



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2022 – 04:07 PM EDT

PDB ID : 5UW0
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 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

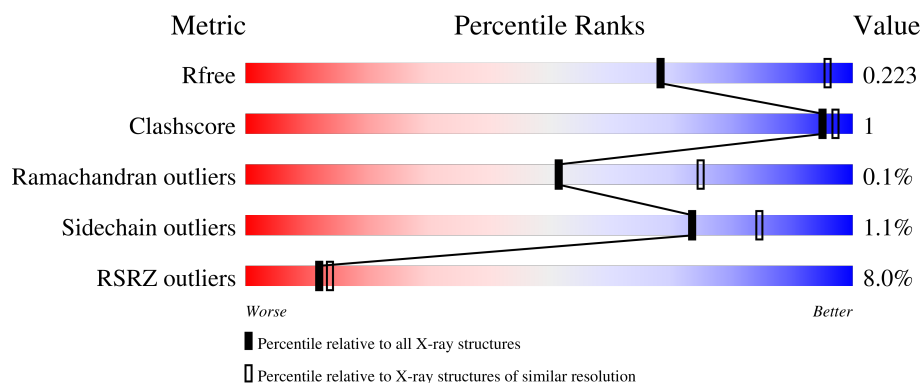
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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	<div> <div>9%</div> <div>84%</div> <div>11%</div> </div>
1	B	720	<div> <div>4%</div> <div>85%</div> <div>11%</div> </div>
1	C	720	<div> <div>6%</div> <div>85%</div> <div>11%</div> </div>
1	D	720	<div> <div>10%</div> <div>83%</div> <div>12%</div> </div>

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

Continued on next page...

Continued from previous page...

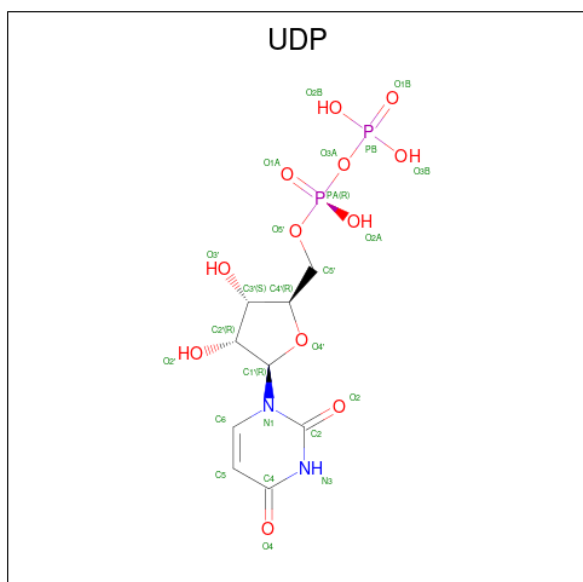
Chain	Residue	Modelled	Actual	Comment	Reference
A	535	SER	ALA	conflict	UNP P27472
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression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

Continued on next page...

Continued from previous page...

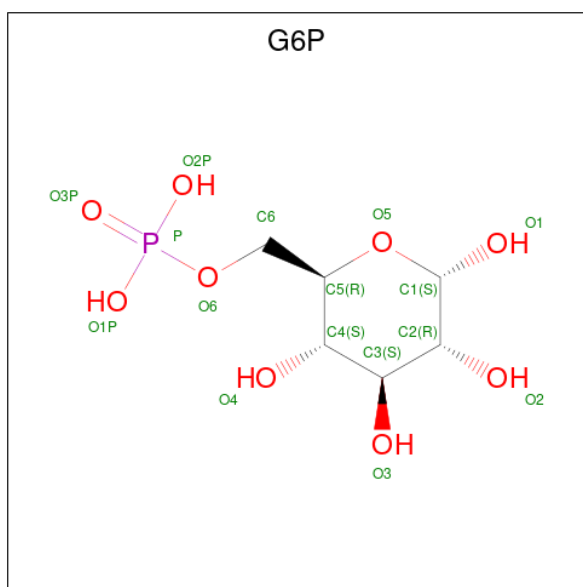
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P27472
C	169	GLN	GLU	engineered mutation	UNP P27472
C	535	SER	ALA	conflict	UNP P27472
D	-19	MET	-	initiating methionine	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression 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 (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



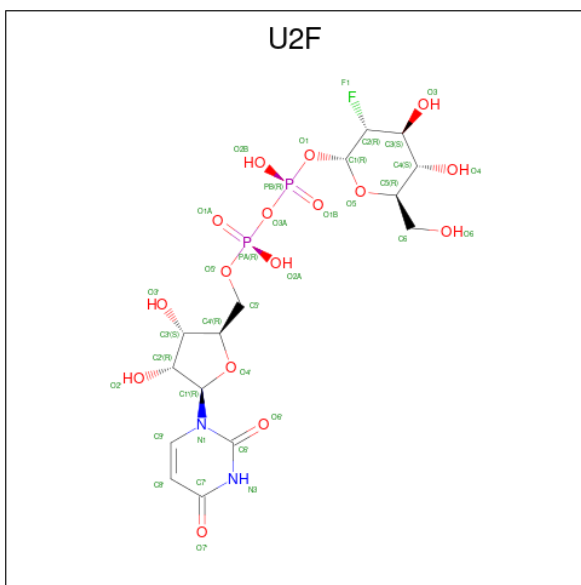
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- 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-2-DEOXY-2-FLUORO-ALPHA-D-GLUCOSE (three-letter code: 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	P	0	0
			36	15	1	2	16	2		

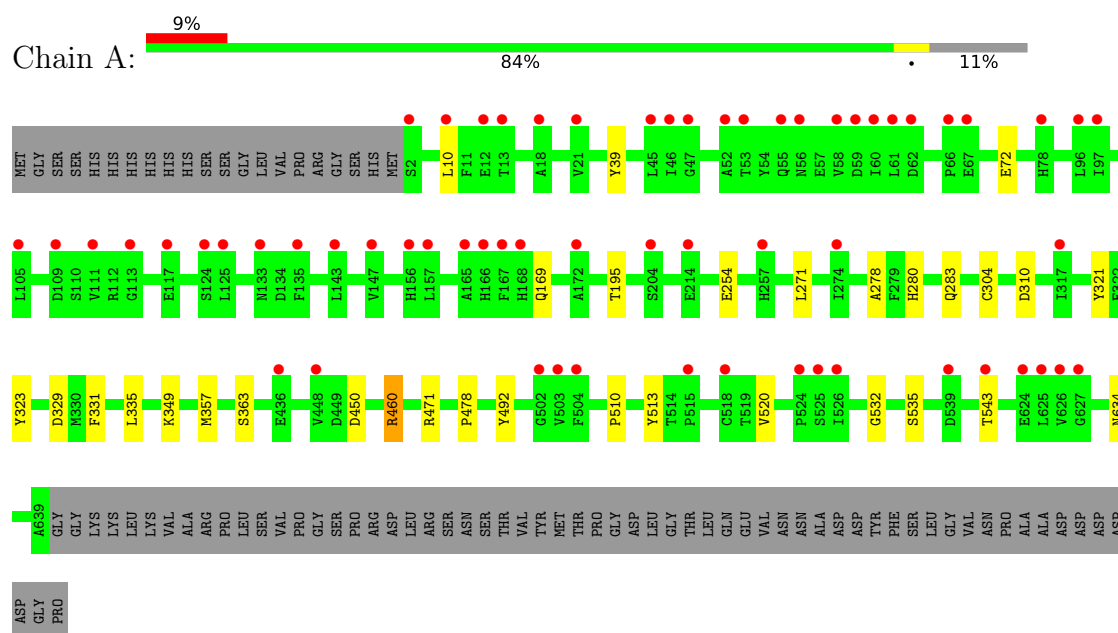
- Molecule 5 is water.

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

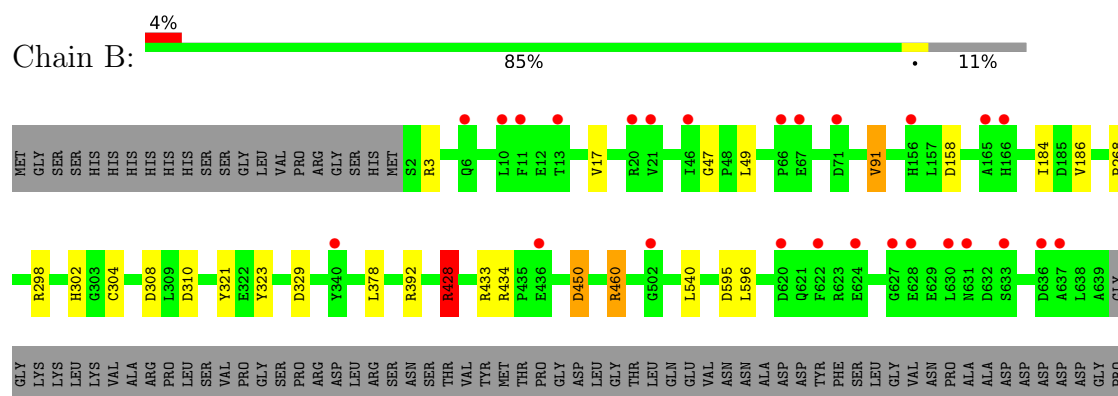
3 Residue-property plots [i](#)

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.

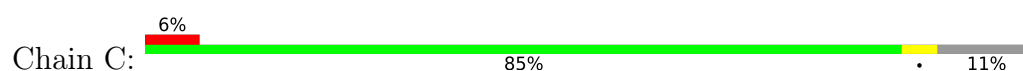
- Molecule 1: Glycogen [starch] synthase isoform 2



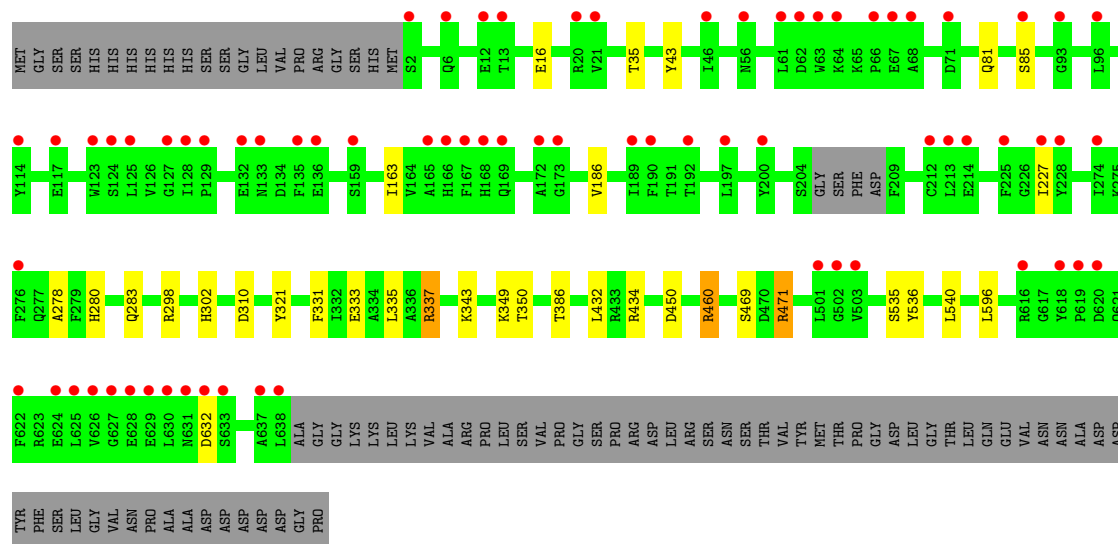
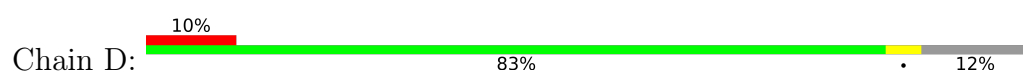
- Molecule 1: Glycogen [starch] synthase isoform 2



- 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	193.52Å 204.71Å 206.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.38 – 2.73 29.84 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.5 (145.38-2.73) 99.6 (29.84-2.73)	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 (5.08%)	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 , 39.2	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, G6P, U2F

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	0.48	0/5184	0.67	2/7048 (0.0%)
1	B	0.53	0/5230	0.74	8/7098 (0.1%)
1	C	0.50	0/5258	0.72	4/7128 (0.1%)
1	D	0.51	0/5146	0.71	5/6994 (0.1%)
All	All	0.50	0/20818	0.71	19/28268 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	471	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	D	471	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	428	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	460	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	C	610	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	298	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	D	337	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	C	460	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	450	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	308	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	C	320	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	460	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	460	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	298	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	460	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	634	ASN	CB-CA-C	-5.11	100.18	110.40
1	C	610	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	392	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	433	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5059	0	4852	14	0
1	B	5105	0	4958	9	0
1	C	5133	0	5024	12	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	50	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 (50) 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:B:450:ASP:OD1	1:B:460:ARG:NH2	2.38	0.56
1:C:396:HIS:HE1	1:C:407:THR:O	1.91	0.52
1:D:227:ILE:HG22	1:D:227:ILE:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	0.46
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:A:195:THR:OG1	1:A:254:GLU:OE1	2.21	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
1:C:326:LYS:NZ	1:C:509:GLU:OE1	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	636/720 (88%)	608 (96%)	27 (4%)	1 (0%)	47 69
1	B	636/720 (88%)	616 (97%)	20 (3%)	0	100 100
1	C	636/720 (88%)	612 (96%)	23 (4%)	1 (0%)	47 69
1	D	629/720 (87%)	601 (96%)	27 (4%)	1 (0%)	47 69
All	All	2537/2880 (88%)	2437 (96%)	97 (4%)	3 (0%)	51 75

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	533/621 (86%)	526 (99%)	7 (1%)	69 82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	542/621 (87%)	535 (99%)	7 (1%)	69	82
1	C	548/621 (88%)	542 (99%)	6 (1%)	73	84
1	D	529/621 (85%)	525 (99%)	4 (1%)	81	89
All	All	2152/2484 (87%)	2128 (99%)	24 (1%)	73	84

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	304	CYS
1	A	310	ASP
1	A	321	TYR
1	A	363	SER
1	A	513	TYR
1	A	543	THR
1	B	91	VAL
1	B	268	PRO
1	B	304	CYS
1	B	310	ASP
1	B	321	TYR
1	B	428	ARG
1	B	595	ASP
1	C	86	ARG
1	C	135	PHE
1	C	321	TYR
1	C	366	VAL
1	C	419	SER
1	C	513	TYR
1	D	16	GLU
1	D	81	GLN
1	D	310	ASP
1	D	321	TYR

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

Mol	Chain	Res	Type
1	A	277	GLN
1	A	477	HIS
1	B	484	ASN
1	C	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	78	HIS
1	C	229	HIS
1	C	396	HIS
1	C	484	ASN
1	C	582	GLN
1	C	586	GLN
1	D	283	GLN
1	D	302	HIS
1	D	403	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](#)

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	$\# Z > 2$
2	UDP	B	801	-	20,26,26	0.75	0	25,40,40	1.11	2 (8%)
2	UDP	D	801	-	20,26,26	0.79	0	25,40,40	1.18	2 (8%)
3	G6P	D	802	-	16,16,16	0.51	0	24,24,24	1.02	2 (8%)
3	G6P	B	802	-	16,16,16	0.53	0	24,24,24	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	U2F	C	801	-	31,38,38	1.26	4 (12%)	39,58,58	2.49	10 (25%)
2	UDP	A	801	-	20,26,26	0.72	0	25,40,40	1.09	2 (8%)
3	G6P	A	802	-	16,16,16	0.60	0	24,24,24	0.83	0
3	G6P	C	802	-	16,16,16	0.54	0	24,24,24	0.81	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	B	801	-	-	6/14/32/32	0/2/2/2
2	UDP	D	801	-	-	6/14/32/32	0/2/2/2
3	G6P	D	802	-	-	3/6/26/26	0/1/1/1
3	G6P	B	802	-	-	0/6/26/26	0/1/1/1
4	U2F	C	801	-	-	5/20/59/59	0/3/3/3
2	UDP	A	801	-	-	8/14/32/32	0/2/2/2
3	G6P	A	802	-	-	4/6/26/26	0/1/1/1
3	G6P	C	802	-	-	0/6/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	801	U2F	C2-C1	3.47	1.56	1.52
4	C	801	U2F	PB-O1	2.95	1.68	1.60
4	C	801	U2F	C2-C3	2.76	1.55	1.52
4	C	801	U2F	O4'-C1'	2.58	1.44	1.41

All (18) 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	6.49	114.61	108.85
4	C	801	U2F	PB-O1-C1	4.74	138.08	119.74
4	C	801	U2F	O5-C1-O1	3.86	116.41	111.36
4	C	801	U2F	O3-C3-C2	3.85	117.32	109.68
4	C	801	U2F	C3-C4-C5	-3.59	103.83	110.24
4	C	801	U2F	F1-C2-C1	3.22	111.17	107.57
4	C	801	U2F	O4-C4-C5	2.74	116.10	109.30
2	D	801	UDP	C3'-C2'-C1'	2.63	104.93	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	UDP	PA-O3A-PB	-2.58	123.96	132.83
2	B	801	UDP	PA-O3A-PB	-2.48	124.31	132.83
3	D	802	G6P	O2P-P-O1P	2.44	116.97	107.64
2	D	801	UDP	PA-O3A-PB	-2.41	124.55	132.83
2	A	801	UDP	C3'-C2'-C1'	2.34	104.51	100.98
4	C	801	U2F	O6-C6-C5	-2.23	103.64	111.29
3	D	802	G6P	O6-P-O3P	-2.07	100.67	106.47
2	B	801	UDP	C3'-C2'-C1'	2.03	104.04	100.98
4	C	801	U2F	PA-O3A-PB	-2.00	125.95	132.83

There are no chirality outliers.

All (32) 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	O4'-C4'-C5'-O5'
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
2	D	801	UDP	O4'-C1'-N1-C6
3	A	802	G6P	C6-O6-P-O1P
3	A	802	G6P	C6-O6-P-O2P
3	D	802	G6P	C6-O6-P-O2P
4	C	801	U2F	O4'-C1'-N1-C9'
4	C	801	U2F	C2'-C1'-N1-C9'
2	A	801	UDP	C3'-C4'-C5'-O5'
2	B	801	UDP	O4'-C4'-C5'-O5'
2	D	801	UDP	O4'-C4'-C5'-O5'
4	C	801	U2F	O5-C5-C6-O6
3	D	802	G6P	C6-O6-P-O3P
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	A	801	UDP	C5'-O5'-PA-O3A
2	A	801	UDP	C5'-O5'-PA-O2A
2	D	801	UDP	C3'-C4'-C5'-O5'
2	D	801	UDP	PB-O3A-PA-O1A
2	B	801	UDP	PB-O3A-PA-O5'
3	A	802	G6P	C6-O6-P-O3P

Continued on next page...

Continued from previous page...

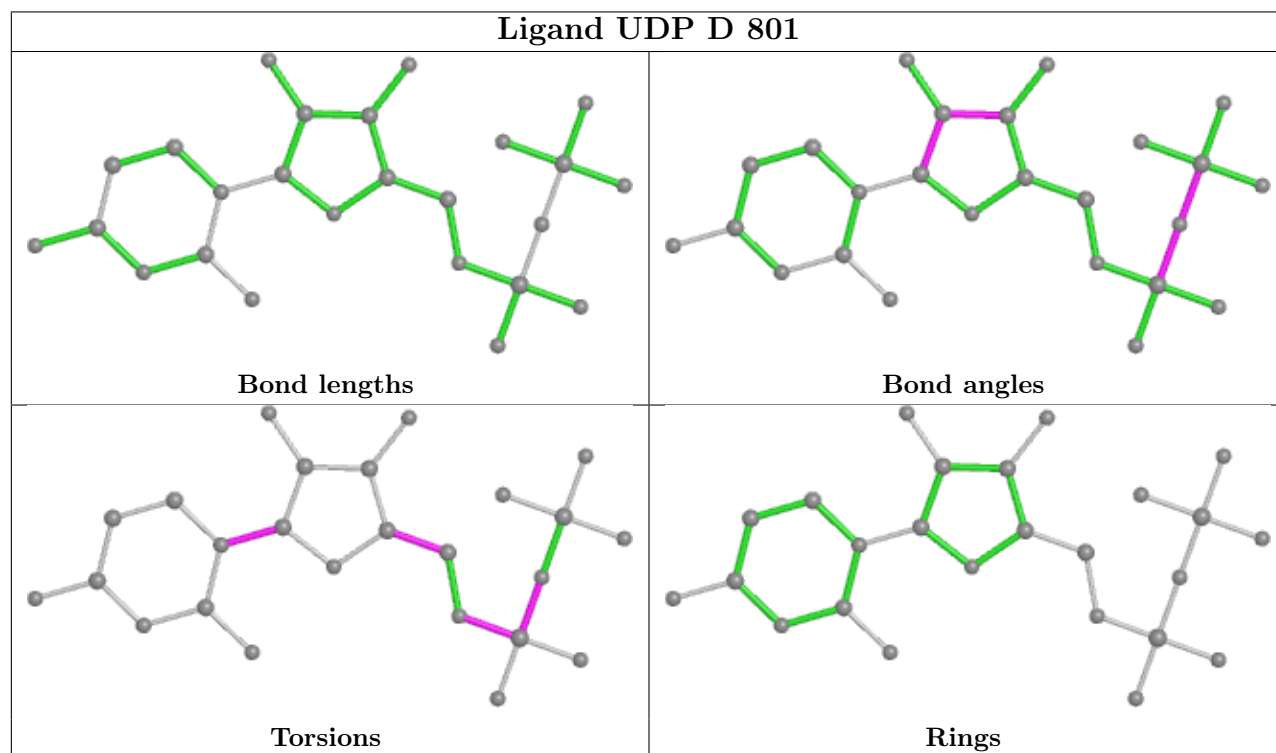
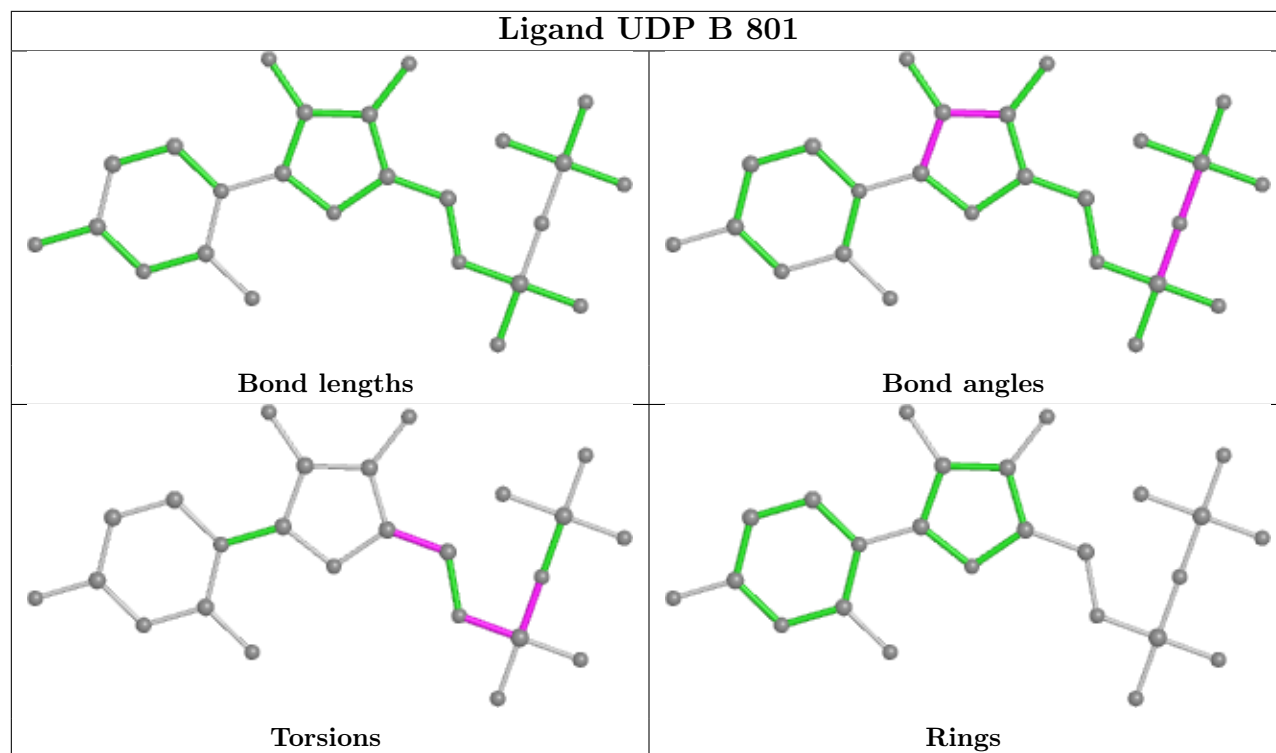
Mol	Chain	Res	Type	Atoms
2	A	801	UDP	PA-O3A-PB-O2B
4	C	801	U2F	O4'-C4'-C5'-O5'
2	B	801	UDP	PB-O3A-PA-O2A
2	D	801	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

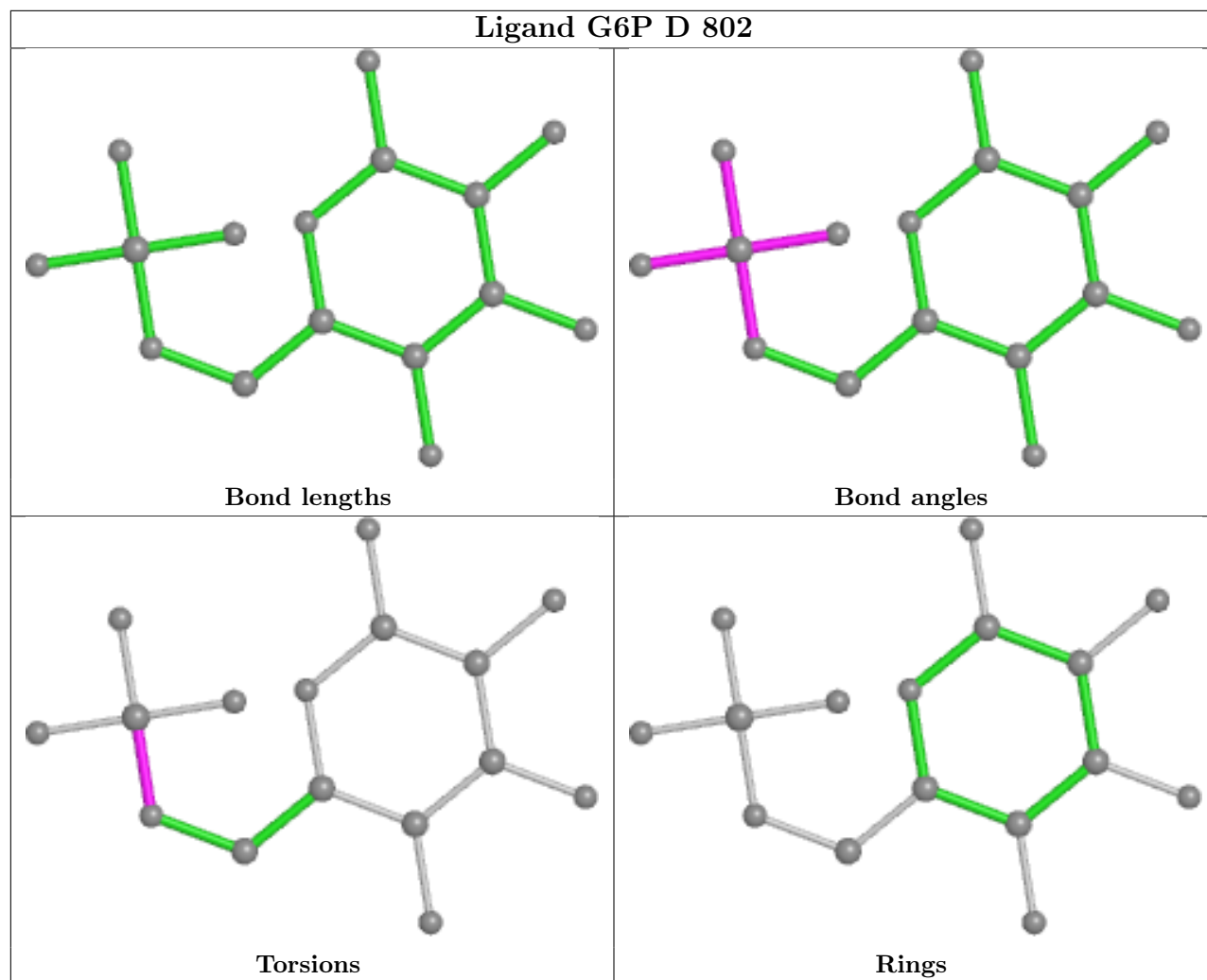
2 monomers are involved in 2 short contacts:

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

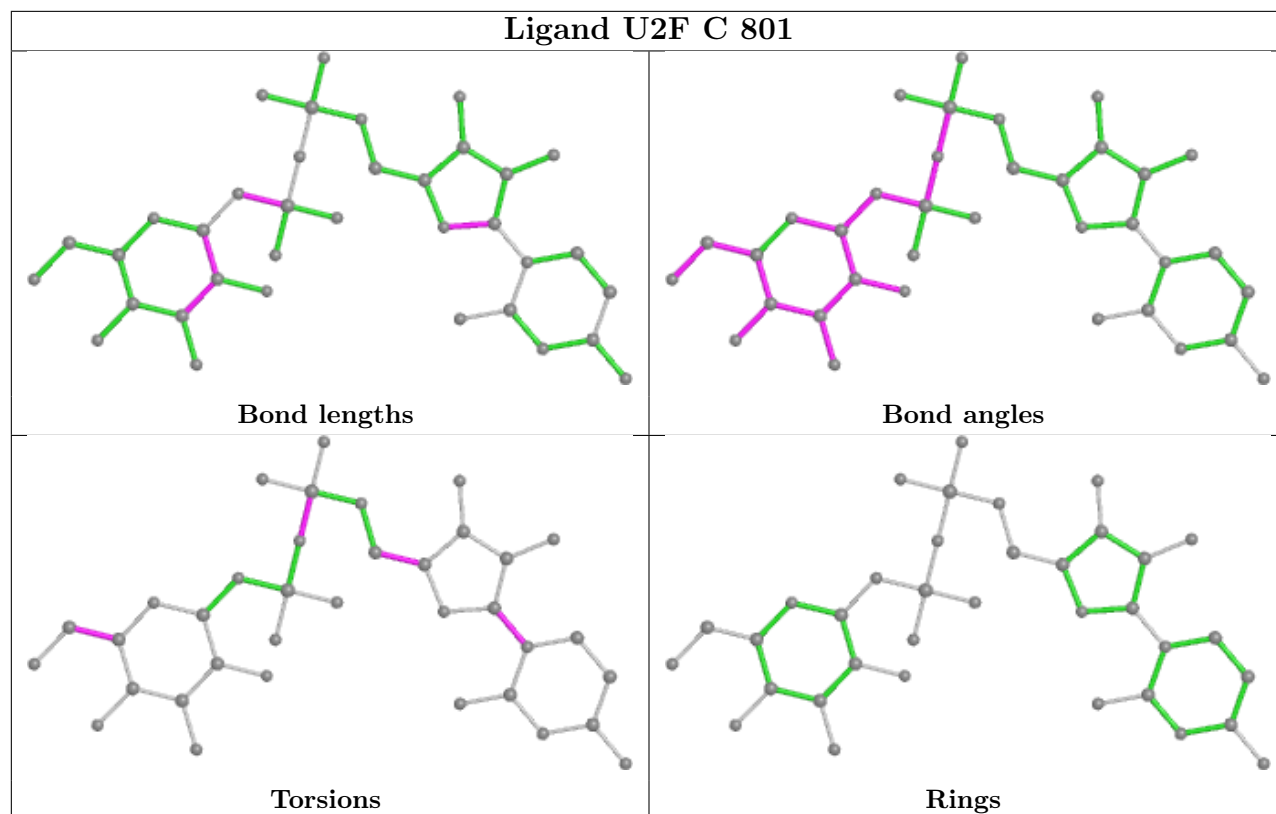
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



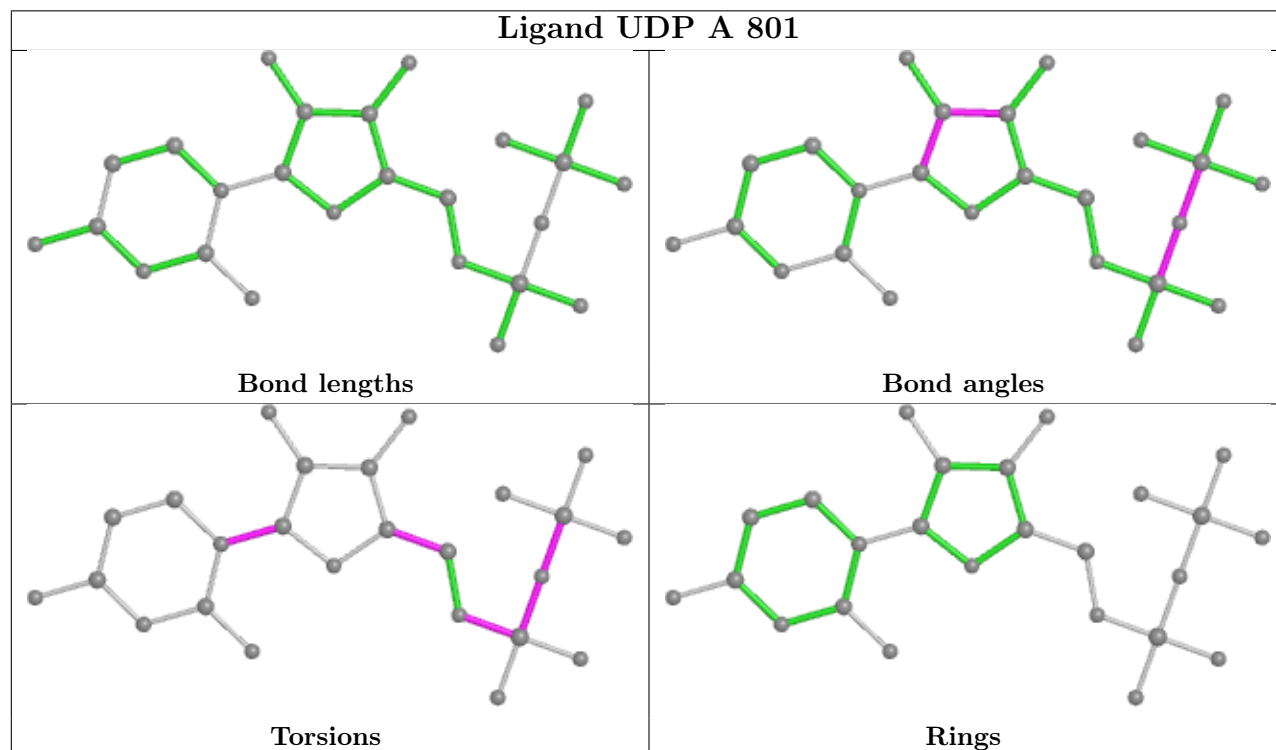
Ligand G6P D 802

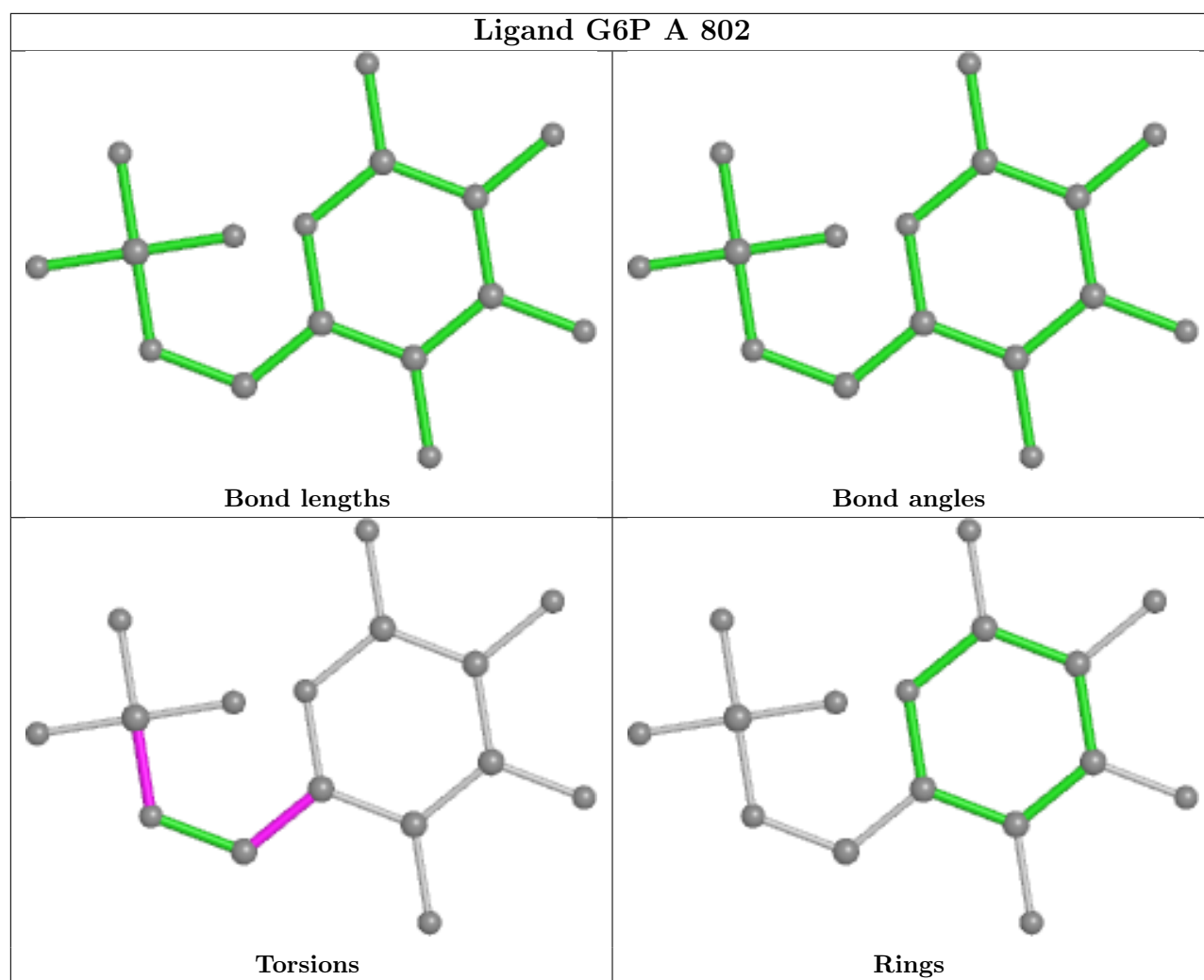


Ligand U2F C 801



Ligand UDP A 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.33	62 (9%) 7 8	44, 80, 160, 181	0
1	B	638/720 (88%)	0.04	26 (4%) 37 41	33, 62, 123, 166	0
1	C	638/720 (88%)	0.22	45 (7%) 16 17	43, 72, 141, 198	0
1	D	633/720 (87%)	0.38	72 (11%) 5 5	37, 81, 158, 188	0
All	All	2547/2880 (88%)	0.24	205 (8%) 12 14	33, 73, 150, 198	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	ALA	8.2
1	D	630	LEU	7.0
1	C	125	LEU	6.5
1	A	135	PHE	6.4
1	A	125	LEU	6.2
1	D	167	PHE	5.5
1	D	629	GLU	5.3
1	D	128	ILE	5.3
1	C	124	SER	5.2
1	D	124	SER	5.2
1	C	135	PHE	5.2
1	B	156	HIS	5.0
1	D	626	VAL	4.8
1	C	128	ILE	4.7
1	D	227	ILE	4.6
1	B	630	LEU	4.6
1	D	274	ILE	4.5
1	D	625	LEU	4.5
1	D	225	PHE	4.5
1	A	96	LEU	4.5
1	C	13	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	13	THR	4.3
1	D	628	GLU	4.3
1	D	624	GLU	4.2
1	A	156	HIS	4.1
1	A	61	LEU	4.0
1	C	129	PRO	4.0
1	D	132	GLU	3.9
1	A	46	ILE	3.9
1	D	61	LEU	3.8
1	B	165	ALA	3.8
1	D	168	HIS	3.8
1	C	133	ASN	3.8
1	C	525	SER	3.8
1	A	503	VAL	3.7
1	C	172	ALA	3.7
1	A	214	GLU	3.7
1	D	125	LEU	3.7
1	B	637	ALA	3.6
1	D	127	GLY	3.6
1	C	55	GLN	3.6
1	D	200	TYR	3.6
1	A	21	VAL	3.6
1	A	78	HIS	3.6
1	A	124	SER	3.6
1	C	624	GLU	3.5
1	D	93	GLY	3.5
1	C	625	LEU	3.5
1	A	165	ALA	3.4
1	D	62	ASP	3.4
1	D	67	GLU	3.4
1	C	66	PRO	3.4
1	A	67	GLU	3.4
1	C	46	ILE	3.3
1	D	166	HIS	3.3
1	D	638	LEU	3.3
1	A	157	LEU	3.3
1	D	620	ASP	3.3
1	D	85	SER	3.3
1	A	204	SER	3.3
1	D	165	ALA	3.3
1	B	166	HIS	3.2
1	D	135	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	625	LEU	3.2
1	D	627	GLY	3.2
1	D	631	ASN	3.2
1	B	67	GLU	3.2
1	D	618	TYR	3.2
1	D	12	GLU	3.2
1	C	626	VAL	3.1
1	A	274	ILE	3.1
1	D	637	ALA	3.1
1	A	626	VAL	3.1
1	D	2	SER	3.1
1	A	13	THR	3.1
1	A	133	ASN	3.1
1	B	11	PHE	3.0
1	C	56	ASN	3.0
1	C	123	TRP	3.0
1	D	117	GLU	3.0
1	D	20	ARG	3.0
1	D	172	ALA	3.0
1	A	55	GLN	3.0
1	D	133	ASN	3.0
1	A	47	GLY	3.0
1	A	45	LEU	2.9
1	A	167	PHE	2.9
1	C	52	ALA	2.9
1	C	11	PHE	2.9
1	C	94	ARG	2.9
1	D	123	TRP	2.9
1	A	502	GLY	2.9
1	A	627	GLY	2.9
1	B	6	GLN	2.9
1	D	213	LEU	2.8
1	B	622	PHE	2.8
1	D	68	ALA	2.8
1	A	53	THR	2.8
1	D	56	ASN	2.8
1	C	526	ILE	2.8
1	B	620	ASP	2.8
1	D	276	PHE	2.7
1	A	111	VAL	2.7
1	C	501	LEU	2.7
1	D	197	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	501	LEU	2.7
1	A	12	GLU	2.7
1	D	173	GLY	2.7
1	D	63	TRP	2.7
1	C	165	ALA	2.7
1	C	524	PRO	2.7
1	D	214	GLU	2.7
1	C	166	HIS	2.6
1	B	10	LEU	2.6
1	A	525	SER	2.6
1	B	21	VAL	2.6
1	D	192	THR	2.6
1	A	172	ALA	2.6
1	D	159	SER	2.6
1	D	632	ASP	2.5
1	A	113	GLY	2.5
1	C	127	GLY	2.5
1	B	20	ARG	2.5
1	C	545	GLN	2.5
1	A	109	ASP	2.5
1	A	624	GLU	2.5
1	D	71	ASP	2.5
1	A	59	ASP	2.5
1	D	96	LEU	2.5
1	D	21	VAL	2.5
1	A	58	VAL	2.5
1	A	518	CYS	2.5
1	A	66	PRO	2.5
1	D	6	GLN	2.5
1	C	126	VAL	2.5
1	C	518	CYS	2.5
1	C	274	ILE	2.4
1	A	448	VAL	2.4
1	D	46	ILE	2.4
1	C	85	SER	2.4
1	D	616	ARG	2.4
1	A	436	GLU	2.4
1	B	633	SER	2.4
1	C	436	GLU	2.4
1	B	631	ASN	2.4
1	C	167	PHE	2.4
1	C	618	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	129	PRO	2.4
1	A	105	LEU	2.4
1	A	543	THR	2.4
1	A	10	LEU	2.4
1	A	143	LEU	2.4
1	A	524	PRO	2.3
1	B	340	TYR	2.3
1	D	66	PRO	2.3
1	A	56	ASN	2.3
1	A	317	ILE	2.3
1	C	503	VAL	2.3
1	B	436	GLU	2.3
1	B	627	GLY	2.3
1	B	636	ASP	2.3
1	A	526	ILE	2.3
1	A	117	GLU	2.3
1	C	131	PRO	2.3
1	D	64	LYS	2.3
1	A	2	SER	2.3
1	D	136	GLU	2.3
1	A	97	ILE	2.3
1	A	539	ASP	2.3
1	A	60	ILE	2.3
1	B	71	ASP	2.3
1	C	60	ILE	2.3
1	C	62	ASP	2.3
1	D	619	PRO	2.2
1	D	114	TYR	2.2
1	A	515	PRO	2.2
1	A	18	ALA	2.2
1	D	622	PHE	2.2
1	B	13	THR	2.2
1	D	502	GLY	2.2
1	B	46	ILE	2.2
1	B	66	PRO	2.2
1	C	628	GLU	2.2
1	D	190	PHE	2.2
1	D	228	TYR	2.2
1	C	147	VAL	2.2
1	C	523	VAL	2.2
1	D	503	VAL	2.2
1	B	628	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	169	GLN	2.2
1	C	86	ARG	2.1
1	D	212	CYS	2.1
1	A	257	HIS	2.1
1	B	624	GLU	2.1
1	A	168	HIS	2.1
1	D	633	SER	2.1
1	C	67	GLU	2.1
1	C	96	LEU	2.1
1	D	189	ILE	2.1
1	A	166	HIS	2.1
1	B	502	GLY	2.1
1	A	62	ASP	2.0
1	A	504	PHE	2.0
1	C	189	ILE	2.0
1	A	147	VAL	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.

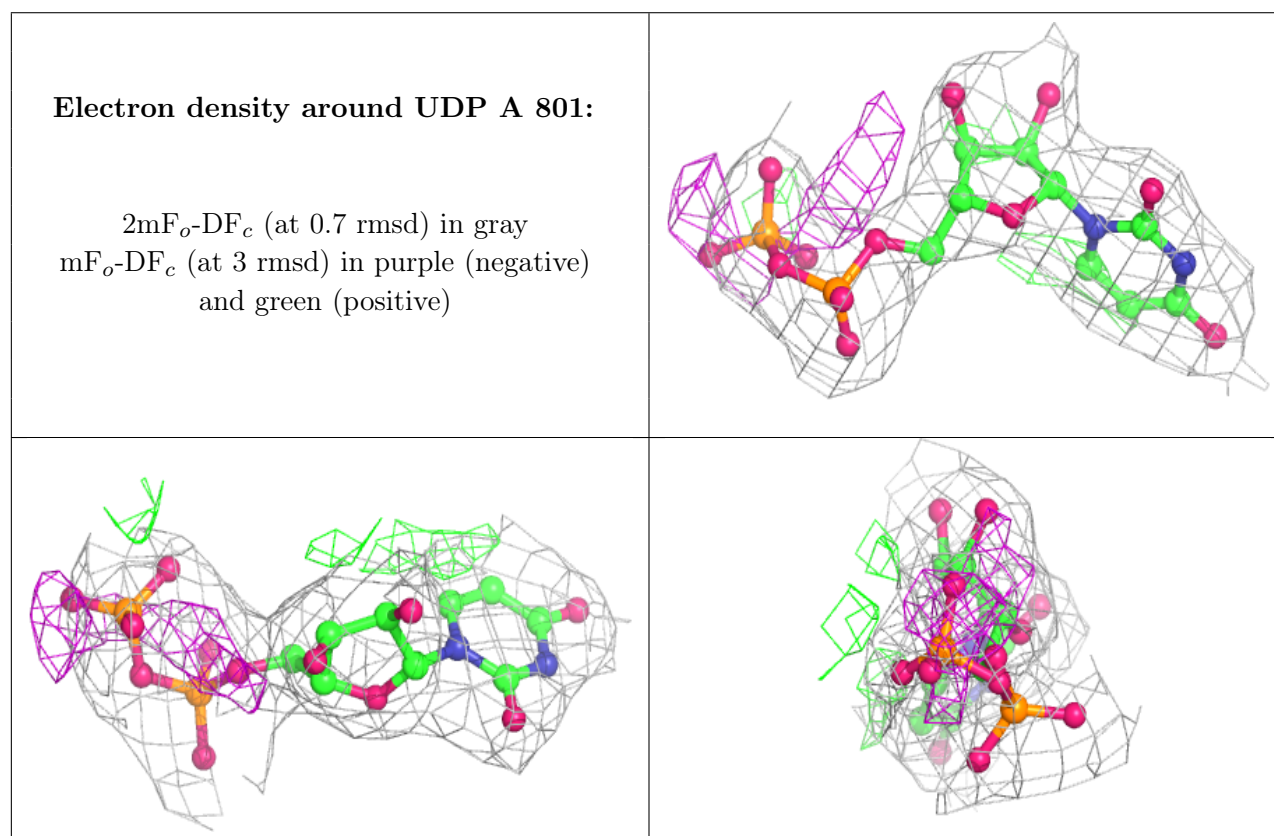
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UDP	A	801	25/25	0.92	0.13	60,77,106,111	0
2	UDP	B	801	25/25	0.92	0.13	46,69,126,128	0
4	U2F	C	801	36/36	0.93	0.16	49,55,61,69	0
2	UDP	D	801	25/25	0.94	0.13	52,71,125,128	0
3	G6P	A	802	16/16	0.96	0.15	44,52,54,55	0
3	G6P	C	802	16/16	0.97	0.14	41,51,54,55	0
3	G6P	D	802	16/16	0.97	0.14	33,37,39,41	0

Continued on next page...

Continued from previous page...

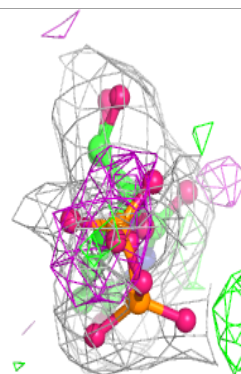
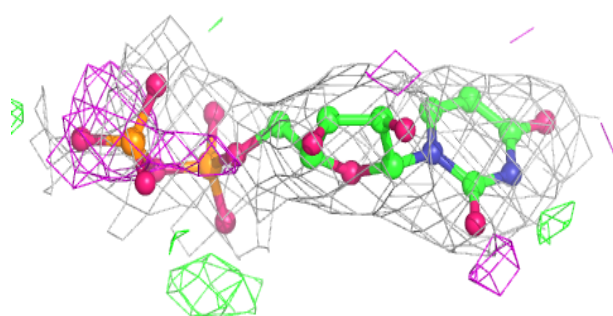
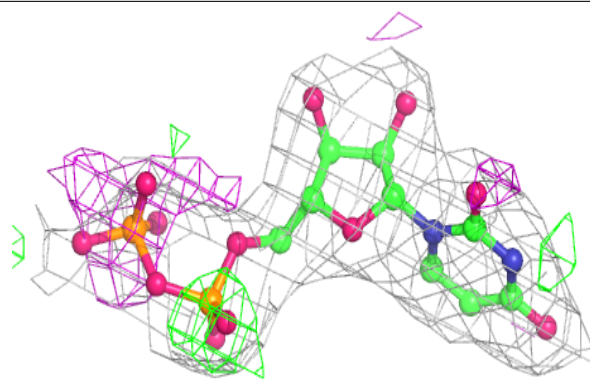
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	G6P	B	802	16/16	0.97	0.13	32,38,39,41	0

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.

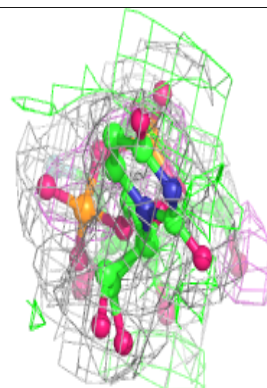
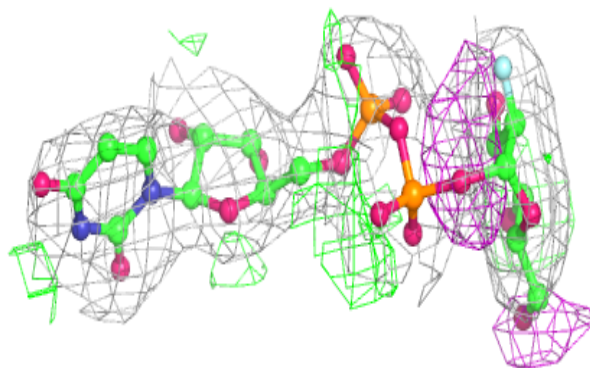
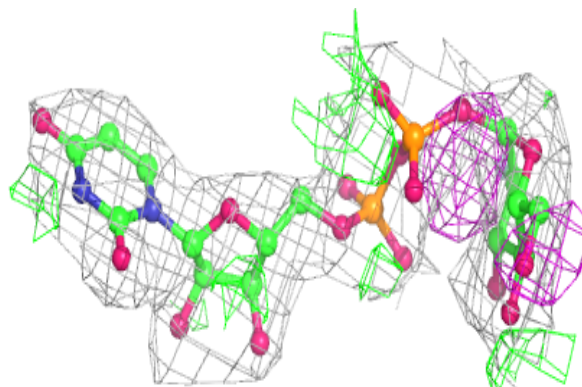


Electron density around UDP B 801:

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

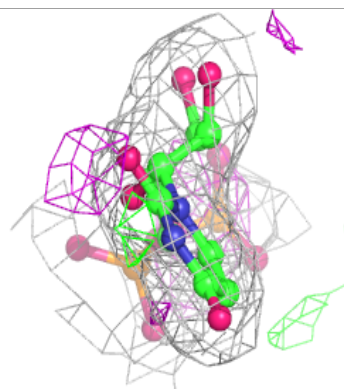
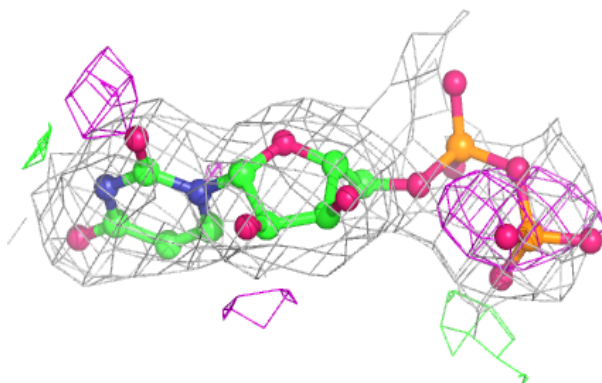
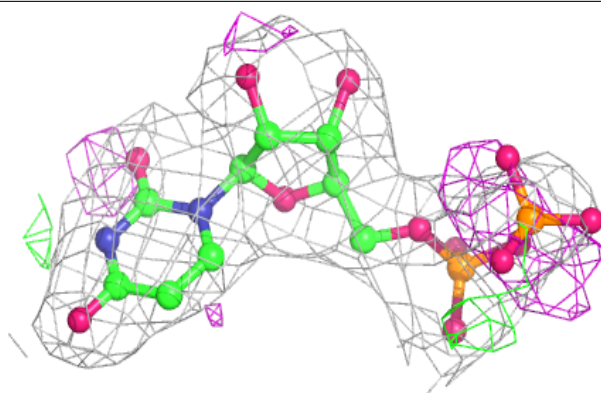
**Electron density around U2F C 801:**

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

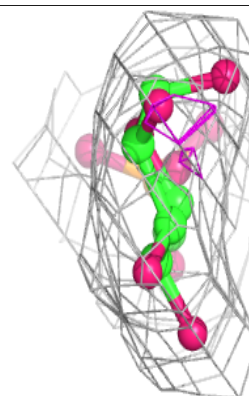
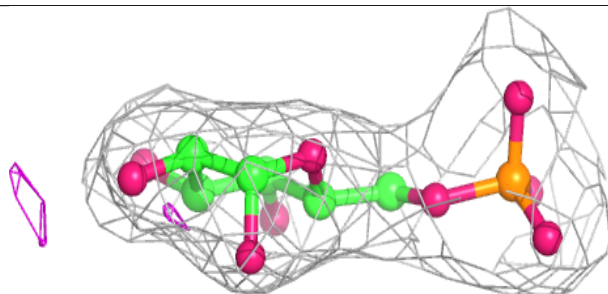
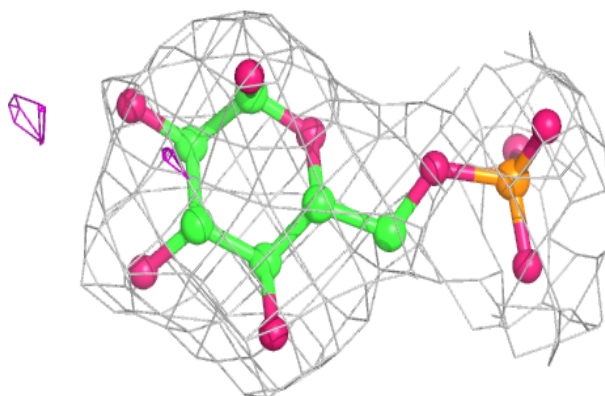


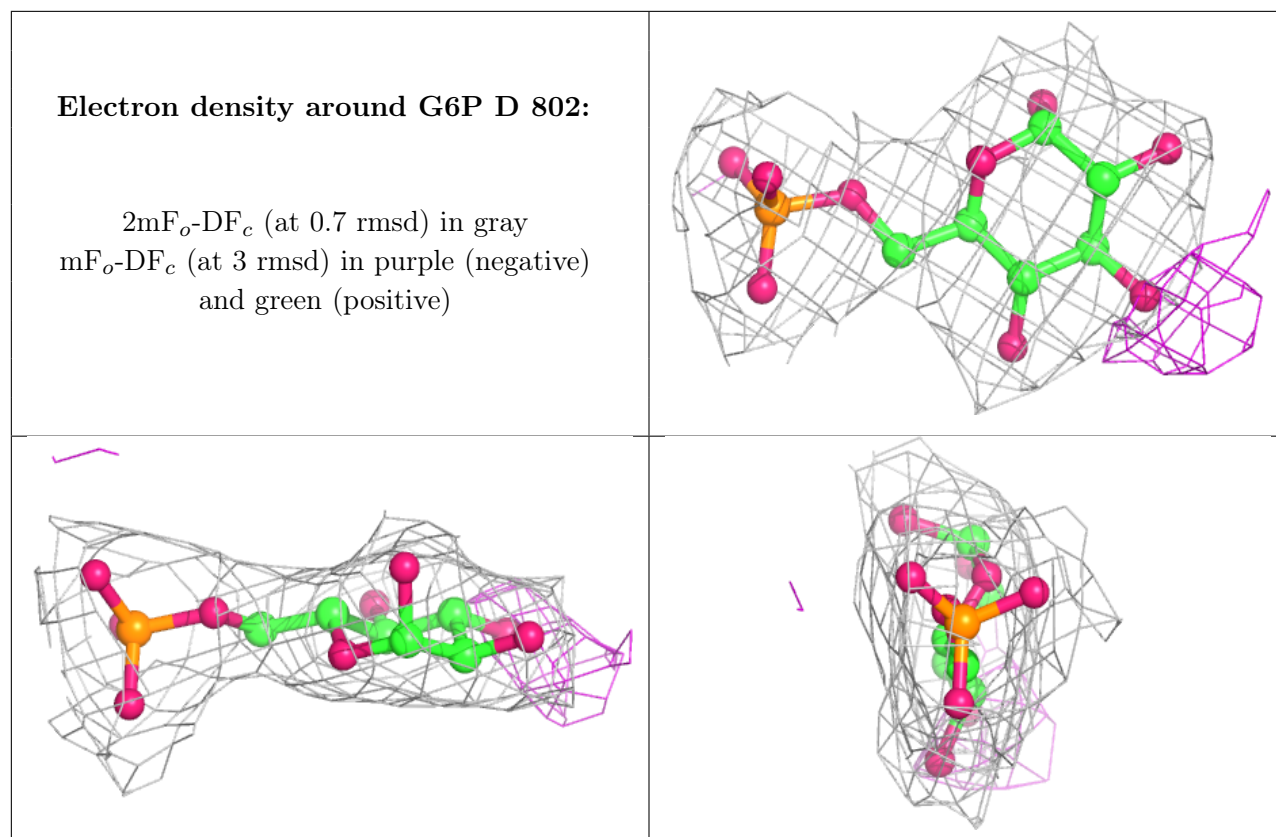
Electron density around UDP D 801:

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

**Electron density around G6P 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.