



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:30 PM UTC

PDB ID : 5UW0 / pdb_00005uw0
Title : Activated state yGsy2p in complex with UDP-2-fluoro-2-deoxy-glucose
Authors : Mahalingan, K.K.; Hurley, T.D.
Deposited on : 2017-02-20
Resolution : 2.73 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

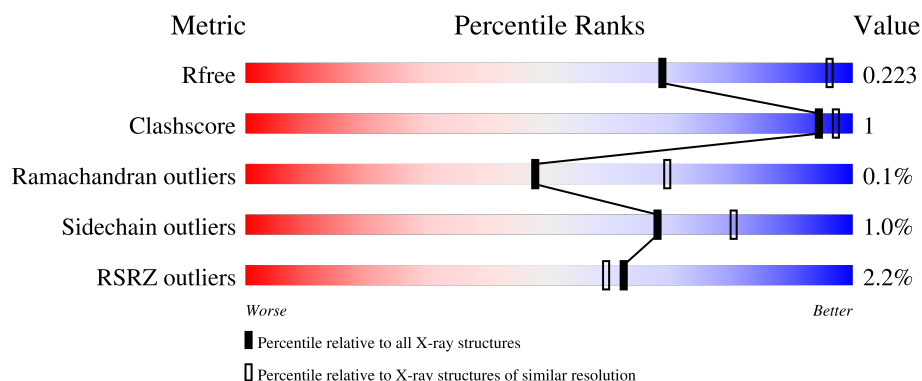
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	
1	B	720	
1	C	720	
1	D	720	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20497 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
			5059	3232	865	943	19			
1	B	638	Total	C	N	O	S	0	0	0
			5105	3260	885	941	19			
1	C	638	Total	C	N	O	S	0	0	0
			5133	3278	895	941	19			
1	D	633	Total	C	N	O	S	0	0	0
			5024	3209	864	932	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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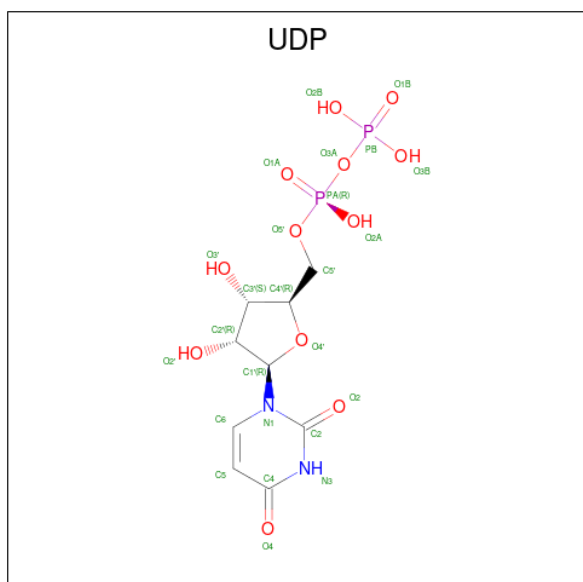
Chain	Residue	Modelled	Actual	Comment	Reference
A	535	SER	ALA	conflict	UNP P27472
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression 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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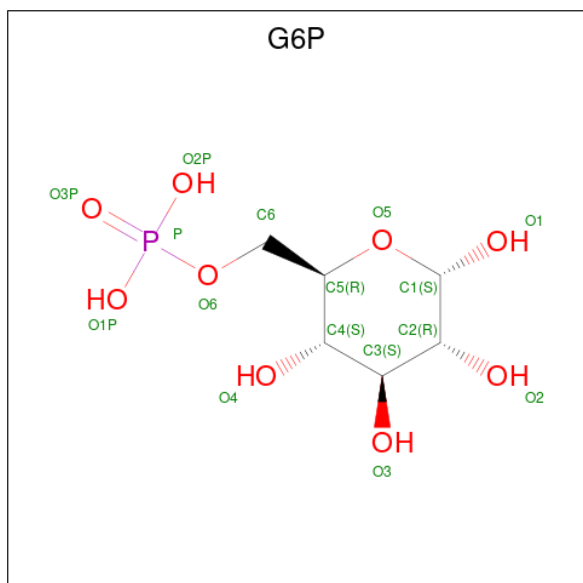
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P27472
C	169	GLN	GLU	engineered mutation	UNP P27472
C	535	SER	ALA	conflict	UNP P27472
D	-19	MET	-	initiating methionine	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression 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 URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



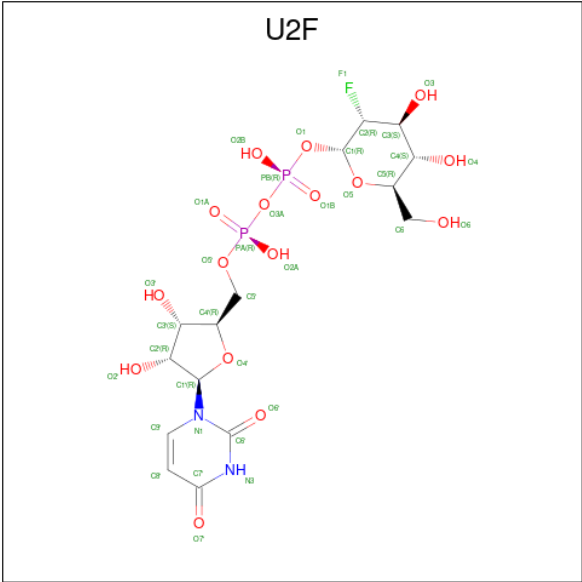
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: 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-2-DEOXY-2-FLUORO-ALPHA-D-GLUCOSE (CCD ID: U2F) (formula: $C_{15}H_{23}FN_2O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	F	N	O	0	0
			36	15	1	2	16		

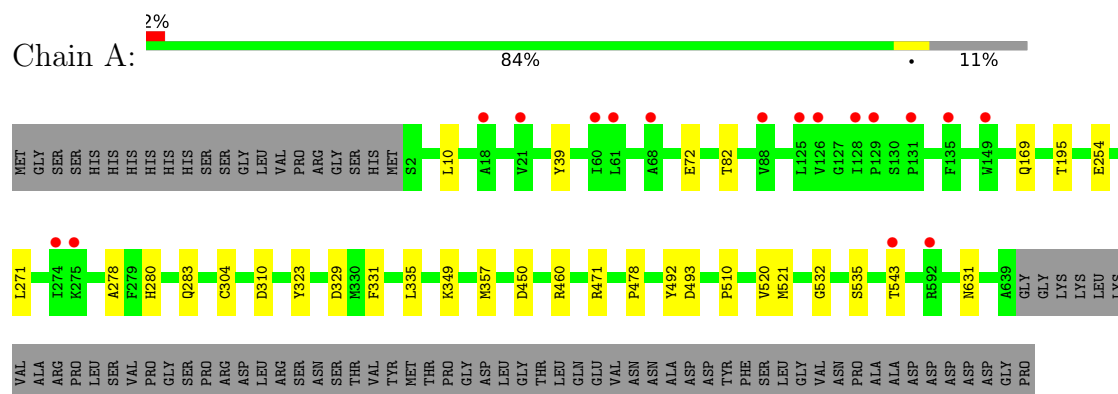
- Molecule 5 is water.

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

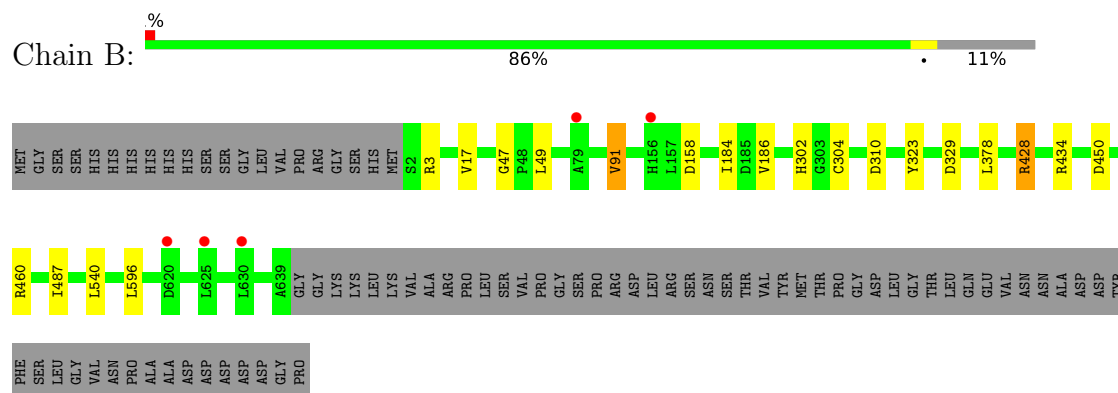
3 Residue-property plots [i](#)

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.

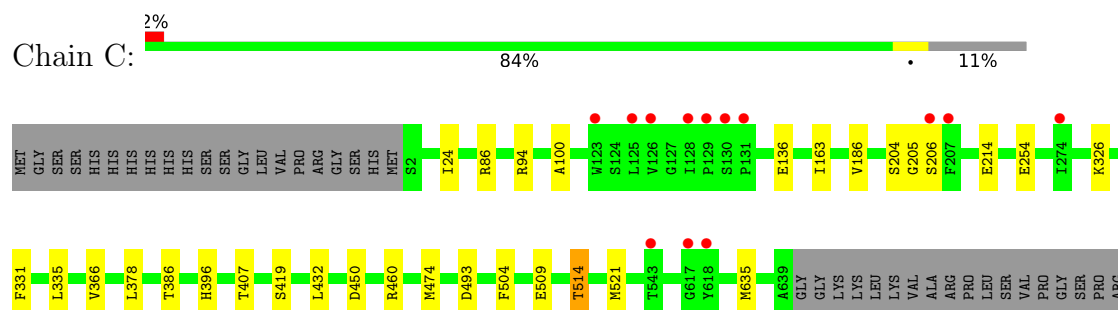
- Molecule 1: Glycogen [starch] synthase isoform 2



- Molecule 1: Glycogen [starch] synthase isoform 2

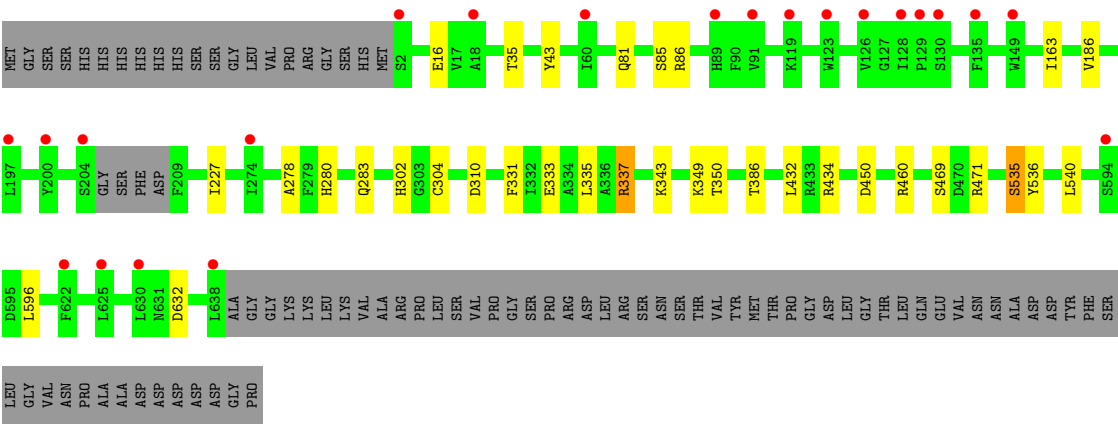
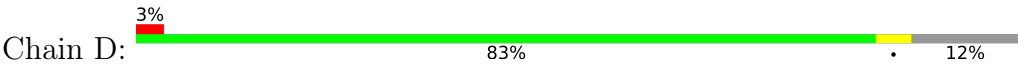


- Molecule 1: Glycogen [starch] synthase isoform 2



ASP	LEU	ARG	SER	SER	ASN	SER	THR	VAL	TYR	MET	THR	PRO	PRO	GLY	ASP	LEU	GLY	THR	LEU	GLN	GLU	VAL	ASN	ASN	ALA	ALA	ASP	ASP	TYR	PHE	SER	SER	LEU	GLY	VAL	ASN	PRO	ALA	ALA	ASP	ASP	ASP	ASP	GLY	PRO
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● 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	193.52Å 204.71Å 206.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.38 – 2.73 145.38 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.5 (145.38-2.73) 99.5 (145.38-2.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.199 , 0.224 0.201 , 0.223	Depositor DCC
R_{free} test set	5465 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20497	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: U2F, UDP, 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	0.67	1/5184 (0.0%)	0.88	0/7048
1	B	0.74	1/5230 (0.0%)	0.90	0/7098
1	C	0.69	0/5258	0.89	1/7128 (0.0%)
1	D	0.72	0/5146	0.89	1/6994 (0.0%)
All	All	0.70	2/20818 (0.0%)	0.89	2/28268 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	487	ILE	N-CA	5.24	1.51	1.45
1	A	631	ASN	CG-OD1	5.14	1.33	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	635	MET	N-CA-C	5.29	116.72	111.07
1	D	535	SER	N-CA-C	-5.26	105.23	110.97

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	5059	0	4852	15	0
1	B	5105	0	4958	9	0
1	C	5133	0	5024	14	0
1	D	5024	0	4833	18	1
2	A	25	0	11	1	0
2	B	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	0	0
4	C	36	0	21	1	0
5	C	1	0	0	0	0
All	All	20497	0	19765	53	1

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 (53) 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	2.22	0.74
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.27	0.67
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.30	0.65
1:D:540:LEU:HD21	1:D:596:LEU:HD13	1.81	0.62
1:B:3:ARG:NH2	1:B:158:ASP:O	2.33	0.61
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.39	0.58
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.40	0.57
1:C:335:LEU:HD13	1:C:474:MET:HE1	1.87	0.56
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.38	0.56
1:A:195:THR:OG1	1:A:254:GLU:OE1	2.21	0.56
1:A:493:ASP:HB2	1:A:521:MET:HE1	1.90	0.54
1:C:396:HIS:HE1	1:C:407:THR:O	1.91	0.52
1:C:493:ASP:HB2	1:C:521:MET:HE1	1.90	0.51
1:D:227:ILE:HG22	1:D:227:ILE:O	2.10	0.50
1:C:504:PHE:CE1	1:C:514:THR:CG2	2.95	0.50
1:D:302:HIS:HD2	1:D:432:LEU:O	1.94	0.50
1:C:204:SER:O	1:C:206:SER:N	2.40	0.50
1:C:378:LEU:HD22	1:C:432:LEU:HD11	1.94	0.49
1:B:540:LEU:HD21	1:B:596:LEU:HD13	1.93	0.49
1:A:510:PRO:O	1:A:532:GLY:HA3	2.13	0.48
1:B:17:VAL:HG22	1:B:47:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.48	0.48
1:D:450:ASP:OD2	1:D:460:ARG:NH2	2.47	0.47
1:A:532:GLY:O	1:A:535:SER:OG	2.25	0.47
1:C:326:LYS:NZ	1:C:509:GLU:OE1	2.49	0.46
1:C:504:PHE:CD1	1:C:514:THR:CG2	2.99	0.46
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.52	0.44
1:C:94:ARG:HD2	1:C:100:ALA:HB1	1.98	0.44
1:A:278:ALA:HB1	1:A:280:HIS:CE1	2.52	0.44
1:D:163:ILE:HB	1:D:186:VAL:HG12	2.00	0.44
1:A:357:MET:O	1:A:478:PRO:HA	2.17	0.43
1:C:24:ILE:HG13	4:C:801:U2F:O6	2.18	0.43
1:D:35:THR:HG21	1:D:43:TYR:CE1	2.52	0.43
1:D:535:SER:OG	1:D:536:TYR:N	2.50	0.43
1:B:378:LEU:HA	1:B:428:ARG:HG3	2.00	0.43
1:D:278:ALA:HB1	1:D:280:HIS:CE1	2.54	0.43
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.53	0.43
1:D:349:LYS:O	1:D:471:ARG:HD3	2.18	0.43
1:D:35:THR:HG21	1:D:43:TYR:CZ	2.54	0.43
1:B:184:ILE:HG22	1:B:186:VAL:HG23	2.00	0.43
1:D:343:LYS:HD3	1:D:469:SER:O	2.18	0.42
1:D:333:GLU:OE2	1:D:337:ARG:HD2	2.19	0.42
1:A:492:TYR:CD1	2:A:801:UDP:C5	3.07	0.42
1:A:271:LEU:HD13	1:A:520:VAL:HG21	2.01	0.42
1:A:10:LEU:HD22	1:A:39:TYR:CE2	2.55	0.42
1:B:302:HIS:O	1:B:434:ARG:NH1	2.48	0.42
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.53	0.41
1:C:163:ILE:HB	1:C:186:VAL:HG12	2.02	0.41
1:C:386:THR:HB	1:D:386:THR:HB	2.02	0.41
1:A:349:LYS:O	1:A:471:ARG:HD3	2.21	0.41
1:A:331:PHE:CZ	1:A:335:LEU:HD11	2.56	0.41
1:B:49:LEU:HD13	1:B:91:VAL:CG1	2.51	0.41
1:D:302:HIS:O	1:D:434:ARG:HD2	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:SER:OG	1:D:85:SER:OG[2_555]	1.86	0.34

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%)	27 (4%)	1 (0%)	43	62
1	B	636/720 (88%)	616 (97%)	20 (3%)	0	100	100
1	C	636/720 (88%)	612 (96%)	23 (4%)	1 (0%)	43	62
1	D	629/720 (87%)	601 (96%)	27 (4%)	1 (0%)	43	62
All	All	2537/2880 (88%)	2437 (96%)	97 (4%)	3 (0%)	48	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	D	632	ASP
1	C	205	GLY

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	533/621 (86%)	528 (99%)	5 (1%)	70	82
1	B	542/621 (87%)	538 (99%)	4 (1%)	76	85
1	C	548/621 (88%)	541 (99%)	7 (1%)	61	75
1	D	529/621 (85%)	523 (99%)	6 (1%)	65	79
All	All	2152/2484 (87%)	2130 (99%)	22 (1%)	68	80

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

Mol	Chain	Res	Type
1	A	72	GLU
1	A	82	THR
1	A	304	CYS
1	A	310	ASP
1	A	543	THR
1	B	91	VAL
1	B	304	CYS
1	B	310	ASP
1	B	428	ARG
1	C	86	ARG
1	C	136	GLU
1	C	214	GLU
1	C	254	GLU
1	C	366	VAL
1	C	419	SER
1	C	514	THR
1	D	16	GLU
1	D	81	GLN
1	D	86	ARG
1	D	304	CYS
1	D	310	ASP
1	D	337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	277	GLN
1	A	477	HIS
1	A	588	ASN
1	B	484	ASN
1	C	50	ASN
1	C	56	ASN
1	C	78	HIS
1	C	161	HIS
1	C	229	HIS
1	C	249	GLN
1	C	380	ASN
1	C	396	HIS
1	C	452	ASN
1	C	585	ASN
1	D	156	HIS
1	D	168	HIS

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Mol	Chain	Res	Type
1	D	283	GLN
1	D	302	HIS
1	D	588	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	U2F	C	801	-	37,38,38	1.38	8 (21%)	53,58,58	2.51	17 (32%)
3	G6P	B	802	-	16,16,16	0.54	0	23,24,24	0.83	0
3	G6P	A	802	-	16,16,16	0.60	0	23,24,24	0.83	0
3	G6P	D	802	-	16,16,16	0.51	0	23,24,24	1.04	2 (8%)
2	UDP	A	801	-	25,26,26	1.23	4 (16%)	38,40,40	1.57	4 (10%)
2	UDP	D	801	-	25,26,26	1.16	3 (12%)	38,40,40	1.63	5 (13%)
3	G6P	C	802	-	16,16,16	0.55	0	23,24,24	0.80	0
2	UDP	B	801	-	25,26,26	1.07	3 (12%)	38,40,40	1.65	5 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	U2F	C	801	-	-	3/22/59/59	0/3/3/3
3	G6P	B	802	-	-	0/6/26/26	0/1/1/1
3	G6P	A	802	-	-	4/6/26/26	0/1/1/1
3	G6P	D	802	-	-	3/6/26/26	0/1/1/1
2	UDP	A	801	-	-	7/16/32/32	0/2/2/2
2	UDP	D	801	-	-	5/16/32/32	0/2/2/2
3	G6P	C	802	-	-	0/6/26/26	0/1/1/1
2	UDP	B	801	-	-	6/16/32/32	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	801	U2F	C2-C1	3.30	1.56	1.52
4	C	801	U2F	PB-O1	2.96	1.68	1.59
2	A	801	UDP	PA-O3A	2.91	1.62	1.59
2	D	801	UDP	PA-O3A	2.87	1.62	1.59
4	C	801	U2F	PA-O3A	2.62	1.62	1.59
2	A	801	UDP	C2-N1	2.53	1.42	1.38
4	C	801	U2F	C2-C3	2.43	1.55	1.52
2	D	801	UDP	C6-C5	2.43	1.40	1.35
2	A	801	UDP	C4-N3	-2.40	1.34	1.38
4	C	801	U2F	C6'-N1	2.40	1.42	1.38
2	B	801	UDP	C6-C5	2.28	1.40	1.35
4	C	801	U2F	PB-O3A	2.25	1.61	1.59
2	B	801	UDP	C2-N1	2.19	1.41	1.38
2	B	801	UDP	PA-O3A	2.19	1.61	1.59
2	A	801	UDP	C6-C5	2.17	1.40	1.35
2	D	801	UDP	C2-N1	2.11	1.41	1.38
4	C	801	U2F	C7'-N3	-2.05	1.35	1.38
4	C	801	U2F	C9'-C8'	2.03	1.39	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	801	U2F	O1-C1-C2	8.77	124.46	108.38
4	C	801	U2F	F1-C2-C3	6.70	114.61	108.81
2	B	801	UDP	C4-N3-C2	-5.04	120.36	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	801	U2F	C7'-N3-C6'	-4.94	120.48	126.61
4	C	801	U2F	N3-C6'-N1	4.94	121.32	114.89
2	B	801	UDP	N3-C2-N1	4.92	121.29	114.89
2	A	801	UDP	C4-N3-C2	-4.75	120.71	126.61
2	D	801	UDP	N3-C2-N1	4.68	120.98	114.89
2	A	801	UDP	N3-C2-N1	4.54	120.81	114.89
2	D	801	UDP	C4-N3-C2	-4.54	120.97	126.61
4	C	801	U2F	O3-C3-C2	4.16	117.32	109.63
4	C	801	U2F	PB-O1-C1	4.14	138.08	121.21
2	A	801	UDP	C5-C4-N3	3.93	120.31	114.80
4	C	801	U2F	O5-C1-O1	3.86	116.41	111.36
4	C	801	U2F	C8'-C7'-N3	3.77	120.09	114.80
4	C	801	U2F	C3-C4-C5	-3.53	103.83	110.23
2	B	801	UDP	C5-C4-N3	3.44	119.62	114.80
2	D	801	UDP	C5-C4-N3	3.30	119.42	114.80
4	C	801	U2F	O7'-C7'-C8'	-3.23	119.59	125.16
2	D	801	UDP	O2-C2-N1	-3.23	118.59	122.80
4	C	801	U2F	F1-C2-C1	3.09	111.17	107.62
2	D	801	UDP	O4-C4-C5	-2.89	120.18	125.16
4	C	801	U2F	O4'-C1'-N1	2.85	114.81	108.36
2	B	801	UDP	O2-C2-N1	-2.84	119.11	122.80
4	C	801	U2F	O4-C4-C5	2.75	116.10	109.32
2	B	801	UDP	O4-C4-C5	-2.75	120.42	125.16
3	D	802	G6P	O2P-P-O1P	2.44	116.97	107.80
4	C	801	U2F	O3A-PB-O1B	-2.36	103.61	110.70
4	C	801	U2F	O6-C6-C5	-2.26	103.64	111.33
2	A	801	UDP	O4-C4-C5	-2.21	121.35	125.16
4	C	801	U2F	C9'-N1-C6'	-2.14	118.40	121.00
3	D	802	G6P	O6-P-O3P	-2.14	100.67	106.44
4	C	801	U2F	O6'-C6'-N3	-2.05	117.70	121.49

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	UDP	C5'-O5'-PA-O2A
2	A	801	UDP	C5'-O5'-PA-O3A
2	A	801	UDP	PB-O3A-PA-O5'
2	B	801	UDP	C3'-C4'-C5'-O5'
2	B	801	UDP	C5'-O5'-PA-O2A
2	B	801	UDP	C5'-O5'-PA-O3A
3	A	802	G6P	C6-O6-P-O1P

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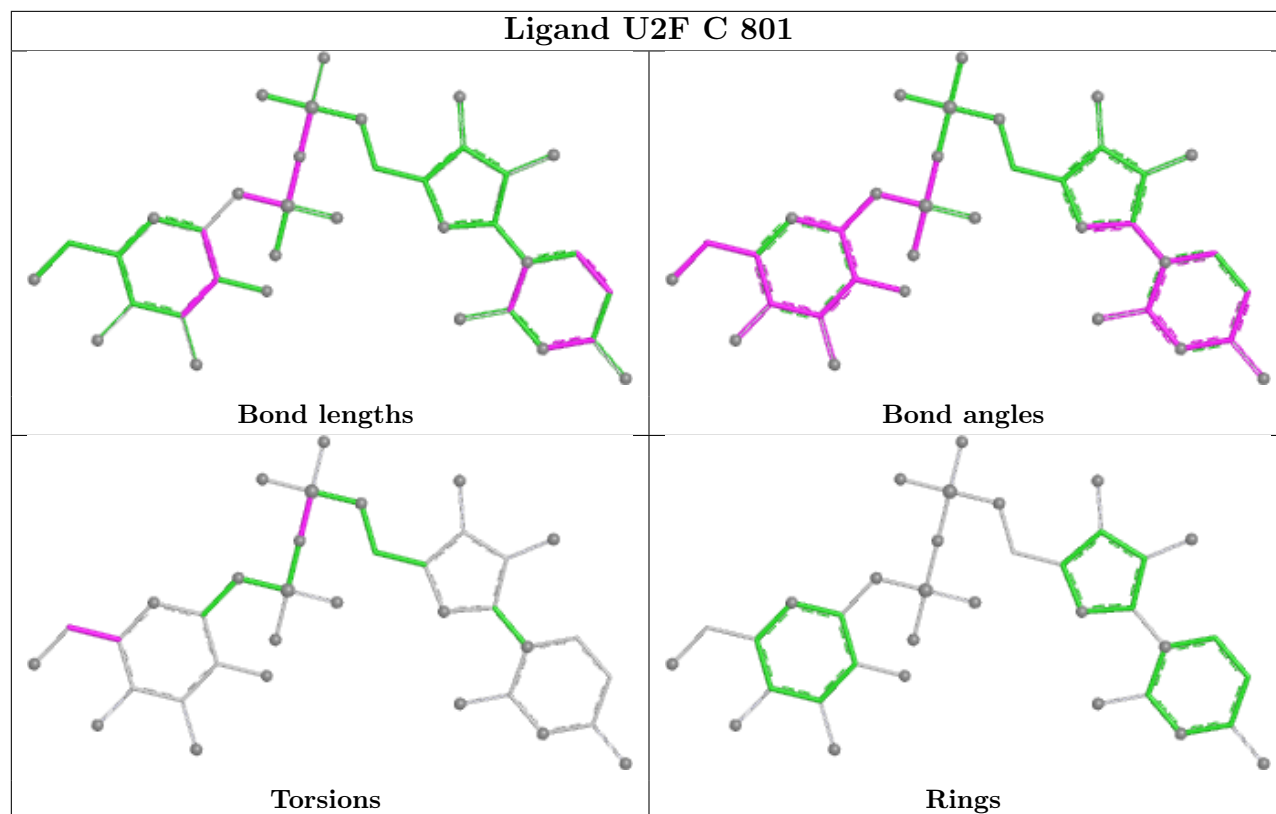
Mol	Chain	Res	Type	Atoms
3	A	802	G6P	C6-O6-P-O2P
3	D	802	G6P	C6-O6-P-O2P
2	B	801	UDP	O4'-C4'-C5'-O5'
2	A	801	UDP	C3'-C4'-C5'-O5'
2	A	801	UDP	O4'-C4'-C5'-O5'
4	C	801	U2F	O5-C5-C6-O6
3	D	802	G6P	C6-O6-P-O3P
2	D	801	UDP	O4'-C4'-C5'-O5'
3	A	802	G6P	O5-C5-C6-O6
2	D	801	UDP	PB-O3A-PA-O5'
4	C	801	U2F	PB-O3A-PA-O5'
3	D	802	G6P	C6-O6-P-O1P
2	D	801	UDP	C5'-O5'-PA-O1A
2	D	801	UDP	PB-O3A-PA-O1A
2	D	801	UDP	C3'-C4'-C5'-O5'
2	B	801	UDP	PB-O3A-PA-O5'
3	A	802	G6P	C6-O6-P-O3P
2	A	801	UDP	PA-O3A-PB-O2B
2	B	801	UDP	PB-O3A-PA-O2A
2	A	801	UDP	O4'-C1'-N1-C6
4	C	801	U2F	PB-O3A-PA-O2A

There are no ring outliers.

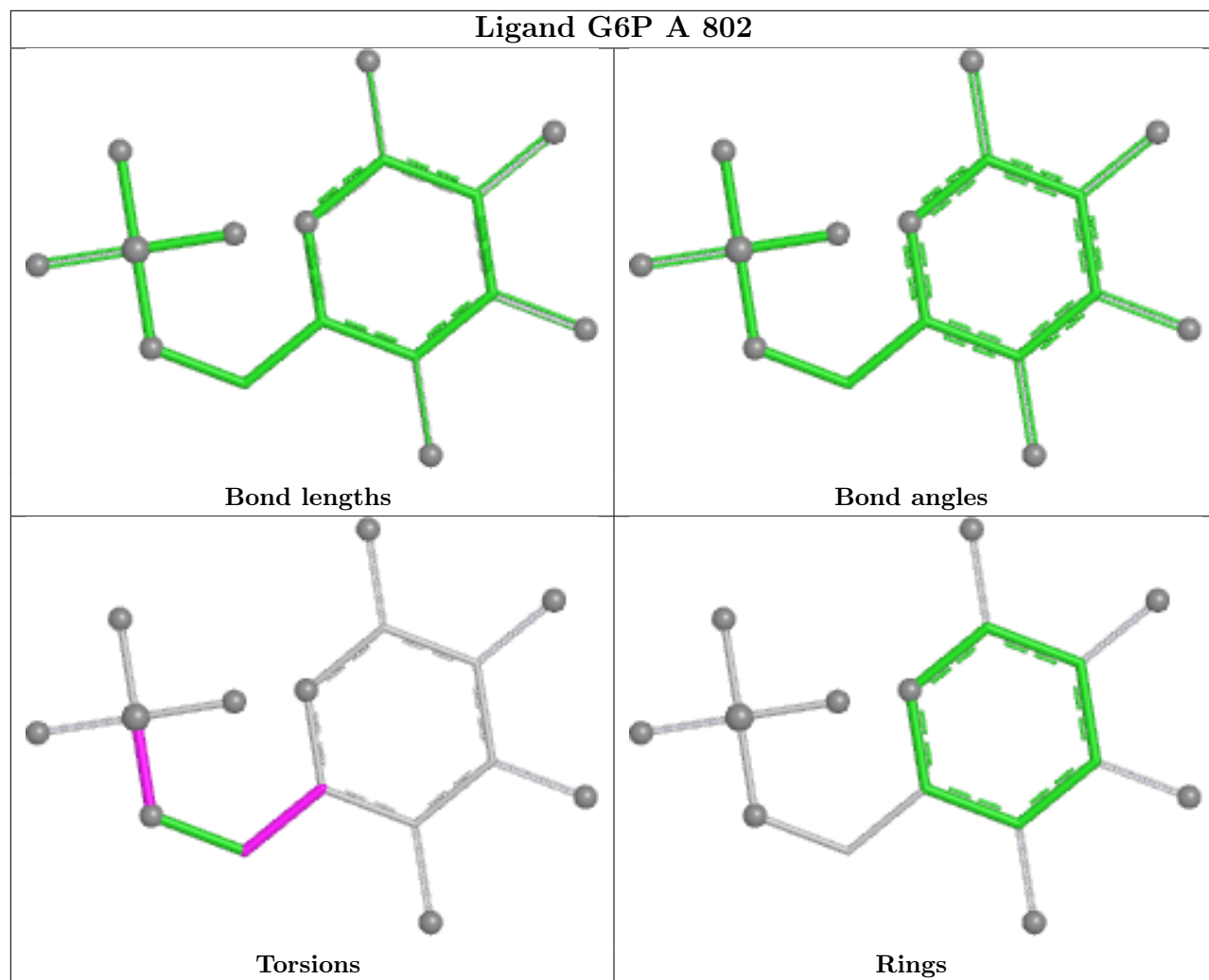
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	801	U2F	1	0
2	A	801	UDP	1	0

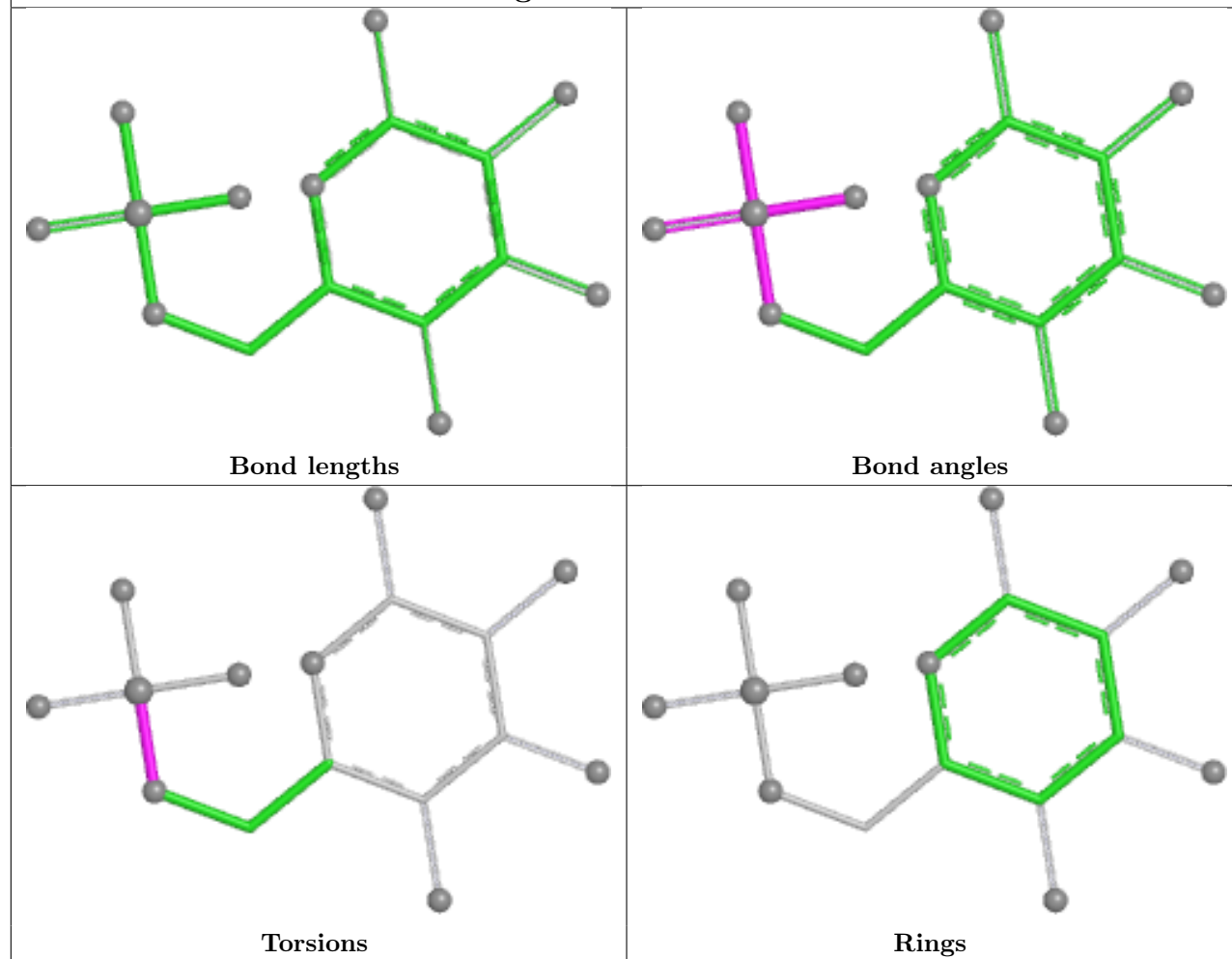
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



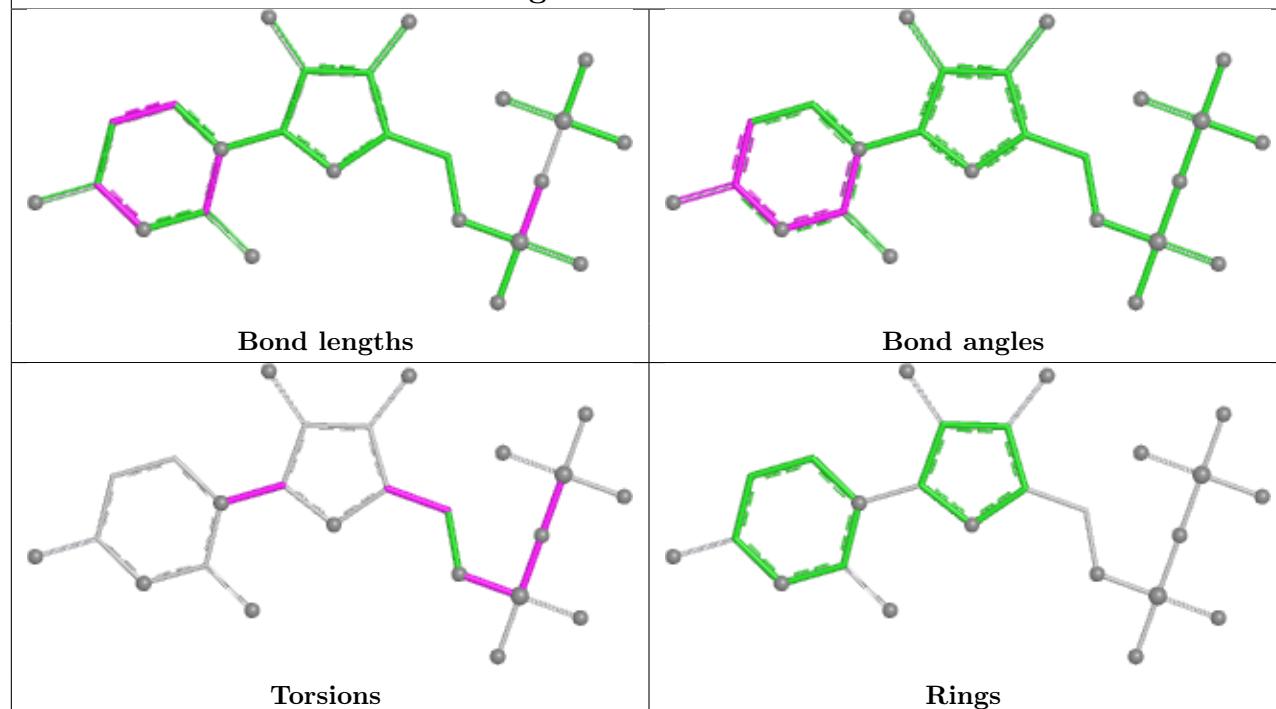
Ligand G6P A 802

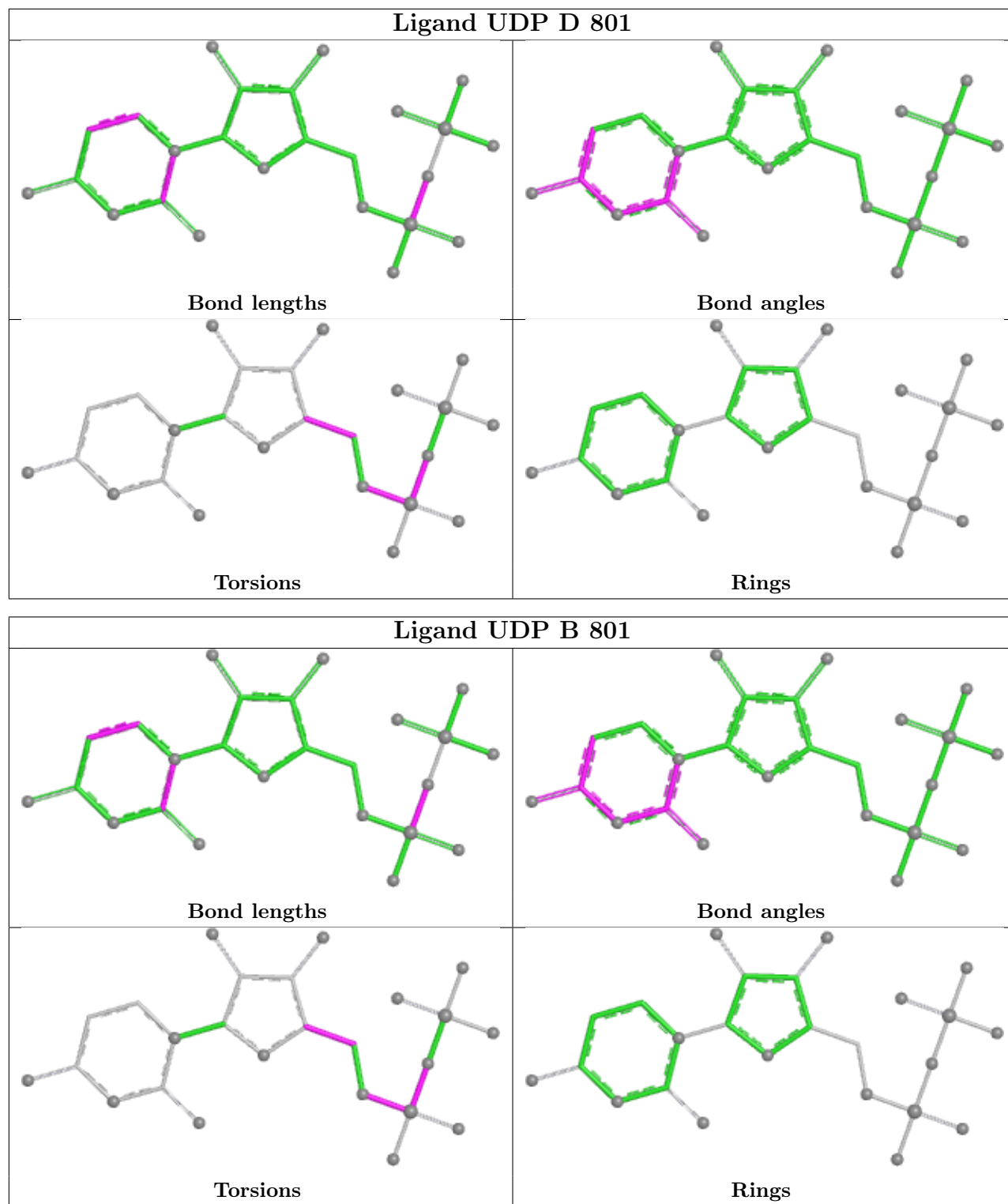


Ligand G6P D 802



Ligand UDP A 801





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.15	17 (2%) 56 53	44, 80, 160, 181	0
1	B	638/720 (88%)	-0.18	5 (0%) 82 82	33, 62, 123, 166	0
1	C	638/720 (88%)	0.02	13 (2%) 65 62	43, 72, 141, 198	0
1	D	633/720 (87%)	0.15	22 (3%) 47 45	37, 81, 158, 188	0
All	All	2547/2880 (88%)	0.03	57 (2%) 62 59	33, 73, 150, 198	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	SER	5.8
1	C	129	PRO	4.9
1	D	630	LEU	4.7
1	C	128	ILE	4.7
1	D	128	ILE	4.3
1	A	274	ILE	4.1
1	D	625	LEU	4.1
1	A	129	PRO	3.9
1	C	125	LEU	3.9
1	C	618	TYR	3.8
1	D	123	TRP	3.6
1	D	638	LEU	3.6
1	A	61	LEU	3.6
1	D	129	PRO	3.4
1	A	125	LEU	3.3
1	B	625	LEU	3.3
1	C	131	PRO	3.3
1	A	275	LYS	3.2
1	C	130	SER	3.1
1	D	274	ILE	3.0
1	D	135	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	149	TRP	2.8
1	A	543	THR	2.8
1	A	592	ARG	2.7
1	C	123	TRP	2.7
1	C	206	SER	2.7
1	A	18	ALA	2.7
1	D	149	TRP	2.6
1	B	630	LEU	2.6
1	A	131	PRO	2.6
1	A	128	ILE	2.5
1	C	207	PHE	2.5
1	C	617	GLY	2.5
1	D	130	SER	2.4
1	D	200	TYR	2.4
1	C	543	THR	2.4
1	C	126	VAL	2.4
1	D	197	LEU	2.4
1	D	594	SER	2.4
1	A	68	ALA	2.4
1	C	274	ILE	2.4
1	B	156	HIS	2.4
1	D	18	ALA	2.3
1	A	126	VAL	2.3
1	D	60	ILE	2.3
1	B	620	ASP	2.2
1	A	21	VAL	2.2
1	A	88	VAL	2.2
1	D	91	VAL	2.2
1	A	60	ILE	2.2
1	D	126	VAL	2.2
1	D	2	SER	2.1
1	D	622	PHE	2.1
1	A	135	PHE	2.1
1	B	79	ALA	2.1
1	D	89	HIS	2.1
1	D	119	LYS	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

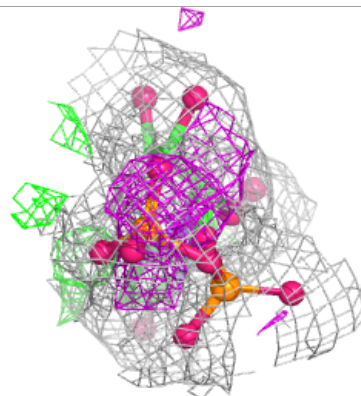
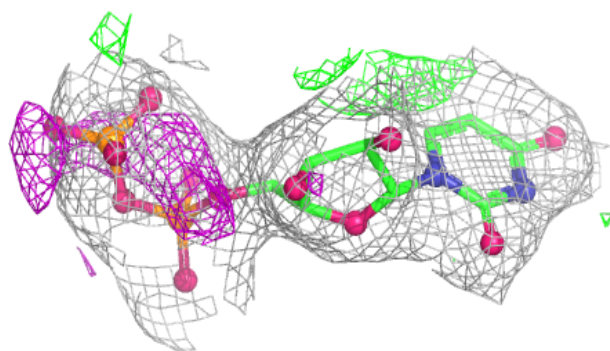
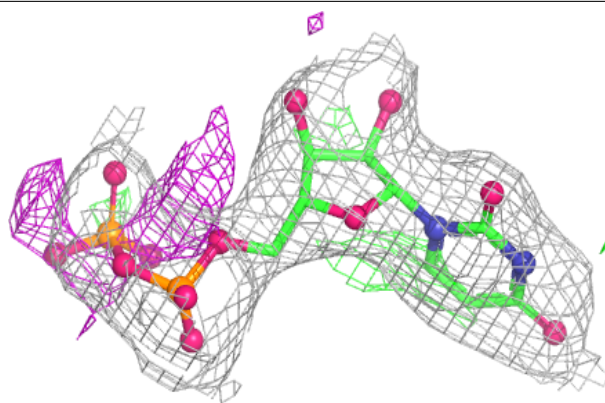
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UDP	A	801	25/25	0.83	0.10	60,77,106,111	0
2	UDP	B	801	25/25	0.88	0.10	46,69,126,128	0
4	U2F	C	801	36/36	0.88	0.11	49,55,61,69	0
2	UDP	D	801	25/25	0.90	0.09	52,71,125,128	0
3	G6P	D	802	16/16	0.97	0.06	33,37,39,41	0
3	G6P	A	802	16/16	0.97	0.06	44,52,54,55	0
3	G6P	B	802	16/16	0.98	0.05	32,38,39,41	0
3	G6P	C	802	16/16	0.98	0.06	41,51,54,55	0

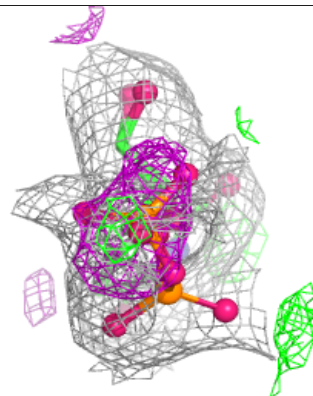
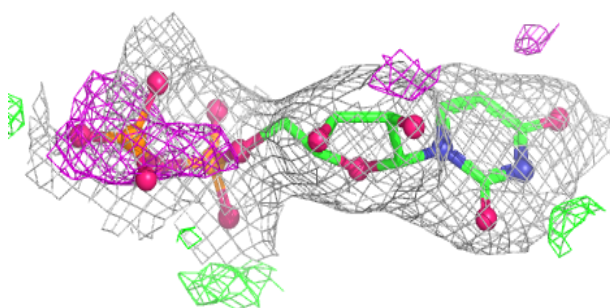
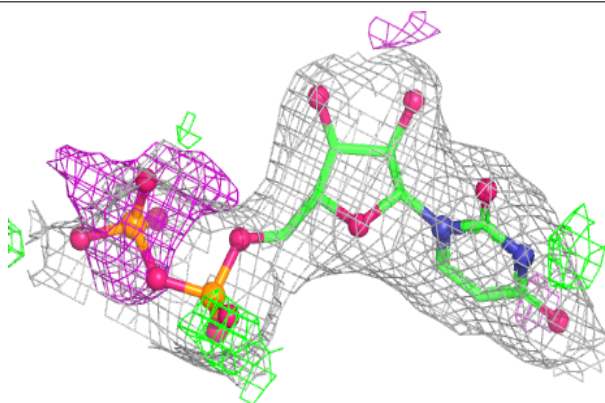
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP A 801:

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

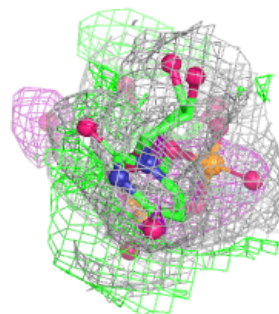
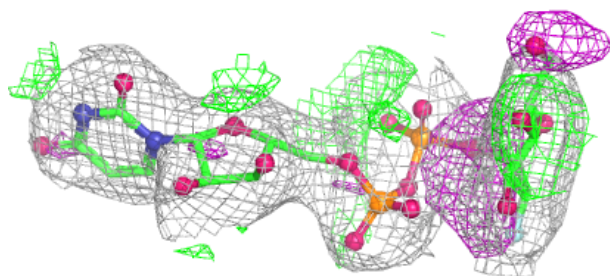
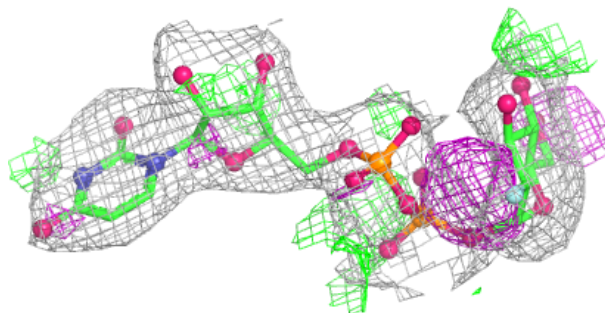
**Electron density around UDP B 801:**

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

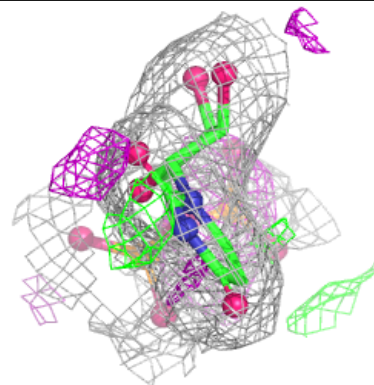
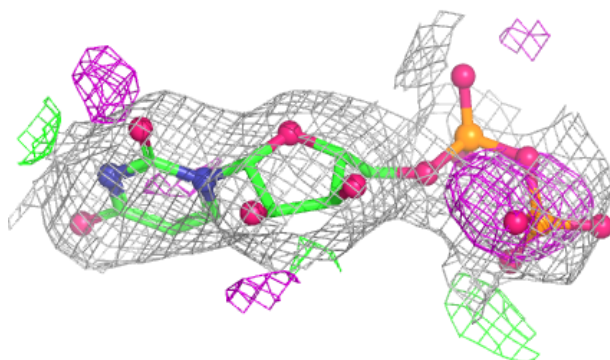
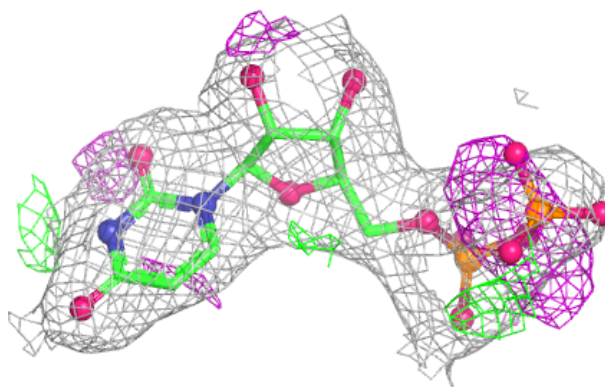


Electron density around U2F C 801:

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

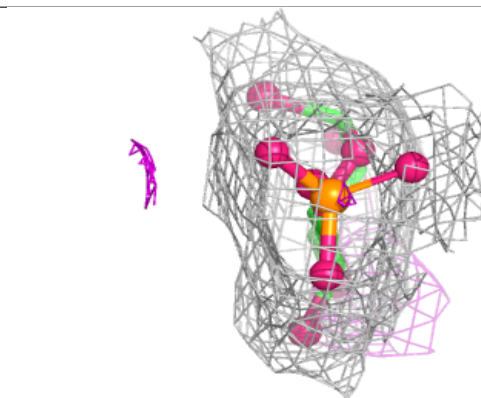
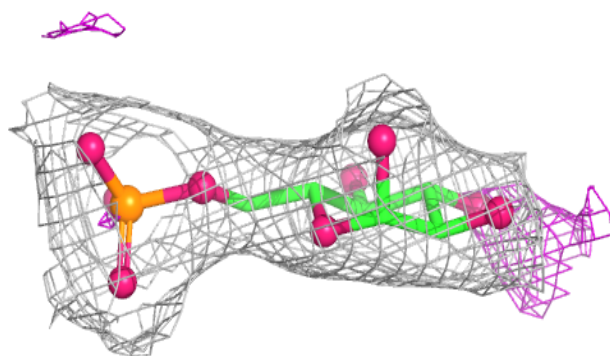
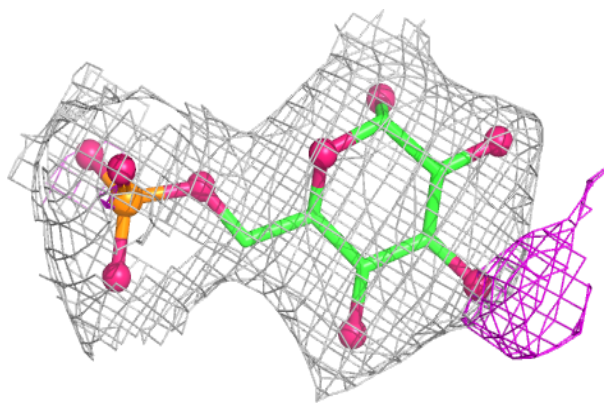
**Electron density around UDP D 801:**

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

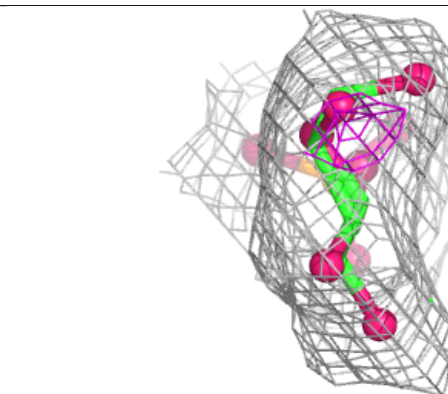
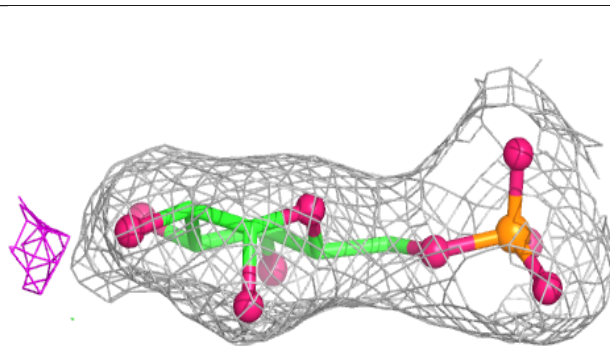
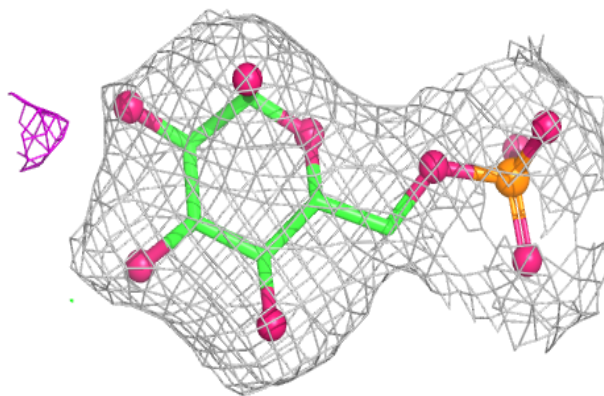


Electron density around G6P D 802:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.