



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:39 PM BST

PDB ID : 5UX7
Title : Activated state yeast Glycogen Synthase in complex with UDP-xylose
Authors : Mahalingan, K.K.; Hurley, T.D.
Deposited on : 2017-02-22
Resolution : 2.69 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

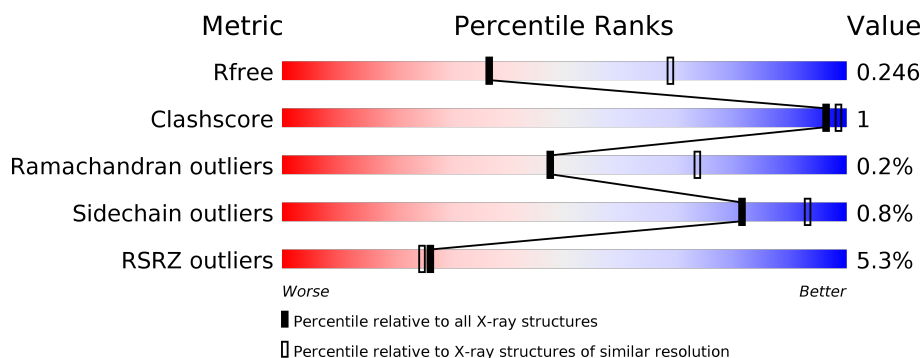
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	720	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>11%</div> </div> </div>
1	B	720	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> </div> </div>
1	C	720	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>11%</div> </div> </div>
1	D	720	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20648 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
			5111	3265	883	944	19			
1	B	638	Total	C	N	O	S	0	0	0
			5131	3278	892	942	19			
1	C	638	Total	C	N	O	S	0	0	0
			5129	3275	893	942	19			
1	D	636	Total	C	N	O	S	0	0	0
			5094	3251	885	939	19			

There are 84 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	535	SER	ALA	conflict	UNP P27472

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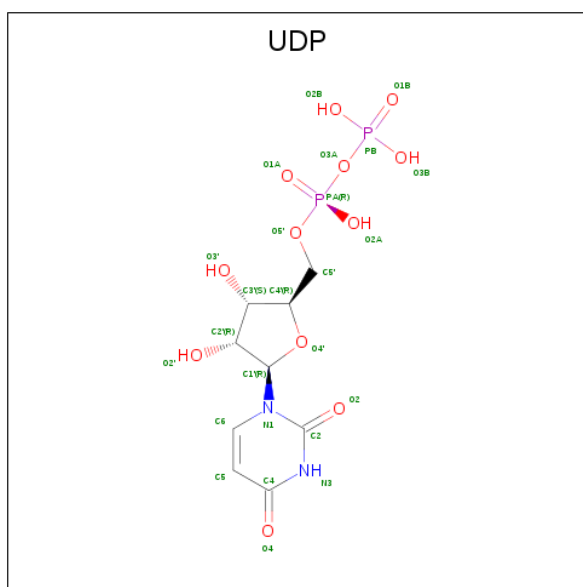
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression 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	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
C	0	HIS	-	expression tag	UNP P27472
C	535	SER	ALA	conflict	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
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	535	SER	ALA	conflict	UNP P27472

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$).



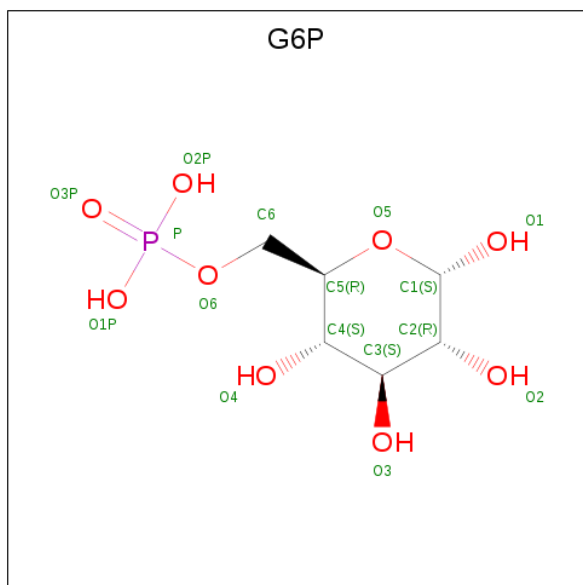
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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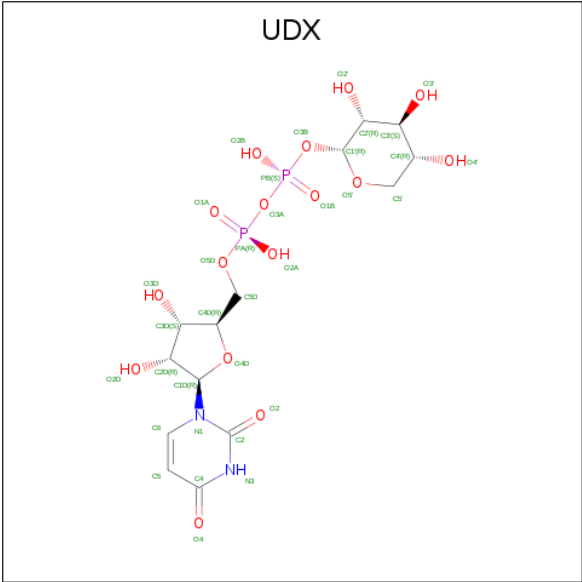
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- 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			

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-XYLOPYRANOSE (three-letter code: UDX) (formula: $C_{14}H_{22}N_2O_{16}P_2$).

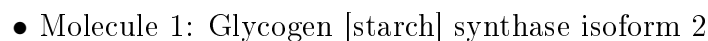


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
4	C	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

- Molecule 5 is water.

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

- Molecule 1: Glycogen [starch] synthase isoform 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.99Å 204.32Å 206.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.30 – 2.69 48.43 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.3 (145.30-2.69) 98.3 (48.43-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.207 , 0.246 0.209 , 0.246	Depositor DCC
R_{free} test set	5560 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20648	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: UDP, UDX, G6P

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	0.44	0/5236	0.65	2/7104 (0.0%)
1	B	0.46	0/5256	0.71	6/7125 (0.1%)
1	C	0.46	0/5254	0.68	2/7124 (0.0%)
1	D	0.45	0/5216	0.70	6/7074 (0.1%)
All	All	0.45	0/20962	0.69	16/28427 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	D	471	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	D	471	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	471	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	D	337	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	460	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	337	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	298	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	298	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	460	ARG	NE-CZ-NH1	5.39	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	460	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	460	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	428	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	298	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	392	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	450	ASP	CB-CG-OD2	5.16	122.95	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	18	ALA	Peptide
1	D	226	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5111	0	4971	13	0
1	B	5131	0	5022	8	0
1	C	5129	0	5011	10	0
1	D	5094	0	4967	12	0
2	A	25	0	11	0	0
2	D	25	0	11	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	1	0
4	B	34	0	20	1	0
4	C	34	0	20	0	0
5	C	1	0	0	0	0
All	All	20648	0	20077	41	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 1.

All (41) 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:280:HIS:CE1	1:D:283:GLN:HG2	2.20	0.77
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.29	0.66
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.35	0.60
1:B:213:LEU:HD21	1:B:254:GLU:HA	1.87	0.57
1:B:349:LYS:O	1:B:471:ARG:HD3	2.06	0.56
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.43	0.52
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.44	0.52
1:B:3:ARG:NH2	1:B:158:ASP:O	2.43	0.51
1:C:221:GLU:HA	1:C:224:ARG:HG2	1.91	0.51
1:C:396:HIS:HE1	1:C:407:THR:O	1.93	0.51
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.92	0.50
1:D:227:ILE:O	1:D:227:ILE:HG22	2.12	0.50
1:C:396:HIS:HD2	1:C:415:GLU:OE2	1.96	0.48
1:B:119:LYS:NZ	1:B:138:ASN:OD1	2.47	0.47
1:B:320:ARG:HH21	4:B:801:UDX:C1'	2.28	0.47
1:D:290:LYS:HE2	3:D:802:G6P:O3P	2.14	0.47
1:A:331:PHE:CZ	1:A:335:LEU:HD11	2.50	0.47
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.96	0.47
1:C:386:THR:HB	1:D:386:THR:HB	1.98	0.46
1:D:302:HIS:HD2	1:D:432:LEU:O	2.00	0.45
1:B:537:MET:CE	1:B:593:LEU:HD21	2.47	0.45
1:A:278:ALA:HB1	1:A:280:HIS:CE1	2.52	0.44
1:D:35:THR:HG21	1:D:43:TYR:CE1	2.53	0.44
1:A:213:LEU:HD21	1:A:254:GLU:HA	1.98	0.44
1:D:209:PHE:O	1:D:213:LEU:HB2	2.18	0.44
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.51	0.43
1:D:349:LYS:O	1:D:471:ARG:HD3	2.18	0.43
1:D:333:GLU:OE2	1:D:337:ARG:HD2	2.19	0.43
1:A:189:ILE:HD11	1:A:610:ARG:HA	2.00	0.43
1:D:213:LEU:HD23	1:D:253:PHE:CE2	2.54	0.42
1:A:213:LEU:HD23	1:A:253:PHE:CE2	2.55	0.42
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.54	0.42
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.01	0.41
1:C:163:ILE:HB	1:C:186:VAL:HG12	2.03	0.41
1:B:623:ARG:CZ	1:B:623:ARG:HB2	2.50	0.41
1:A:124:SER:O	1:A:125:LEU:HB2	2.21	0.41
1:A:492:TYR:O	1:A:496:VAL:HG23	2.21	0.41
1:A:199:ARG:HG2	1:A:508:TYR:CE2	2.55	0.41
1:D:377:ALA:HB1	1:D:428:ARG:HE	1.85	0.41
1:A:299:GLY:HA2	1:A:375:VAL:HG21	2.02	0.40
1:C:23:GLY:O	1:C:27:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/720 (88%)	605 (95%)	27 (4%)	4 (1%)	25	50
1	B	636/720 (88%)	614 (96%)	22 (4%)	0	100	100
1	C	636/720 (88%)	614 (96%)	22 (4%)	0	100	100
1	D	632/720 (88%)	616 (98%)	14 (2%)	2 (0%)	41	66
All	All	2540/2880 (88%)	2449 (96%)	85 (3%)	6 (0%)	47	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	LEU
1	A	126	VAL
1	D	204	SER
1	A	205	GLY
1	D	40	LYS
1	A	169	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	
1	A	544/621 (88%)	542 (100%)	2 (0%)	91	97
1	B	548/621 (88%)	542 (99%)	6 (1%)	73	90
1	C	547/621 (88%)	542 (99%)	5 (1%)	78	92
1	D	542/621 (87%)	537 (99%)	5 (1%)	78	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2181/2484 (88%)	2163 (99%)	18 (1%)	81	93

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	TYR
1	A	595	ASP
1	B	310	ASP
1	B	321	TYR
1	B	363	SER
1	B	428	ARG
1	B	471	ARG
1	B	595	ASP
1	C	250	ILE
1	C	310	ASP
1	C	321	TYR
1	C	363	SER
1	C	513	TYR
1	D	180	ARG
1	D	310	ASP
1	D	321	TYR
1	D	471	ARG
1	D	595	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	277	GLN
1	A	339	ASN
1	A	477	HIS
1	B	403	ASN
1	C	396	HIS
1	C	582	GLN
1	D	168	HIS
1	D	484	ASN
1	D	621	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	802	-	16,16,16	0.60	0	24,24,24	1.05	2 (8%)
3	G6P	A	802	-	16,16,16	0.58	0	24,24,24	0.77	0
3	G6P	B	802	-	16,16,16	0.55	0	24,24,24	0.91	1 (4%)
4	UDX	C	801	-	29,36,36	0.80	0	38,55,55	1.51	4 (10%)
2	UDP	A	801	-	20,26,26	1.12	2 (10%)	25,40,40	1.35	3 (12%)
2	UDP	D	801	-	20,26,26	0.82	0	25,40,40	1.15	2 (8%)
3	G6P	C	802	-	16,16,16	0.51	0	24,24,24	0.85	0
4	UDX	B	801	-	29,36,36	0.72	0	38,55,55	1.29	4 (10%)

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	D	802	-	-	1/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G6P	A	802	-	-	0/6/26/26	0/1/1/1
3	G6P	B	802	-	-	1/6/26/26	0/1/1/1
4	UDX	C	801	-	-	6/19/54/54	0/3/3/3
2	UDP	A	801	-	-	7/14/32/32	0/2/2/2
2	UDP	D	801	-	-	3/14/32/32	0/2/2/2
3	G6P	C	802	-	-	1/6/26/26	0/1/1/1
4	UDX	B	801	-	-	6/19/54/54	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	UDP	PB-O1B	3.46	1.61	1.50
2	A	801	UDP	O4'-C1'	2.14	1.44	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	801	UDX	C5'-C4'-C3'	5.15	116.00	109.67
4	C	801	UDX	O5'-C1'-C2'	-3.68	104.39	110.04
4	B	801	UDX	C3D-C2D-C1D	3.53	106.29	100.98
2	A	801	UDP	PA-O3A-PB	-3.36	121.29	132.83
2	A	801	UDP	O3B-PB-O2B	3.26	120.08	107.64
4	C	801	UDX	PA-O3A-PB	-3.14	122.06	132.83
4	C	801	UDX	O5'-C5'-C4'	3.01	115.41	110.77
2	D	801	UDP	PA-O3A-PB	-2.91	122.85	132.83
4	B	801	UDX	PA-O3A-PB	-2.76	123.35	132.83
3	D	802	G6P	O2P-P-O1P	2.73	118.08	107.64
3	D	802	G6P	O6-P-O3P	-2.35	99.88	106.47
4	B	801	UDX	O5'-C1'-C2'	-2.27	106.56	110.04
4	B	801	UDX	O3B-C1'-C2'	2.26	112.53	108.38
3	B	802	G6P	O2P-P-O6	-2.26	100.73	106.73
2	A	801	UDP	C3'-C2'-C1'	2.16	104.24	100.98
2	D	801	UDP	O2B-PB-O1B	2.10	118.92	110.68

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	802	G6P	C6-O6-P-O3P
4	C	801	UDX	C1'-O3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
2	A	801	UDP	C5'-O5'-PA-O2A
2	A	801	UDP	C5'-O5'-PA-O3A
2	D	801	UDP	C2'-C1'-N1-C6
2	D	801	UDP	O4'-C1'-N1-C6
3	C	802	G6P	C4-C5-C6-O6
4	B	801	UDX	C5D-O5D-PA-O3A
4	B	801	UDX	C5D-O5D-PA-O1A
4	C	801	UDX	C2'-C1'-O3B-PB
2	A	801	UDP	C3'-C4'-C5'-O5'
4	B	801	UDX	C4D-C5D-O5D-PA
4	B	801	UDX	C1'-O3B-PB-O3A
4	C	801	UDX	C5D-O5D-PA-O3A
4	C	801	UDX	C1'-O3B-PB-O1B
2	A	801	UDP	PB-O3A-PA-O1A
2	A	801	UDP	C5'-O5'-PA-O1A
4	B	801	UDX	C5D-O5D-PA-O2A
4	C	801	UDX	PA-O3A-PB-O1B
4	C	801	UDX	PA-O3A-PB-O2B
2	A	801	UDP	PB-O3A-PA-O2A
2	A	801	UDP	O4'-C4'-C5'-O5'
4	B	801	UDX	PB-O3A-PA-O2A
3	B	802	G6P	C6-O6-P-O1P
2	D	801	UDP	PA-O3A-PB-O3B

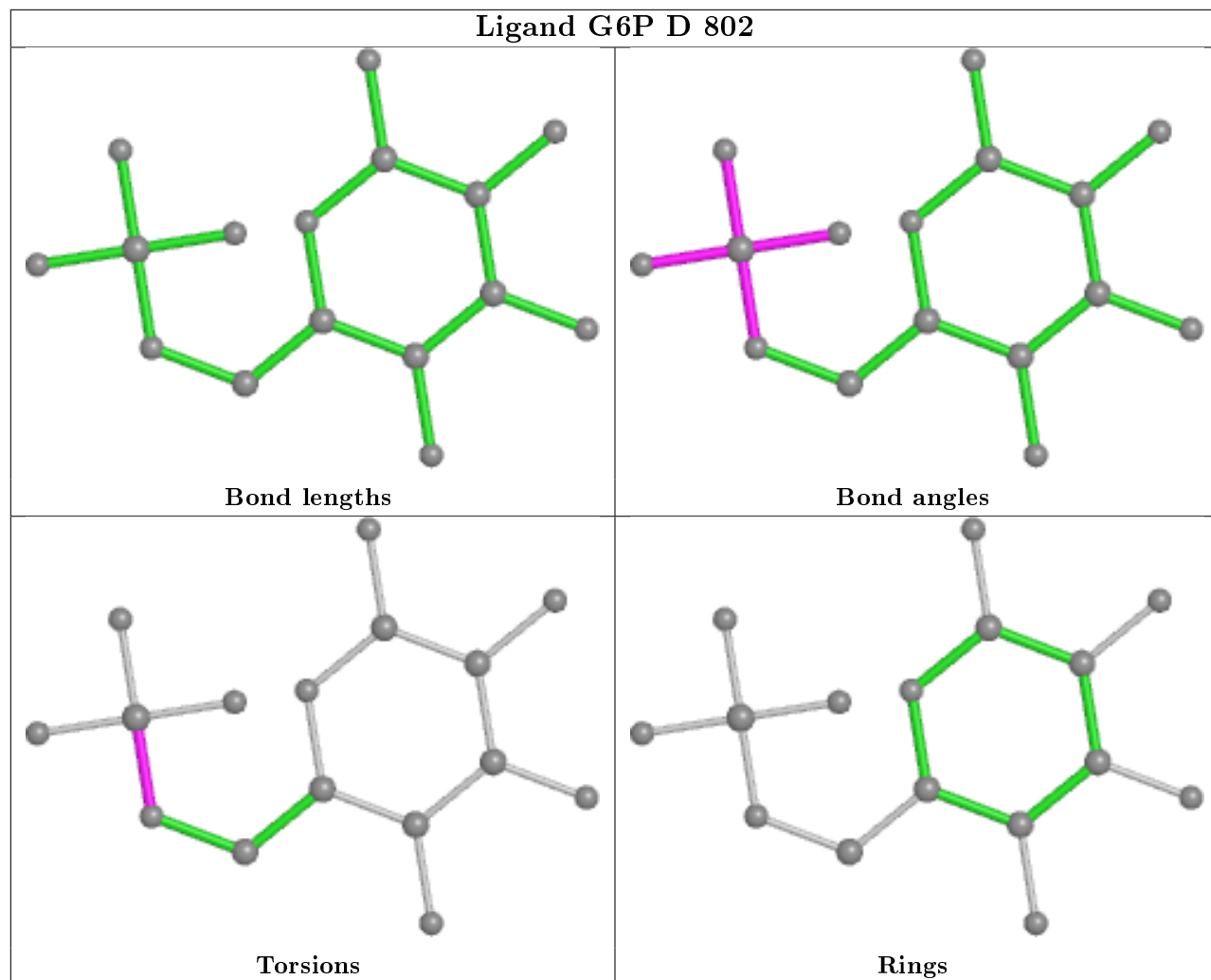
There are no ring outliers.

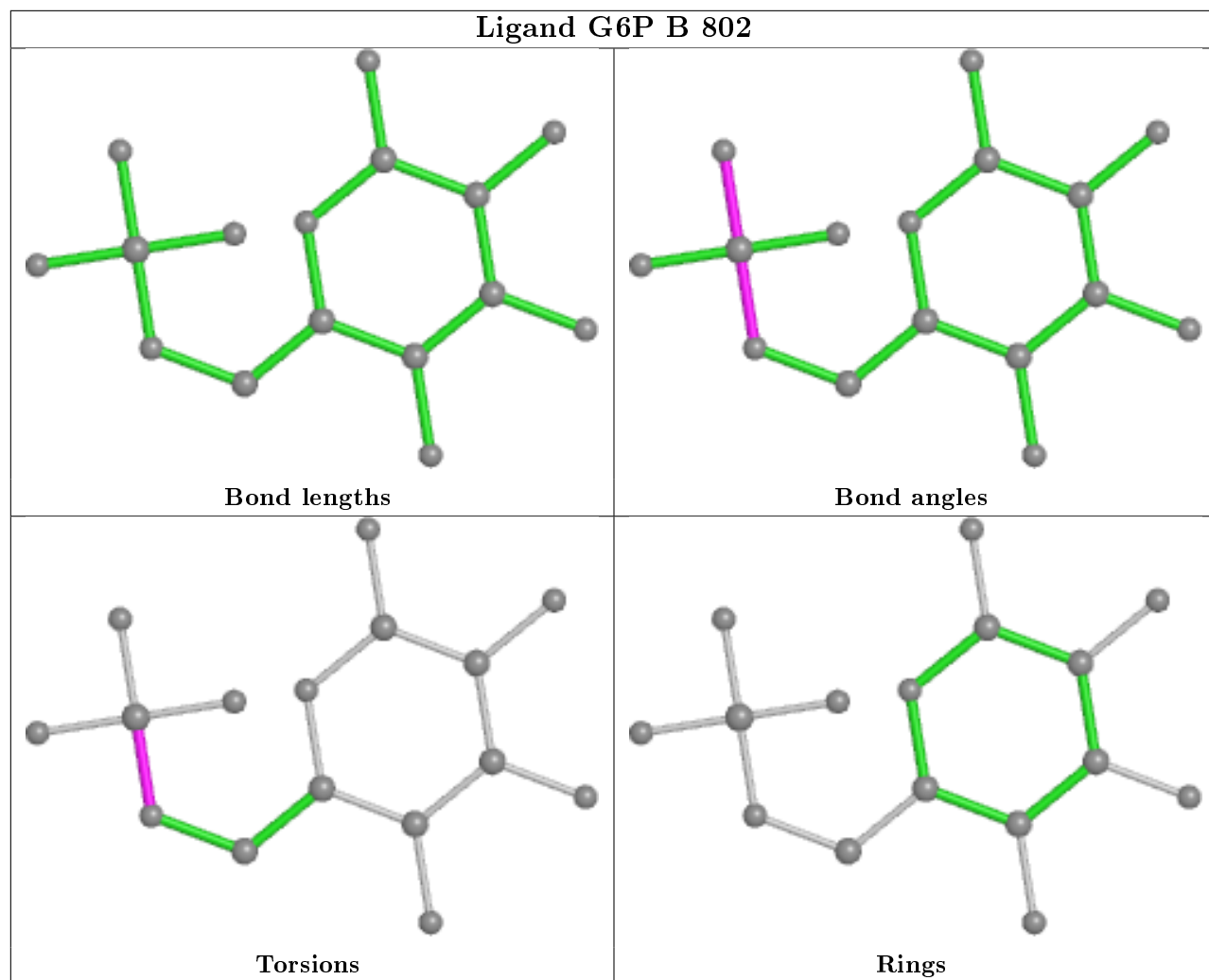
2 monomers are involved in 2 short contacts:

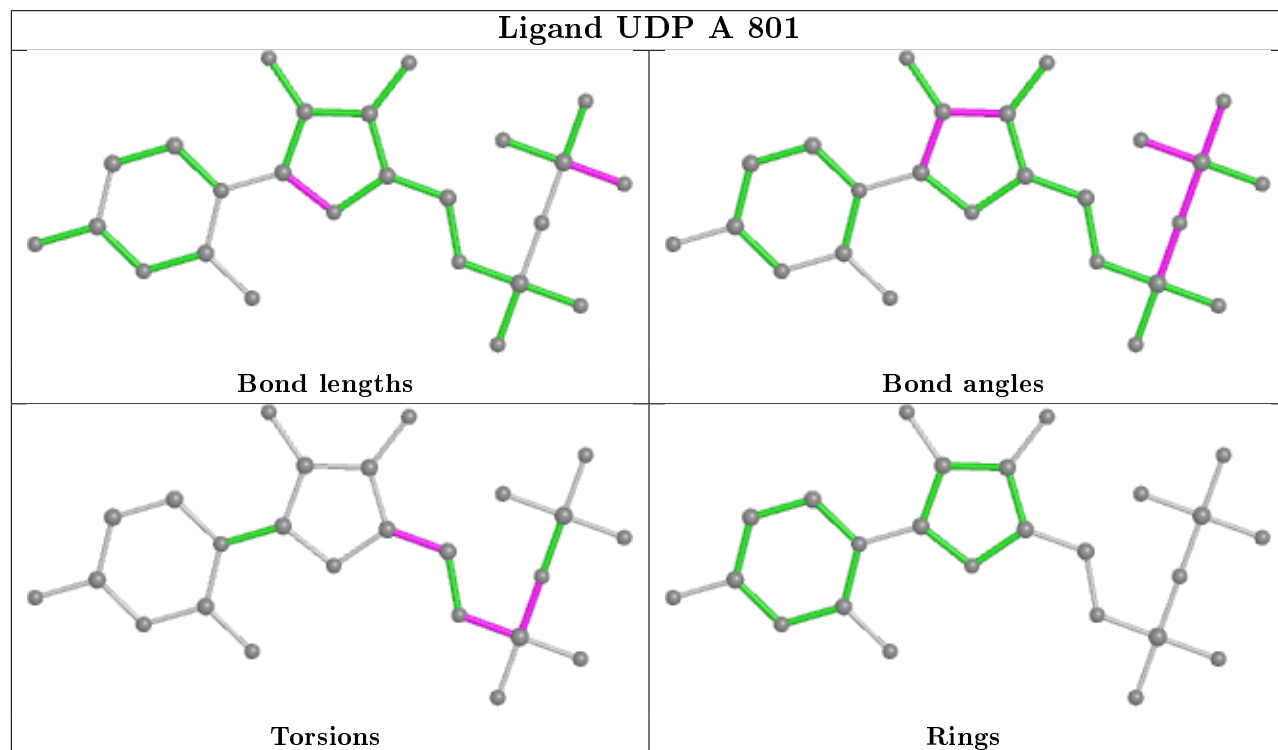
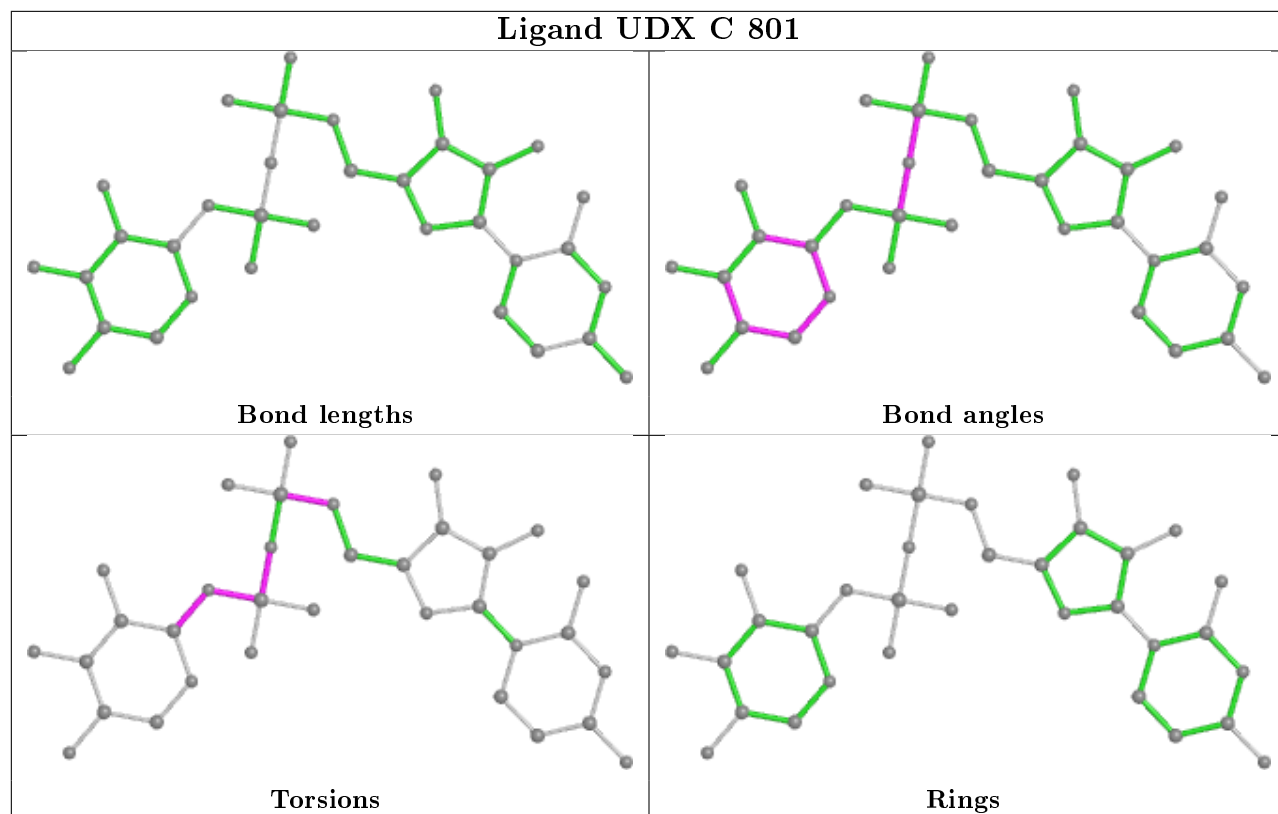
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	802	G6P	1	0
4	B	801	UDX	1	0

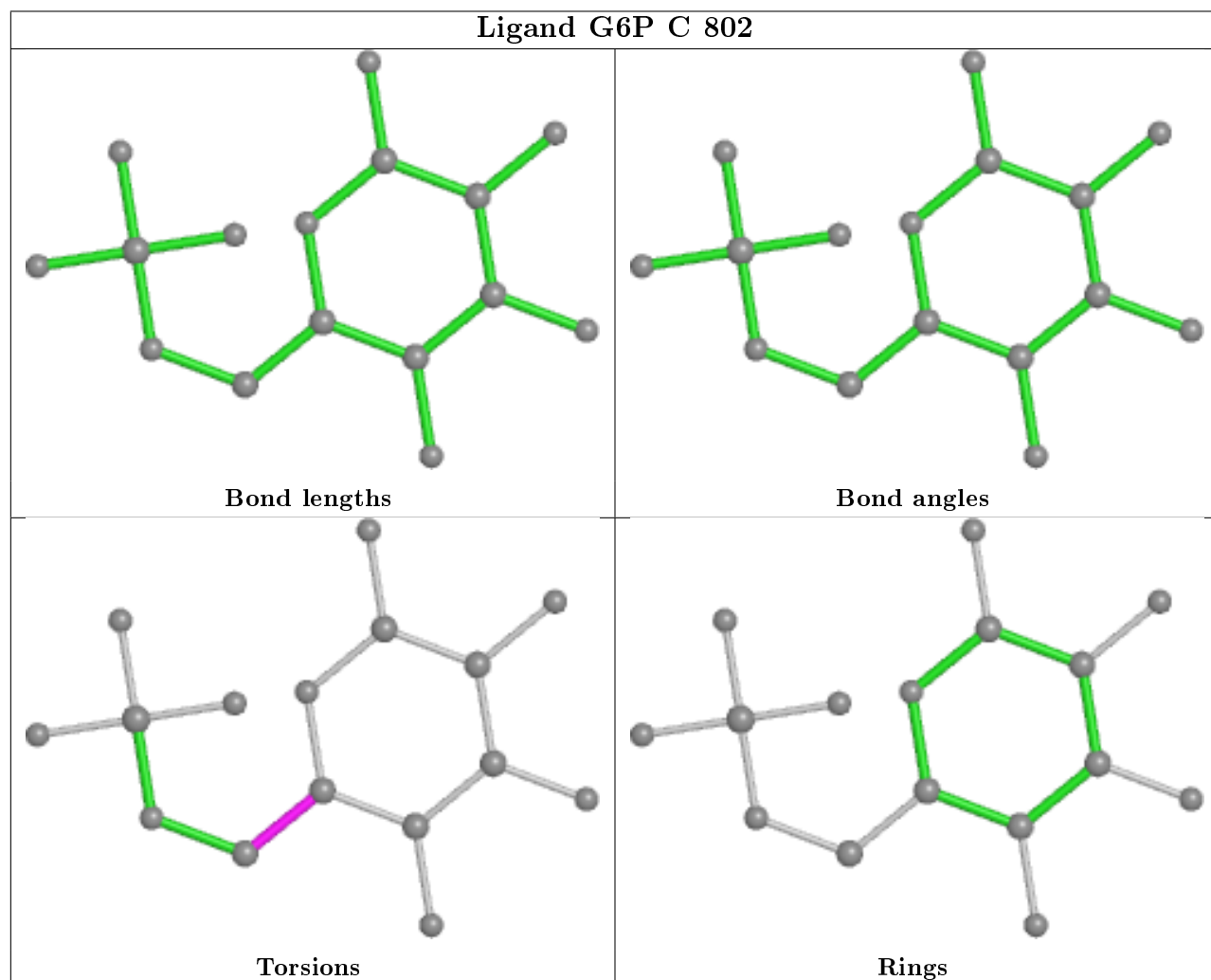
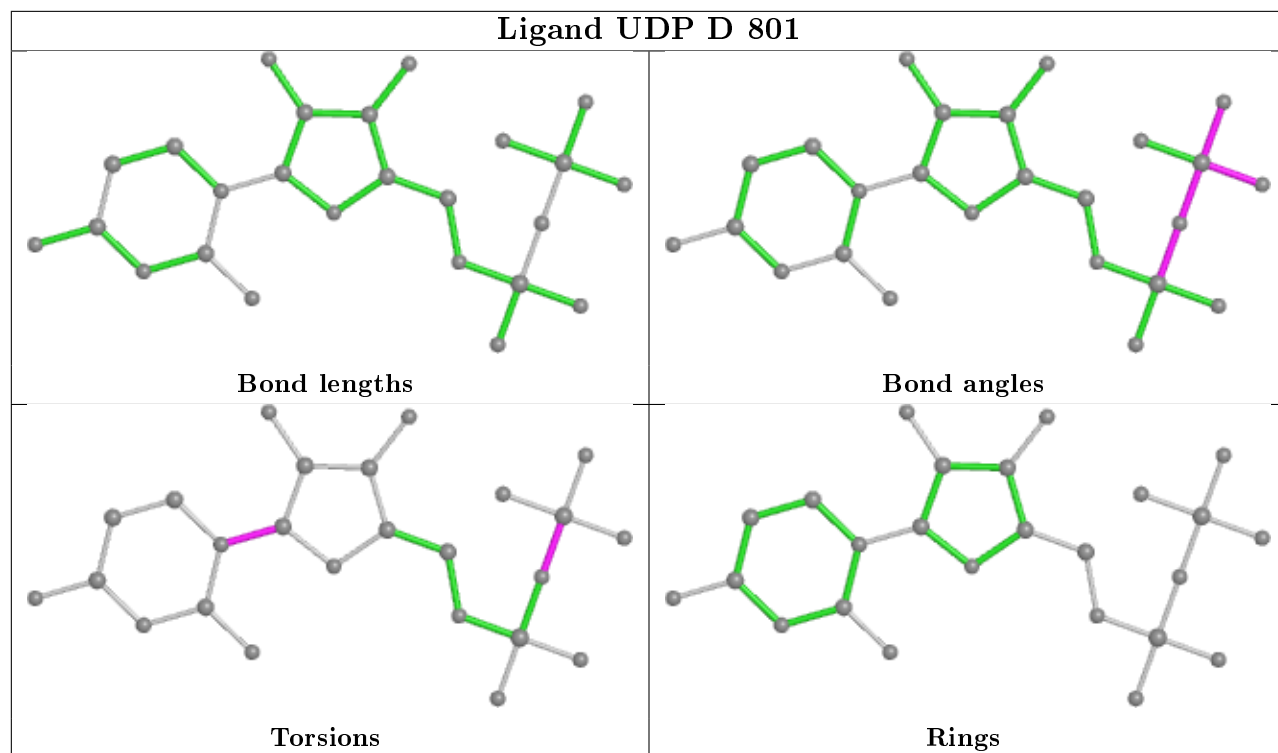
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

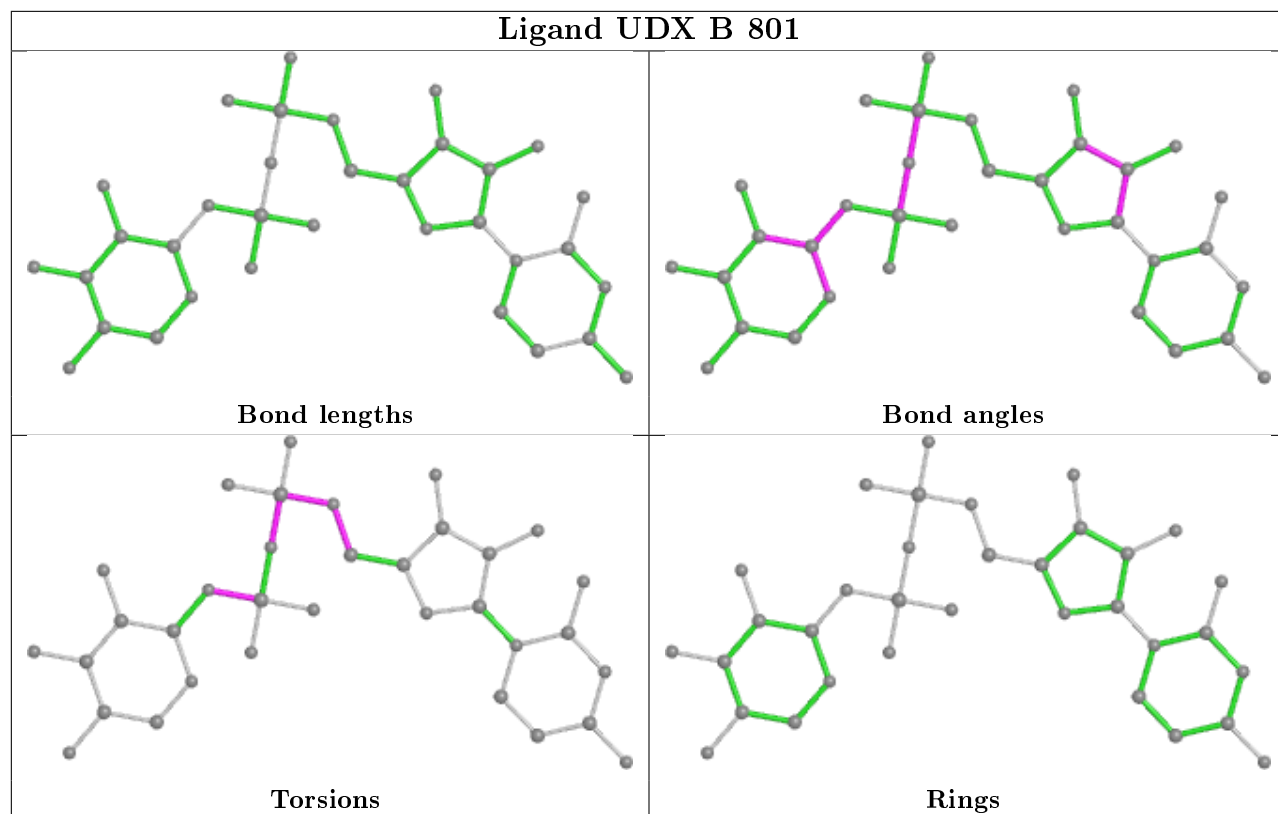
equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	638/720 (88%)	0.21	35 (5%) 25 24	41, 73, 140, 168	0
1	B	638/720 (88%)	0.05	14 (2%) 62 63	30, 61, 142, 185	2 (0%)
1	C	638/720 (88%)	0.17	31 (4%) 29 28	39, 70, 130, 178	0
1	D	636/720 (88%)	0.35	54 (8%) 10 9	34, 77, 178, 203	0
All	All	2550/2880 (88%)	0.19	134 (5%) 26 25	30, 70, 151, 203	2 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	8.5
1	B	624	GLU	7.2
1	D	128	ILE	6.6
1	D	630	LEU	6.6
1	D	627	GLY	6.5
1	D	639	ALA	6.3
1	D	622	PHE	6.2
1	D	626	VAL	5.7
1	A	61	LEU	5.4
1	C	128	ILE	5.2
1	C	91	VAL	4.9
1	A	543	THR	4.8
1	D	629	GLU	4.8
1	A	92	TYR	4.3
1	D	64	LYS	4.3
1	D	124	SER	4.2
1	D	127	GLY	4.1
1	A	63	TRP	4.1
1	C	125	LEU	4.0
1	D	61	LEU	3.9
1	C	124	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	78	HIS	3.8
1	A	69	PHE	3.8
1	D	129	PRO	3.7
1	D	125	LEU	3.6
1	D	227	ILE	3.6
1	D	637	ALA	3.6
1	C	149	TRP	3.5
1	A	90	PHE	3.5
1	C	83	MET	3.5
1	A	68	ALA	3.5
1	A	91	VAL	3.5
1	A	52	ALA	3.4
1	B	543	THR	3.4
1	D	624	GLU	3.4
1	A	96	LEU	3.4
1	D	625	LEU	3.4
1	D	225	PHE	3.3
1	C	206	SER	3.3
1	D	628	GLU	3.3
1	C	229	HIS	3.3
1	D	11	PHE	3.2
1	D	90	PHE	3.2
1	B	71	ASP	3.2
1	B	630	LEU	3.2
1	B	86	ARG	3.2
1	D	93	GLY	3.1
1	D	623	ARG	3.1
1	D	197	LEU	3.0
1	A	60	ILE	3.0
1	C	48	PRO	3.0
1	D	633	SER	3.0
1	D	614	LEU	3.0
1	B	90	PHE	3.0
1	C	138	ASN	2.9
1	A	157	LEU	2.9
1	A	199	ARG	2.9
1	B	61	LEU	2.9
1	A	79	ALA	2.9
1	C	126	VAL	2.9
1	D	67	GLU	2.8
1	C	135	PHE	2.8
1	A	59	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	62	ASP	2.8
1	C	544	ASN	2.8
1	D	132	GLU	2.8
1	A	49	LEU	2.8
1	C	129	PRO	2.8
1	B	67	GLU	2.7
1	D	615	ARG	2.7
1	B	85	SER	2.7
1	C	106	PHE	2.7
1	C	142	LEU	2.7
1	D	620	ASP	2.6
1	D	617	GLY	2.6
1	A	76	VAL	2.6
1	C	132	GLU	2.6
1	A	77	GLN	2.6
1	B	623	ARG	2.6
1	D	204	SER	2.6
1	D	133	ASN	2.6
1	C	228	TYR	2.5
1	D	122	LEU	2.5
1	D	638	LEU	2.5
1	D	59	ASP	2.5
1	C	113	GLY	2.5
1	D	113	GLY	2.5
1	D	76	VAL	2.5
1	A	85	SER	2.5
1	A	64	LYS	2.4
1	A	88	VAL	2.4
1	D	149	TRP	2.4
1	D	618	TYR	2.4
1	A	544	ASN	2.4
1	D	45	LEU	2.4
1	C	543	THR	2.4
1	B	88	VAL	2.4
1	D	596	LEU	2.3
1	A	67	GLU	2.3
1	D	150	PHE	2.3
1	C	63	TRP	2.3
1	D	631	ASN	2.3
1	D	274	ILE	2.3
1	A	214	GLU	2.3
1	D	549	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	106	PHE	2.3
1	C	87	GLY	2.3
1	D	228	TYR	2.3
1	D	601	ARG	2.3
1	C	92	TYR	2.2
1	A	104	ILE	2.2
1	C	88	VAL	2.2
1	A	93	GLY	2.2
1	C	146	THR	2.2
1	D	632	ASP	2.2
1	C	131	PRO	2.2
1	A	206	SER	2.2
1	D	231	TYR	2.1
1	B	637	ALA	2.1
1	C	123	TRP	2.1
1	A	126	VAL	2.1
1	C	549	TYR	2.1
1	D	619	PRO	2.1
1	C	18	ALA	2.1
1	A	106	PHE	2.1
1	B	87	GLY	2.1
1	A	66	PRO	2.1
1	C	108	LEU	2.1
1	A	153	GLU	2.1
1	D	147	VAL	2.0
1	A	376	ARG	2.0
1	C	154	VAL	2.0
1	A	135	PHE	2.0
1	D	156	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

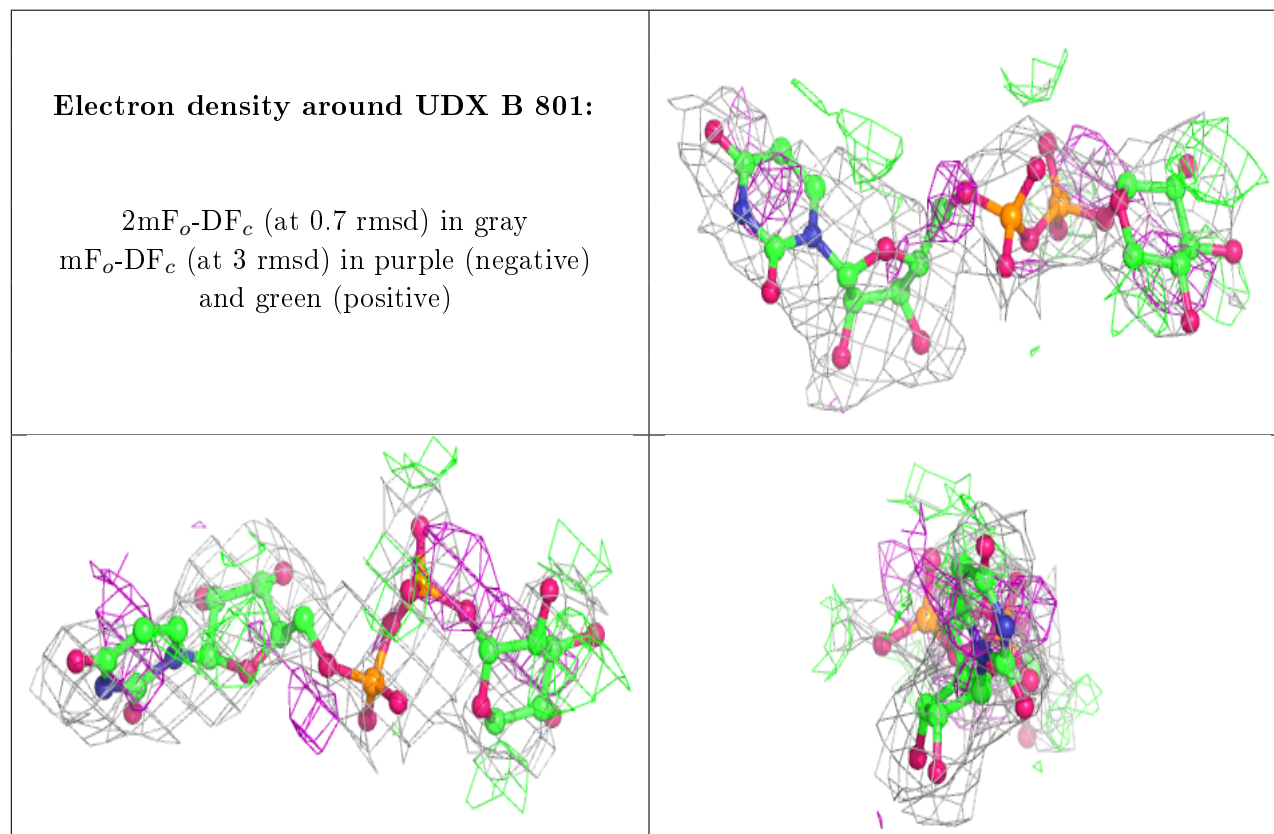
There are no monosaccharides in this entry.

6.4 Ligands [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, 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.

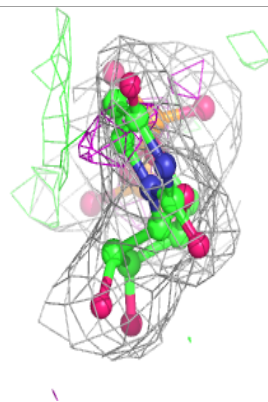
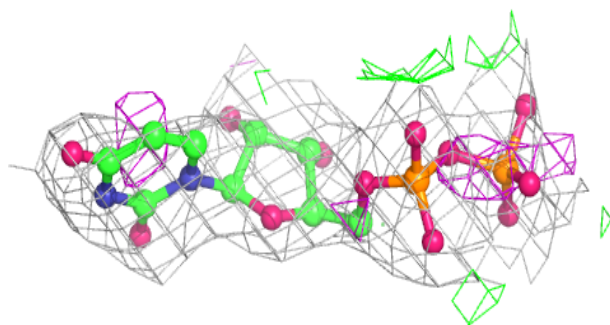
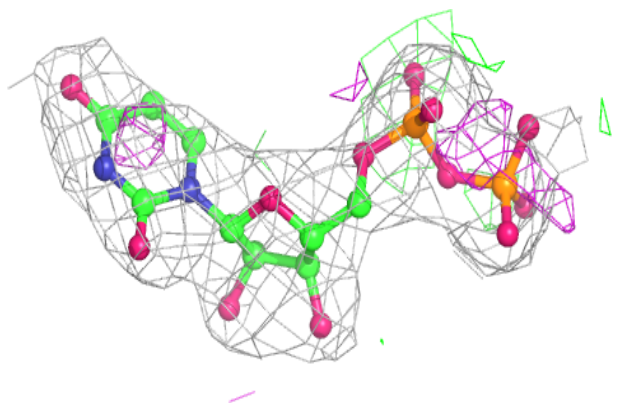
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	UDX	B	801	34/34	0.74	0.29	59,99,116,119	0
2	UDP	D	801	25/25	0.87	0.17	52,69,115,121	0
4	UDX	C	801	34/34	0.89	0.19	54,71,82,84	0
2	UDP	A	801	25/25	0.89	0.18	56,63,88,95	0
3	G6P	A	802	16/16	0.98	0.13	36,40,41,41	0
3	G6P	B	802	16/16	0.98	0.13	22,23,26,27	0
3	G6P	C	802	16/16	0.98	0.12	33,36,37,38	0
3	G6P	D	802	16/16	0.98	0.11	23,25,31,32	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.

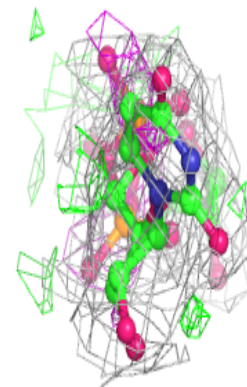
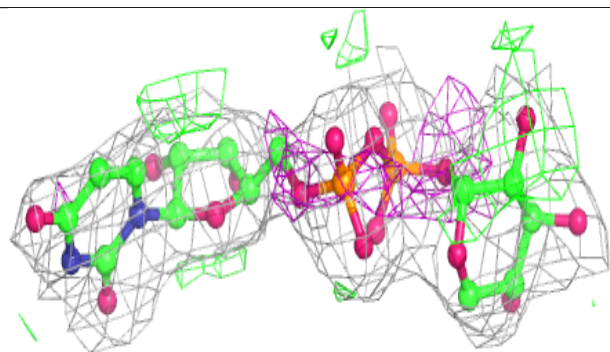
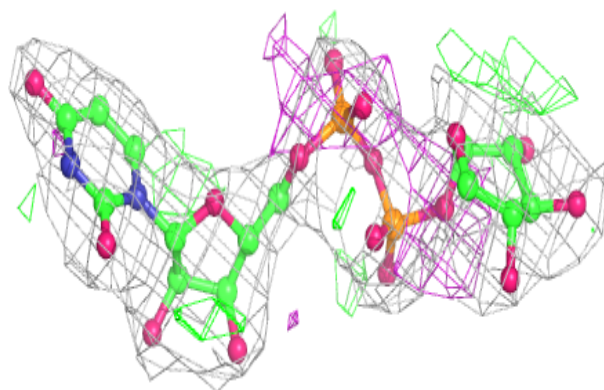


Electron density around UDP D 801:

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

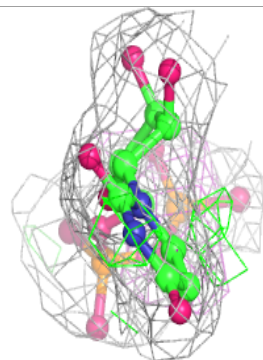
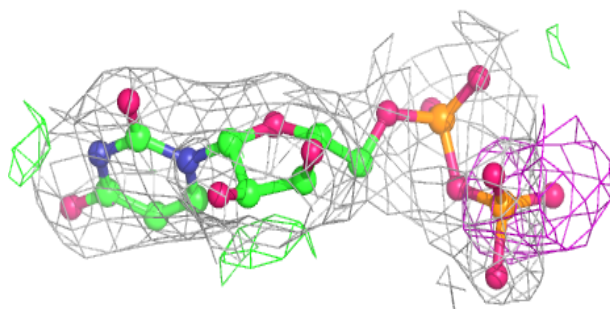
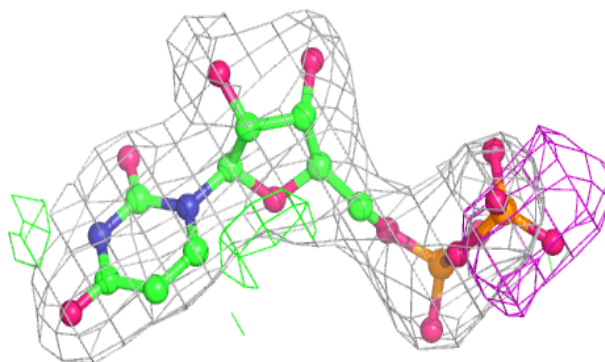
**Electron density around UDX C 801:**

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

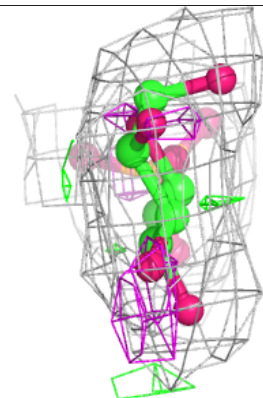
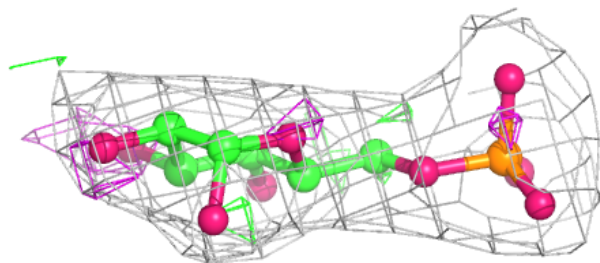
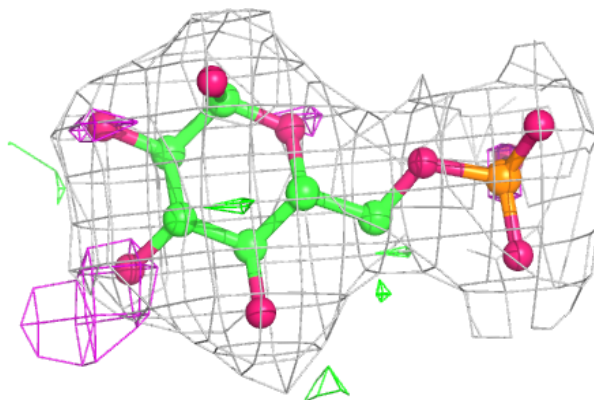


Electron density around UDP A 801:

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

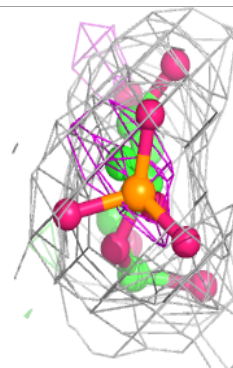
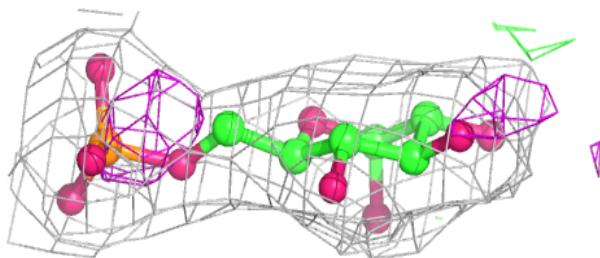
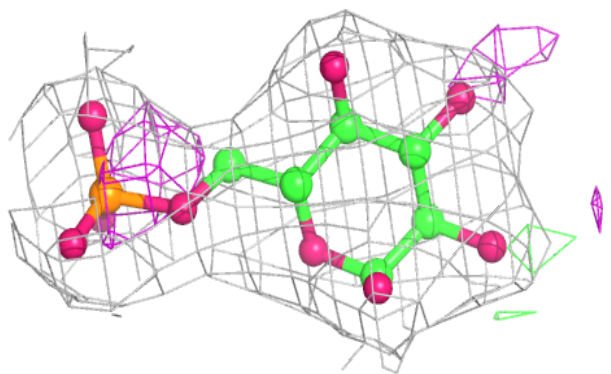
**Electron density around G6P B 802:**

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

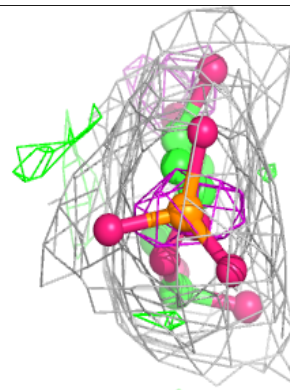
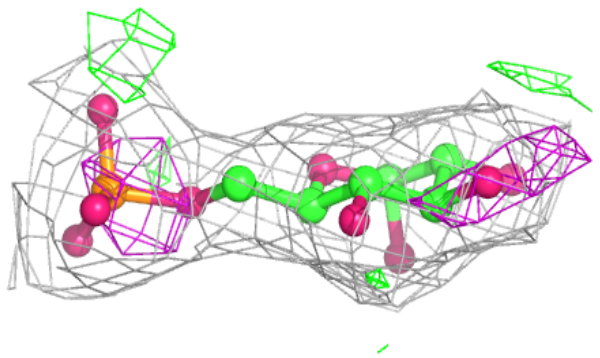
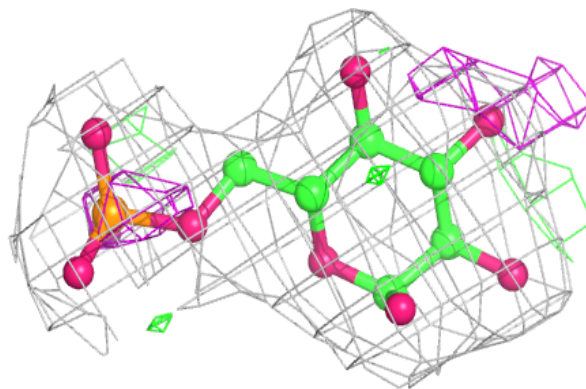


Electron density around G6P C 802:

$2mF_o-DF_c$ (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.