



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:53 PM BST

PDB ID : 4KQM  
Title : Crystal structure of yeast glycogen synthase E169Q mutant in complex with glucose and UDP  
Authors : Chikwana, V.M.; Hurley, T.D.  
Deposited on : 2013-05-15  
Resolution : 2.77 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](mailto: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.

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

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

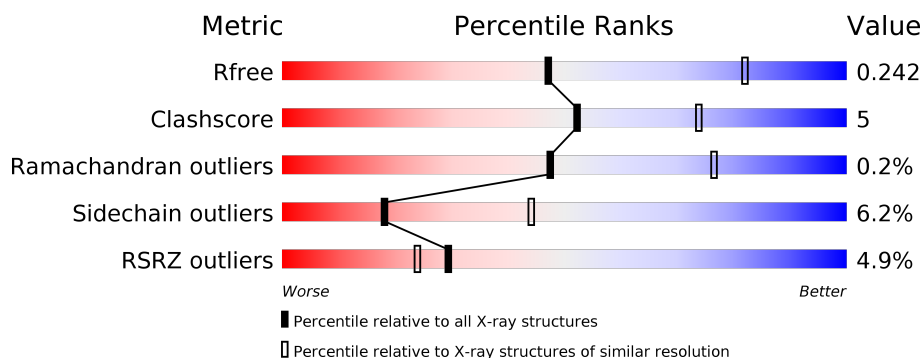
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	724	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	724	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	724	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	724	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20825 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 Gsy2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5157	3292	903	943	19			
1	B	638	Total	C	N	O	S	0	1	0
			5163	3296	904	944	19			
1	C	638	Total	C	N	O	S	0	0	0
			5157	3292	903	943	19			
1	D	635	Total	C	N	O	S	0	0	0
			5132	3276	900	937	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP E7NKU1
A	-17	GLY	-	expression tag	UNP E7NKU1
A	-16	SER	-	expression tag	UNP E7NKU1
A	-15	SER	-	expression tag	UNP E7NKU1
A	-14	HIS	-	expression tag	UNP E7NKU1
A	-13	HIS	-	expression tag	UNP E7NKU1
A	-12	HIS	-	expression tag	UNP E7NKU1
A	-11	HIS	-	expression tag	UNP E7NKU1
A	-10	HIS	-	expression tag	UNP E7NKU1
A	-9	HIS	-	expression tag	UNP E7NKU1
A	-8	SER	-	expression tag	UNP E7NKU1
A	-7	SER	-	expression tag	UNP E7NKU1
A	-6	GLY	-	expression tag	UNP E7NKU1
A	-5	LEU	-	expression tag	UNP E7NKU1
A	-4	VAL	-	expression tag	UNP E7NKU1
A	-3	PRO	-	expression tag	UNP E7NKU1
A	-2	ARG	-	expression tag	UNP E7NKU1
A	-1	GLY	-	expression tag	UNP E7NKU1
A	0	SER	-	expression tag	UNP E7NKU1
A	169	GLN	GLU	engineered mutation	UNP E7NKU1
B	-18	MET	-	initiating methionine	UNP E7NKU1

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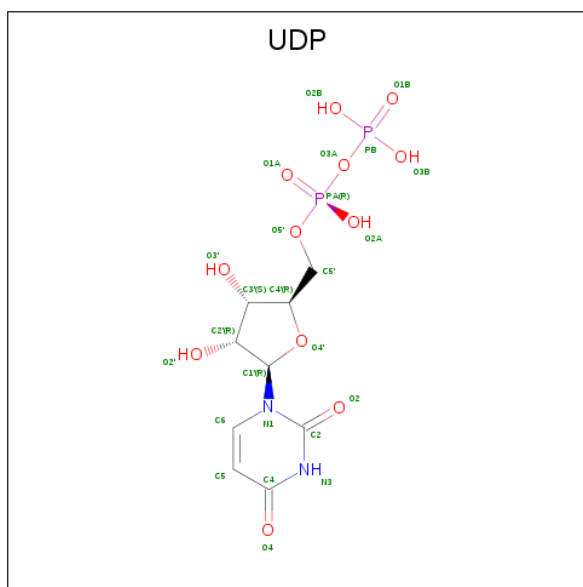
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP E7NKU1
B	-16	SER	-	expression tag	UNP E7NKU1
B	-15	SER	-	expression tag	UNP E7NKU1
B	-14	HIS	-	expression tag	UNP E7NKU1
B	-13	HIS	-	expression tag	UNP E7NKU1
B	-12	HIS	-	expression tag	UNP E7NKU1
B	-11	HIS	-	expression tag	UNP E7NKU1
B	-10	HIS	-	expression tag	UNP E7NKU1
B	-9	HIS	-	expression tag	UNP E7NKU1
B	-8	SER	-	expression tag	UNP E7NKU1
B	-7	SER	-	expression tag	UNP E7NKU1
B	-6	GLY	-	expression tag	UNP E7NKU1
B	-5	LEU	-	expression tag	UNP E7NKU1
B	-4	VAL	-	expression tag	UNP E7NKU1
B	-3	PRO	-	expression tag	UNP E7NKU1
B	-2	ARG	-	expression tag	UNP E7NKU1
B	-1	GLY	-	expression tag	UNP E7NKU1
B	0	SER	-	expression tag	UNP E7NKU1
B	169	GLN	GLU	engineered mutation	UNP E7NKU1
C	-18	MET	-	initiating methionine	UNP E7NKU1
C	-17	GLY	-	expression tag	UNP E7NKU1
C	-16	SER	-	expression tag	UNP E7NKU1
C	-15	SER	-	expression tag	UNP E7NKU1
C	-14	HIS	-	expression tag	UNP E7NKU1
C	-13	HIS	-	expression tag	UNP E7NKU1
C	-12	HIS	-	expression tag	UNP E7NKU1
C	-11	HIS	-	expression tag	UNP E7NKU1
C	-10	HIS	-	expression tag	UNP E7NKU1
C	-9	HIS	-	expression tag	UNP E7NKU1
C	-8	SER	-	expression tag	UNP E7NKU1
C	-7	SER	-	expression tag	UNP E7NKU1
C	-6	GLY	-	expression tag	UNP E7NKU1
C	-5	LEU	-	expression tag	UNP E7NKU1
C	-4	VAL	-	expression tag	UNP E7NKU1
C	-3	PRO	-	expression tag	UNP E7NKU1
C	-2	ARG	-	expression tag	UNP E7NKU1
C	-1	GLY	-	expression tag	UNP E7NKU1
C	0	SER	-	expression tag	UNP E7NKU1
C	169	GLN	GLU	engineered mutation	UNP E7NKU1
D	-18	MET	-	initiating methionine	UNP E7NKU1
D	-17	GLY	-	expression tag	UNP E7NKU1
D	-16	SER	-	expression tag	UNP E7NKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP E7NKU1
D	-14	HIS	-	expression tag	UNP E7NKU1
D	-13	HIS	-	expression tag	UNP E7NKU1
D	-12	HIS	-	expression tag	UNP E7NKU1
D	-11	HIS	-	expression tag	UNP E7NKU1
D	-10	HIS	-	expression tag	UNP E7NKU1
D	-9	HIS	-	expression tag	UNP E7NKU1
D	-8	SER	-	expression tag	UNP E7NKU1
D	-7	SER	-	expression tag	UNP E7NKU1
D	-6	GLY	-	expression tag	UNP E7NKU1
D	-5	LEU	-	expression tag	UNP E7NKU1
D	-4	VAL	-	expression tag	UNP E7NKU1
D	-3	PRO	-	expression tag	UNP E7NKU1
D	-2	ARG	-	expression tag	UNP E7NKU1
D	-1	GLY	-	expression tag	UNP E7NKU1
D	0	SER	-	expression tag	UNP E7NKU1
D	169	GLN	GLU	engineered mutation	UNP E7NKU1

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



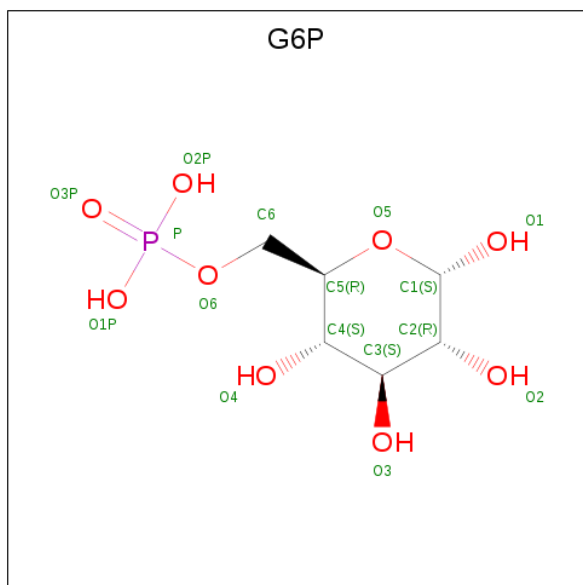
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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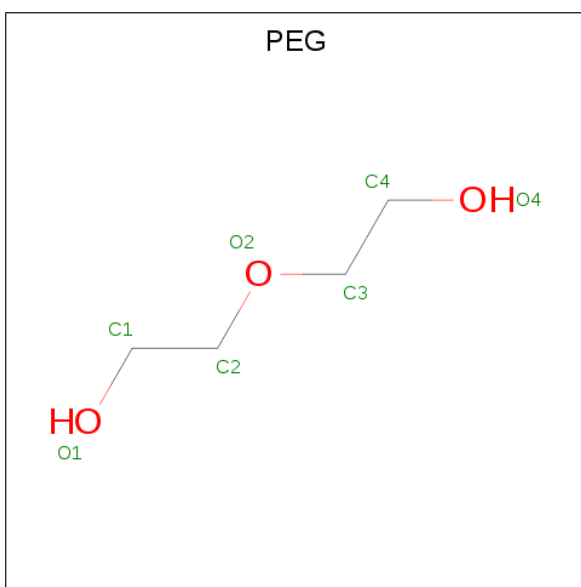
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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



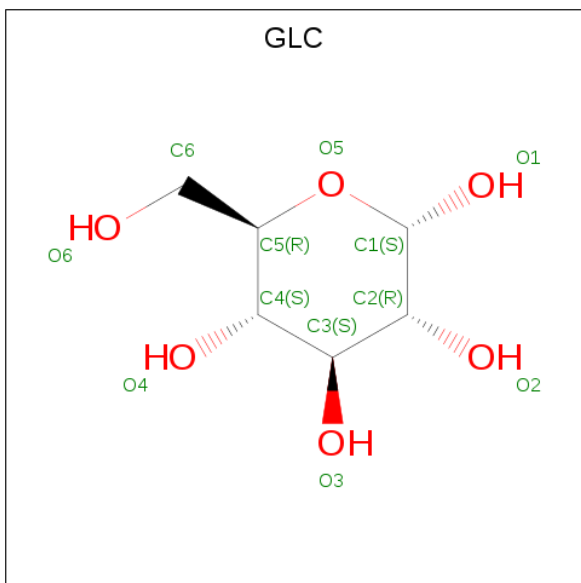
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	O	P	16	6	9
			1	6	9	1			
3	B	1	Total	C	O	P	16	6	9
			1	6	9	1			
3	C	1	Total	C	O	P	16	6	9
			1	6	9	1			
3	D	1	Total	C	O	P	16	6	9
			1	6	9	1			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



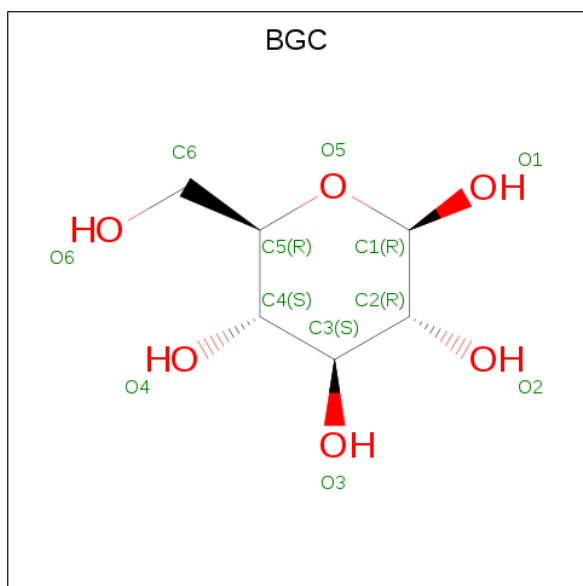
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 6 is beta-D-glucopyranose (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



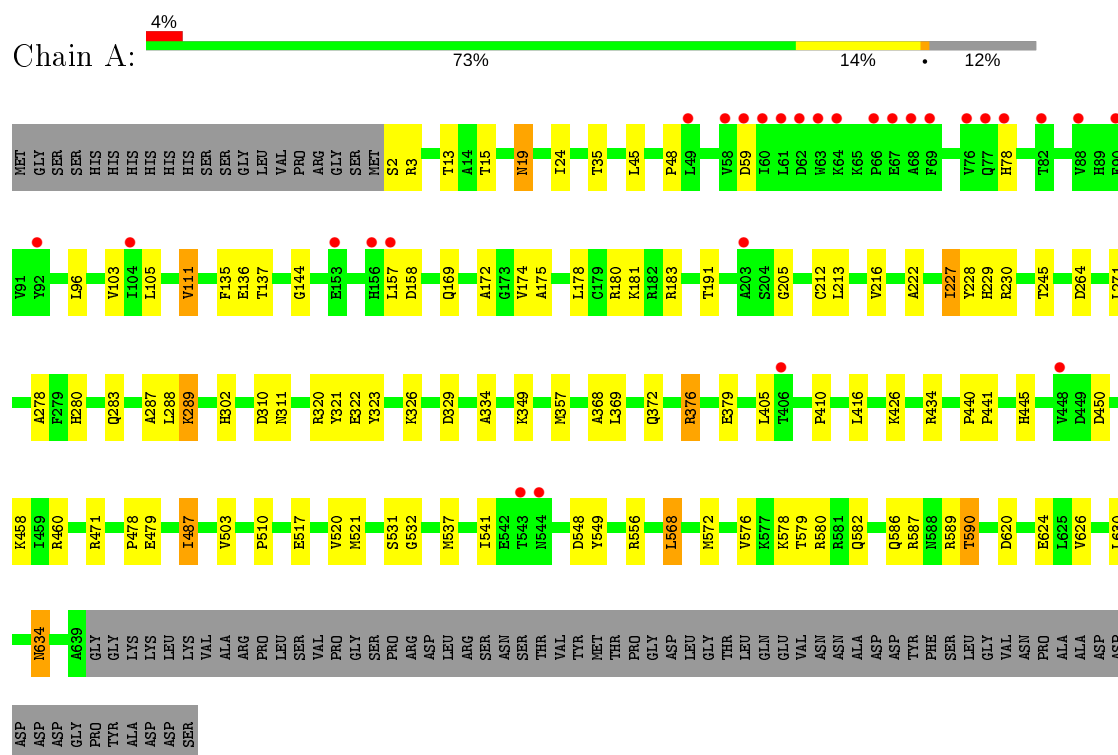
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			12	6	6		



### 3 Residue-property plots [i](#)

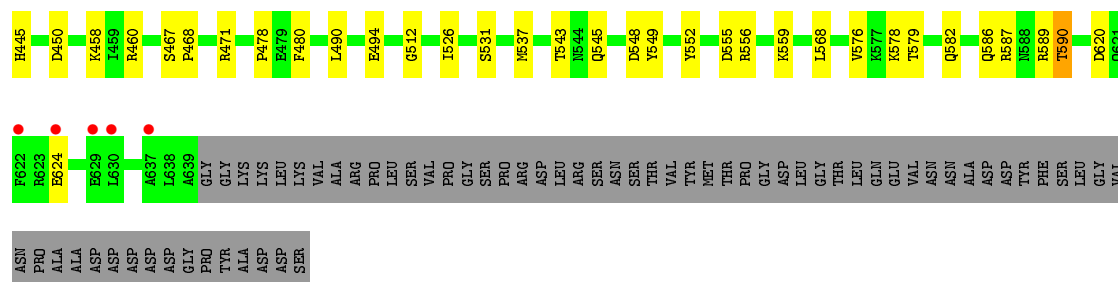
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Gsy2p

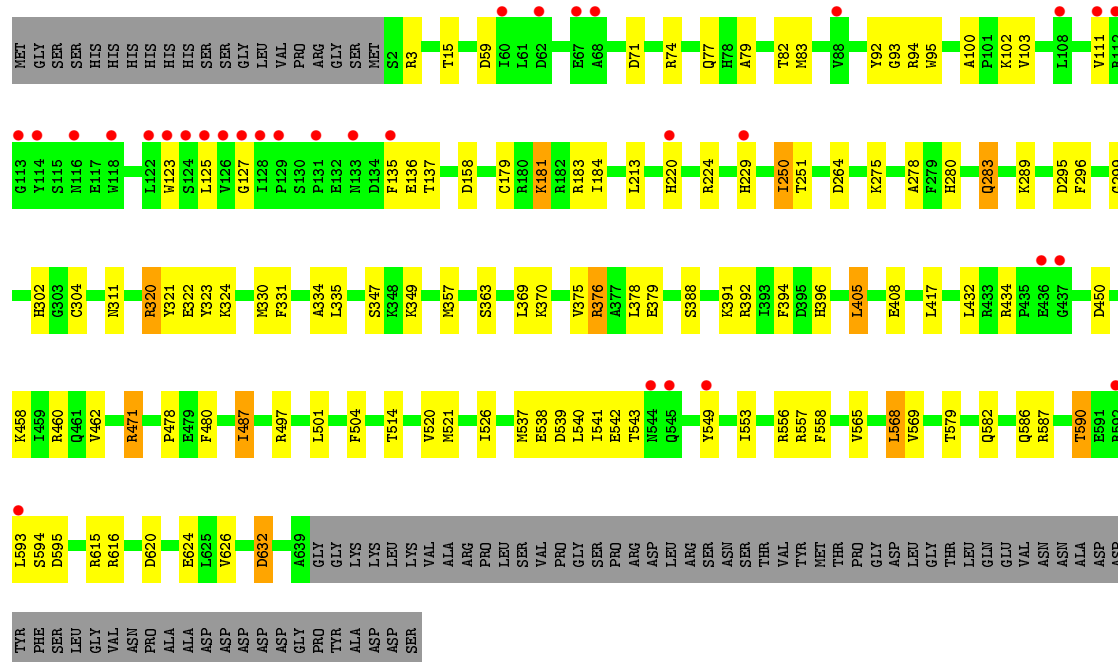


#### • Molecule 1: Gsy2p

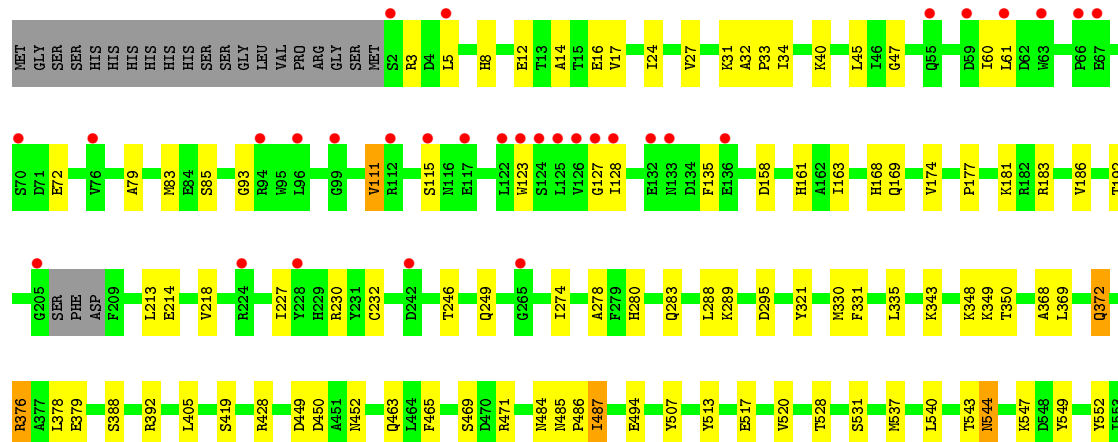


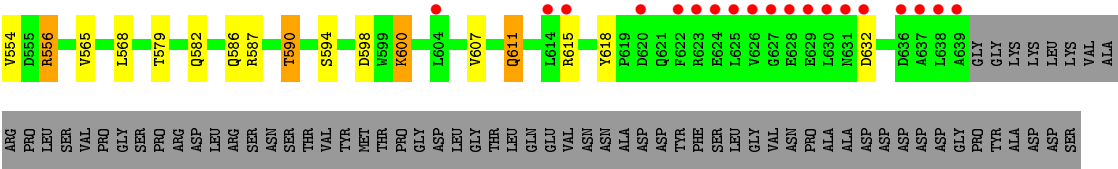


- Molecule 1: Gsy2p



- Molecule 1: Gsy2p





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.71Å 204.44Å 206.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.77 48.41 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.41-2.77) 98.7 (48.41-2.77)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.201 , 0.241 0.201 , 0.242	Depositor DCC
$R_{free}$ test set	5074 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20825	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GLC, UDP, BGC, PEG, 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	0.42	0/5282	0.59	0/7155
1	B	0.51	0/5291	0.67	0/7167
1	C	0.44	0/5282	0.61	0/7155
1	D	0.45	0/5255	0.59	0/7117
All	All	0.46	0/21110	0.62	0/28594

There are no bond length outliers.

There are no bond angle outliers.

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	5157	0	5072	60	0
1	B	5163	0	5080	57	0
1	C	5157	0	5072	64	0
1	D	5132	0	5053	54	1
2	A	25	0	11	0	0
2	B	25	0	11	1	0
2	C	25	0	11	3	0
2	D	25	0	11	0	0
3	A	16	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	11	1	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
4	A	7	0	10	1	0
4	B	7	0	10	1	0
4	C	7	0	10	2	0
4	D	7	0	10	1	0
5	C	12	0	6	0	0
6	C	12	0	6	0	0
All	All	20825	0	20417	226	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 5.

All (226) 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:B:283:GLN:HG2	1:C:280:HIS:CE1	2.00	0.96
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.07	0.88
1:B:280:HIS:CE1	1:C:283:GLN:HG2	2.10	0.86
1:A:379:GLU:HG2	4:B:803:PEG:H41	1.65	0.78
1:B:349:LYS:HE2	1:B:576:VAL:O	1.85	0.77
1:A:586:GLN:O	1:A:590:THR:HG22	1.85	0.76
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.21	0.75
1:B:199:ARG:HG2	1:B:199:ARG:HH11	1.52	0.74
1:B:192:THR:HG22	1:B:246:THR:HG22	1.69	0.74
1:D:586:GLN:O	1:D:590:THR:HG22	1.87	0.74
1:A:19:ASN:HD22	1:A:19:ASN:H	1.40	0.69
1:A:320:ARG:HG3	1:A:326:LYS:HD2	1.73	0.69
1:C:320:ARG:NH2	1:C:322:GLU:OE2	2.25	0.69
1:D:543:THR:O	1:D:544:ASN:HB2	1.92	0.69
1:C:520:VAL:HA	1:C:594:SER:HB3	1.76	0.68
1:B:199:ARG:CG	1:B:199:ARG:HH11	2.07	0.68
1:C:586:GLN:O	1:C:590:THR:HG22	1.93	0.68
1:A:280:HIS:CE1	1:D:283:GLN:CG	2.77	0.67
1:C:391:LYS:HD3	4:C:805:PEG:H41	1.76	0.67
1:B:128:ILE:HG12	1:B:232:CYS:HB3	1.78	0.66
1:B:94:ARG:HD2	1:B:100:ALA:HB1	1.79	0.65
1:A:19:ASN:N	1:A:19:ASN:HD22	1.94	0.64
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.29	0.64
1:B:192:THR:CG2	1:B:246:THR:HG22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.79	0.63
1:A:24:ILE:HD11	1:A:169:GLN:CG	2.29	0.63
1:B:579:THR:H	1:B:582:GLN:NE2	1.97	0.62
1:C:379:GLU:HG2	4:D:803:PEG:H11	1.83	0.61
1:C:378:LEU:HD22	1:C:432:LEU:HD11	1.83	0.61
1:A:283:GLN:HG3	3:A:802:G6P:O1	2.01	0.60
1:B:377:ALA:HB1	1:B:428:ARG:NH1	2.16	0.60
1:A:24:ILE:HD11	1:A:169:GLN:HG3	1.83	0.59
1:C:587:ARG:HA	1:C:590:THR:HG23	1.83	0.59
1:D:579:THR:H	1:D:582:GLN:NE2	2.01	0.59
1:A:369:LEU:HA	1:A:487:ILE:HD11	1.85	0.58
1:B:548:ASP:O	1:B:589:ARG:NH1	2.31	0.58
1:B:586:GLN:O	1:B:590:THR:HG22	2.03	0.58
1:C:304:CYS:SG	1:C:434:ARG:HD3	2.43	0.58
1:D:598:ASP:OD2	1:D:600:LYS:HB2	2.03	0.58
1:D:61:LEU:HD12	1:D:93:GLY:HA2	1.86	0.57
1:B:227:ILE:HD12	1:B:230:ARG:HD2	1.86	0.56
1:B:18:ALA:HB2	1:B:105:LEU:HD22	1.86	0.56
4:A:803:PEG:H12	1:B:379:GLU:HG2	1.88	0.56
1:B:549:TYR:O	1:B:590:THR:HB	2.06	0.56
1:D:513:TYR:O	1:D:517:GLU:HB2	2.06	0.56
1:A:549:TYR:O	1:A:590:THR:HB	2.06	0.55
1:D:579:THR:H	1:D:582:GLN:HE21	1.52	0.55
1:D:549:TYR:O	1:D:590:THR:HB	2.05	0.55
1:B:410:PRO:HG2	1:B:416:LEU:HD21	1.89	0.54
1:B:89:HIS:HD2	1:B:110:SER:HB2	1.72	0.54
1:A:175:ALA:HA	1:A:178:LEU:HD12	1.90	0.54
1:A:264:ASP:O	1:A:634:ASN:HB2	2.08	0.54
1:A:579:THR:H	1:A:582:GLN:NE2	2.06	0.54
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.90	0.53
1:D:227:ILE:HG13	1:D:230:ARG:HD2	1.90	0.53
1:B:320:ARG:HG3	1:B:322:GLU:HG3	1.91	0.53
1:A:103:VAL:HG12	1:A:105:LEU:HG	1.90	0.53
1:D:547:LYS:HG2	1:D:552:TYR:CD1	2.44	0.52
1:D:372:GLN:NE2	1:D:486:PRO:O	2.42	0.52
1:C:320:ARG:NH1	2:C:803:UDP:O3B	2.43	0.52
1:B:213:LEU:HA	1:B:216:VAL:HG13	1.92	0.51
1:D:368:ALA:O	1:D:487:ILE:HD11	2.09	0.51
1:D:27:VAL:O	1:D:31:LYS:HB2	2.10	0.51
1:D:388:SER:HB3	1:D:392:ARG:NH1	2.26	0.51
1:A:372:GLN:NE2	1:A:376:ARG:HH11	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:O	1:A:478:PRO:HA	2.09	0.51
1:A:24:ILE:HD11	1:A:169:GLN:HG2	1.92	0.50
1:C:620:ASP:O	1:C:624:GLU:HG2	2.10	0.50
1:D:3:ARG:NH2	1:D:158:ASP:O	2.45	0.50
1:A:334:ALA:CB	1:A:568:LEU:HD13	2.41	0.50
1:D:5:LEU:O	1:D:8:HIS:HD2	1.94	0.50
1:B:179:CYS:HA	1:B:184:ILE:HD12	1.93	0.50
1:D:123:TRP:O	1:D:127:GLY:HA2	2.11	0.50
1:D:349:LYS:O	1:D:471:ARG:HD3	2.12	0.50
1:B:620:ASP:O	1:B:624:GLU:HG2	2.12	0.50
1:C:579:THR:H	1:C:582:GLN:NE2	2.09	0.50
1:D:449:ASP:OD2	1:D:452:ASN:HB2	2.11	0.50
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.45	0.49
1:A:78:HIS:HB3	1:A:157:LEU:HD13	1.93	0.49
1:C:579:THR:H	1:C:582:GLN:HE21	1.58	0.49
1:A:410:PRO:HG2	1:A:416:LEU:HD21	1.94	0.49
1:B:579:THR:H	1:B:582:GLN:HE21	1.59	0.49
1:A:302:HIS:O	1:A:434:ARG:HD2	2.12	0.49
1:C:95:TRP:HB2	1:C:103:VAL:HG21	1.95	0.49
1:C:92:TYR:OH	1:C:102:LYS:HD2	2.12	0.48
1:C:137:THR:HG21	1:C:229:HIS:CD2	2.48	0.48
1:D:520:VAL:HA	1:D:594:SER:HB2	1.94	0.48
1:D:295:ASP:CG	1:D:376:ARG:HH22	2.17	0.48
1:A:227:ILE:HD12	1:A:230:ARG:HD2	1.96	0.48
1:B:349:LYS:O	1:B:471:ARG:HD3	2.13	0.48
1:A:289:LYS:N	1:A:289:LYS:HD2	2.29	0.48
1:D:587:ARG:HA	1:D:590:THR:HG23	1.96	0.48
1:A:580:ARG:HE	3:A:802:G6P:H62	1.78	0.48
1:C:250:ILE:HG22	1:C:251:THR:N	2.29	0.48
1:C:538:GLU:HG3	1:C:553:ILE:HD13	1.95	0.48
1:A:191:THR:OG1	1:A:245:THR:OG1	2.31	0.47
1:D:368:ALA:C	1:D:487:ILE:HD11	2.35	0.47
1:B:490:LEU:HD22	1:B:494:GLU:HB3	1.95	0.47
1:C:59:ASP:O	1:C:93:GLY:HA3	2.14	0.47
1:B:555:ASP:HB3	1:B:559:LYS:HD2	1.97	0.47
1:A:368:ALA:O	1:A:487:ILE:HD11	2.14	0.47
1:B:59:ASP:HB2	1:B:96:LEU:HD21	1.96	0.47
1:A:626:VAL:HG11	1:A:630:LEU:HD11	1.95	0.47
1:A:13:THR:HG22	1:A:172:ALA:HB1	1.95	0.47
1:B:199:ARG:CG	1:B:199:ARG:NH1	2.70	0.47
1:B:283:GLN:CG	1:C:280:HIS:CE1	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.97	0.47
1:A:222:ALA:HB1	1:A:228:TYR:HA	1.97	0.47
1:B:103:VAL:HG12	1:B:105:LEU:HG	1.95	0.47
1:B:445:HIS:ND1	1:B:478:PRO:HD2	2.29	0.47
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.49	0.47
1:C:3:ARG:NH2	1:C:158:ASP:O	2.47	0.47
1:D:174:VAL:O	1:D:177:PRO:HD2	2.15	0.47
1:A:572:MET:O	1:A:576:VAL:HG23	2.14	0.47
1:D:24:ILE:HD11	1:D:169:GLN:HG3	1.97	0.47
1:A:278:ALA:HB1	1:A:280:HIS:CE1	2.50	0.47
1:C:311:ASN:OD1	1:C:349:LYS:NZ	2.46	0.47
1:A:372:GLN:HE21	1:A:376:ARG:NH1	2.12	0.46
1:A:548:ASP:O	1:A:589:ARG:NH1	2.43	0.46
1:B:3:ARG:NH2	1:B:158:ASP:O	2.48	0.46
1:B:578:LYS:HA	1:B:582:GLN:NE2	2.30	0.46
1:C:278:ALA:HB1	1:C:280:HIS:CE1	2.50	0.46
1:C:458:LYS:O	1:C:462:VAL:HG22	2.15	0.46
1:B:480:PHE:CD1	2:B:801:UDP:C4	3.03	0.46
1:A:620:ASP:O	1:A:624:GLU:HG2	2.16	0.46
1:D:507:TYR:HB2	1:D:556:ARG:NH2	2.31	0.46
1:D:607:VAL:O	1:D:611:GLN:HG2	2.15	0.46
1:D:5:LEU:HD21	1:D:618:TYR:HD1	1.81	0.46
1:B:103:VAL:CG1	1:B:105:LEU:HG	2.46	0.46
1:B:95:TRP:HB2	1:B:103:VAL:HG21	1.98	0.46
1:C:504:PHE:CE1	1:C:514:THR:CG2	2.99	0.46
1:A:372:GLN:HE21	1:A:376:ARG:HH11	1.62	0.46
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.98	0.46
1:D:543:THR:O	1:D:544:ASN:CB	2.62	0.46
1:C:370:LYS:HB3	1:C:370:LYS:HE2	1.78	0.46
1:A:311:ASN:OD1	1:A:349:LYS:HD3	2.16	0.46
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.98	0.46
1:B:467:SER:HB2	1:B:468:PRO:HD2	1.97	0.46
1:A:578:LYS:HA	1:A:582:GLN:NE2	2.31	0.45
1:B:283:GLN:HG3	3:B:802:G6P:O1	2.16	0.45
1:B:526:ILE:HG12	1:B:552:TYR:HB2	1.97	0.45
1:C:125:LEU:HD22	1:C:181:LYS:HD2	1.99	0.45
1:C:394:PHE:CE1	1:D:379:GLU:HG3	2.51	0.45
1:B:587:ARG:HA	1:B:590:THR:CG2	2.47	0.45
1:D:278:ALA:HB1	1:D:280:HIS:CE1	2.51	0.45
1:A:19:ASN:N	1:A:19:ASN:ND2	2.63	0.45
1:C:586:GLN:O	1:C:590:THR:CG2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HG21	1:B:229:HIS:HD2	1.81	0.45
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.52	0.45
1:C:330:MET:HG2	1:C:565:VAL:HG22	1.99	0.45
1:A:213:LEU:O	1:A:216:VAL:HG22	2.17	0.45
1:C:388:SER:HB3	1:C:392:ARG:NH1	2.32	0.45
1:D:528:THR:HG22	1:D:554:VAL:HB	1.98	0.45
1:B:440:PRO:HA	1:B:441:PRO:HD3	1.90	0.44
1:C:334:ALA:CB	1:C:568:LEU:HD13	2.47	0.44
1:B:170:TRP:HB2	1:B:233:ILE:HG22	1.98	0.44
4:C:805:PEG:H31	1:D:379:GLU:HG2	2.00	0.44
1:C:557:ARG:HD3	1:C:558:PHE:CE2	2.52	0.44
1:B:119:LYS:NZ	1:B:138:ASN:OD1	2.50	0.44
1:D:34:ILE:HD12	1:D:600:LYS:HA	2.00	0.44
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.53	0.44
1:B:302:HIS:HB2	1:B:432:LEU:HD22	2.00	0.44
1:C:264:ASP:CG	1:C:616:ARG:HH12	2.20	0.44
1:C:357:MET:O	1:C:478:PRO:HA	2.18	0.44
1:B:304:CYS:SG	1:B:440:PRO:HD3	2.58	0.44
1:A:517:GLU:O	1:A:521:MET:HG2	2.17	0.43
1:A:271:LEU:HD13	1:A:520:VAL:HG21	2.01	0.43
1:D:14:ALA:HB2	1:D:168:HIS:HB2	2.00	0.43
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.50	0.43
1:C:295:ASP:HB3	1:C:376:ARG:HH22	1.83	0.43
1:B:418:LYS:O	1:B:421:ASP:HB2	2.18	0.43
1:C:123:TRP:O	1:C:127:GLY:HA2	2.18	0.43
1:C:179:CYS:HA	1:C:184:ILE:HD12	2.00	0.43
1:A:283:GLN:CG	1:D:280:HIS:CE1	2.99	0.43
1:C:299:GLY:HA2	1:C:375:VAL:HG21	2.00	0.43
1:C:549:TYR:O	1:C:590:THR:HB	2.19	0.43
1:D:330:MET:HG2	1:D:565:VAL:HG22	2.01	0.43
1:A:15:THR:HA	1:A:48:PRO:HD2	2.00	0.43
1:B:79:ALA:O	1:B:83:MET:HG2	2.19	0.43
1:A:445:HIS:NE2	1:A:479:GLU:OE1	2.46	0.43
1:A:587:ARG:HA	1:A:590:THR:HG23	2.01	0.43
1:C:71:ASP:HA	1:C:74:ARG:HG2	2.01	0.43
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.51	0.43
1:D:79:ALA:O	1:D:83:MET:HG2	2.19	0.43
1:A:3:ARG:NH2	1:A:158:ASP:O	2.51	0.42
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.54	0.42
1:A:503:VAL:HG21	1:A:572:MET:HE2	2.02	0.42
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:ARG:CZ	1:C:521:MET:HG2	2.49	0.42
1:C:369:LEU:HA	1:C:487:ILE:HD11	2.02	0.42
1:D:463:GLN:HG2	1:D:465:PHE:HE2	1.83	0.42
1:C:137:THR:HG21	1:C:229:HIS:HD2	1.84	0.42
1:D:72:GLU:O	1:D:161:HIS:HE1	2.03	0.42
1:D:615:ARG:CZ	1:D:632:ASP:HB3	2.49	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.88	0.42
1:A:379:GLU:HG3	1:B:394:PHE:CE1	2.54	0.42
1:C:349:LYS:O	1:C:471:ARG:HG3	2.19	0.42
1:C:549:TYR:HB3	1:C:593:LEU:HD11	2.02	0.42
1:D:484:ASN:O	1:D:485:ASN:C	2.57	0.42
1:C:320:ARG:HH11	2:C:803:UDP:PB	2.43	0.41
1:C:396:HIS:CE1	1:C:405:LEU:HG	2.55	0.41
1:C:615:ARG:CZ	1:C:632:ASP:HB3	2.50	0.41
1:D:343:LYS:HD3	1:D:469:SER:O	2.20	0.41
1:C:565:VAL:O	1:C:569:VAL:HG23	2.20	0.41
1:A:287:ALA:HB2	3:A:802:G6P:H2	2.03	0.41
1:A:510:PRO:O	1:A:532:GLY:HA3	2.20	0.41
1:C:299:GLY:O	1:C:302:HIS:HD2	2.03	0.41
1:C:79:ALA:O	1:C:83:MET:HG2	2.20	0.41
1:D:32:ALA:N	1:D:33:PRO:HD2	2.35	0.41
1:B:25:TYR:CE1	1:B:95:TRP:HZ2	2.39	0.41
1:C:501:LEU:HD21	1:C:526:ILE:HD11	2.02	0.41
1:C:480:PHE:CD1	2:C:803:UDP:C4	3.09	0.41
1:C:94:ARG:HD2	1:C:100:ALA:HB1	2.03	0.41
1:C:296:PHE:CE1	1:C:487:ILE:HG23	2.55	0.41
1:C:323:TYR:OH	1:C:458:LYS:CG	2.69	0.41
1:D:369:LEU:HD23	1:D:487:ILE:HD12	2.01	0.41
1:A:137:THR:HG21	1:A:229:HIS:HD2	1.86	0.41
1:A:440:PRO:HA	1:A:441:PRO:HD3	1.90	0.40
1:B:24:ILE:CD1	1:B:169:GLN:HG3	2.51	0.40
1:C:250:ILE:CG2	1:C:251:THR:N	2.84	0.40
1:C:74:ARG:NH1	1:C:77:GLN:OE1	2.54	0.40
1:D:192:THR:CG2	1:D:246:THR:HG22	2.52	0.40
1:B:234:GLU:HG2	1:B:259:LEU:HD21	2.03	0.40
1:B:278:ALA:HB1	1:B:280:HIS:CE1	2.56	0.40
1:D:17:VAL:HB	1:D:47:GLY:HA3	2.04	0.40
1:C:504:PHE:CD1	1:C:514:THR:CG2	3.05	0.40

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]	1.92	0.28

## 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	636/724 (88%)	610 (96%)	24 (4%)	2 (0%)	41	70
1	B	637/724 (88%)	620 (97%)	16 (2%)	1 (0%)	47	76
1	C	636/724 (88%)	611 (96%)	25 (4%)	0	100	100
1	D	631/724 (87%)	600 (95%)	29 (5%)	2 (0%)	41	70
All	All	2540/2896 (88%)	2441 (96%)	94 (4%)	5 (0%)	47	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLY
1	D	111	VAL
1	D	544	ASN
1	A	111	VAL
1	B	512	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	553/624 (89%)	523 (95%)	30 (5%)	22	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	554/624 (89%)	519 (94%)	35 (6%)	18	43
1	C	553/624 (89%)	516 (93%)	37 (7%)	16	40
1	D	550/624 (88%)	514 (94%)	36 (6%)	17	41
All	All	2210/2496 (88%)	2072 (94%)	138 (6%)	18	44

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	19	ASN
1	A	35	THR
1	A	45	LEU
1	A	111	VAL
1	A	135	PHE
1	A	136	GLU
1	A	180	ARG
1	A	181	LYS
1	A	183	ARG
1	A	212	CYS
1	A	227	ILE
1	A	288	LEU
1	A	289	LYS
1	A	310	ASP
1	A	321	TYR
1	A	322	GLU
1	A	376	ARG
1	A	405	LEU
1	A	426	LYS
1	A	458	LYS
1	A	471	ARG
1	A	487	ILE
1	A	531	SER
1	A	537	MET
1	A	541	ILE
1	A	556	ARG
1	A	568	LEU
1	A	590	THR
1	A	634	ASN
1	B	15	THR
1	B	34	ILE
1	B	40	LYS

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	60	ILE
1	B	82	THR
1	B	111	VAL
1	B	123	TRP
1	B	156	HIS
1	B	183	ARG
1	B	199	ARG
1	B	216	VAL
1	B	227	ILE
1	B	249	GLN
1	B	274	ILE
1	B	289	LYS
1	B	291	GLU
1	B	295	ASP
1	B	321	TYR
1	B	348	LYS
1	B	372[A]	GLN
1	B	372[B]	GLN
1	B	376	ARG
1	B	391	LYS
1	B	403	ASN
1	B	428	ARG
1	B	436	GLU
1	B	458	LYS
1	B	531	SER
1	B	537	MET
1	B	543	THR
1	B	545	GLN
1	B	556	ARG
1	B	568	LEU
1	B	590	THR
1	C	15	THR
1	C	82	THR
1	C	111	VAL
1	C	135	PHE
1	C	136	GLU
1	C	181	LYS
1	C	183	ARG
1	C	213	LEU
1	C	220	HIS
1	C	224	ARG

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Mol	Chain	Res	Type
1	C	250	ILE
1	C	275	LYS
1	C	283	GLN
1	C	289	LYS
1	C	320	ARG
1	C	321	TYR
1	C	324	LYS
1	C	347	SER
1	C	363	SER
1	C	376	ARG
1	C	405	LEU
1	C	408	GLU
1	C	417	LEU
1	C	471	ARG
1	C	487	ILE
1	C	537	MET
1	C	539	ASP
1	C	540	LEU
1	C	541	ILE
1	C	542	GLU
1	C	543	THR
1	C	556	ARG
1	C	568	LEU
1	C	590	THR
1	C	595	ASP
1	C	626	VAL
1	C	632	ASP
1	D	12	GLU
1	D	16	GLU
1	D	40	LYS
1	D	45	LEU
1	D	60	ILE
1	D	111	VAL
1	D	115	SER
1	D	135	PHE
1	D	181	LYS
1	D	183	ARG
1	D	213	LEU
1	D	214	GLU
1	D	218	VAL
1	D	249	GLN
1	D	274	ILE

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Mol	Chain	Res	Type
1	D	288	LEU
1	D	289	LYS
1	D	321	TYR
1	D	348	LYS
1	D	372	GLN
1	D	376	ARG
1	D	378	LEU
1	D	405	LEU
1	D	419	SER
1	D	428	ARG
1	D	450	ASP
1	D	487	ILE
1	D	494	GLU
1	D	531	SER
1	D	537	MET
1	D	540	LEU
1	D	556	ARG
1	D	568	LEU
1	D	590	THR
1	D	600	LYS
1	D	611	GLN

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

Mol	Chain	Res	Type
1	A	372	GLN
1	A	484	ASN
1	A	582	GLN
1	A	621	GLN
1	A	634	ASN
1	B	7	ASN
1	B	19	ASN
1	B	89	HIS
1	B	582	GLN
1	C	6	GLN
1	C	89	HIS
1	C	249	GLN
1	C	362	ASN
1	C	582	GLN
1	D	8	HIS
1	D	38	GLN
1	D	249	GLN

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Mol	Chain	Res	Type
1	D	582	GLN
1	D	611	GLN
1	D	631	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

14 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	0.78	0	25,40,40	1.17	2 (8%)
3	G6P	A	802	-	16,16,16	0.52	0	24,24,24	0.88	2 (8%)
2	UDP	A	801	-	20,26,26	0.91	0	25,40,40	1.20	2 (8%)
4	PEG	A	803	-	6,6,6	0.48	0	5,5,5	0.28	0
4	PEG	D	803	-	6,6,6	0.42	0	5,5,5	0.37	0
3	G6P	D	802	-	16,16,16	0.50	0	24,24,24	0.98	1 (4%)
4	PEG	B	803	-	6,6,6	0.45	0	5,5,5	0.42	0
2	UDP	D	801	-	20,26,26	0.85	0	25,40,40	1.15	1 (4%)
5	GLC	C	801	-	12,12,12	0.53	0	17,17,17	0.83	0
3	G6P	B	802	-	16,16,16	0.49	0	24,24,24	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UDP	C	803	-	20,26,26	0.93	1 (5%)	25,40,40	1.21	2 (8%)
3	G6P	C	804	-	16,16,16	0.58	0	24,24,24	0.87	1 (4%)
4	PEG	C	805	-	6,6,6	0.39	0	5,5,5	0.38	0
6	BGC	C	802	-	12,12,12	0.49	0	17,17,17	0.84	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	-	-	5/14/32/32	0/2/2/2
3	G6P	A	802	-	-	1/6/26/26	0/1/1/1
2	UDP	A	801	-	-	8/14/32/32	0/2/2/2
4	PEG	A	803	-	-	3/4/4/4	-
4	PEG	D	803	-	-	3/4/4/4	-
3	G6P	D	802	-	-	0/6/26/26	0/1/1/1
4	PEG	B	803	-	-	3/4/4/4	-
2	UDP	D	801	-	-	5/14/32/32	0/2/2/2
5	GLC	C	801	-	-	0/2/22/22	0/1/1/1
3	G6P	B	802	-	-	2/6/26/26	0/1/1/1
2	UDP	C	803	-	-	8/14/32/32	0/2/2/2
3	G6P	C	804	-	-	0/6/26/26	0/1/1/1
4	PEG	C	805	-	-	3/4/4/4	-
6	BGC	C	802	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	803	UDP	O4'-C1'	2.25	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	UDP	C3'-C2'-C1'	3.22	105.83	100.98
2	A	801	UDP	PA-O3A-PB	-3.04	122.40	132.83
2	D	801	UDP	PA-O3A-PB	-3.01	122.51	132.83
2	B	801	UDP	PA-O3A-PB	-2.61	123.86	132.83
2	A	801	UDP	C3'-C2'-C1'	2.50	104.75	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	803	UDP	O3B-PB-O3A	-2.46	96.37	104.64
3	A	802	G6P	O2P-P-O1P	2.33	116.56	107.64
3	A	802	G6P	O2P-P-O6	-2.33	100.53	106.73
2	C	803	UDP	O3B-PB-O2B	2.10	115.66	107.64
3	D	802	G6P	O3-C3-C4	-2.07	105.56	110.35
3	C	804	G6P	O2P-P-O1P	2.07	115.53	107.64

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	UDP	C2'-C1'-N1-C6
2	B	801	UDP	O4'-C1'-N1-C6
3	B	802	G6P	C4-C5-C6-O6
2	A	801	UDP	O4'-C1'-N1-C6
2	A	801	UDP	C3'-C4'-C5'-O5'
2	A	801	UDP	C5'-O5'-PA-O2A
2	A	801	UDP	C5'-O5'-PA-O3A
2	A	801	UDP	PA-O3A-PB-O3B
2	D	801	UDP	C2'-C1'-N1-C6
2	D	801	UDP	O4'-C1'-N1-C6
2	C	803	UDP	C2'-C1'-N1-C6
2	C	803	UDP	O4'-C1'-N1-C6
2	C	803	UDP	C5'-O5'-PA-O2A
2	C	803	UDP	PB-O3A-PA-O5'
2	A	801	UDP	O4'-C4'-C5'-O5'
2	C	803	UDP	O4'-C4'-C5'-O5'
4	D	803	PEG	O1-C1-C2-O2
4	D	803	PEG	O2-C3-C4-O4
4	B	803	PEG	O1-C1-C2-O2
4	A	803	PEG	O2-C3-C4-O4
4	C	805	PEG	O1-C1-C2-O2
2	B	801	UDP	PA-O3A-PB-O1B
2	D	801	UDP	PA-O3A-PB-O1B
4	C	805	PEG	C4-C3-O2-C2
2	C	803	UDP	C5'-O5'-PA-O3A
4	D	803	PEG	C4-C3-O2-C2
4	A	803	PEG	C1-C2-O2-C3
2	C	803	UDP	C5'-O5'-PA-O1A
4	B	803	PEG	C1-C2-O2-C3
4	A	803	PEG	C4-C3-O2-C2
2	C	803	UDP	C3'-C4'-C5'-O5'

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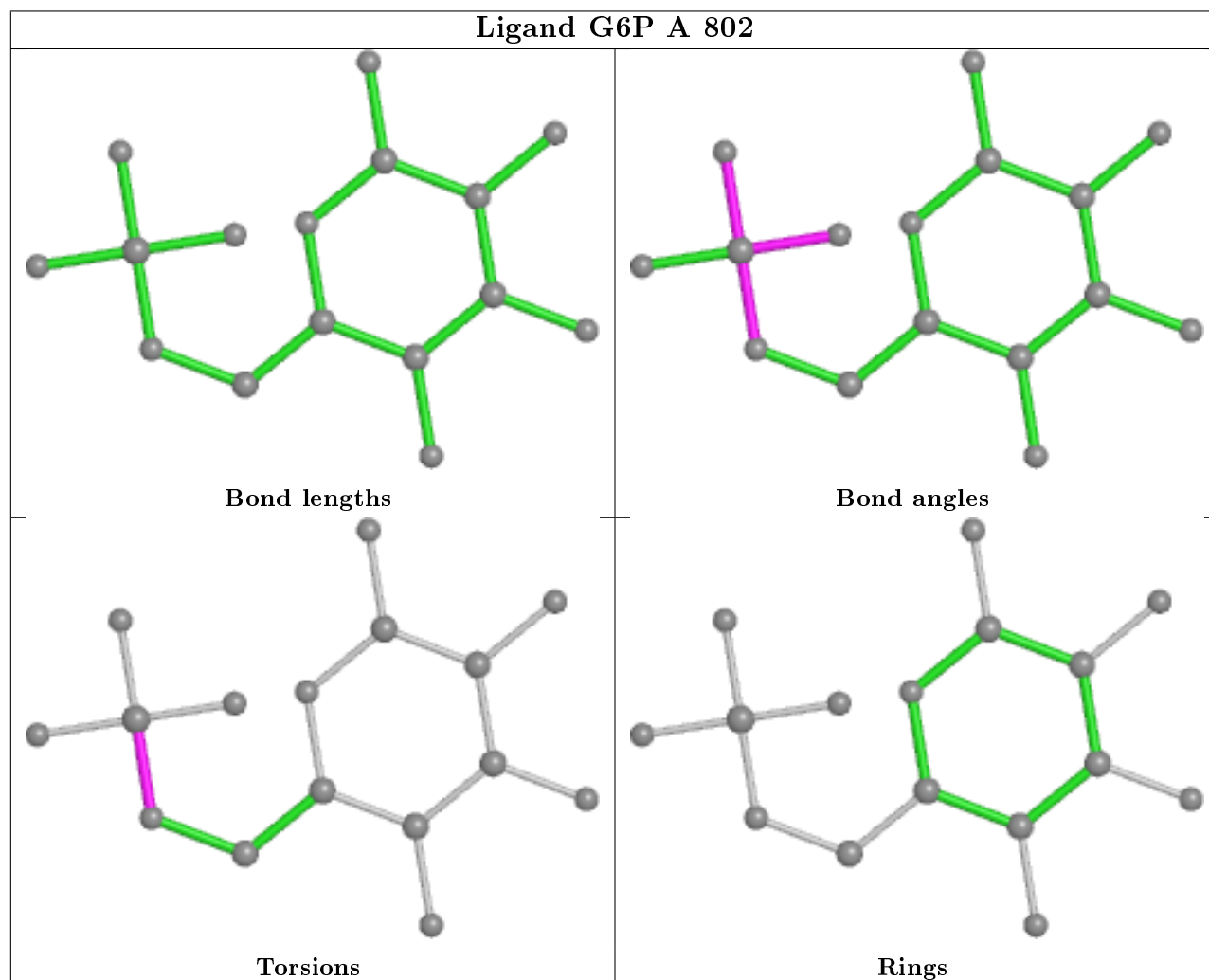
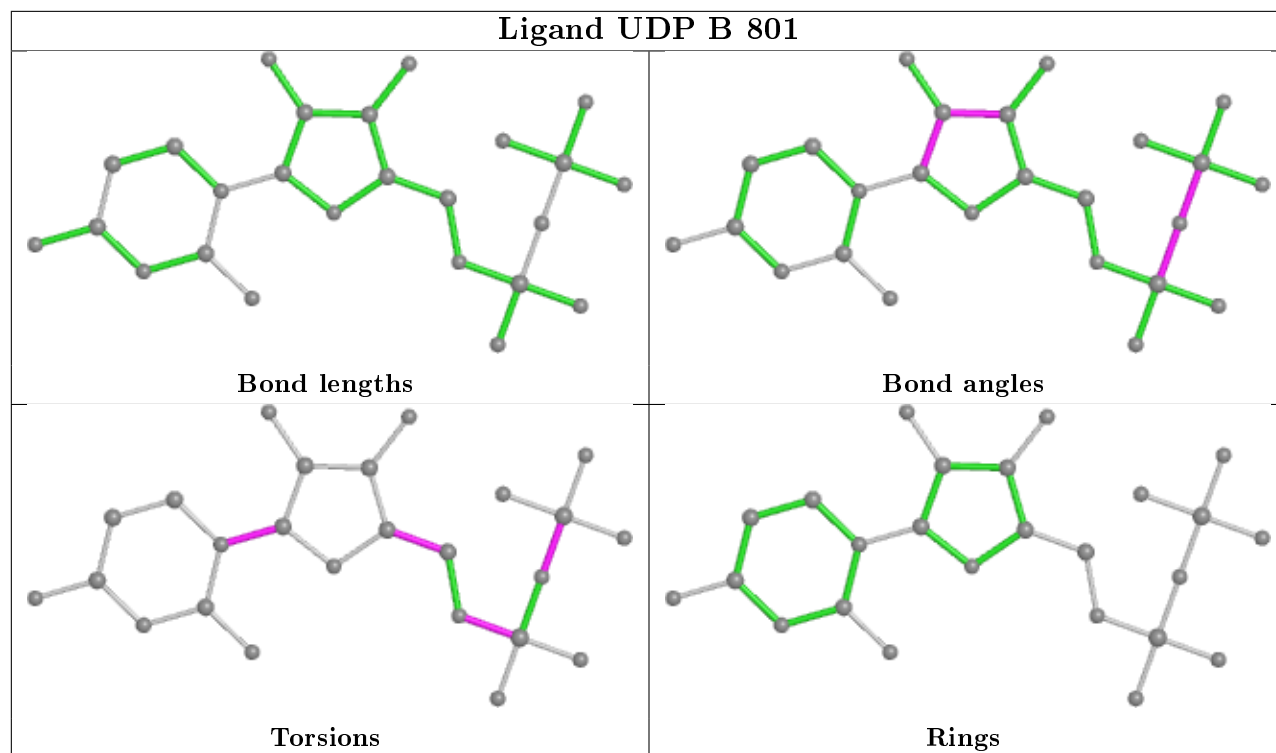
Mol	Chain	Res	Type	Atoms
3	B	802	G6P	O5-C5-C6-O6
3	A	802	G6P	C6-O6-P-O3P
2	A	801	UDP	PA-O3A-PB-O2B
4	C	805	PEG	C1-C2-O2-C3
2	B	801	UDP	O4'-C4'-C5'-O5'
2	D	801	UDP	O4'-C4'-C5'-O5'
4	B	803	PEG	C4-C3-O2-C2
2	B	801	UDP	C5'-O5'-PA-O1A
2	D	801	UDP	C5'-O5'-PA-O1A
2	A	801	UDP	PA-O3A-PB-O1B

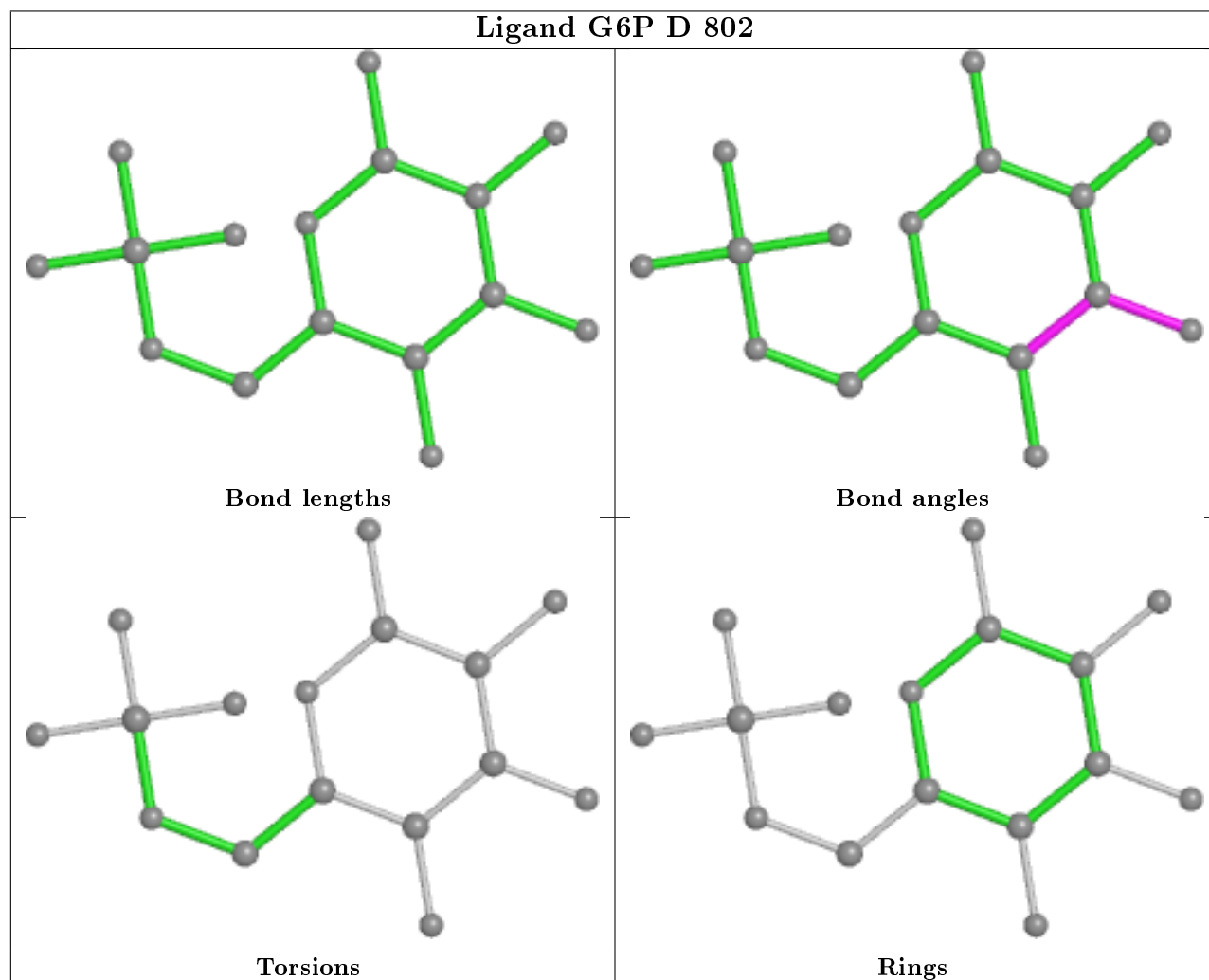
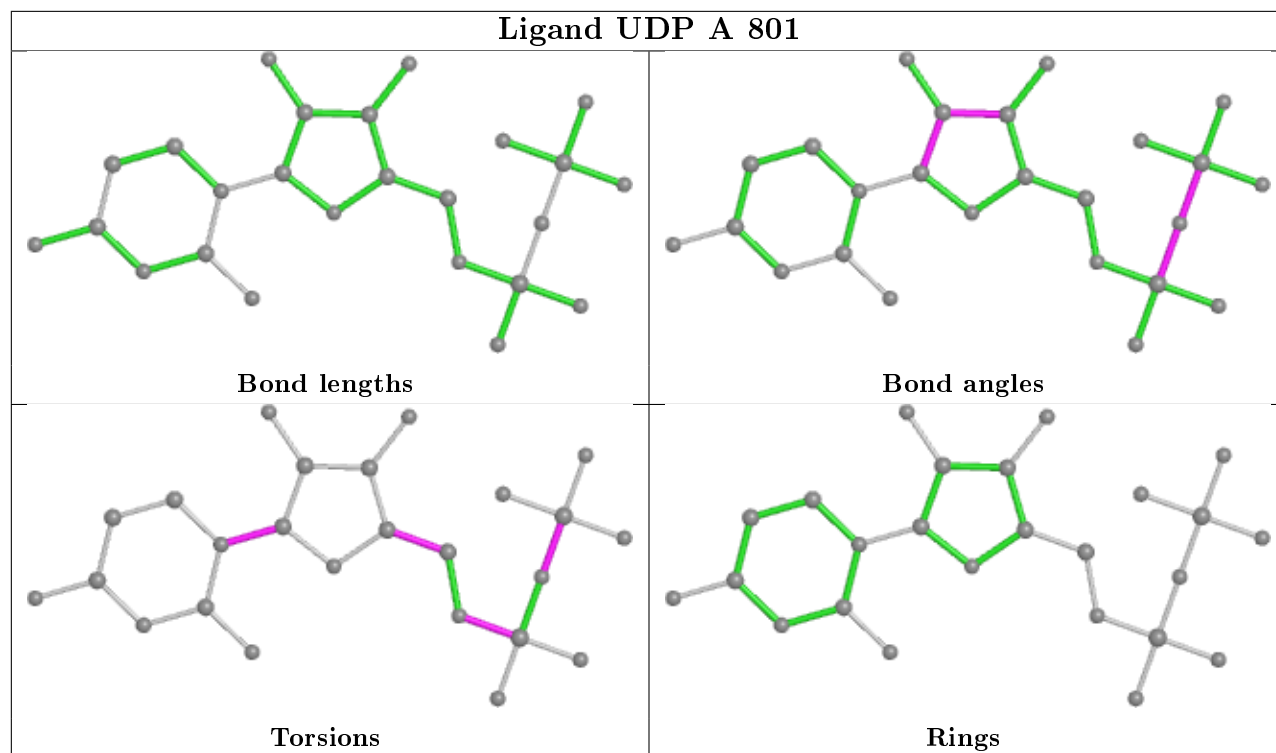
There are no ring outliers.

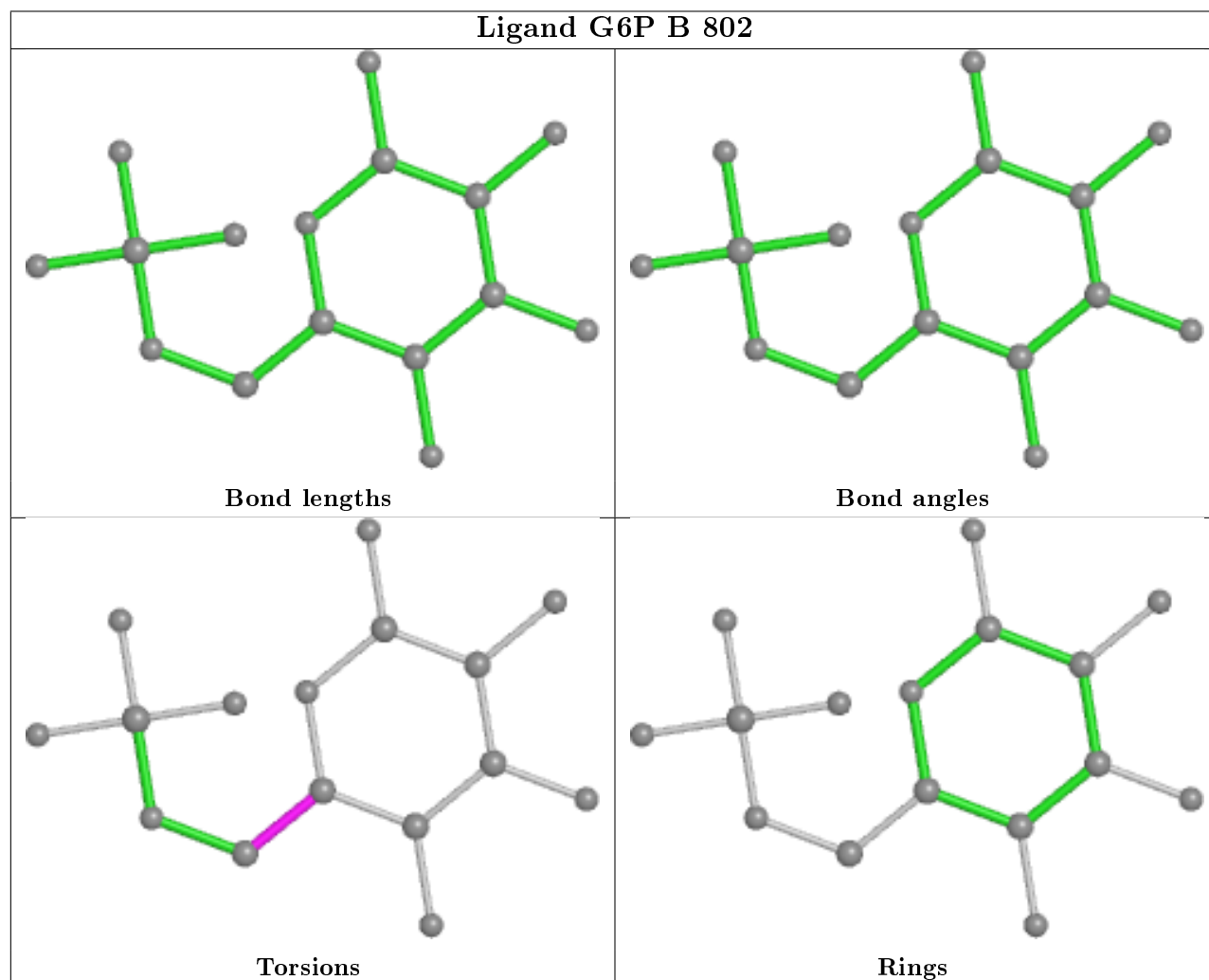
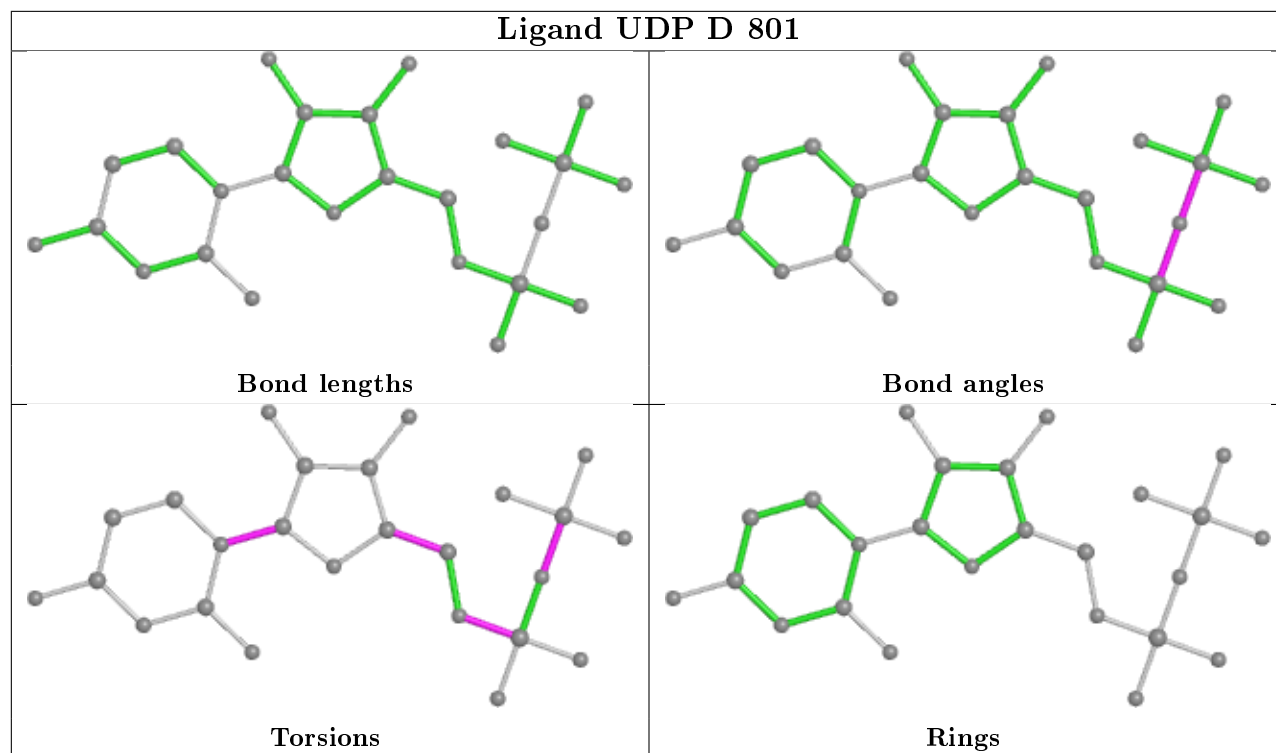
8 monomers are involved in 13 short contacts:

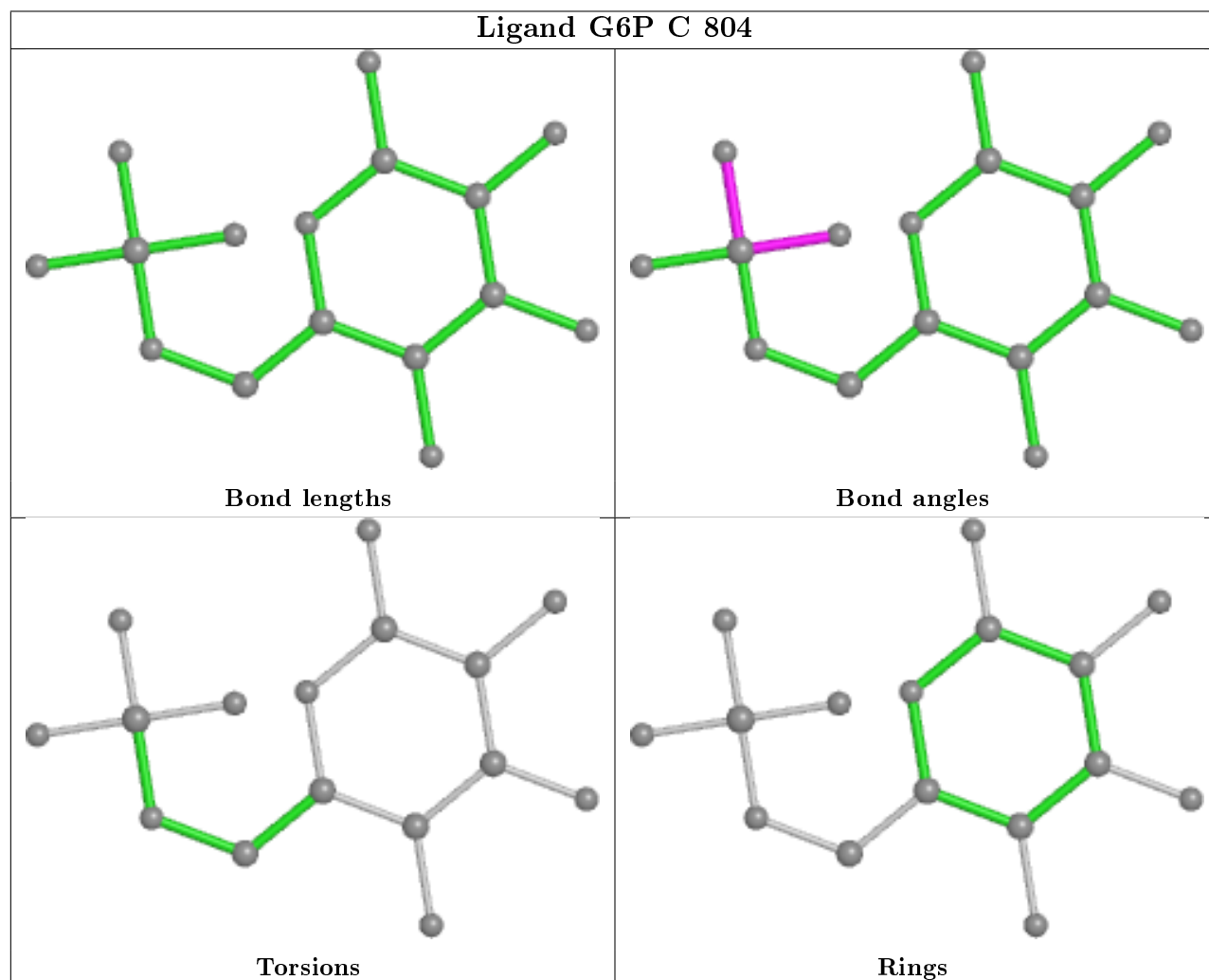
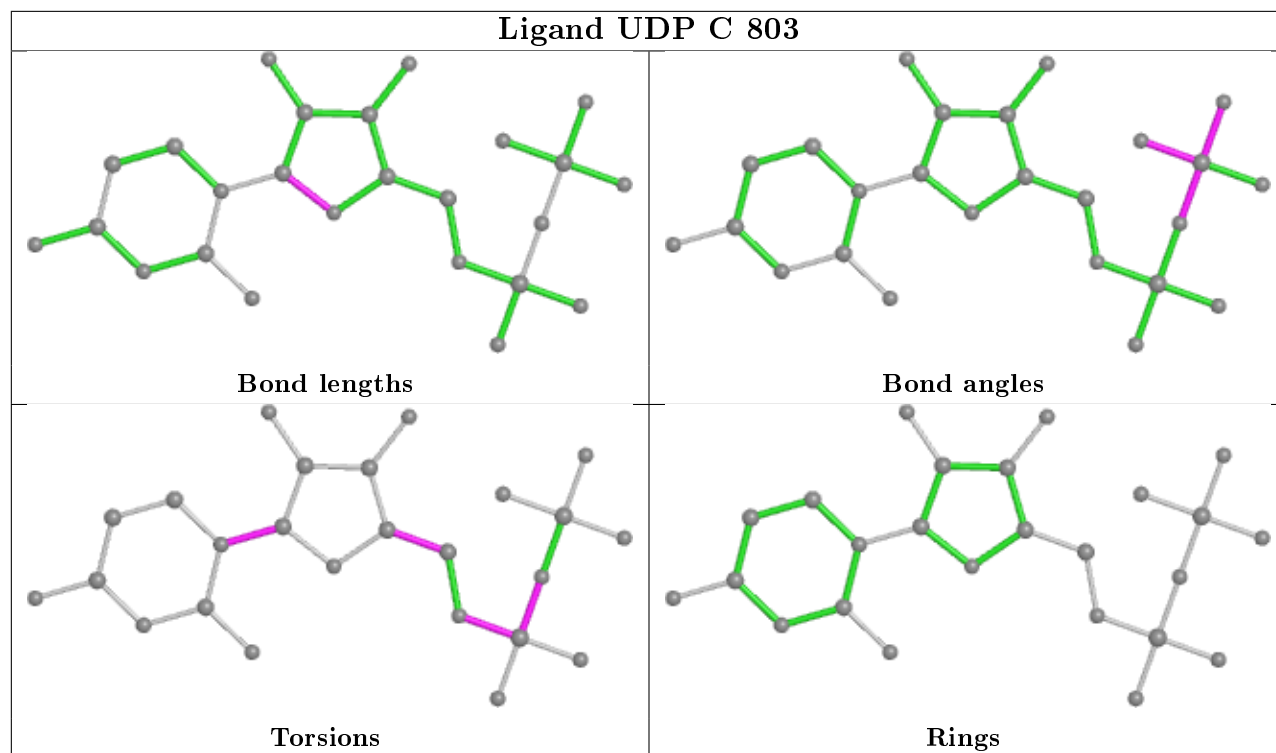
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	UDP	1	0
3	A	802	G6P	3	0
4	A	803	PEG	1	0
4	D	803	PEG	1	0
4	B	803	PEG	1	0
3	B	802	G6P	1	0
2	C	803	UDP	3	0
4	C	805	PEG	2	0

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











## 5.7 Other polymers

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	638/724 (88%)	0.25	28 (4%) 34 28	41, 61, 110, 139	0
1	B	638/724 (88%)	0.04	15 (2%) 59 54	33, 53, 106, 139	0
1	C	638/724 (88%)	0.22	32 (5%) 28 23	40, 59, 111, 142	1 (0%)
1	D	635/724 (87%)	0.38	50 (7%) 12 9	35, 72, 137, 165	0
All	All	2549/2896 (88%)	0.22	125 (4%) 29 24	33, 59, 123, 165	1 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	630	LEU	7.2
1	D	637	ALA	6.5
1	D	626	VAL	6.1
1	D	627	GLY	5.5
1	C	128	ILE	5.5
1	D	122	LEU	5.5
1	D	622	PHE	5.2
1	D	125	LEU	5.2
1	D	128	ILE	5.1
1	D	629	GLU	5.0
1	D	628	GLU	4.9
1	D	132	GLU	4.5
1	A	61	LEU	4.5
1	B	624	GLU	4.5
1	D	126	VAL	4.2
1	C	129	PRO	4.2
1	C	133	ASN	4.1
1	D	123	TRP	4.0
1	D	638	LEU	4.0
1	D	631	ASN	4.0
1	D	620	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	135	PHE	3.9
1	D	133	ASN	3.9
1	B	630	LEU	3.9
1	A	60	ILE	3.9
1	D	205	GLY	3.9
1	C	125	LEU	3.8
1	C	68	ALA	3.7
1	A	62	ASP	3.7
1	A	543	THR	3.7
1	D	76	VAL	3.7
1	D	624	GLU	3.7
1	A	92	TYR	3.6
1	D	625	LEU	3.6
1	B	2	SER	3.5
1	A	76	VAL	3.5
1	D	615	ARG	3.5
1	C	116	ASN	3.4
1	C	123	TRP	3.4
1	C	114	TYR	3.4
1	D	61	LEU	3.4
1	C	126	VAL	3.4
1	D	55	GLN	3.4
1	A	69	PHE	3.3
1	C	549	TYR	3.3
1	A	157	LEU	3.3
1	D	70	SER	3.2
1	D	614	LEU	3.2
1	D	124	SER	3.2
1	A	63	TRP	3.1
1	D	59	ASP	3.1
1	C	124	SER	2.9
1	C	88	VAL	2.9
1	C	60	ILE	2.8
1	C	436	GLU	2.8
1	D	639	ALA	2.8
1	C	111	VAL	2.8
1	C	118	TRP	2.8
1	A	104	ILE	2.8
1	D	94	ARG	2.8
1	A	64	LYS	2.7
1	B	65	LYS	2.7
1	C	62	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	622	PHE	2.7
1	A	88	VAL	2.7
1	A	448	VAL	2.7
1	D	2	SER	2.7
1	B	637	ALA	2.7
1	A	90	PHE	2.7
1	A	58	VAL	2.6
1	A	77	GLN	2.6
1	A	68	ALA	2.6
1	D	623	ARG	2.6
1	B	71	ASP	2.6
1	C	131	PRO	2.6
1	A	66	PRO	2.5
1	B	67	GLU	2.5
1	A	544	ASN	2.5
1	D	136	GLU	2.5
1	C	127	GLY	2.5
1	B	61	LEU	2.4
1	D	5	LEU	2.4
1	A	406	THR	2.4
1	B	629	GLU	2.4
1	A	82	THR	2.4
1	C	113	GLY	2.4
1	D	112	ARG	2.4
1	D	117	GLU	2.4
1	D	63	TRP	2.4
1	C	544	ASN	2.4
1	A	156	HIS	2.3
1	D	632	ASP	2.3
1	D	99	GLY	2.3
1	D	115	SER	2.3
1	A	49	LEU	2.3
1	A	59	ASP	2.3
1	D	127	GLY	2.3
1	C	545	GLN	2.2
1	B	132	GLU	2.2
1	C	592	ARG	2.2
1	B	5	LEU	2.2
1	A	67	GLU	2.2
1	C	112	ARG	2.2
1	C	122	LEU	2.2
1	A	153	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	229	HIS	2.1
1	C	67	GLU	2.1
1	C	220	HIS	2.1
1	D	224	ARG	2.1
1	D	66	PRO	2.1
1	D	228	TYR	2.1
1	A	203	ALA	2.1
1	D	636	ASP	2.1
1	C	593	LEU	2.1
1	D	67	GLU	2.1
1	D	242	ASP	2.1
1	D	604	LEU	2.0
1	B	78	HIS	2.0
1	D	265	GLY	2.0
1	B	64	LYS	2.0
1	B	74	ARG	2.0
1	C	437	GLY	2.0
1	C	108	LEU	2.0
1	D	96	LEU	2.0
1	A	78	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

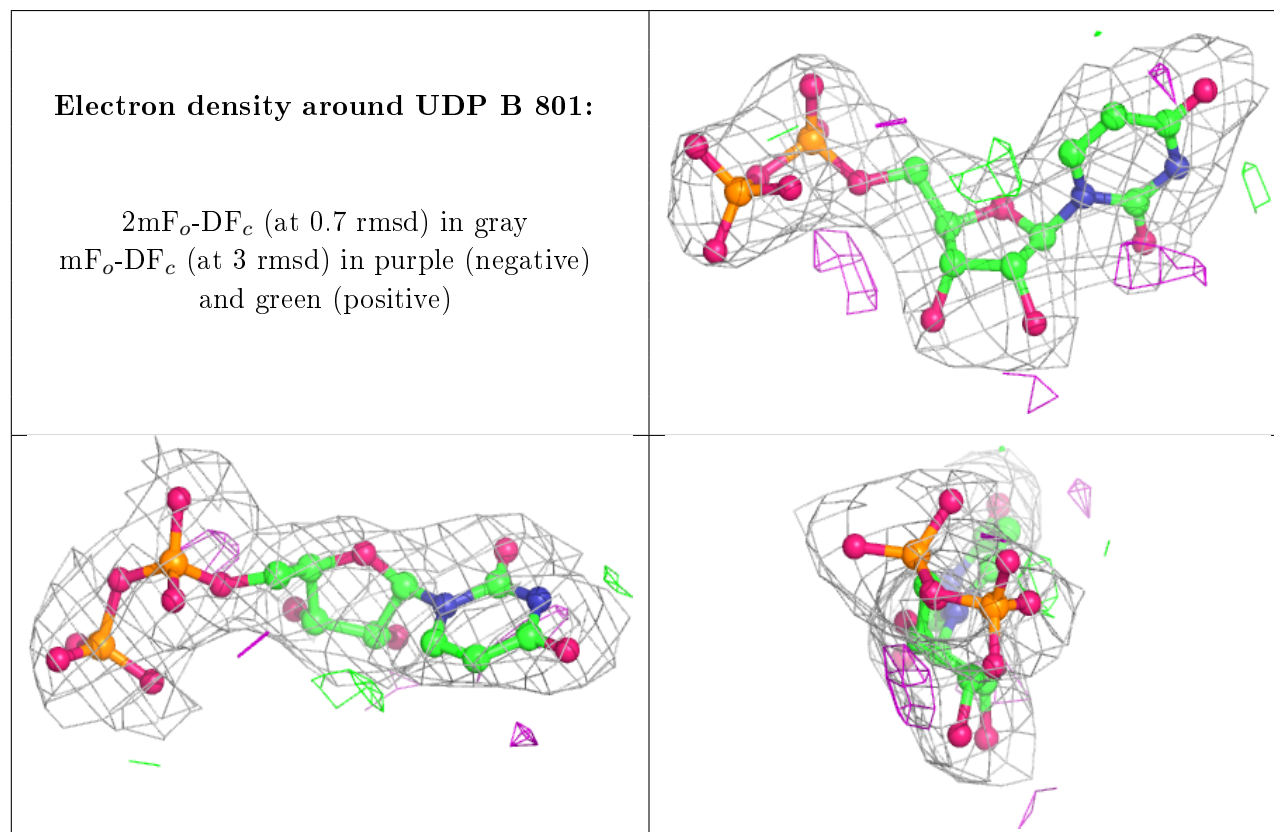
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	A	803	7/7	0.86	0.18	73,77,85,85	0
4	PEG	B	803	7/7	0.91	0.26	68,69,76,76	0
4	PEG	D	803	7/7	0.93	0.21	55,65,75,78	0

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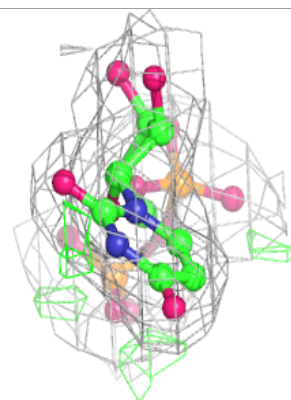
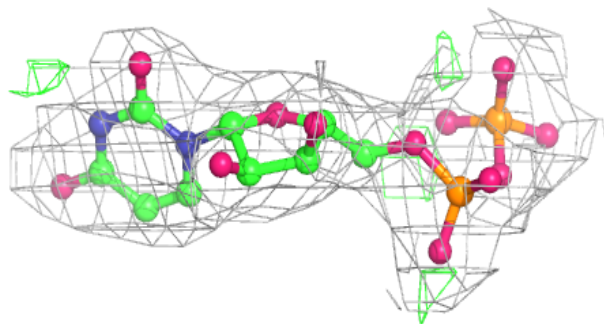
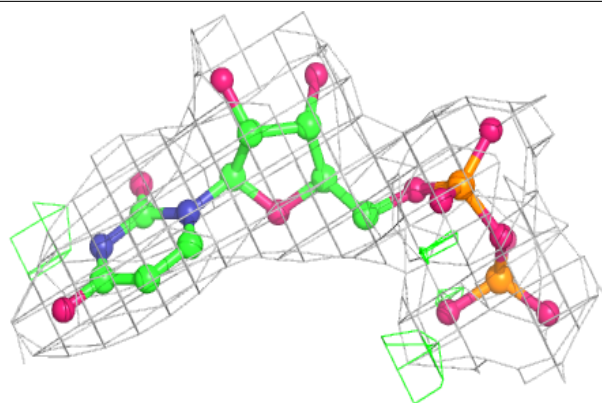
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	C	805	7/7	0.94	0.13	62,69,77,78	0
2	UDP	B	801	25/25	0.97	0.15	46,57,85,89	0
2	UDP	C	803	25/25	0.97	0.19	39,51,55,59	0
2	UDP	A	801	25/25	0.97	0.14	47,59,72,73	0
5	GLC	C	801	12/12	0.98	0.15	46,49,51,53	12
3	G6P	B	802	16/16	0.98	0.17	36,41,45,47	0
3	G6P	C	804	16/16	0.98	0.14	43,47,49,52	0
2	UDP	D	801	25/25	0.98	0.12	48,58,70,71	0
6	BGC	C	802	12/12	0.98	0.16	53,57,59,60	12
3	G6P	D	802	16/16	0.99	0.16	35,40,44,46	0
3	G6P	A	802	16/16	0.99	0.17	42,48,52,52	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.

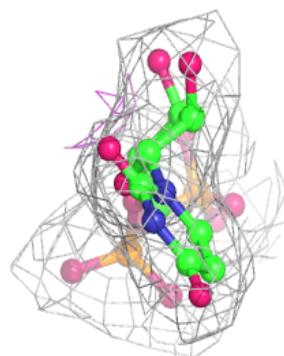
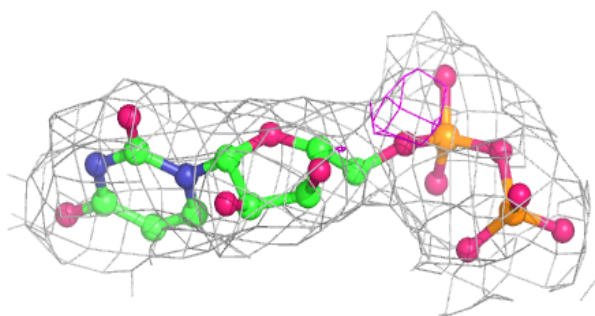
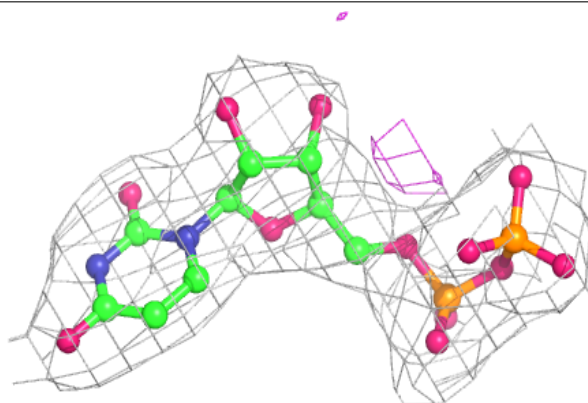


**Electron density around UDP C 803:**

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

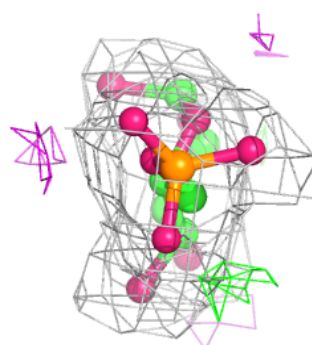
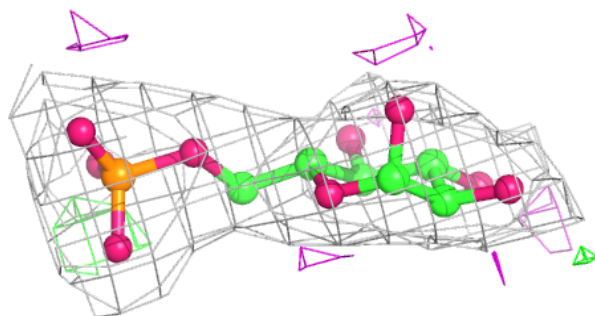
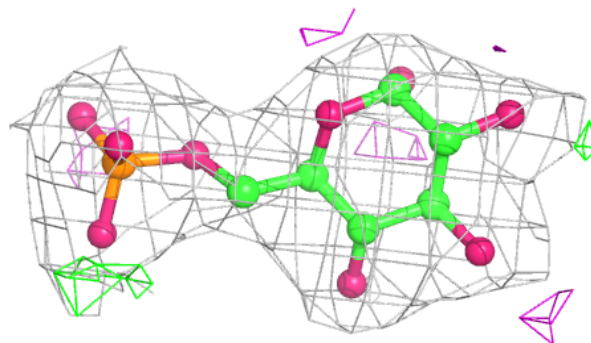
**Electron density around UDP A 801:**

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

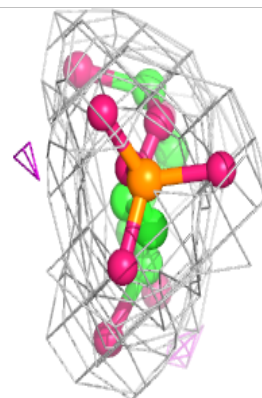
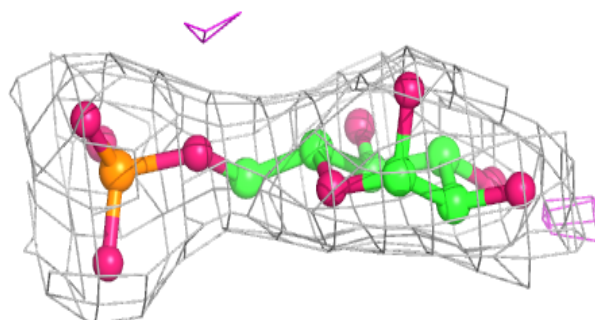
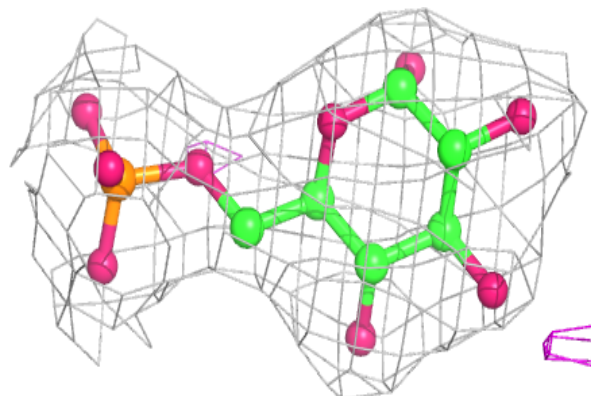


**Electron density around G6P B 802:**

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

**Electron density around G6P C 804:**

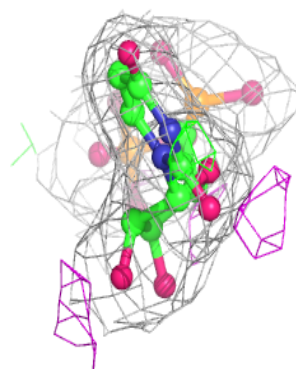
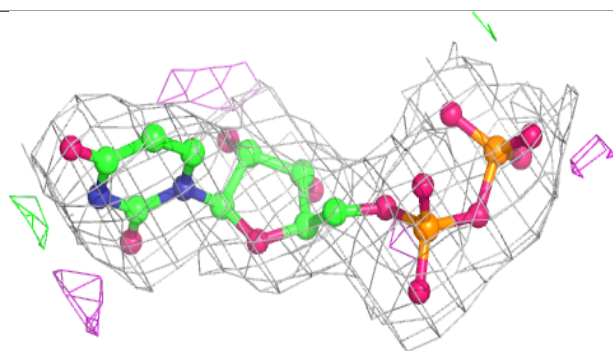
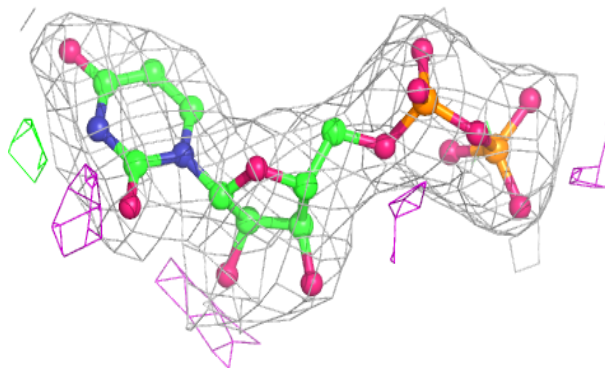
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



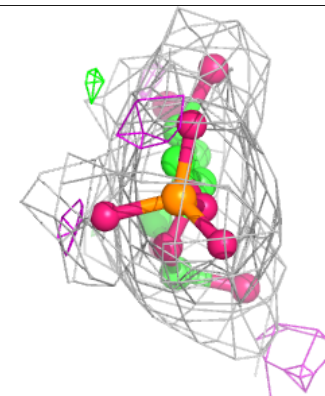
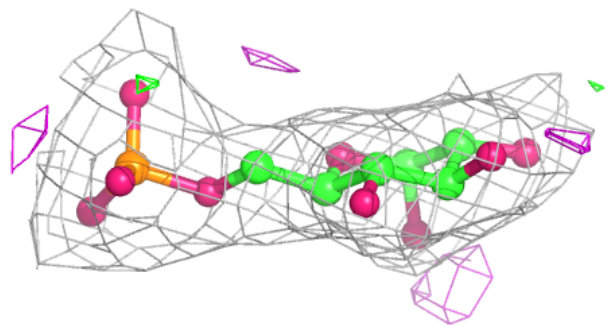
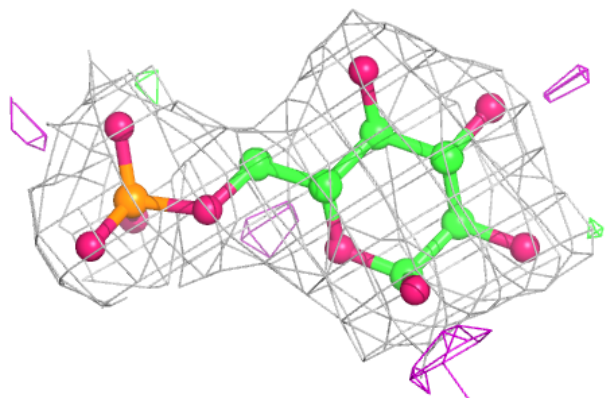


**Electron density around UDP D 801:**

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

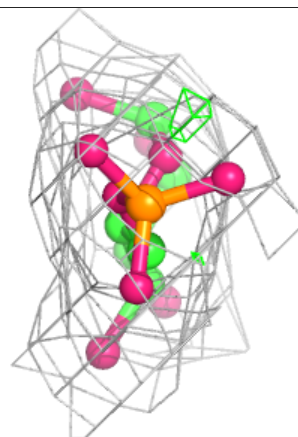
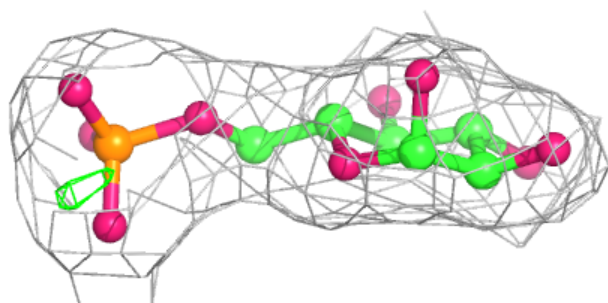
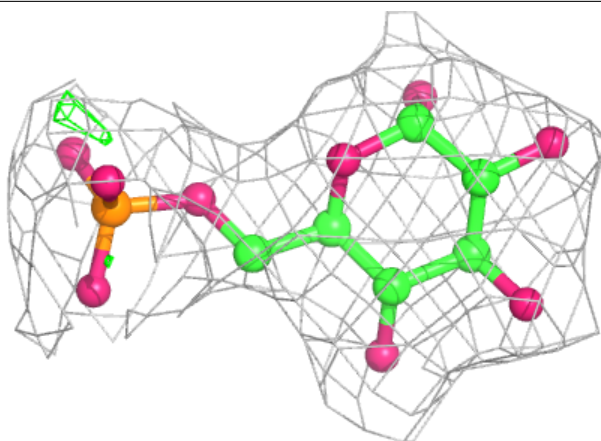
**Electron density around G6P D 802:**

$2mF_o-DF_c$  (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.