



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2022 – 06:07 PM EDT

PDB ID : 5VNC
Title : Glycogen synthase in complex with UDP and glucosamine
Authors : Mahalingan, K.K.; Hurley, T.D.
Deposited on : 2017-04-30
Resolution : 2.98 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 : 2.27
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) : 2.27

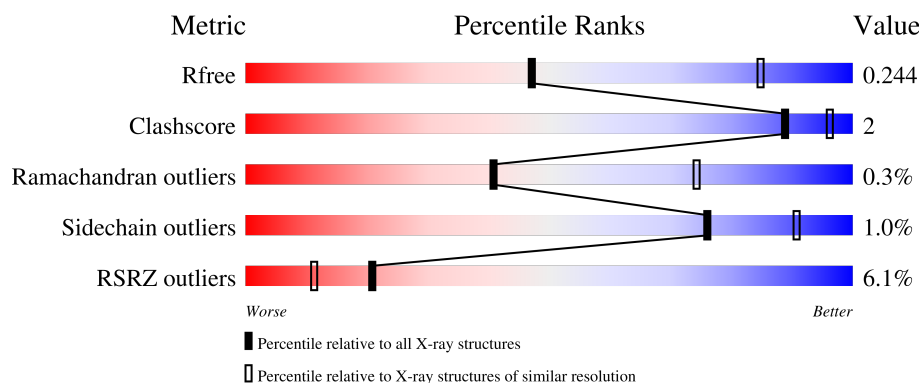
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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

Mol	Chain	Length	Quality of chain
1	A	720	<div> <div>6%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
1	B	720	<div> <div>4%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>
1	C	720	<div> <div>5%</div> <div>82%</div> <div>6%</div> <div>11%</div> </div>
1	D	720	<div> <div>7%</div> <div>83%</div> <div>6%</div> <div>12%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20386 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
			4980	3185	853	924	18			
1	B	636	Total	C	N	O	S	0	0	0
			5097	3256	889	933	19			
1	C	638	Total	C	N	O	S	0	0	0
			5127	3272	894	942	19			
1	D	636	Total	C	N	O	S	0	0	0
			5005	3195	865	927	18			

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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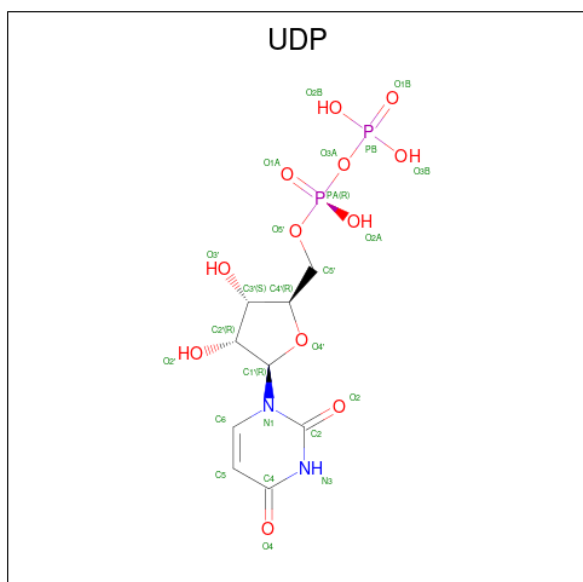
Chain	Residue	Modelled	Actual	Comment	Reference
A	535	SER	ALA	engineered mutation	UNP P27472
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	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	engineered mutation	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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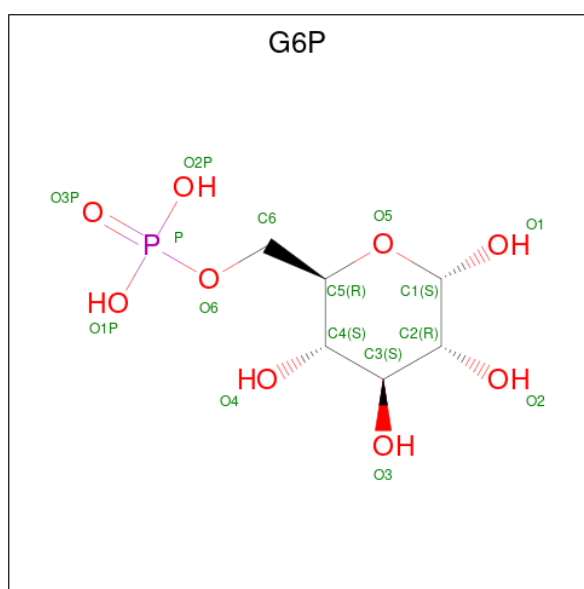
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P27472
C	169	GLN	GLU	engineered mutation	UNP P27472
C	535	SER	ALA	engineered mutation	UNP P27472
D	-19	MET	-	initiating methionine	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	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	engineered mutation	UNP P27472

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



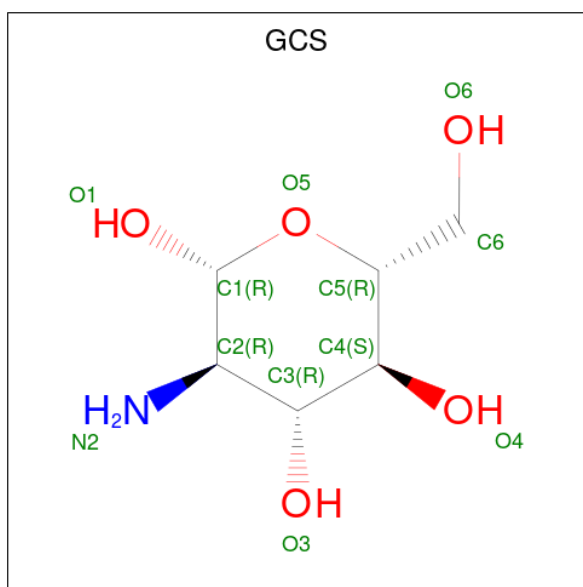
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- 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 2-amino-2-deoxy-beta-D-glucopyranose (three-letter code: GCS) (formula: $C_6H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			12	6	1	5		

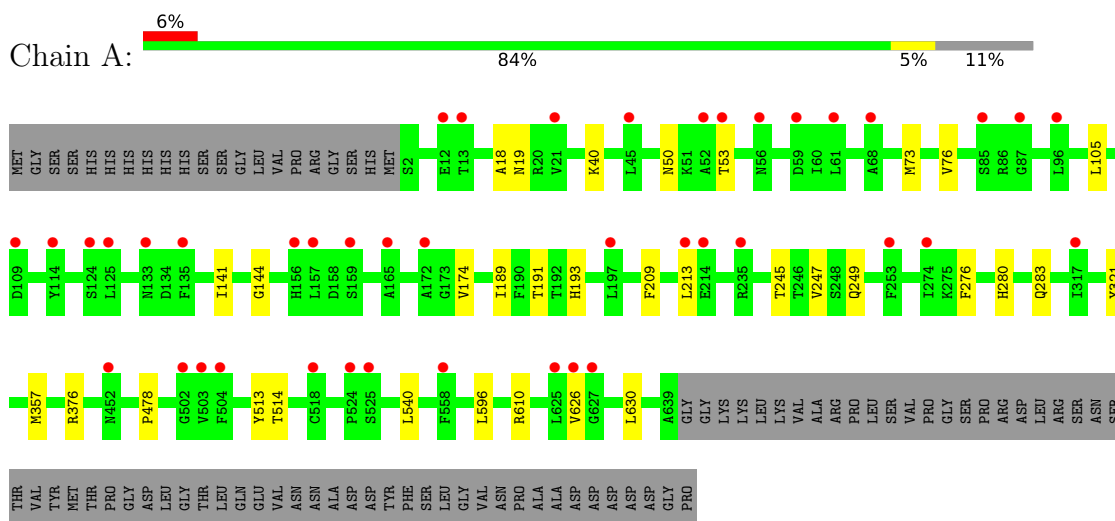
- Molecule 5 is water.

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

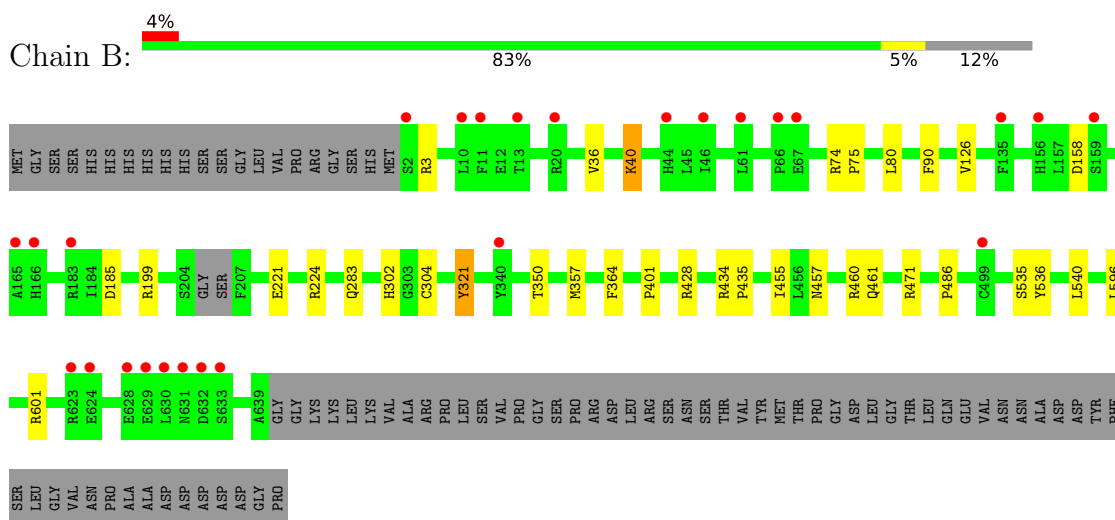
3 Residue-property plots [i](#)

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.

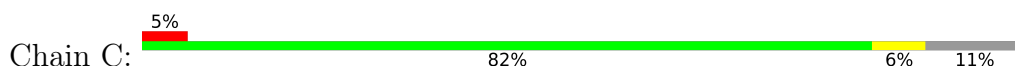
- Molecule 1: Glycogen [starch] synthase isoform 2

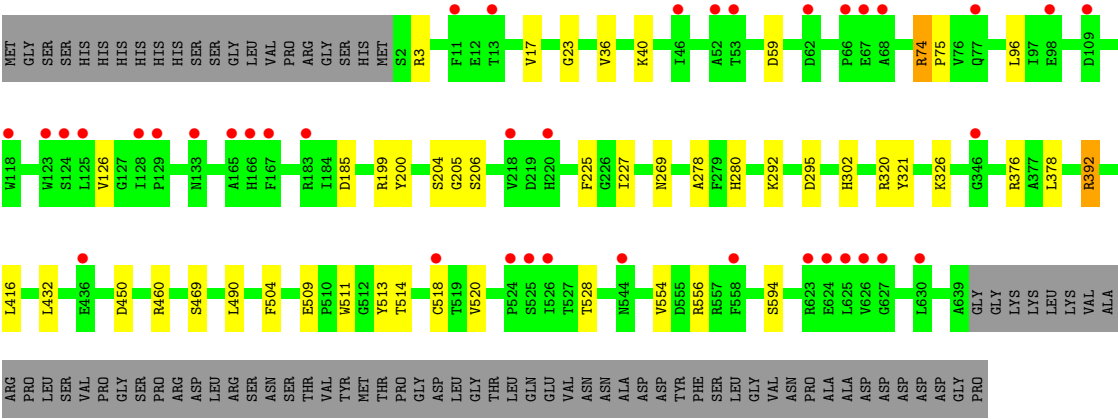


- Molecule 1: Glycogen [starch] synthase isoform 2

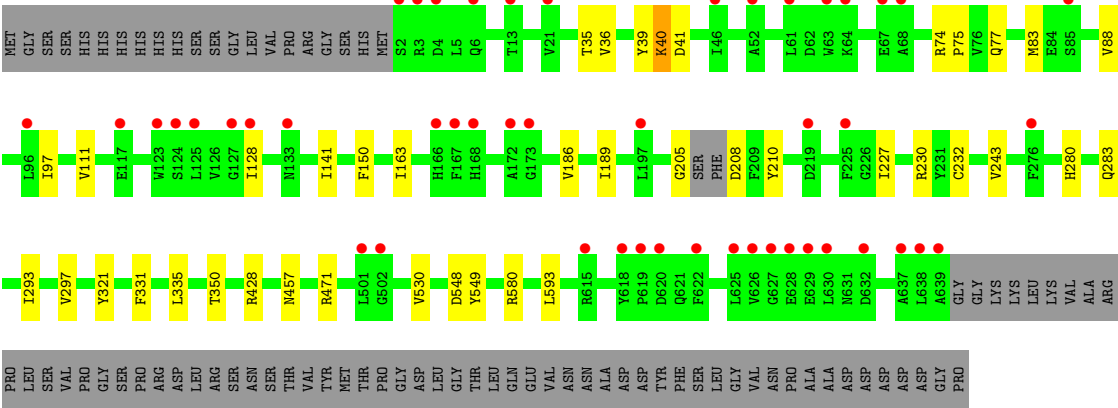
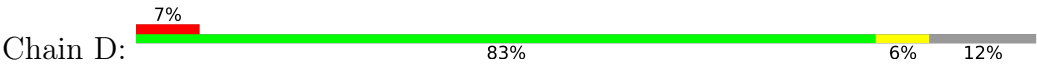


- Molecule 1: Glycogen [starch] synthase isoform 2





● 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	193.04Å 204.70Å 205.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.98 29.95 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.98) 99.7 (29.95-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.196 , 0.244 0.197 , 0.244	Depositor DCC
R_{free} test set	4474 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20386	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G6P, UDP, GCS

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	0.46	0/5101	0.67	1/6943 (0.0%)
1	B	0.51	0/5220	0.75	1/7079 (0.0%)
1	C	0.50	0/5251	0.72	4/7119 (0.1%)
1	D	0.48	0/5124	0.71	0/6964
All	All	0.49	0/20696	0.71	6/28105 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	320	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	199	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	428	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	376	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	392	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4980	0	4753	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5097	0	4972	20	0
1	C	5127	0	5015	22	0
1	D	5005	0	4823	20	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
2	C	25	0	11	1	0
2	D	25	0	11	0	0
3	A	16	0	11	1	0
3	B	16	0	11	1	0
3	C	16	0	11	0	0
3	D	16	0	11	1	0
4	C	12	0	13	0	0
5	B	1	0	0	0	0
All	All	20386	0	19664	76	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 (76) 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:D:580:ARG:NH1	3:D:802:G6P:O1P	2.26	0.67
1:C:204:SER:O	1:C:206:SER:N	2.28	0.66
1:B:283:GLN:HG2	1:C:280:HIS:CE1	2.32	0.65
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.31	0.64
1:B:357:MET:HE3	1:B:455:ILE:HD11	1.80	0.63
1:C:200:TYR:CE2	1:C:227:ILE:HD11	2.36	0.60
1:B:357:MET:CE	1:B:455:ILE:HD11	2.31	0.59
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.38	0.59
1:C:200:TYR:CZ	1:C:227:ILE:HD11	2.42	0.55
1:B:221:GLU:OE2	1:B:224:ARG:NH1	2.41	0.54
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.40	0.54
1:C:520:VAL:HA	1:C:594:SER:HB3	1.89	0.53
1:C:295:ASP:OD2	1:C:376:ARG:NH2	2.42	0.53
1:C:292:LYS:HD3	1:C:490:LEU:HD21	1.90	0.53
1:D:39:TYR:O	1:D:41:ASP:N	2.42	0.53
1:B:536:TYR:OH	1:B:601:ARG:NH2	2.43	0.52
1:D:227:ILE:CG2	1:D:230:ARG:CB	2.88	0.52
1:C:378:LEU:HD22	1:C:432:LEU:HD11	1.92	0.52
1:D:128:ILE:HD12	1:D:232:CYS:HB3	1.92	0.51
1:C:225:PHE:HB3	1:C:227:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ALA:HB1	1:C:280:HIS:CE1	2.47	0.49
1:A:141:ILE:HA	1:A:174:VAL:HG21	1.94	0.49
1:D:74:ARG:NH1	1:D:77:GLN:OE1	2.44	0.49
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.47	0.49
1:C:23:GLY:N	2:C:802:UDP:O3B	2.41	0.49
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.95	0.48
1:A:19:ASN:N	1:A:19:ASN:OD1	2.47	0.47
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.49	0.47
1:D:293:ILE:O	1:D:297:VAL:HG23	2.15	0.46
1:B:80:LEU:HD22	1:B:90:PHE:CE2	2.50	0.46
1:B:3:ARG:NH2	1:B:158:ASP:O	2.49	0.45
1:B:457:ASN:OD1	1:B:460:ARG:NH1	2.49	0.45
1:C:74:ARG:N	1:C:75:PRO:CD	2.79	0.45
1:B:540:LEU:HD21	1:B:601:ARG:NH2	2.31	0.45
1:B:283:GLN:HG3	3:B:802:G6P:O1	2.16	0.45
1:D:88:VAL:HG23	1:D:111:VAL:HG23	1.99	0.45
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.50	0.44
1:B:126:VAL:HG12	1:B:126:VAL:O	2.17	0.44
1:D:74:ARG:N	1:D:75:PRO:CD	2.79	0.44
1:A:73:MET:O	1:A:76:VAL:HG12	2.17	0.44
1:A:50:ASN:ND2	1:A:53:THR:OG1	2.50	0.44
1:C:528:THR:HG22	1:C:554:VAL:HG12	1.99	0.44
1:D:549:TYR:HB3	1:D:593:LEU:HD22	2.00	0.44
1:D:205:GLY:O	1:D:208:ASP:N	2.51	0.43
1:A:193:HIS:ND1	1:A:247:VAL:HG11	2.33	0.43
1:B:350:THR:OG1	1:B:471:ARG:NH1	2.52	0.43
1:B:36:VAL:O	1:B:40:LYS:N	2.51	0.43
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.99	0.43
1:B:74:ARG:N	1:B:75:PRO:CD	2.82	0.43
1:D:83:MET:HE1	1:D:150:PHE:HA	2.00	0.42
1:A:357:MET:O	1:A:478:PRO:HA	2.19	0.42
1:A:283:GLN:HG3	3:A:802:G6P:O1	2.19	0.42
1:C:326:LYS:NZ	1:C:509:GLU:OE1	2.53	0.42
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.53	0.42
1:A:209:PHE:O	1:A:213:LEU:HB3	2.20	0.42
1:A:626:VAL:HG11	1:A:630:LEU:HD11	2.01	0.42
1:B:321:TYR:CZ	1:B:455:ILE:HD12	2.55	0.42
1:B:540:LEU:HD23	1:B:596:LEU:HD13	2.02	0.42
1:C:504:PHE:CD1	1:C:514:THR:CG2	3.03	0.42
1:A:191:THR:HA	1:A:245:THR:O	2.20	0.42
1:D:210:TYR:CZ	1:D:530:VAL:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:HIS:O	1:B:434:ARG:HD2	2.20	0.41
1:D:36:VAL:O	1:D:40:LYS:N	2.53	0.41
1:A:626:VAL:O	1:A:626:VAL:HG12	2.19	0.41
1:B:434:ARG:HB2	1:B:435:PRO:HD2	2.02	0.41
1:C:269:ASN:HB2	1:C:511:TRP:CD1	2.56	0.41
1:D:428:ARG:HD3	1:D:428:ARG:HA	1.87	0.41
1:B:364:PHE:CE2	1:B:486:PRO:HD2	2.56	0.41
1:C:59:ASP:HB2	1:C:96:LEU:HD21	2.02	0.41
1:C:392:ARG:NH1	1:C:416:LEU:O	2.54	0.41
1:A:18:ALA:HB2	1:A:105:LEU:CD2	2.51	0.41
1:C:302:HIS:HB2	1:C:432:LEU:HD22	2.03	0.41
1:D:189:ILE:HG23	1:D:243:VAL:HG13	2.02	0.41
1:A:144:GLY:HA3	1:A:174:VAL:HG23	2.03	0.41
1:C:36:VAL:O	1:C:40:LYS:N	2.52	0.40
1:A:540:LEU:HD23	1:A:596:LEU:HD13	2.03	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%)	608 (96%)	26 (4%)	2 (0%)	41	74
1	B	632/720 (88%)	601 (95%)	29 (5%)	2 (0%)	41	74
1	C	636/720 (88%)	598 (94%)	36 (6%)	2 (0%)	41	74
1	D	632/720 (88%)	597 (94%)	34 (5%)	1 (0%)	47	80
All	All	2536/2880 (88%)	2404 (95%)	125 (5%)	7 (0%)	41	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	401	PRO
1	D	40	LYS
1	C	205	GLY
1	A	40	LYS
1	C	17	VAL
1	B	40	LYS
1	A	276	PHE

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	516/621 (83%)	512 (99%)	4 (1%)	81	92
1	B	541/621 (87%)	536 (99%)	5 (1%)	78	91
1	C	547/621 (88%)	540 (99%)	7 (1%)	69	88
1	D	523/621 (84%)	517 (99%)	6 (1%)	73	90
All	All	2127/2484 (86%)	2105 (99%)	22 (1%)	76	91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	321	TYR
1	A	513	TYR
1	A	514	THR
1	B	199	ARG
1	B	304	CYS
1	B	321	TYR
1	B	461	GLN
1	B	535	SER
1	C	74	ARG
1	C	126	VAL
1	C	321	TYR
1	C	469	SER
1	C	513	TYR
1	C	518	CYS

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Mol	Chain	Res	Type
1	C	556	ARG
1	D	35	THR
1	D	97	ILE
1	D	141	ILE
1	D	321	TYR
1	D	457	ASN
1	D	548	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	B	396	HIS
1	B	452	ASN
1	B	634	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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
2	UDP	D	801	-	20,26,26	0.78	0	25,40,40	1.08	1 (4%)
3	G6P	B	802	-	16,16,16	0.53	0	24,24,24	0.96	1 (4%)
3	G6P	C	803	-	16,16,16	0.58	0	24,24,24	0.92	1 (4%)
2	UDP	C	802	-	20,26,26	0.82	1 (5%)	25,40,40	1.30	3 (12%)
4	GCS	C	801	-	12,12,12	0.71	0	16,17,17	0.87	1 (6%)
3	G6P	D	802	-	16,16,16	0.54	0	24,24,24	0.89	1 (4%)
2	UDP	B	801	-	20,26,26	0.77	0	25,40,40	1.04	1 (4%)
2	UDP	A	801	-	20,26,26	0.75	0	25,40,40	1.22	3 (12%)
3	G6P	A	802	-	16,16,16	0.60	0	24,24,24	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	D	801	-	-	2/14/32/32	0/2/2/2
3	G6P	B	802	-	-	0/6/26/26	0/1/1/1
3	G6P	C	803	-	-	0/6/26/26	0/1/1/1
2	UDP	C	802	-	-	4/14/32/32	0/2/2/2
4	GCS	C	801	-	-	0/2/22/22	0/1/1/1
3	G6P	D	802	-	-	1/6/26/26	0/1/1/1
2	UDP	B	801	-	-	5/14/32/32	0/2/2/2
2	UDP	A	801	-	-	8/14/32/32	0/2/2/2
3	G6P	A	802	-	-	1/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	802	UDP	O4'-C1'	2.10	1.44	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	UDP	C3'-C2'-C1'	3.25	105.87	100.98
2	A	801	UDP	C3'-C2'-C1'	3.20	105.80	100.98
2	D	801	UDP	C3'-C2'-C1'	3.03	105.54	100.98
2	B	801	UDP	C3'-C2'-C1'	2.73	105.09	100.98
2	A	801	UDP	PA-O3A-PB	-2.65	123.74	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	UDP	PA-O3A-PB	-2.56	124.04	132.83
3	B	802	G6P	O2P-P-O1P	2.46	117.03	107.64
4	C	801	GCS	C3-C2-N2	-2.41	106.11	111.05
3	D	802	G6P	O2P-P-O1P	2.29	116.40	107.64
3	C	803	G6P	O2P-P-O1P	2.17	115.93	107.64
2	C	802	UDP	O3B-PB-O2B	2.07	115.54	107.64
2	A	801	UDP	O3B-PB-O2B	2.01	115.33	107.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

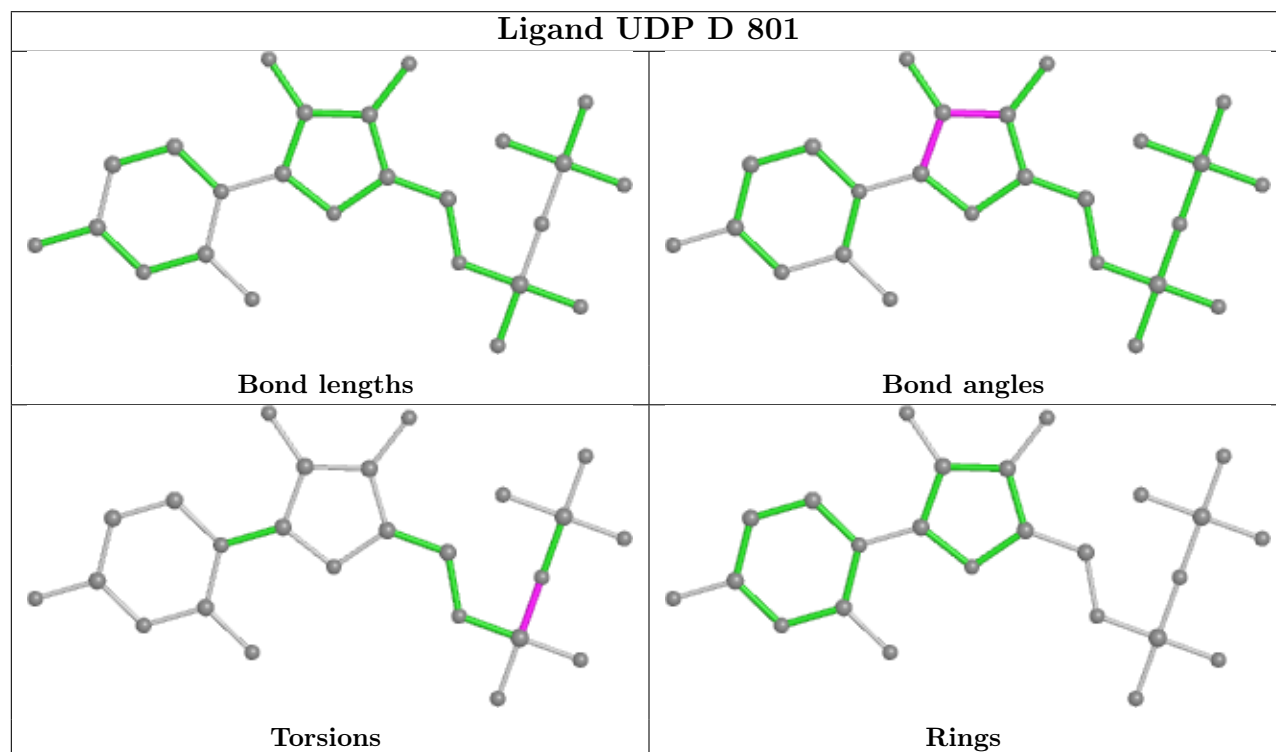
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	G6P	1	0
2	C	802	UDP	1	0
3	D	802	G6P	1	0

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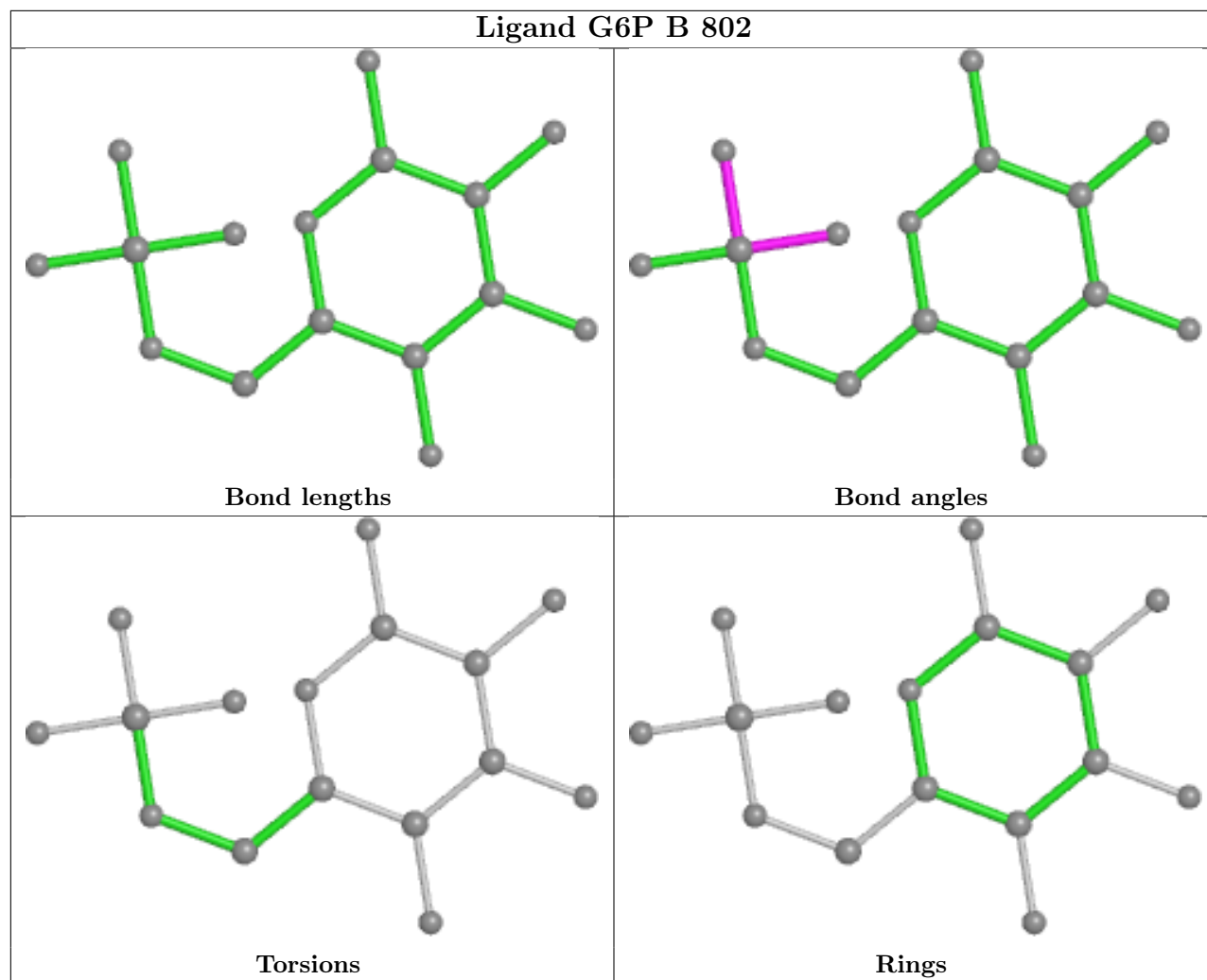
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	G6P	1	0

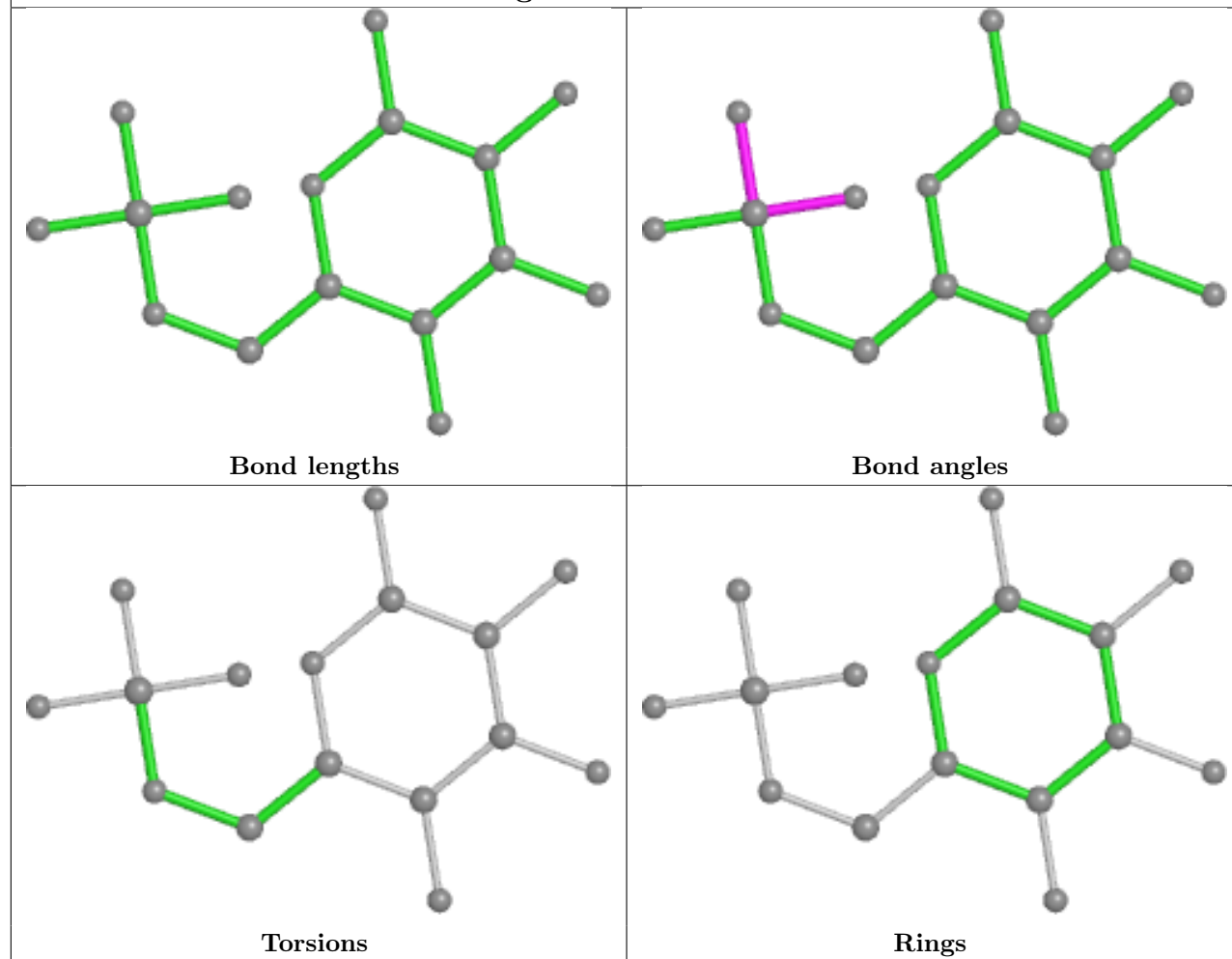
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



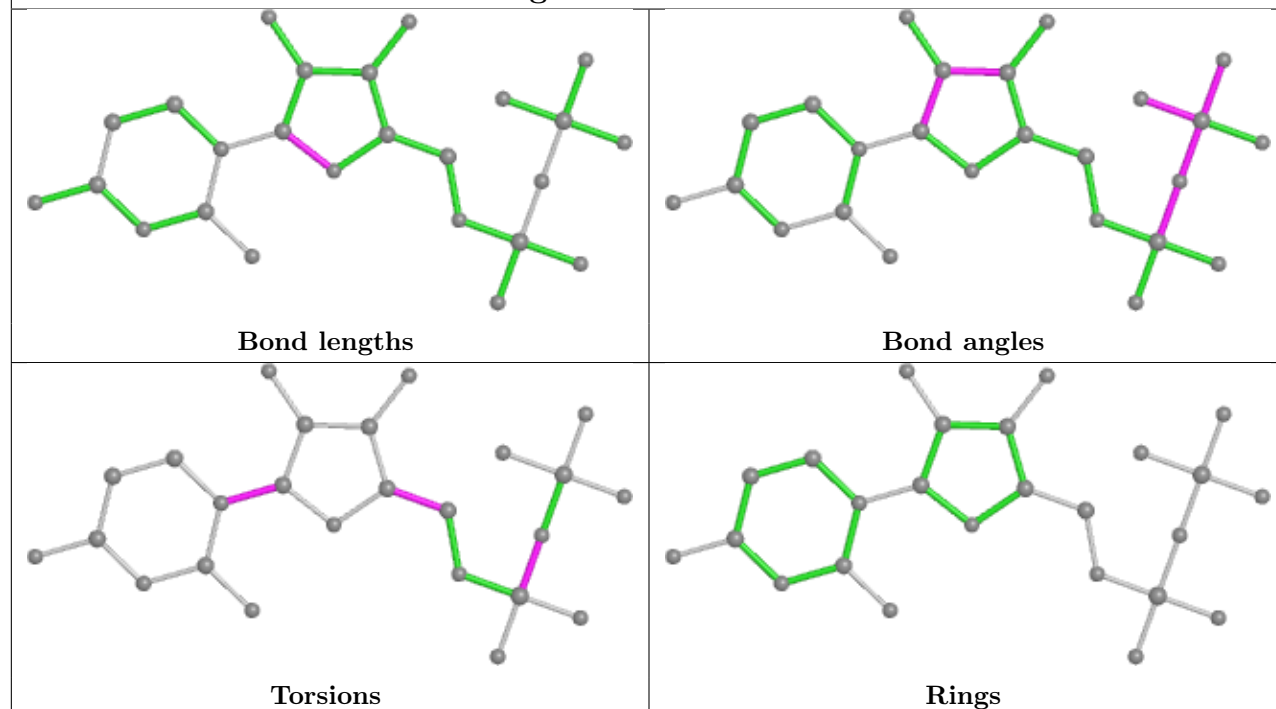
Ligand G6P B 802

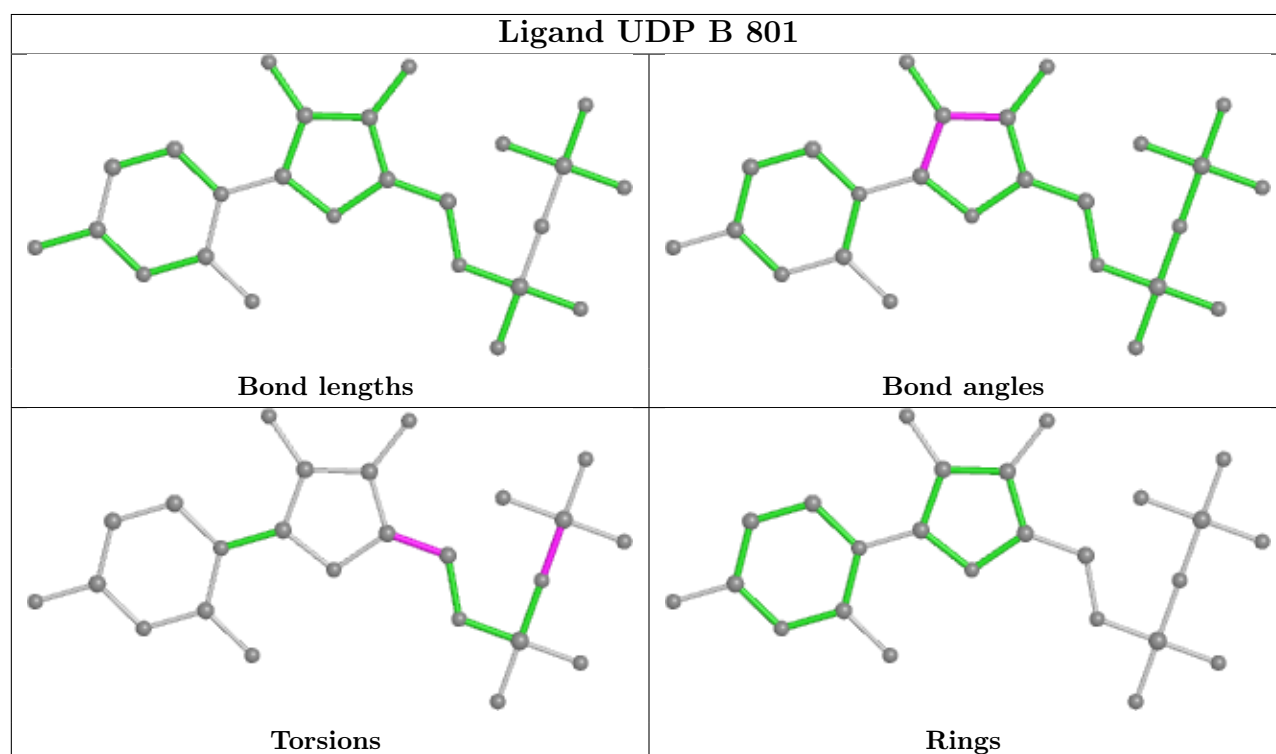
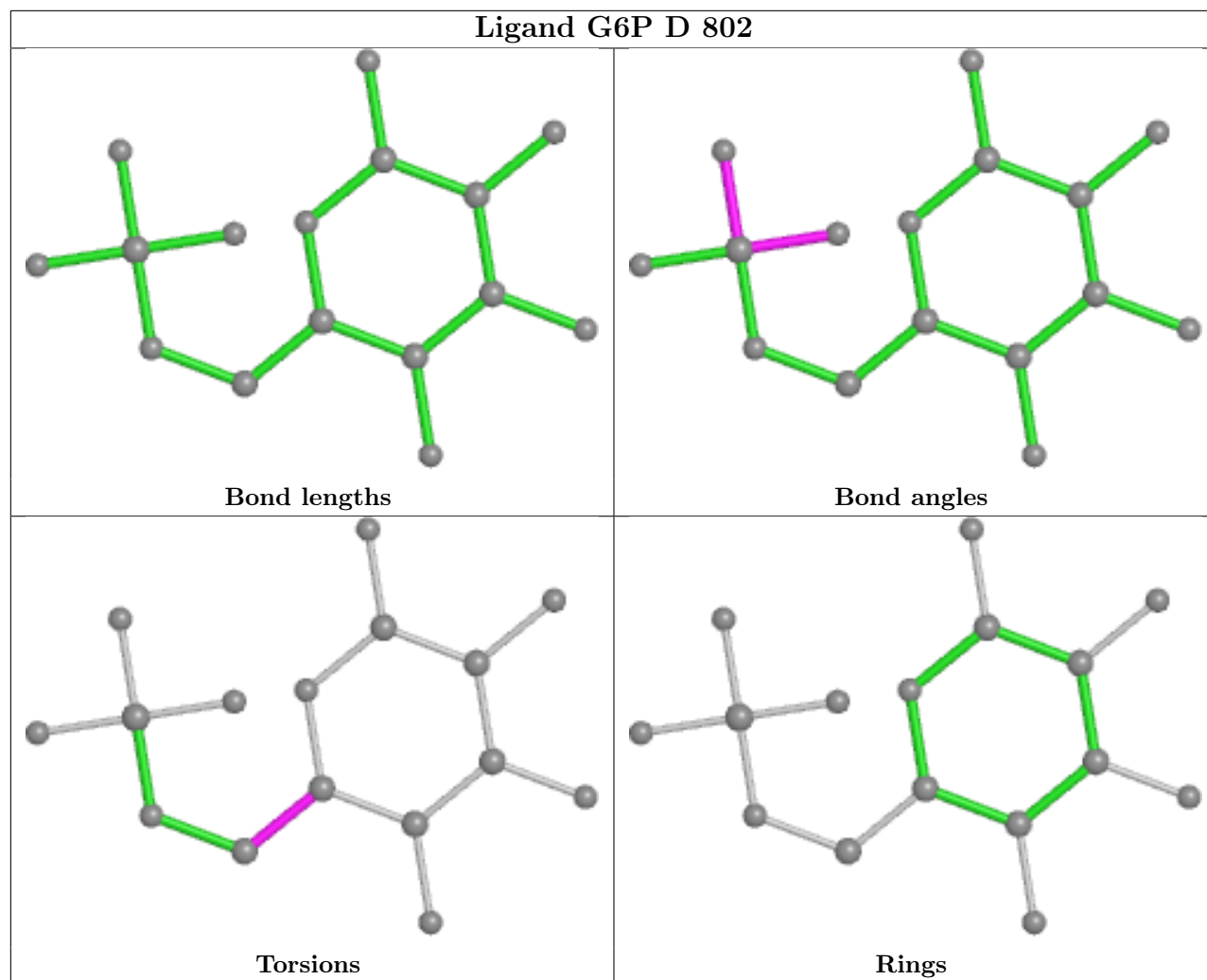


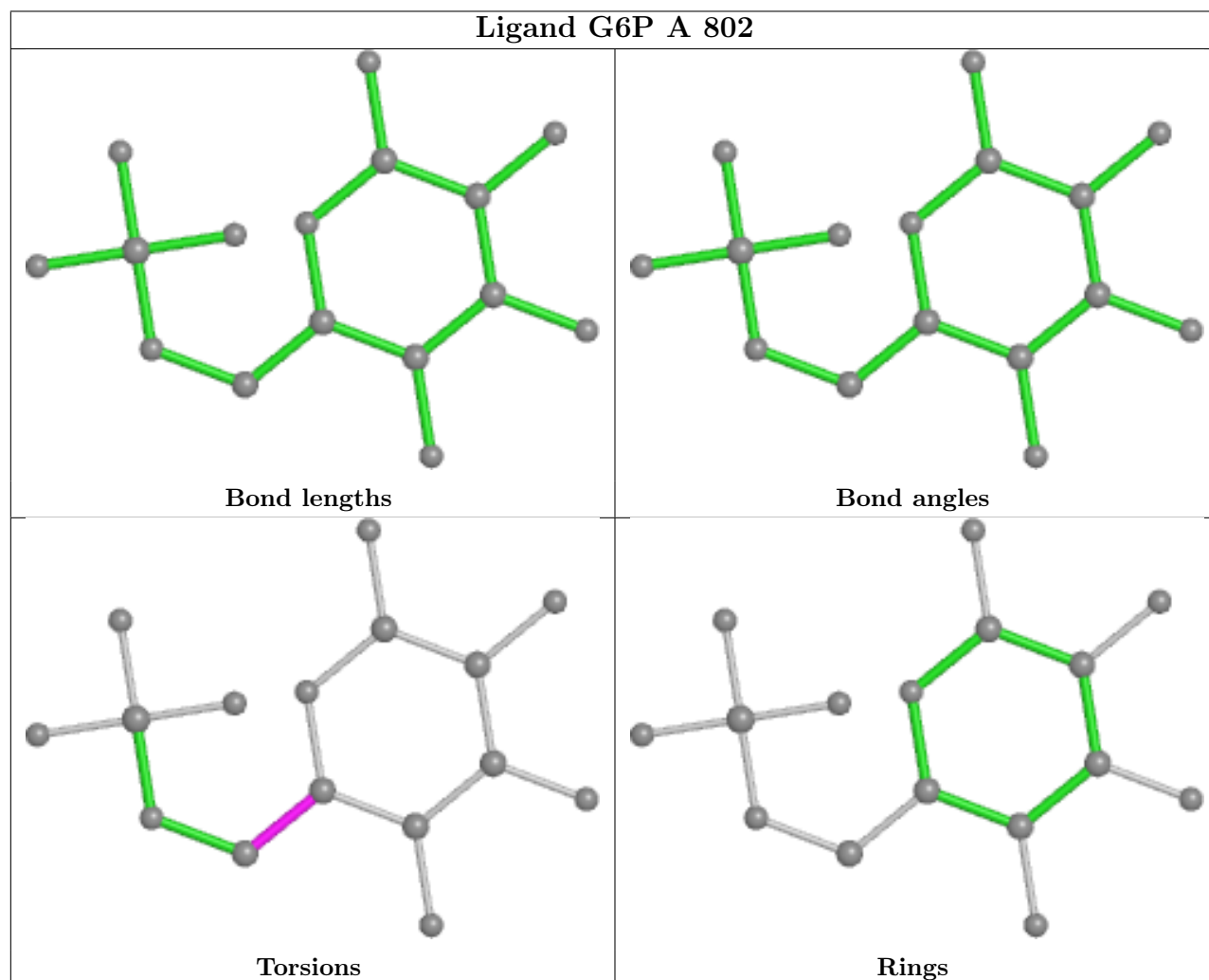
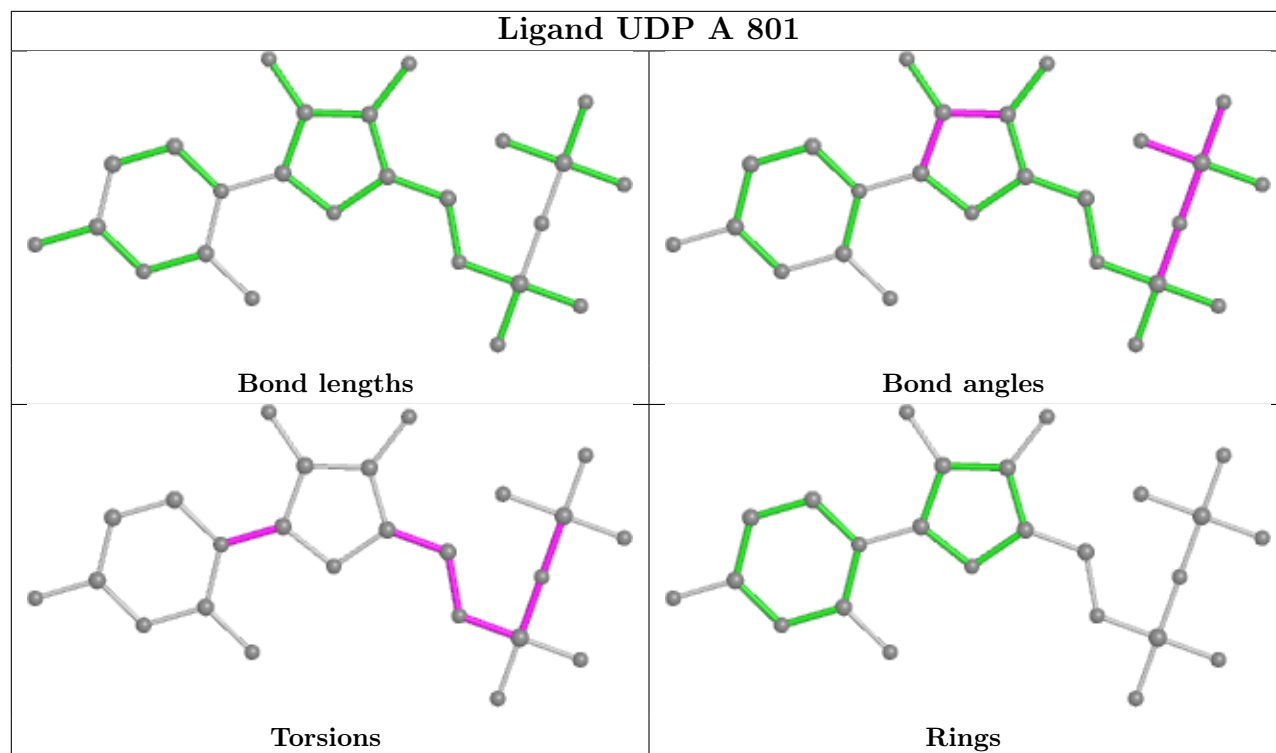
Ligand G6P C 803



Ligand UDP C 802







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%)	0.28	42 (6%) 18 9	54, 89, 159, 179	0
1	B	636/720 (88%)	0.06	26 (4%) 37 22	42, 72, 125, 162	0
1	C	638/720 (88%)	0.21	39 (6%) 21 11	54, 80, 139, 160	0
1	D	636/720 (88%)	0.32	48 (7%) 14 7	46, 89, 157, 173	0
All	All	2548/2880 (88%)	0.22	155 (6%) 21 11	42, 82, 151, 179	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	7.0
1	A	96	LEU	6.8
1	D	630	LEU	5.7
1	A	52	ALA	5.4
1	D	618	TYR	5.1
1	C	124	SER	4.9
1	D	124	SER	4.8
1	D	167	PHE	4.8
1	C	525	SER	4.8
1	C	125	LEU	4.7
1	C	123	TRP	4.6
1	C	624	GLU	4.5
1	C	52	ALA	4.4
1	D	13	THR	4.4
1	D	639	ALA	4.3
1	A	627	GLY	4.3
1	D	620	ASP	4.2
1	C	626	VAL	4.1
1	D	629	GLU	4.1
1	B	630	LEU	4.0
1	A	626	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	61	LEU	4.0
1	A	56	ASN	3.9
1	A	525	SER	3.9
1	C	128	ILE	3.9
1	D	619	PRO	3.8
1	B	624	GLU	3.7
1	C	13	THR	3.7
1	D	622	PHE	3.6
1	B	631	ASN	3.6
1	C	218	VAL	3.6
1	A	61	LEU	3.6
1	D	125	LEU	3.6
1	A	133	ASN	3.5
1	B	628	GLU	3.4
1	C	544	ASN	3.4
1	A	625	LEU	3.3
1	C	625	LEU	3.3
1	A	502	GLY	3.2
1	D	64	LYS	3.2
1	C	518	CYS	3.2
1	D	172	ALA	3.1
1	A	214	GLU	3.1
1	D	166	HIS	3.1
1	C	183	ARG	3.0
1	D	68	ALA	3.0
1	A	504	PHE	3.0
1	D	276	PHE	3.0
1	A	274	ILE	3.0
1	D	123	TRP	3.0
1	A	53	THR	3.0
1	D	85	SER	3.0
1	D	173	GLY	3.0
1	B	165	ALA	3.0
1	C	165	ALA	2.9
1	D	219	ASP	2.9
1	B	166	HIS	2.9
1	D	197	LEU	2.9
1	A	156	HIS	2.9
1	C	524	PRO	2.9
1	D	626	VAL	2.9
1	A	503	VAL	2.9
1	D	502	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	159	SER	2.9
1	C	46	ILE	2.8
1	B	623	ARG	2.8
1	D	501	LEU	2.8
1	D	133	ASN	2.8
1	B	183	ARG	2.8
1	C	627	GLY	2.7
1	D	168	HIS	2.7
1	C	62	ASP	2.7
1	D	627	GLY	2.7
1	A	114	TYR	2.7
1	D	225	PHE	2.7
1	C	623	ARG	2.7
1	A	135	PHE	2.7
1	C	436	GLU	2.7
1	D	127	GLY	2.7
1	B	156	HIS	2.6
1	C	67	GLU	2.6
1	D	6	GLN	2.6
1	D	21	VAL	2.6
1	D	628	GLU	2.6
1	C	346	GLY	2.6
1	B	67	GLU	2.6
1	D	128	ILE	2.6
1	B	11	PHE	2.6
1	B	340	TYR	2.6
1	A	68	ALA	2.6
1	A	165	ALA	2.6
1	C	630	LEU	2.5
1	C	53	THR	2.5
1	C	98	GLU	2.5
1	B	633	SER	2.5
1	D	96	LEU	2.5
1	A	85	SER	2.5
1	C	66	PRO	2.4
1	D	3	ARG	2.4
1	A	109	ASP	2.4
1	D	615	ARG	2.4
1	D	625	LEU	2.4
1	A	524	PRO	2.4
1	D	63	TRP	2.4
1	C	11	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2	SER	2.4
1	C	68	ALA	2.4
1	A	125	LEU	2.4
1	B	13	THR	2.4
1	C	166	HIS	2.4
1	A	59	ASP	2.4
1	A	452	ASN	2.3
1	C	109	ASP	2.3
1	B	632	ASP	2.3
1	D	117	GLU	2.3
1	A	124	SER	2.3
1	D	67	GLU	2.3
1	A	558	PHE	2.3
1	B	46	ILE	2.2
1	C	118	TRP	2.2
1	A	21	VAL	2.2
1	C	167	PHE	2.2
1	A	518	CYS	2.2
1	B	135	PHE	2.2
1	B	44	HIS	2.2
1	C	220	HIS	2.2
1	A	317	ILE	2.2
1	B	629	GLU	2.2
1	D	632	ASP	2.1
1	A	235	ARG	2.1
1	C	129	PRO	2.1
1	B	499	CYS	2.1
1	A	213	LEU	2.1
1	A	172	ALA	2.1
1	A	253	PHE	2.1
1	A	13	THR	2.1
1	D	52	ALA	2.1
1	D	637	ALA	2.1
1	A	87	GLY	2.1
1	B	66	PRO	2.1
1	B	61	LEU	2.1
1	C	526	ILE	2.1
1	D	4	ASP	2.1
1	B	20	ARG	2.1
1	C	133	ASN	2.1
1	A	45	LEU	2.0
1	A	197	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	157	LEU	2.0
1	C	558	PHE	2.0
1	B	159	SER	2.0
1	C	77	GLN	2.0
1	A	12	GLU	2.0
1	D	46	ILE	2.0
1	B	10	LEU	2.0
1	D	638	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](#)

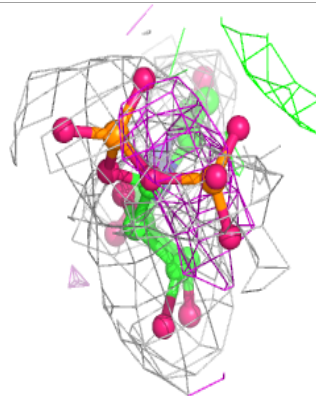
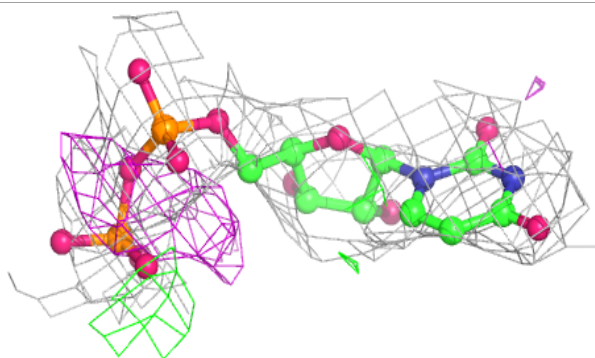
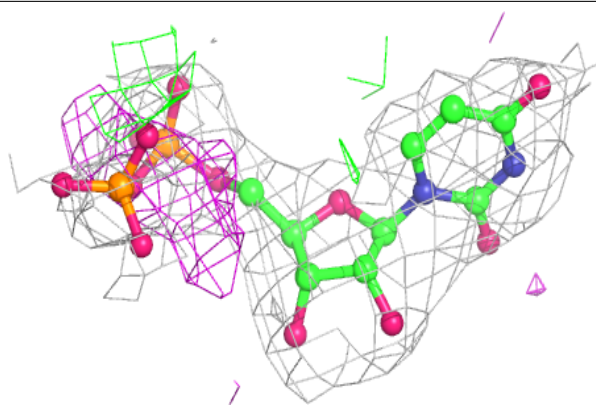
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	UDP	B	801	25/25	0.85	0.22	93,115,165,169	0
2	UDP	A	801	25/25	0.90	0.16	78,93,103,106	0
2	UDP	D	801	25/25	0.93	0.14	80,100,127,130	0
2	UDP	C	802	25/25	0.95	0.17	68,84,90,95	0
3	G6P	A	802	16/16	0.97	0.13	51,59,62,63	0
3	G6P	B	802	16/16	0.97	0.12	40,48,50,52	0
3	G6P	C	803	16/16	0.97	0.16	55,68,72,74	0
3	G6P	D	802	16/16	0.97	0.15	43,51,55,56	0
4	GCS	C	801	12/12	0.97	0.16	57,60,66,68	0

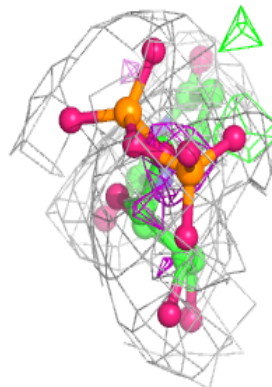
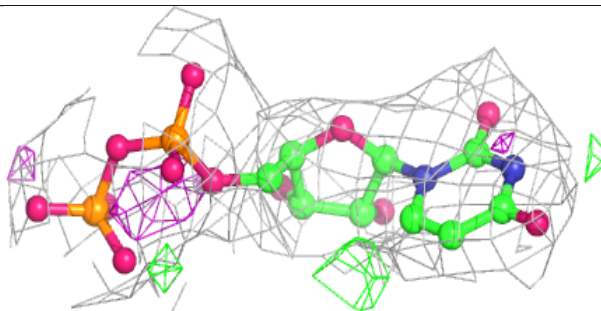
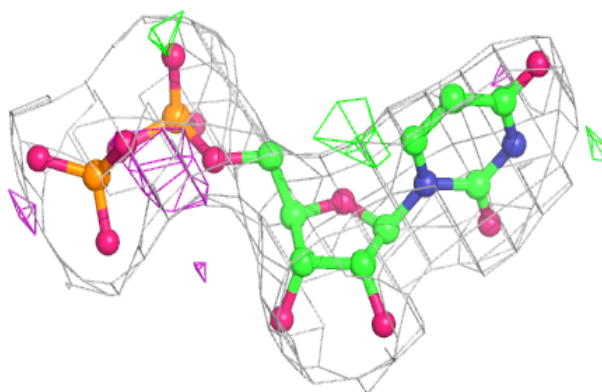
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP 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)

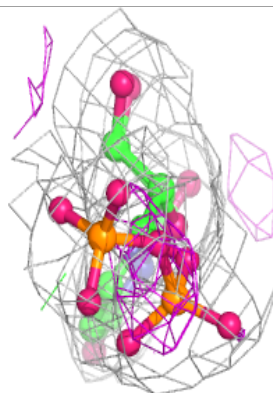
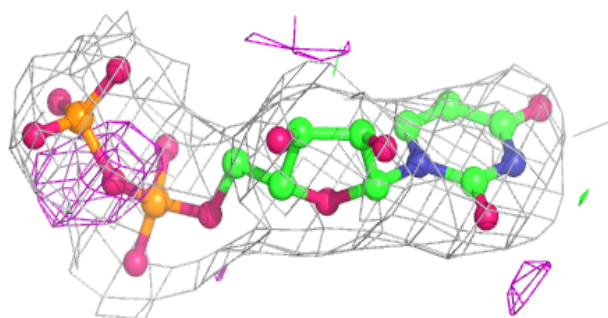
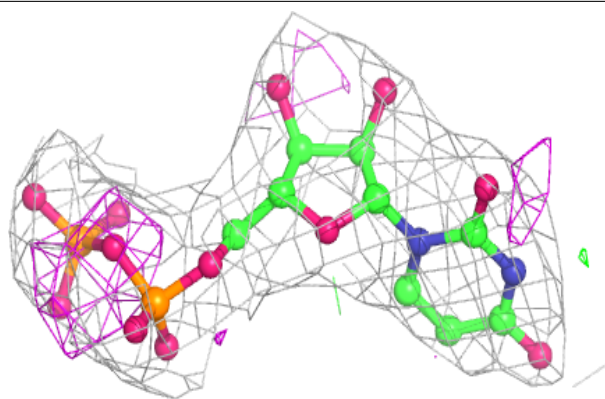
**Electron density around UDP A 801:**

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

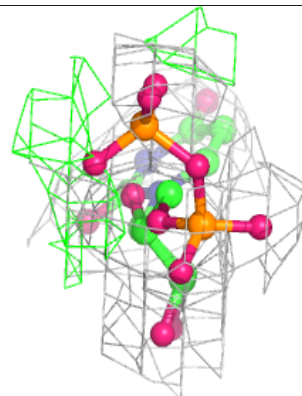
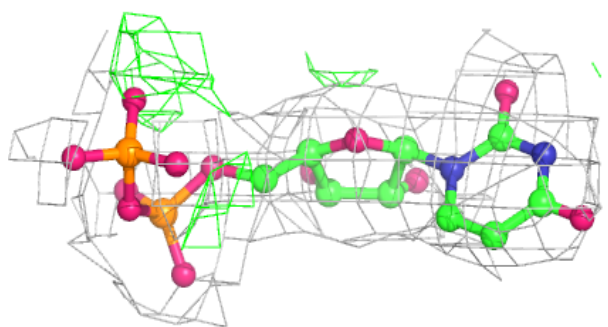
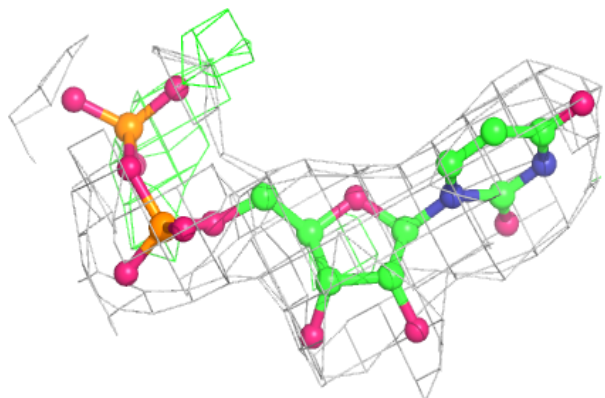


Electron density around UDP D 801:

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

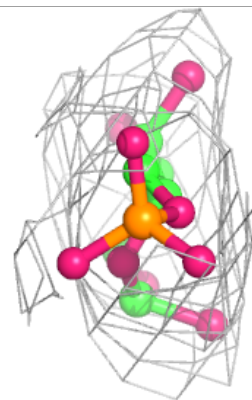
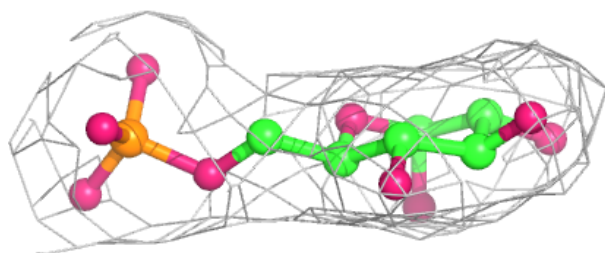
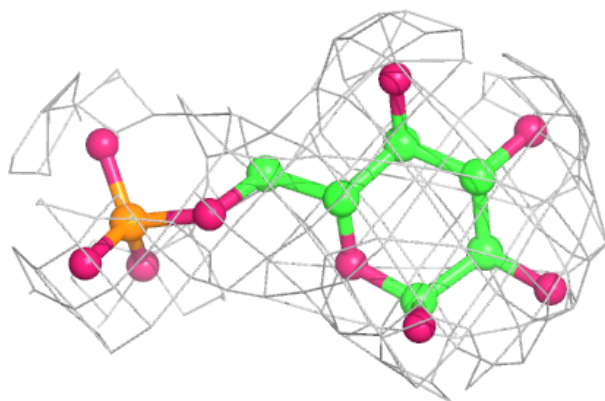
**Electron density around UDP C 802:**

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

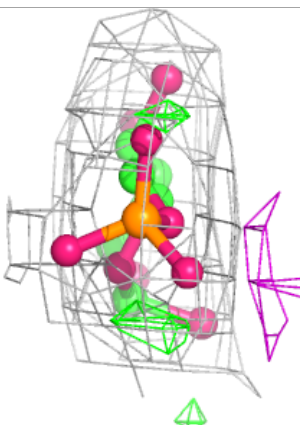
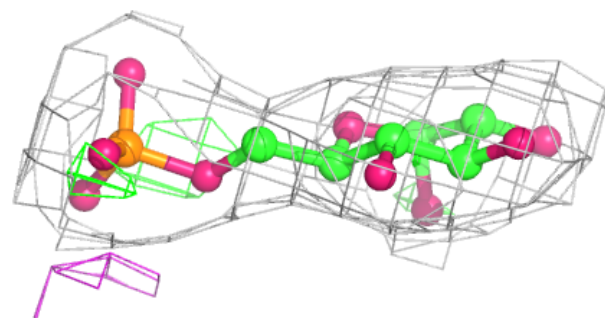
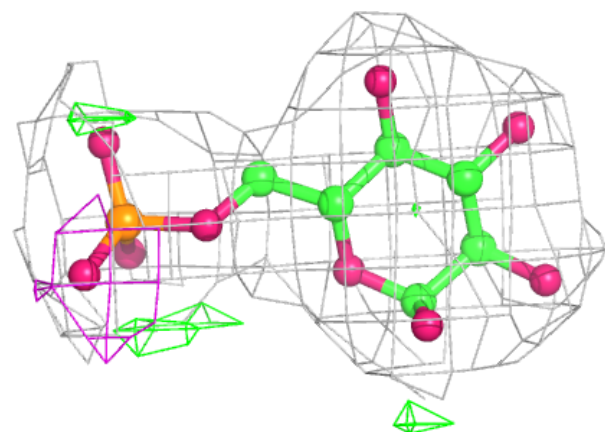


Electron density around G6P A 802:

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

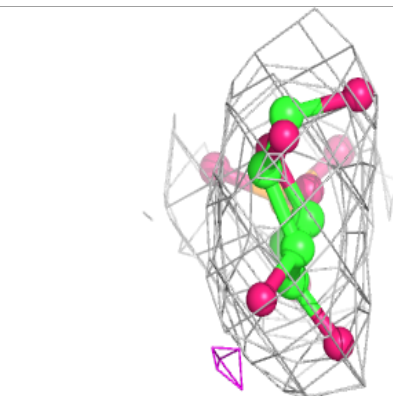
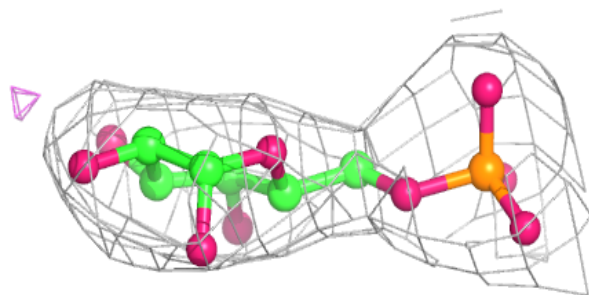
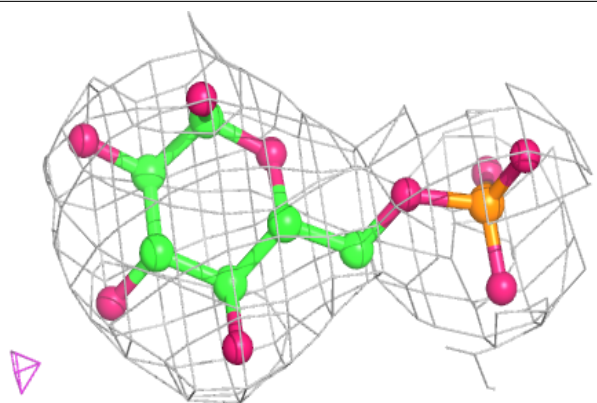
**Electron density around G6P B 802:**

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

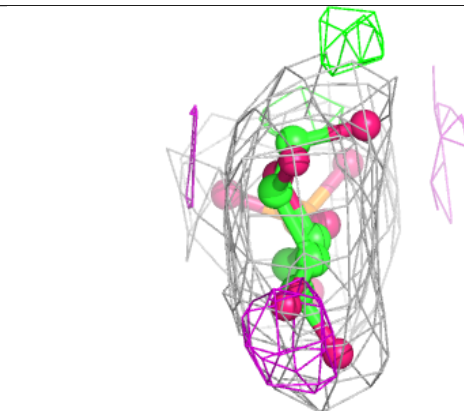
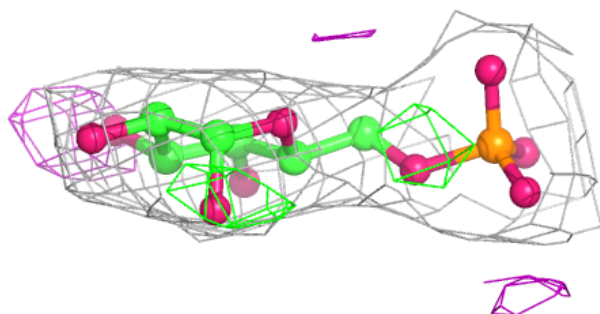
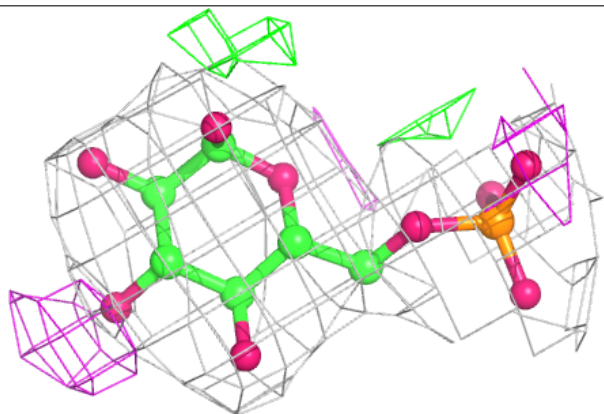


Electron density around G6P C 803:

$2mF_o-DF_c$ (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.