P27472
D	-12	HIS	-	expression tag	UNP P27472
D	-11	HIS	-	expression tag	UNP P27472
D	-10	HIS	-	expression tag	UNP P27472
D	-9	SER	-	expression tag	UNP P27472
D	-8	SER	-	expression tag	UNP P27472
D	-7	GLY	-	expression tag	UNP P27472
D	-6	LEU	-	expression tag	UNP P27472
D	-5	VAL	-	expression tag	UNP P27472
D	-4	PRO	-	expression tag	UNP P27472
D	-3	ARG	-	expression tag	UNP P27472
D	-2	GLY	-	expression tag	UNP P27472
D	-1	SER	-	expression tag	UNP P27472
D	0	HIS	-	expression tag	UNP P27472
D	169	GLN	GLU	engineered mutation	UNP P27472
D	535	SER	ALA	conflict	UNP P27472

- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



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

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



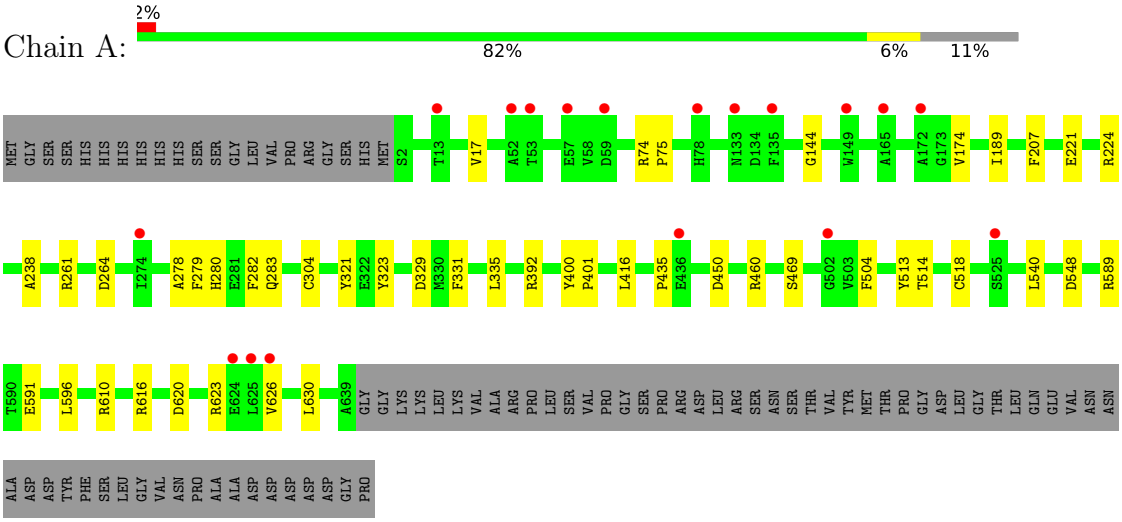
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		

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.

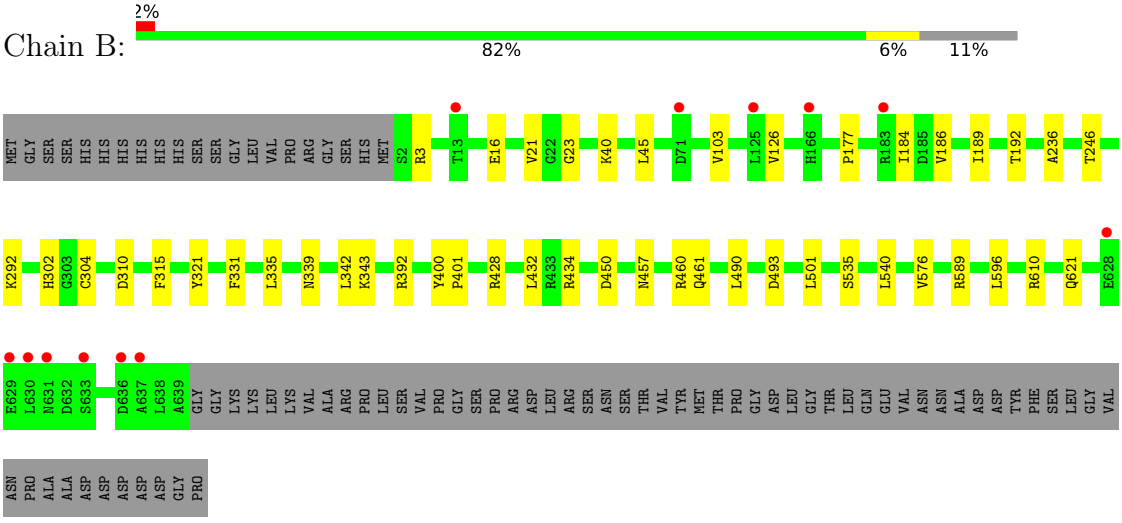
• Molecule 1: Glycogen [starch] synthase isoform 2

Chain A:



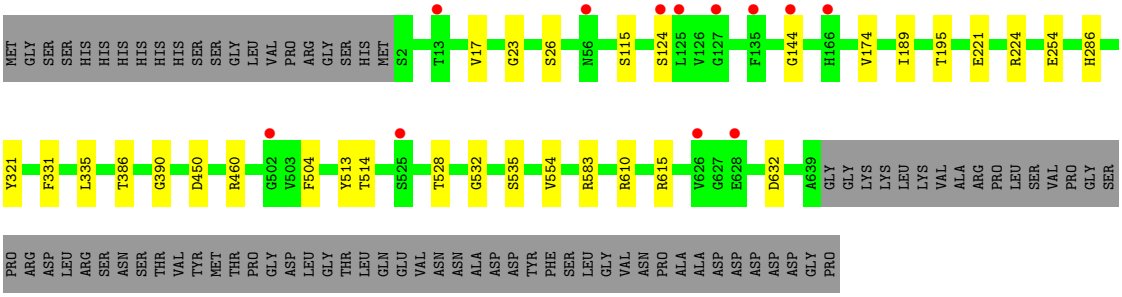
• Molecule 1: Glycogen [starch] synthase isoform 2

Chain B:



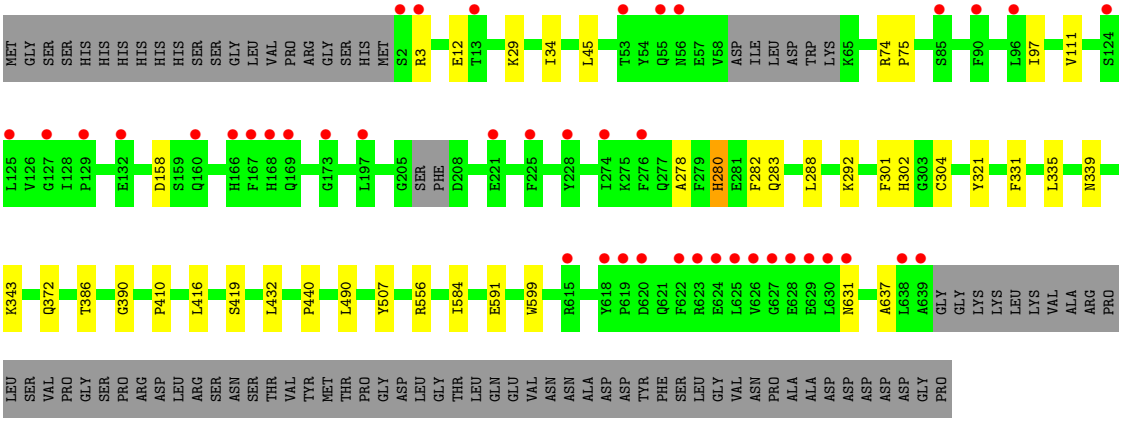
• Molecule 1: Glycogen [starch] synthase isoform 2

Chain C:



• Molecule 1: Glycogen [starch] synthase isoform 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	193.66Å 206.45Å 205.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.50 – 3.26 29.50 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.2 (145.50-3.26) 98.4 (29.50-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.185 , 0.230 0.188 , 0.226	Depositor DCC
R_{free} test set	3255 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	85.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20503	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: G6P, 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	0.47	0/5164	0.68	0/7023
1	B	0.53	0/5242	0.73	3/7109 (0.0%)
1	C	0.50	0/5234	0.70	0/7100
1	D	0.51	0/5149	0.70	0/6984
All	All	0.50	0/20789	0.70	3/28216 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	589	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	428	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	392	ARG	NE-CZ-NH1	5.43	123.02	120.30

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	5039	0	4829	21	0
1	B	5117	0	4995	20	0
1	C	5110	0	4979	14	0
1	D	5029	0	4887	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	22	0	0
2	B	36	0	22	0	0
2	C	36	0	22	0	0
2	D	36	0	22	0	0
3	A	16	0	11	1	0
3	B	16	0	11	0	0
3	C	16	0	11	2	0
3	D	16	0	11	0	0
All	All	20503	0	19822	70	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 2.

All (70) 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:450:ASP:OD1	1:C:460:ARG:NH2	2.21	0.73
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.26	0.68
1:D:292:LYS:HD2	1:D:490:LEU:HD21	1.75	0.68
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.33	0.61
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.36	0.61
1:B:540:LEU:HD23	1:B:596:LEU:HD13	1.84	0.59
1:B:292:LYS:HD2	1:B:490:LEU:HD21	1.86	0.58
1:D:34:ILE:HG21	1:D:599:TRP:HB3	1.87	0.57
1:A:278:ALA:HB2	1:D:584:ILE:HD13	1.91	0.53
1:B:126:VAL:HG11	1:B:177:PRO:HB3	1.91	0.52
1:C:195:THR:OG1	1:C:254:GLU:OE2	2.18	0.52
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.91	0.52
1:B:184:ILE:HG22	1:B:186:VAL:HG23	1.92	0.51
1:B:339:ASN:O	1:B:343:LYS:HG3	2.11	0.51
1:B:16:GLU:HG2	1:B:21:VAL:HB	1.92	0.51
1:A:331:PHE:CZ	1:A:335:LEU:HD11	2.45	0.51
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.93	0.51
1:D:3:ARG:NH2	1:D:158:ASP:O	2.44	0.50
1:B:342:LEU:HD21	1:B:576:VAL:HG11	1.93	0.50
1:A:238:ALA:O	1:A:261:ARG:NH1	2.45	0.50
1:B:302:HIS:O	1:B:434:ARG:NH1	2.44	0.50
1:A:626:VAL:HG11	1:A:630:LEU:HD11	1.93	0.49
1:C:221:GLU:HA	1:C:224:ARG:HG2	1.95	0.49
1:A:221:GLU:OE2	1:A:224:ARG:NH2	2.46	0.49
1:C:390:GLY:CA	1:D:386:THR:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ASN:O	1:D:343:LYS:HG3	2.14	0.47
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.97	0.47
1:B:192:THR:HG22	1:B:246:THR:HG22	1.96	0.46
1:A:264:ASP:CG	1:A:616:ARG:HH12	2.18	0.46
1:D:282:PHE:CD2	1:D:591:GLU:HG3	2.50	0.46
1:A:283:GLN:HG3	3:A:802:G6P:O1	2.15	0.46
1:C:615:ARG:HE	1:C:632:ASP:HB3	1.79	0.46
1:A:540:LEU:HD23	1:A:596:LEU:HD13	1.98	0.46
1:D:302:HIS:HD2	1:D:432:LEU:O	1.98	0.46
1:C:583:ARG:NH1	3:C:802:G6P:O2P	2.48	0.45
1:B:331:PHE:CZ	1:B:335:LEU:HD11	2.52	0.45
1:B:315:PHE:CE1	1:B:501:LEU:HD23	2.51	0.45
1:C:504:PHE:CE1	1:C:514:THR:HG22	2.51	0.45
1:B:3:ARG:O	1:B:621:GLN:NE2	2.50	0.45
1:B:177:PRO:HG3	1:B:236:ALA:HB1	1.99	0.45
1:D:12:GLU:HB3	1:D:45:LEU:HD23	1.97	0.45
1:A:400:TYR:CD1	1:A:401:PRO:HA	2.52	0.44
1:C:286:HIS:NE2	3:C:802:G6P:O1P	2.43	0.44
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.99	0.44
1:A:392:ARG:HD2	1:A:416:LEU:HA	1.99	0.44
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.53	0.44
1:C:532:GLY:O	1:C:535:SER:OG	2.30	0.43
1:B:400:TYR:CD1	1:B:401:PRO:HA	2.53	0.43
1:C:528:THR:HG22	1:C:554:VAL:HB	2.00	0.43
1:C:386:THR:HG21	1:D:390:GLY:CA	2.49	0.43
1:A:504:PHE:CE1	1:A:514:THR:HG22	2.53	0.43
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.54	0.43
1:A:279:PHE:O	1:A:282:PHE:HD1	2.03	0.42
1:D:301:PHE:CD2	1:D:440:PRO:HG2	2.54	0.42
1:D:74:ARG:N	1:D:75:PRO:CD	2.82	0.42
1:D:631:ASN:HB3	1:D:637:ALA:HB1	2.02	0.42
1:D:278:ALA:HB1	1:D:280:HIS:CE1	2.54	0.42
1:B:457:ASN:OD1	1:B:460:ARG:NH1	2.53	0.41
1:A:74:ARG:N	1:A:75:PRO:CD	2.83	0.41
1:D:410:PRO:HG2	1:D:416:LEU:HD21	2.02	0.41
1:B:292:LYS:CD	1:B:490:LEU:HD21	2.50	0.41
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.56	0.41
1:D:507:TYR:HB2	1:D:556:ARG:NH1	2.36	0.41
1:D:29:LYS:HG3	1:D:97:ILE:HD13	2.03	0.41
1:A:548:ASP:O	1:A:589:ARG:HD2	2.21	0.40
1:A:620:ASP:OD1	1:A:623:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:HIS:HB2	1:B:432:LEU:HD22	2.03	0.40
1:A:282:PHE:CE1	1:A:591:GLU:HG3	2.57	0.40
1:C:144:GLY:HA3	1:C:174:VAL:HB	2.03	0.40
1:B:45:LEU:HB2	1:B:103:VAL:HG12	2.03	0.40

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	636/720 (88%)	590 (93%)	43 (7%)	3 (0%)	29	62
1	B	636/720 (88%)	592 (93%)	42 (7%)	2 (0%)	41	72
1	C	636/720 (88%)	591 (93%)	42 (7%)	3 (0%)	29	62
1	D	624/720 (87%)	586 (94%)	36 (6%)	2 (0%)	41	72
All	All	2532/2880 (88%)	2359 (93%)	163 (6%)	10 (0%)	34	67

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	C	23	GLY
1	A	207	PHE
1	B	23	GLY
1	B	40	LYS
1	C	115	SER
1	A	435	PRO
1	D	280	HIS
1	C	17	VAL
1	D	111	VAL

5.3.2 Protein sidechains (i)

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	529/621 (85%)	524 (99%)	5 (1%)	78 87
1	B	546/621 (88%)	540 (99%)	6 (1%)	73 84
1	C	544/621 (88%)	540 (99%)	4 (1%)	84 90
1	D	534/621 (86%)	529 (99%)	5 (1%)	78 87
All	All	2153/2484 (87%)	2133 (99%)	20 (1%)	78 87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	CYS
1	A	321	TYR
1	A	469	SER
1	A	513	TYR
1	A	518	CYS
1	B	304	CYS
1	B	310	ASP
1	B	321	TYR
1	B	461	GLN
1	B	493	ASP
1	B	535	SER
1	C	26	SER
1	C	124	SER
1	C	321	TYR
1	C	513	TYR
1	D	288	LEU
1	D	304	CYS
1	D	321	TYR
1	D	372	GLN
1	D	419	SER

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	402	HIS
1	A	477	HIS
1	B	42	HIS
1	B	402	HIS
1	B	621	GLN
1	B	634	ASN
1	C	81	GLN
1	C	396	HIS
1	C	582	GLN
1	D	138	ASN
1	D	211	ASN
1	D	302	HIS

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

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	$\#\|Z\| > 2$
3	G6P	C	802	-	16,16,16	0.60	0	24,24,24	1.05	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GDU	B	801	-	35,38,38	0.99	3 (8%)	53,58,58	1.61	9 (16%)
2	GDU	A	801	-	35,38,38	0.93	3 (8%)	53,58,58	1.55	8 (15%)
3	G6P	B	802	-	16,16,16	0.59	0	24,24,24	0.95	0
2	GDU	C	801	-	35,38,38	0.99	3 (8%)	53,58,58	1.51	9 (16%)
3	G6P	A	802	-	16,16,16	0.63	0	24,24,24	1.05	2 (8%)
3	G6P	D	802	-	16,16,16	0.61	0	24,24,24	2.08	4 (16%)
2	GDU	D	801	-	35,38,38	0.97	3 (8%)	53,58,58	1.45	6 (11%)

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
3	G6P	C	802	-	-	2/6/26/26	0/1/1/1
2	GDU	B	801	-	-	8/23/59/59	0/3/3/3
2	GDU	A	801	-	-	6/23/59/59	0/3/3/3
3	G6P	B	802	-	-	0/6/26/26	0/1/1/1
2	GDU	C	801	-	-	9/23/59/59	0/3/3/3
3	G6P	A	802	-	-	2/6/26/26	0/1/1/1
3	G6P	D	802	-	-	3/6/26/26	0/1/1/1
2	GDU	D	801	-	-	9/23/59/59	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	GDU	C2-N1	2.80	1.42	1.38
2	B	801	GDU	C2-N1	2.76	1.42	1.38
2	C	801	GDU	C2-N1	2.72	1.42	1.38
2	A	801	GDU	C2-N1	2.54	1.42	1.38
2	B	801	GDU	C4-N3	-2.36	1.34	1.38
2	D	801	GDU	C6-C5	2.36	1.40	1.35
2	D	801	GDU	C4-N3	-2.29	1.34	1.38
2	B	801	GDU	C6-C5	2.25	1.40	1.35
2	A	801	GDU	C4-N3	-2.20	1.34	1.38
2	C	801	GDU	C4-N3	-2.17	1.34	1.38
2	C	801	GDU	C2-N3	-2.06	1.34	1.38
2	A	801	GDU	C6-C5	2.06	1.39	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	802	G6P	C6-C5-C4	5.80	124.19	112.09
3	D	802	G6P	O6-C6-C5	5.26	127.11	108.99
2	B	801	GDU	N3-C2-N1	5.04	121.57	114.89
2	B	801	GDU	C4-N3-C2	-4.92	120.09	126.58
2	A	801	GDU	N3-C2-N1	4.91	121.41	114.89
2	D	801	GDU	N3-C2-N1	4.70	121.13	114.89
2	A	801	GDU	C4-N3-C2	-4.55	120.58	126.58
2	C	801	GDU	C4-N3-C2	-4.47	120.68	126.58
2	D	801	GDU	C4-N3-C2	-4.46	120.70	126.58
2	C	801	GDU	N3-C2-N1	4.21	120.48	114.89
2	B	801	GDU	PB-O3A-PA	-3.93	119.33	132.83
2	C	801	GDU	C5-C4-N3	3.74	120.43	114.84
2	B	801	GDU	C5-C4-N3	3.43	119.97	114.84
2	A	801	GDU	C5-C4-N3	3.33	119.83	114.84
2	D	801	GDU	C5-C4-N3	3.32	119.81	114.84
3	D	802	G6P	O5-C5-C6	-2.93	100.75	106.67
2	C	801	GDU	PB-O3A-PA	-2.84	123.09	132.83
2	C	801	GDU	O4-C4-C5	-2.77	120.29	125.16
2	A	801	GDU	PB-O3A-PA	-2.77	123.33	132.83
3	D	802	G6P	C4-C3-C2	2.72	115.58	110.82
2	A	801	GDU	O4-C4-C5	-2.71	120.39	125.16
2	D	801	GDU	O4-C4-C5	-2.67	120.47	125.16
2	D	801	GDU	C3D-C2D-C1D	2.52	106.22	101.43
2	A	801	GDU	C1'-C2'-C3'	2.50	115.21	110.00
2	B	801	GDU	O4-C4-C5	-2.48	120.80	125.16
2	C	801	GDU	O2B-PB-O1B	2.44	124.29	112.24
2	D	801	GDU	PB-O3A-PA	-2.40	124.59	132.83
2	B	801	GDU	C3D-C2D-C1D	2.34	105.86	101.43
2	B	801	GDU	O2A-PA-O1A	2.32	123.70	112.24
2	C	801	GDU	O2A-PA-O1A	2.28	123.50	112.24
2	A	801	GDU	C3D-C2D-C1D	2.26	105.72	101.43
3	A	802	G6P	O2-C2-C3	2.19	115.41	110.35
2	C	801	GDU	O2-C2-N3	-2.15	117.49	121.50
2	B	801	GDU	O2-C2-N3	-2.14	117.51	121.50
2	C	801	GDU	C3D-C2D-C1D	2.14	105.49	101.43
2	A	801	GDU	C6-N1-C2	-2.06	118.36	120.99
3	A	802	G6P	O2P-P-O1P	2.05	115.48	107.64
2	B	801	GDU	O2B-PB-O1B	2.03	122.27	112.24
3	C	802	G6P	O5-C1-C2	-2.02	106.69	110.28
3	C	802	G6P	O3-C3-C4	-2.01	105.69	110.35

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GDU	C5D-O5D-PA-O1A
2	B	801	GDU	C5D-O5D-PA-O3A
2	C	801	GDU	C3D-C4D-C5D-O5D
2	C	801	GDU	C5D-O5D-PA-O2A
2	C	801	GDU	C5D-O5D-PA-O3A
2	D	801	GDU	C3D-C4D-C5D-O5D
2	D	801	GDU	O4D-C4D-C5D-O5D
2	D	801	GDU	C5D-O5D-PA-O3A
2	D	801	GDU	O5'-C1'-O3B-PB
3	A	802	G6P	C4-C5-C6-O6
3	A	802	G6P	O5-C5-C6-O6
3	C	802	G6P	C4-C5-C6-O6
3	D	802	G6P	C4-C5-C6-O6
3	D	802	G6P	O5-C5-C6-O6
2	D	801	GDU	O5'-C5'-C6'-O6'
2	B	801	GDU	C3D-C4D-C5D-O5D
2	B	801	GDU	O4D-C4D-C5D-O5D
2	D	801	GDU	C4'-C5'-C6'-O6'
2	C	801	GDU	O5'-C5'-C6'-O6'
2	C	801	GDU	O4D-C4D-C5D-O5D
2	B	801	GDU	C4'-C5'-C6'-O6'
2	C	801	GDU	C4'-C5'-C6'-O6'
2	B	801	GDU	O5'-C5'-C6'-O6'
2	B	801	GDU	PB-O3A-PA-O1A
2	A	801	GDU	PB-O3A-PA-O5D
2	C	801	GDU	PB-O3A-PA-O5D
2	D	801	GDU	PB-O3A-PA-O5D
2	B	801	GDU	C5D-O5D-PA-O2A
2	D	801	GDU	C5D-O5D-PA-O2A
2	D	801	GDU	C1'-O3B-PB-O3A
2	C	801	GDU	O5'-C1'-O3B-PB
3	C	802	G6P	O5-C5-C6-O6
2	A	801	GDU	O4D-C1D-N1-C6
2	A	801	GDU	C2D-C1D-N1-C6
2	B	801	GDU	PB-O3A-PA-O5D
3	D	802	G6P	C6-O6-P-O2P
2	C	801	GDU	PB-O3A-PA-O1A
2	A	801	GDU	O4D-C4D-C5D-O5D
2	A	801	GDU	O4D-C1D-N1-C2

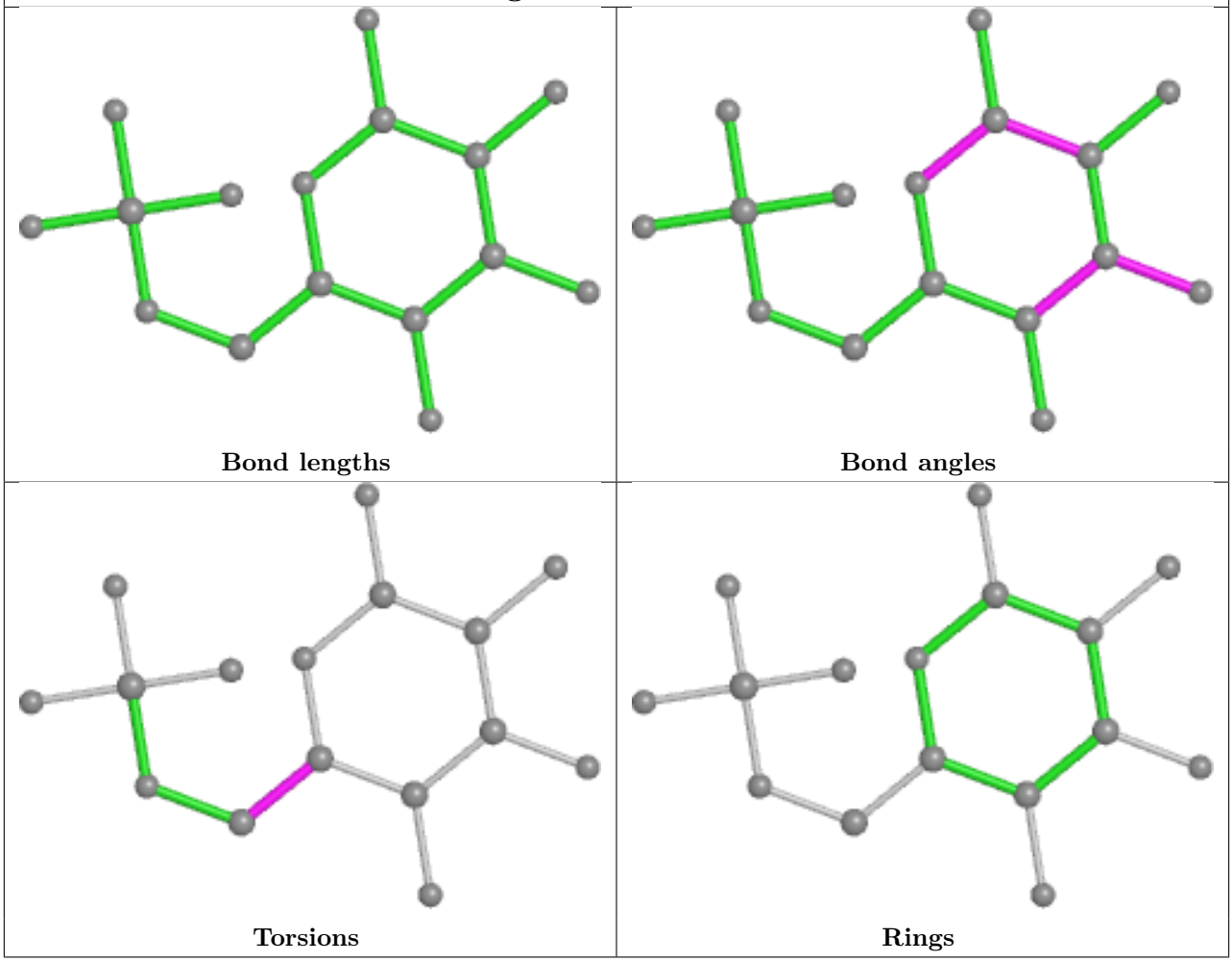
There are no ring outliers.

2 monomers are involved in 3 short contacts:

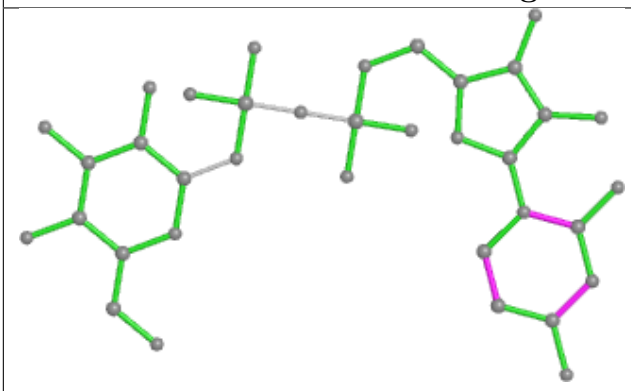
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	G6P	2	0
3	A	802	G6P	1	0

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 then 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.

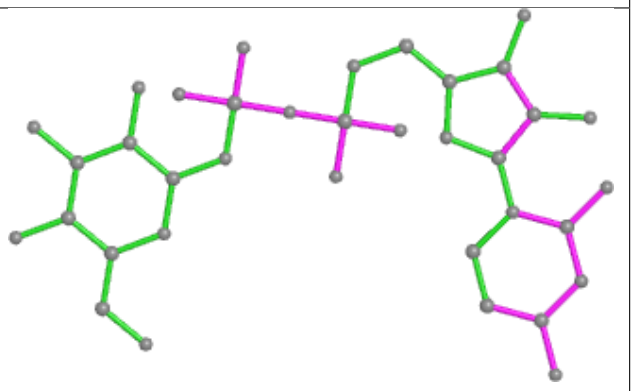
Ligand G6P C 802



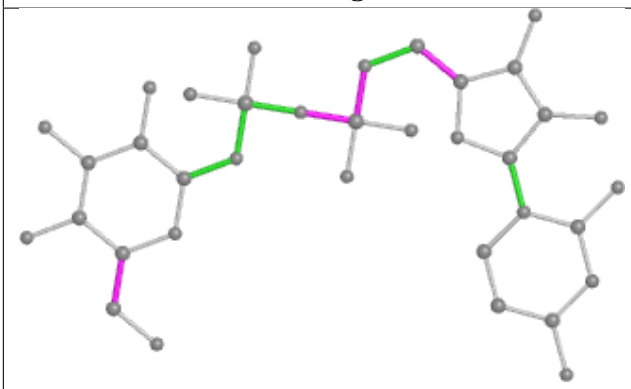
Ligand GDU B 801



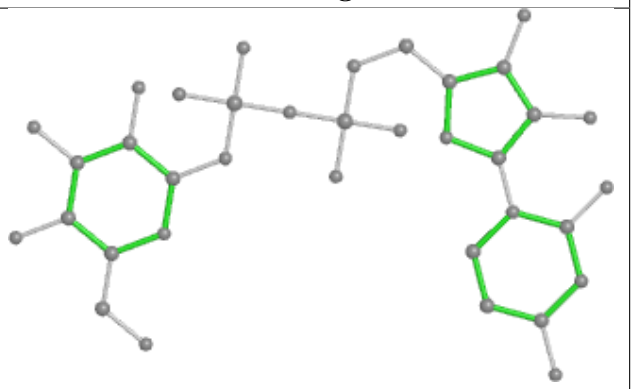
Bond lengths



Bond angles

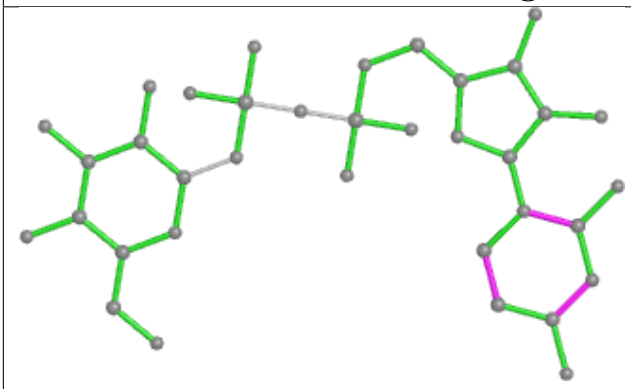


Torsions

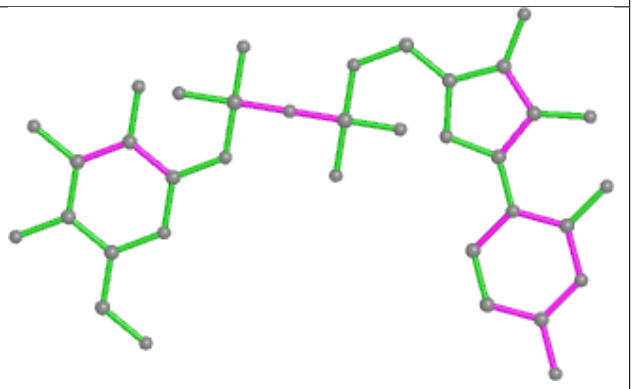


Rings

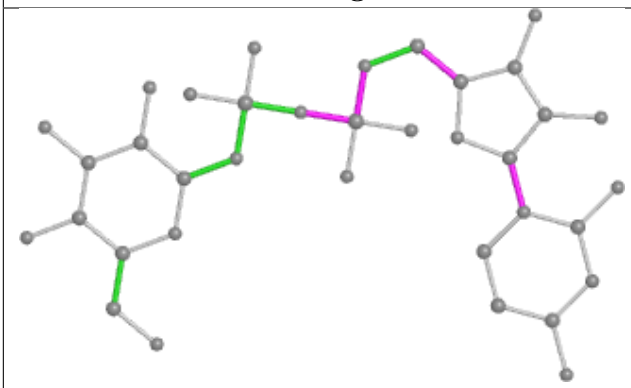
Ligand GDU A 801



Bond lengths



Bond angles



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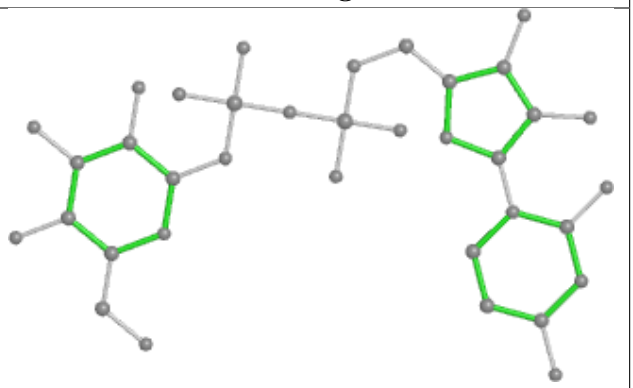
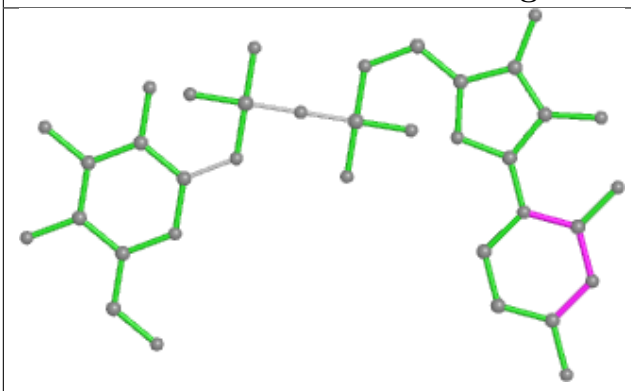
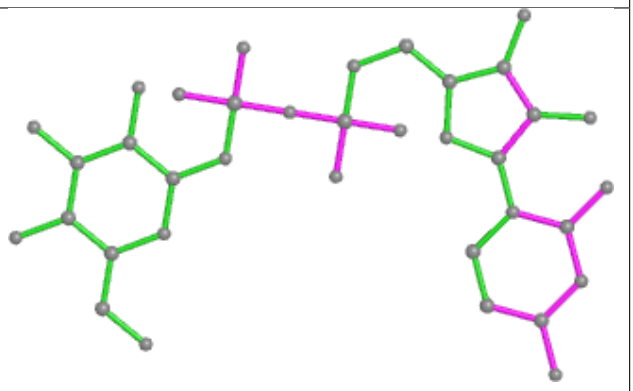


Rings

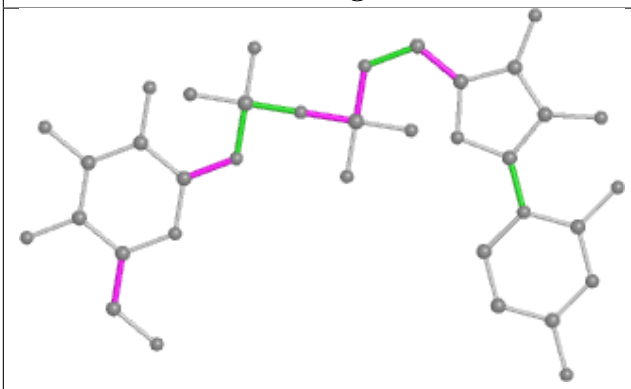
Ligand GDU C 801



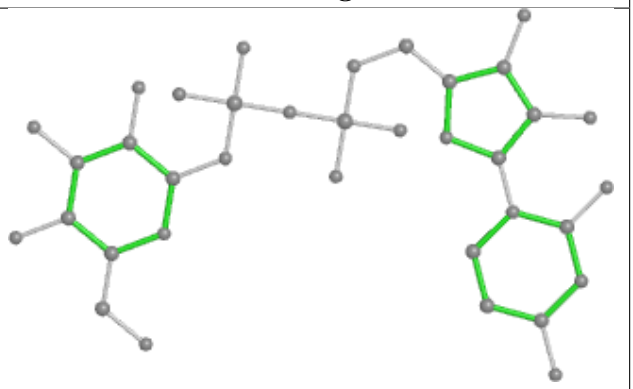
Bond lengths



Bond angles

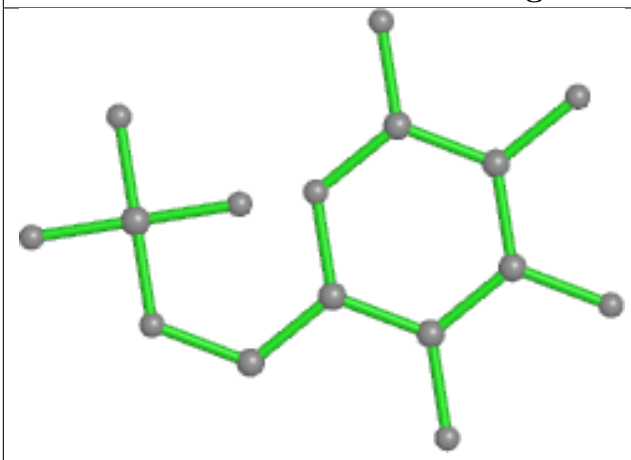


Torsions



Rings

Ligand G6P A 802



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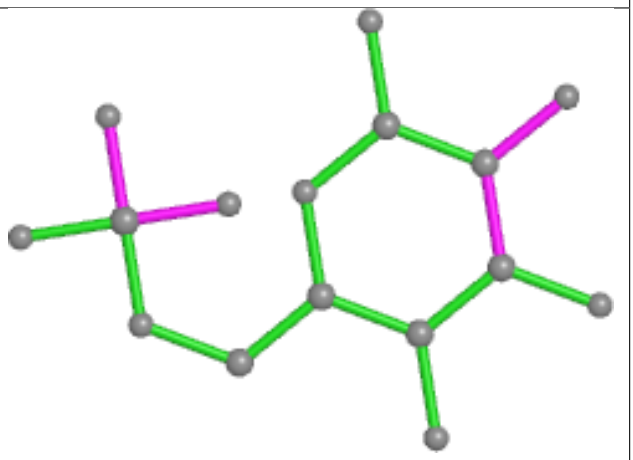
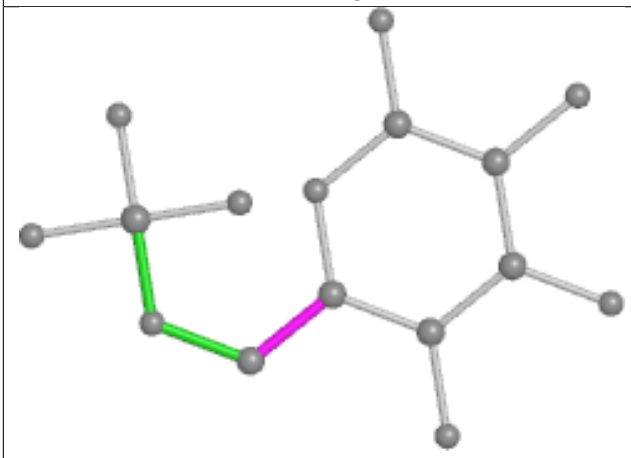
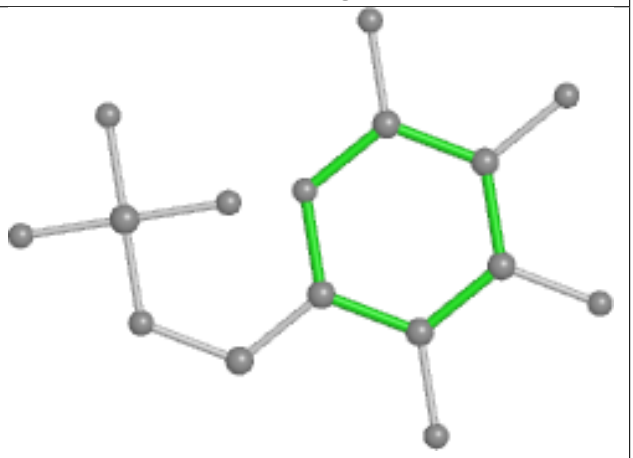


Bond angles

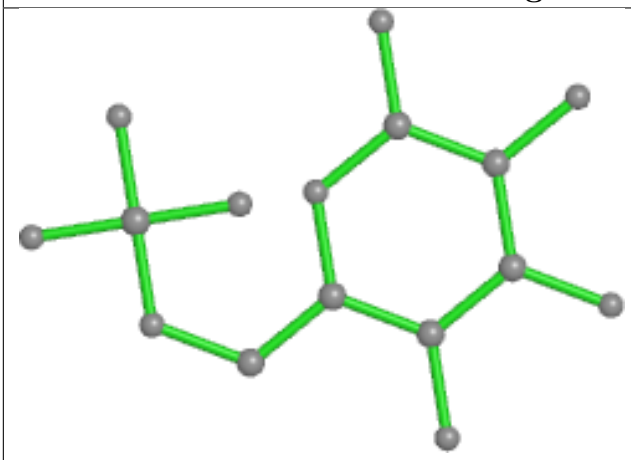


Torsions

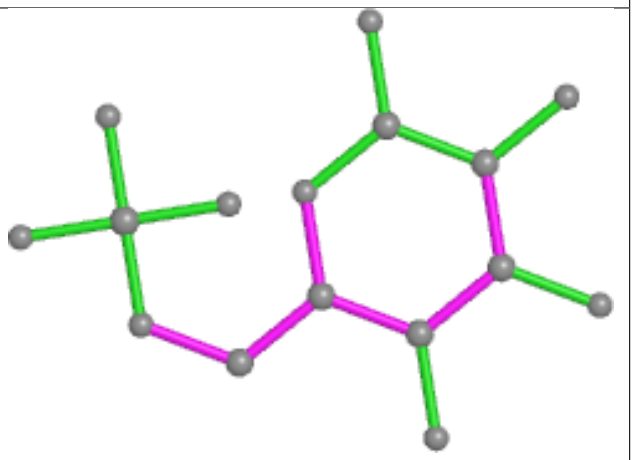


Rings

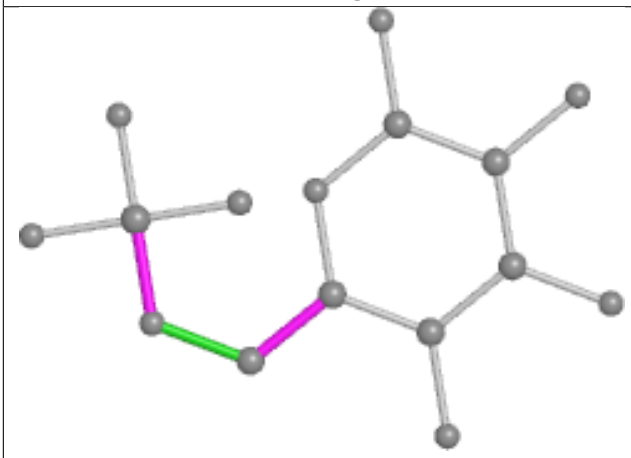
Ligand G6P D 802



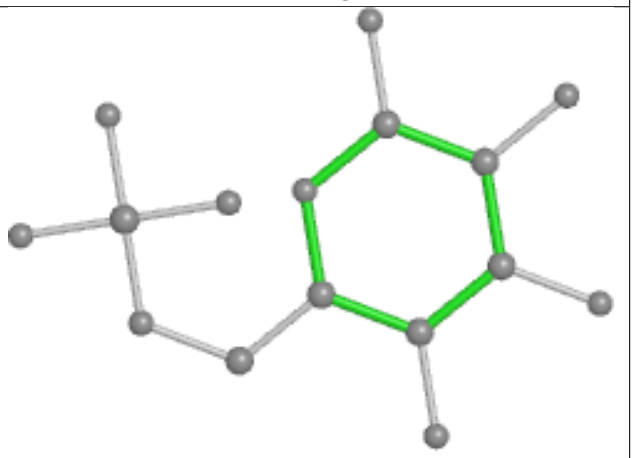
Bond lengths



Bond angles

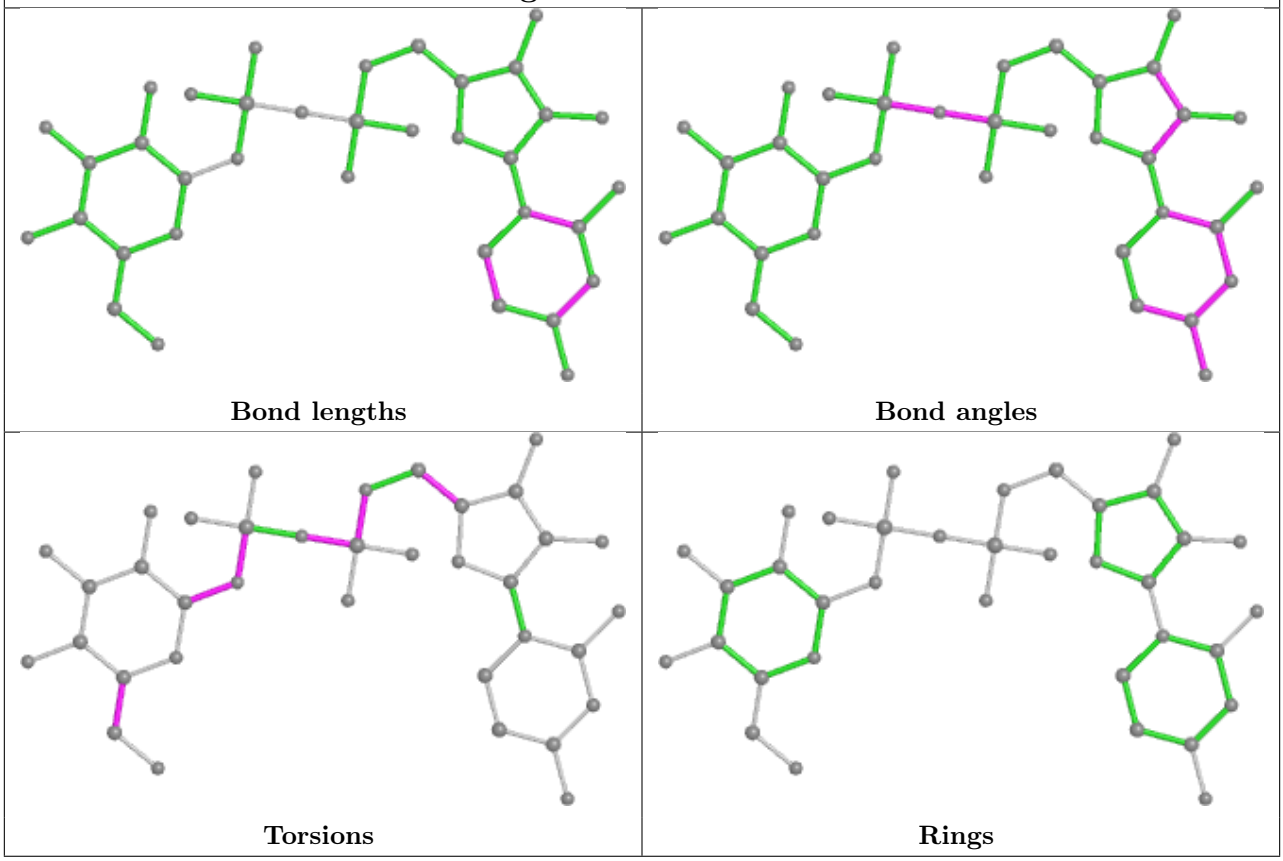


Torsions



Rings

Ligand GDU D 801



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, 95^{th} 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	638/720 (88%)	-0.01	18 (2%)	53	50	66, 106, 194, 213	0
1	B	638/720 (88%)	-0.21	12 (1%)	66	64	47, 86, 153, 184	0
1	C	638/720 (88%)	-0.13	12 (1%)	66	64	58, 96, 163, 190	0
1	D	630/720 (87%)	0.11	42 (6%)	17	17	53, 105, 191, 212	0
All	All	2544/2880 (88%)	-0.06	84 (3%)	46	43	47, 98, 182, 213	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	4.9
1	D	629	GLU	4.9
1	D	639	ALA	4.5
1	C	525	SER	4.3
1	D	624	GLU	4.3
1	D	630	LEU	4.3
1	D	619	PRO	4.2
1	A	57	GLU	4.0
1	D	622	PHE	3.9
1	C	13	THR	3.8
1	D	618	TYR	3.7
1	D	167	PHE	3.6
1	D	129	PRO	3.6
1	D	628	GLU	3.4
1	A	625	LEU	3.4
1	D	625	LEU	3.3
1	B	630	LEU	3.2
1	D	626	VAL	3.0
1	A	52	ALA	3.0
1	A	135	PHE	3.0
1	C	125	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	638	LEU	2.9
1	B	71	ASP	2.9
1	A	78	HIS	2.9
1	D	125	LEU	2.9
1	B	166	HIS	2.8
1	D	620	ASP	2.8
1	D	85	SER	2.8
1	A	626	VAL	2.8
1	D	627	GLY	2.8
1	D	127	GLY	2.8
1	D	631	ASN	2.7
1	D	168	HIS	2.7
1	D	132	GLU	2.7
1	A	502	GLY	2.7
1	D	166	HIS	2.7
1	C	626	VAL	2.6
1	B	13	THR	2.6
1	C	56	ASN	2.6
1	B	636	ASP	2.6
1	D	90	PHE	2.5
1	D	276	PHE	2.5
1	D	13	THR	2.5
1	D	221	GLU	2.4
1	A	53	THR	2.4
1	D	225	PHE	2.4
1	C	124	SER	2.4
1	A	133	ASN	2.4
1	D	124	SER	2.4
1	C	502	GLY	2.4
1	D	169	GLN	2.3
1	D	160	GLN	2.3
1	B	633	SER	2.3
1	B	183	ARG	2.3
1	D	96	LEU	2.3
1	D	615	ARG	2.3
1	A	165	ALA	2.3
1	C	628	GLU	2.3
1	D	53	THR	2.3
1	B	637	ALA	2.2
1	C	127	GLY	2.2
1	D	56	ASN	2.2
1	D	55	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	2.2
1	A	59	ASP	2.2
1	A	436	GLU	2.1
1	A	149	TRP	2.1
1	B	631	ASN	2.1
1	D	3	ARG	2.1
1	D	623	ARG	2.1
1	A	624	GLU	2.1
1	B	629	GLU	2.1
1	C	144	GLY	2.1
1	D	197	LEU	2.1
1	B	628	GLU	2.1
1	A	13	THR	2.1
1	D	274	ILE	2.1
1	A	525	SER	2.1
1	C	166	HIS	2.0
1	C	135	PHE	2.0
1	A	274	ILE	2.0
1	D	228	TYR	2.0
1	D	173	GLY	2.0
1	B	125	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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
2	GDU	A	801	36/36	0.91	0.21	89,112,126,127	0
2	GDU	B	801	36/36	0.94	0.16	64,86,139,145	0

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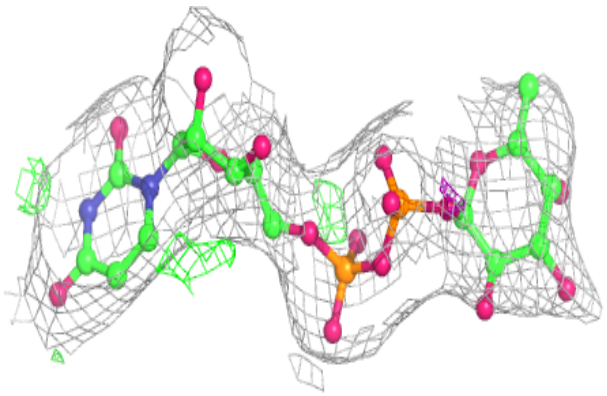
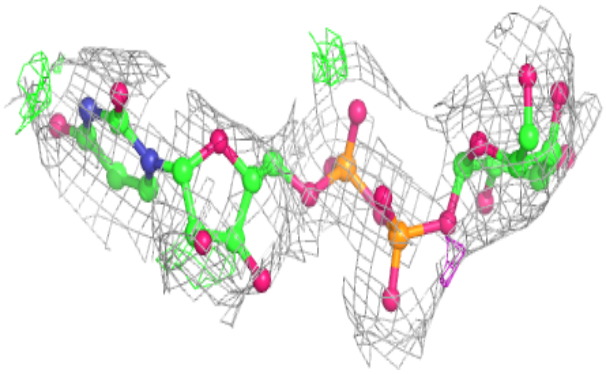
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GDU	C	801	36/36	0.94	0.15	71,78,86,88	0
2	GDU	D	801	36/36	0.94	0.16	70,99,148,152	0
3	G6P	A	802	16/16	0.95	0.17	61,65,70,70	0
3	G6P	C	802	16/16	0.96	0.19	54,58,62,63	0
3	G6P	D	802	16/16	0.96	0.16	40,47,51,52	0
3	G6P	B	802	16/16	0.97	0.17	40,45,47,49	0

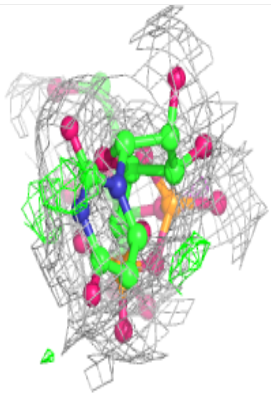
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDU A 801:

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

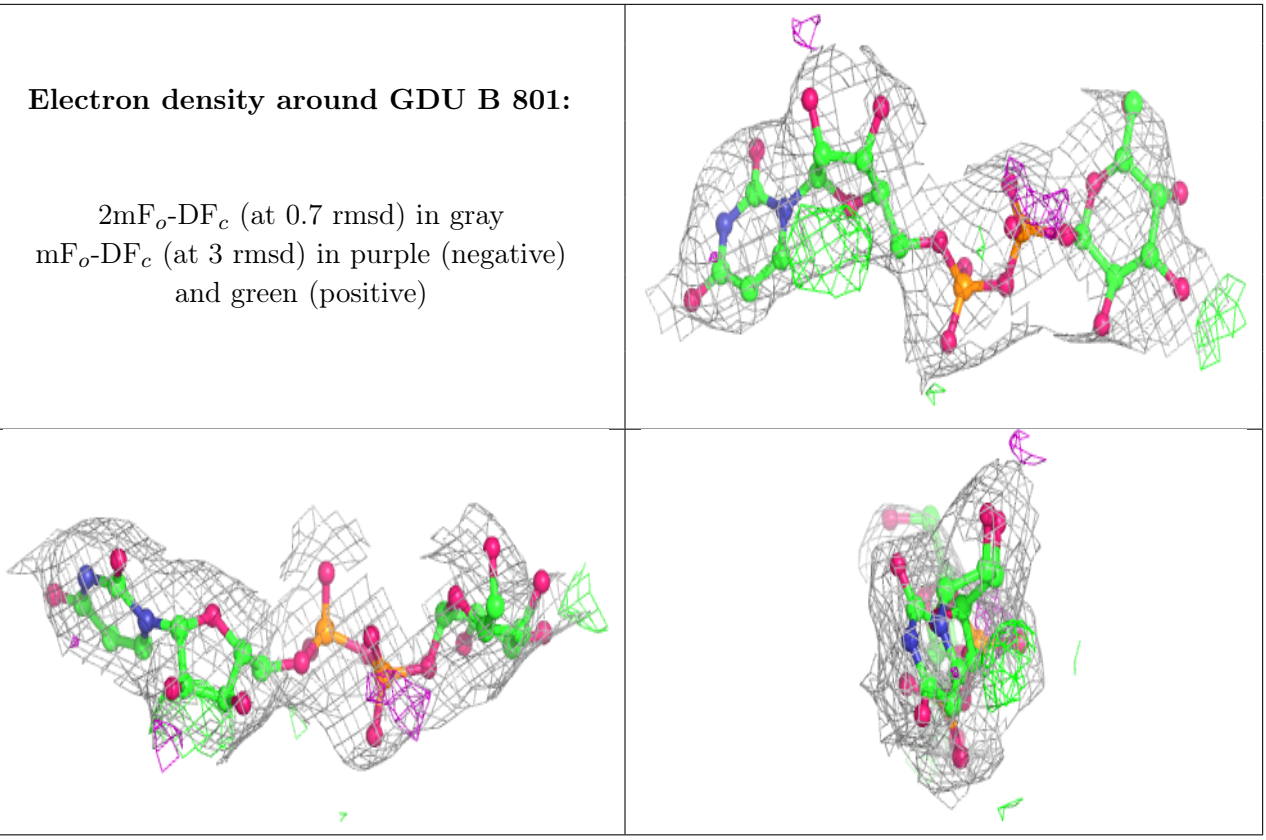






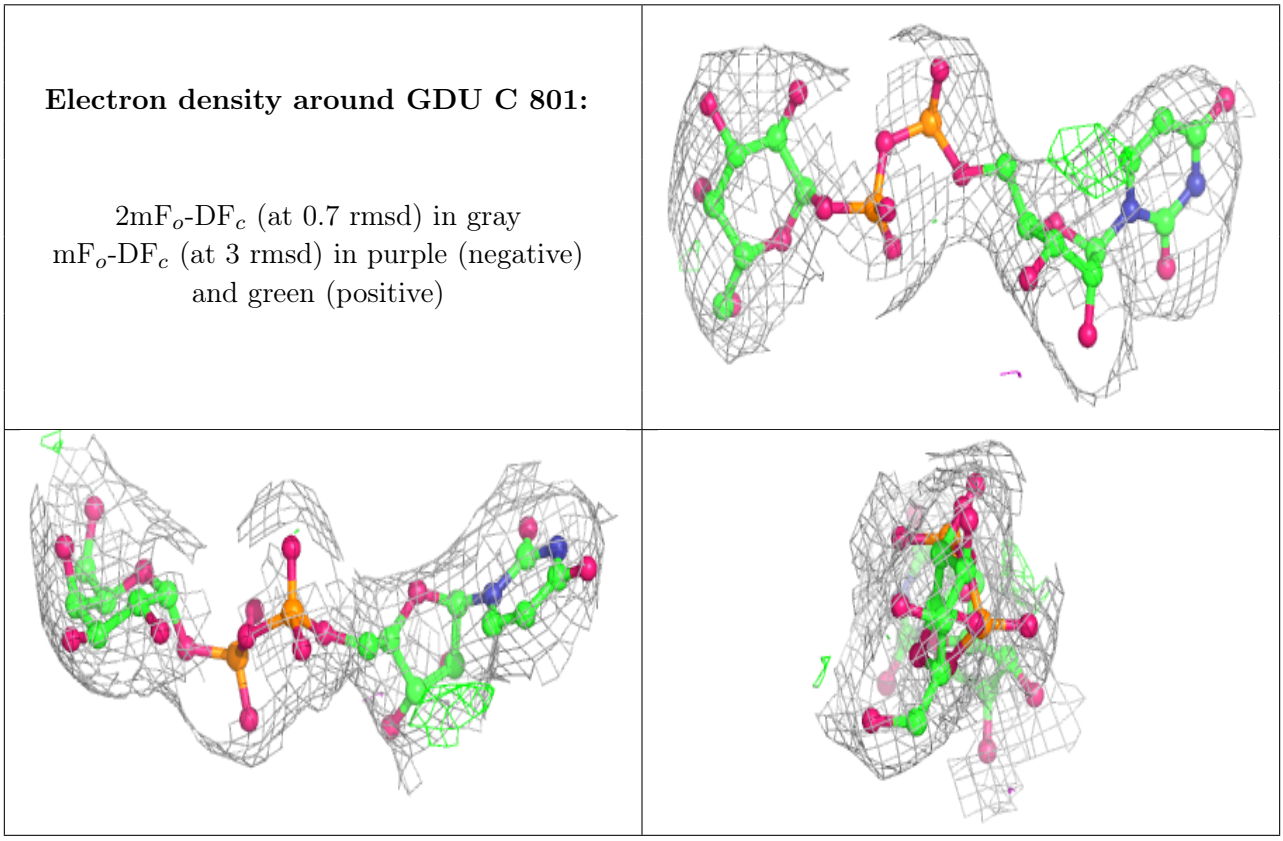
Electron density around GDU B 801:

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



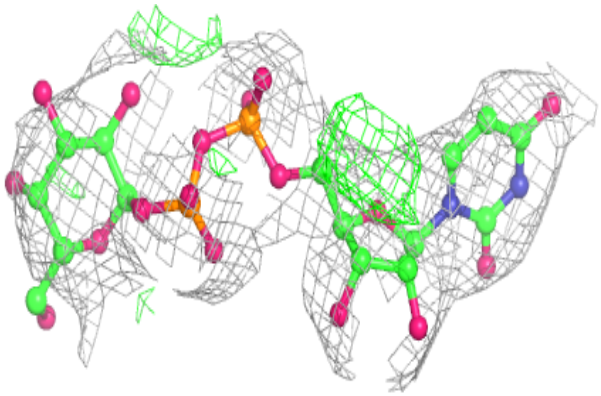
Electron density around GDU C 801:

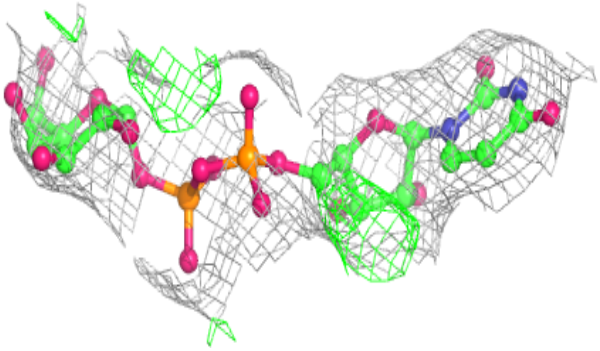
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

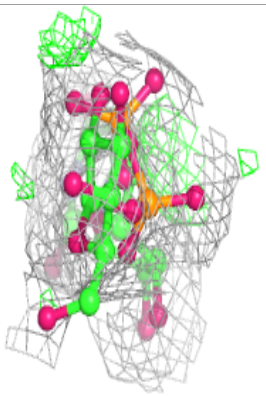


Electron density around GDU D 801:

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

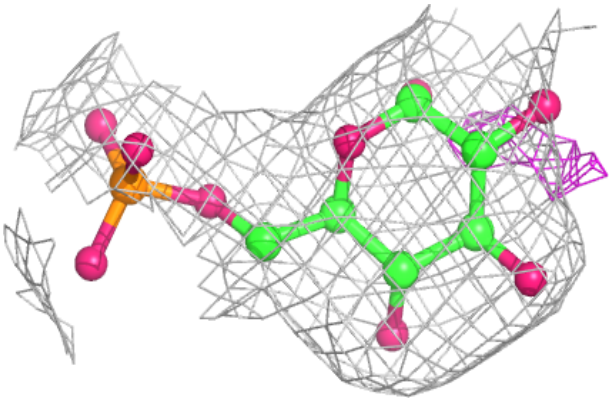


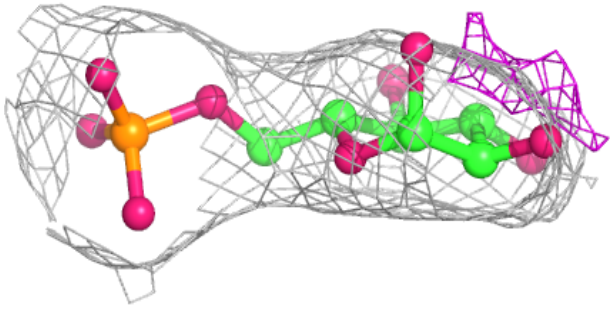


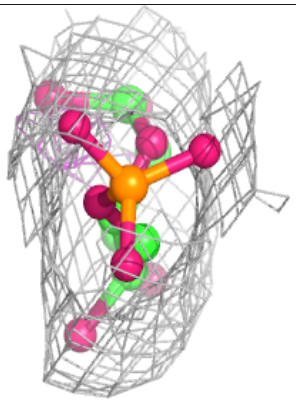


Electron density around G6P A 802:

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

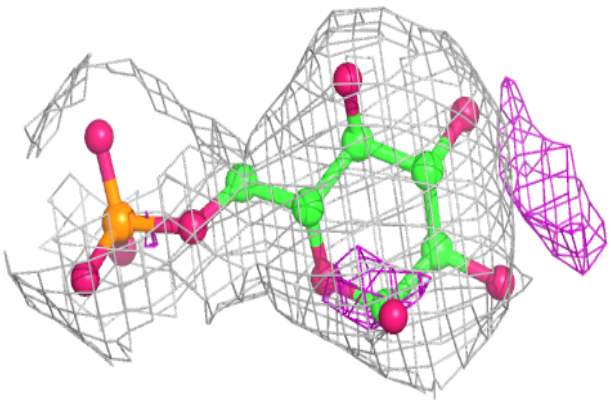


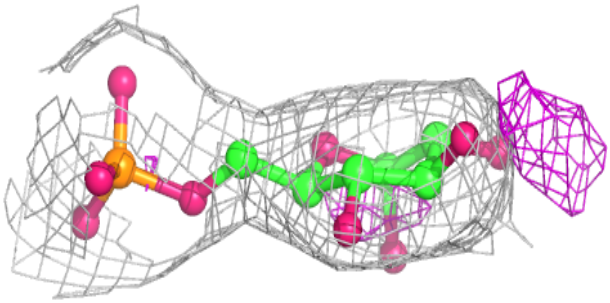


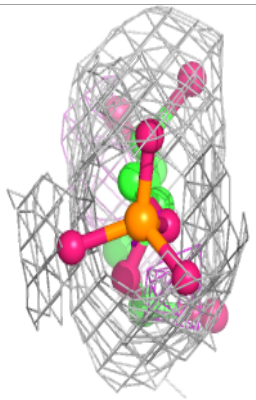


Electron density around G6P C 802:

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

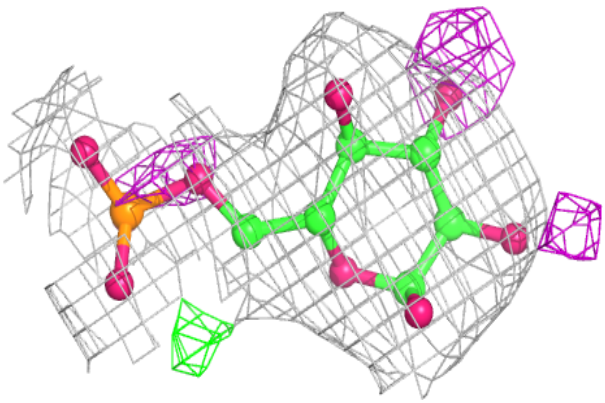


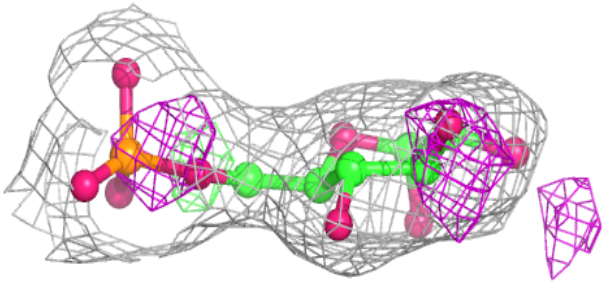


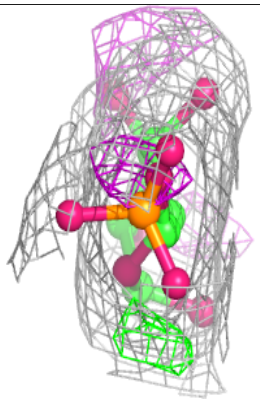


Electron density around G6P D 802:

$2mF_o$-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.