



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:56 AM UTC

PDB ID : 4KQ2 / pdb_00004kq2
Title : Glucose1,2cyclic phosphate bound activated state of Yeast Glycogen Synthase
Authors : Chikwana, V.M.; Hurley, T.D.
Deposited on : 2013-05-14
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

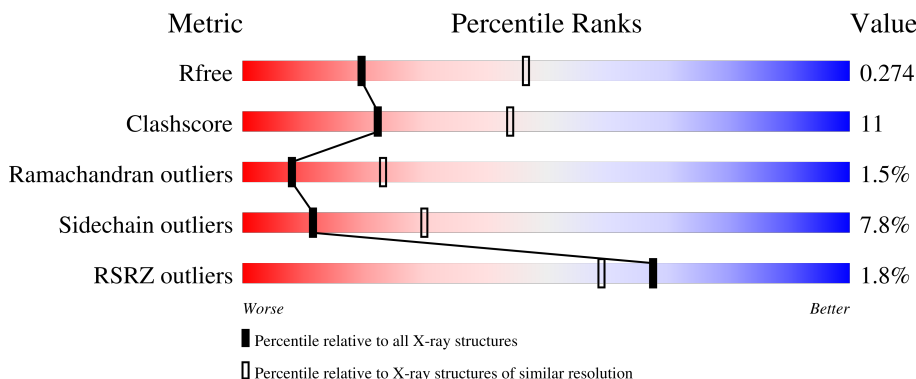
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	724	2% 65% 20% • 12%
1	B	724	% 65% 20% • 12%
1	C	724	2% 63% 22% • 12%
1	D	724	% 61% 24% • 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20806 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
			5145	3286	896	944	19			
1	B	638	Total	C	N	O	S	0	3	0
			5163	3298	900	946	19			
1	C	638	Total	C	N	O	S	0	1	0
			5154	3291	898	946	19			
1	D	636	Total	C	N	O	S	0	2	0
			5146	3284	897	946	19			

There are 84 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	589	ALA	ARG	engineered mutation	UNP E7NKU1
A	592	ALA	ARG	engineered mutation	UNP E7NKU1

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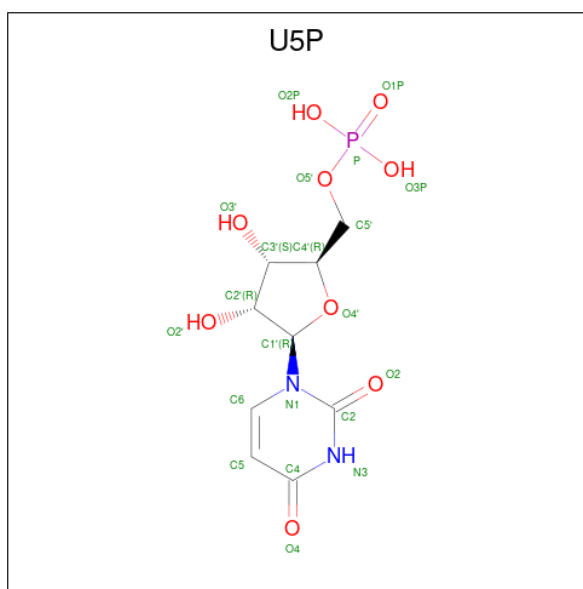
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP E7NKU1
B	-17	GLY	-	expression tag	UNP E7NKU1
B	-16	SER	-	expression tag	UNP E7NKU1
B	-15	SER	-	expression tag	UNP E7NKU1
B	-14	HIS	-	expression tag	UNP E7NKU1
B	-13	HIS	-	expression tag	UNP E7NKU1
B	-12	HIS	-	expression 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	589	ALA	ARG	engineered mutation	UNP E7NKU1
B	592	ALA	ARG	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	589	ALA	ARG	engineered mutation	UNP E7NKU1
C	592	ALA	ARG	engineered mutation	UNP E7NKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP E7NKU1
D	-17	GLY	-	expression tag	UNP E7NKU1
D	-16	SER	-	expression tag	UNP E7NKU1
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	589	ALA	ARG	engineered mutation	UNP E7NKU1
D	592	ALA	ARG	engineered mutation	UNP E7NKU1

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: $C_9H_{13}N_2O_9P$).



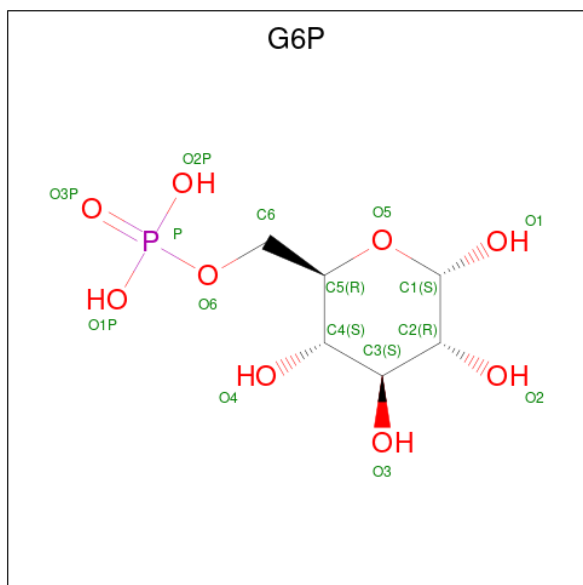
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

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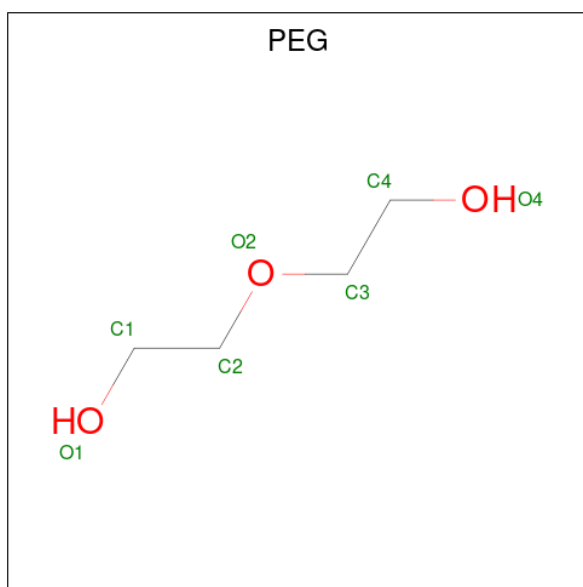
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- 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 DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

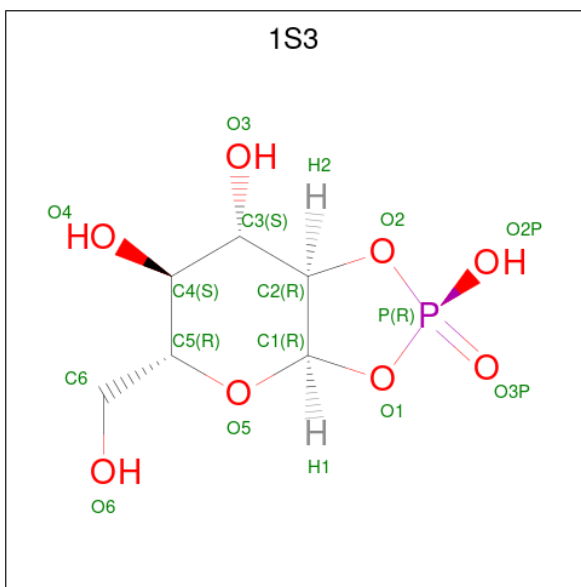


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ba	0	0
			2	2		
5	B	2	Total	Ba	0	0
			2	2		
5	C	1	Total	Ba	0	0
			1	1		
5	D	2	Total	Ba	0	0
			2	2		

- Molecule 6 is (2R,3aR,5R,6S,7S,7aR)-5-(hydroxymethyl)tetrahydro-3aH-[1,3,2]dioxaphospholo[4,5-b]pyran-2,6,7-triol 2-oxide (CCD ID: 1S3) (formula: C₆H₁₁O₈P).

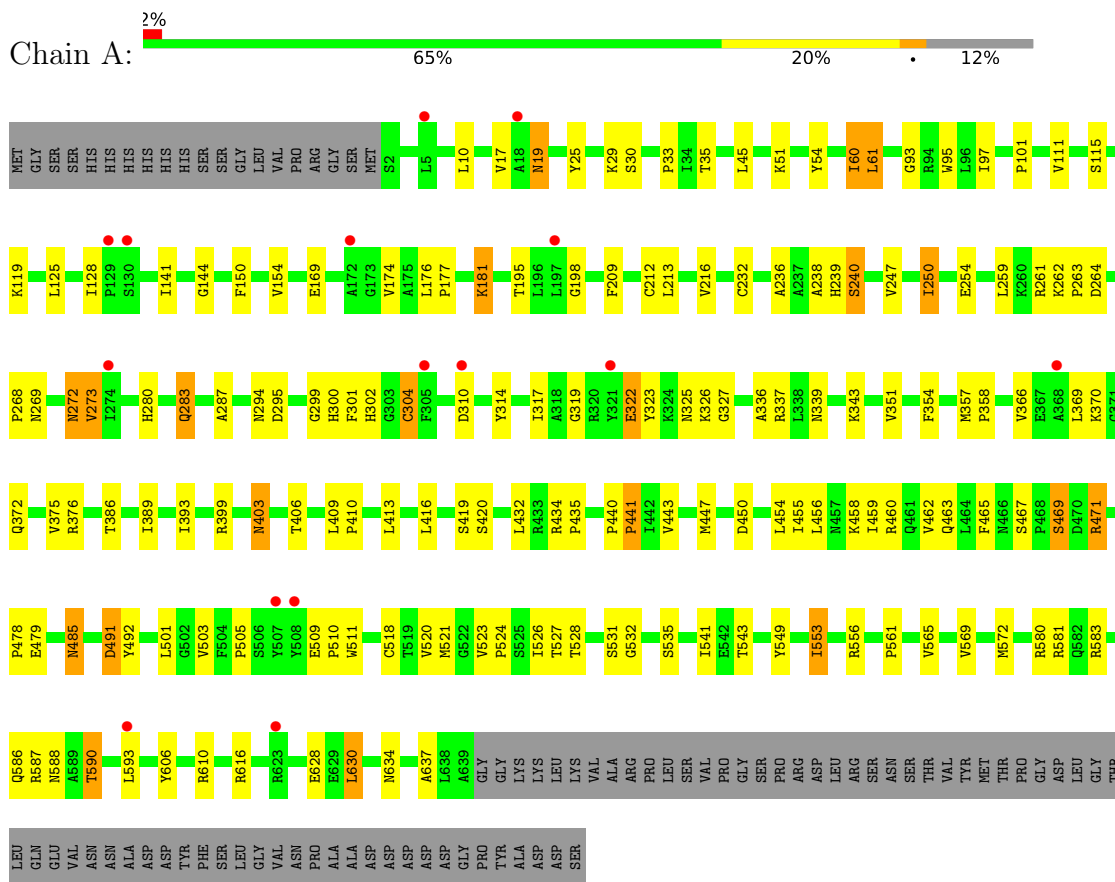


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	P	0	0
			15	6	8	1		

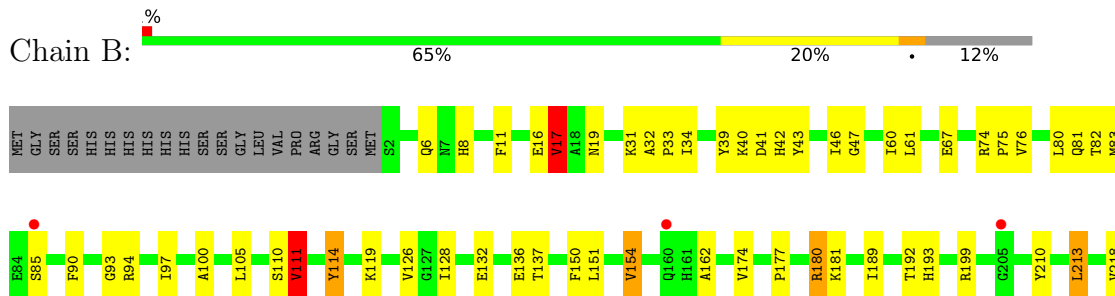
3 Residue-property plots [i](#)

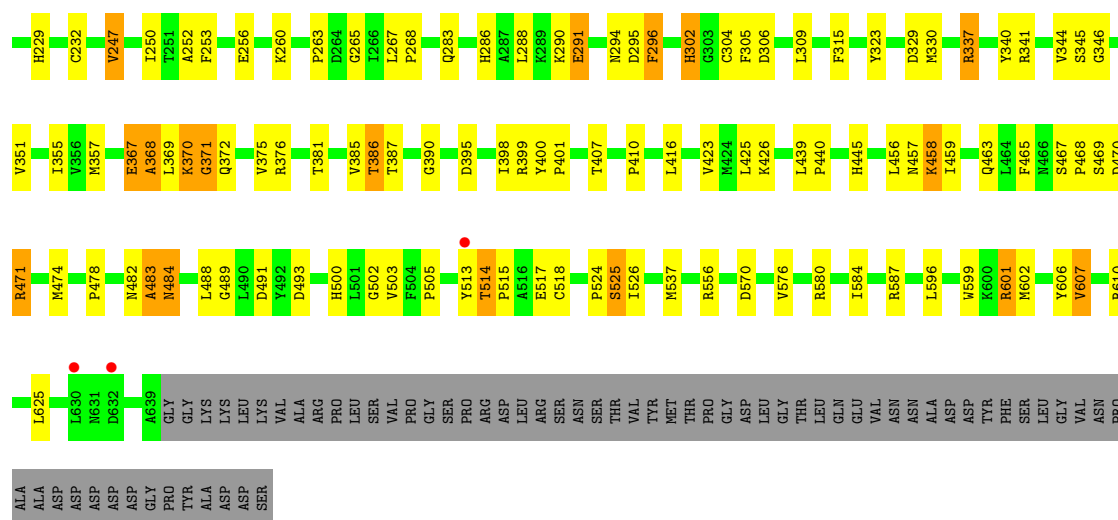
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Gsy2p

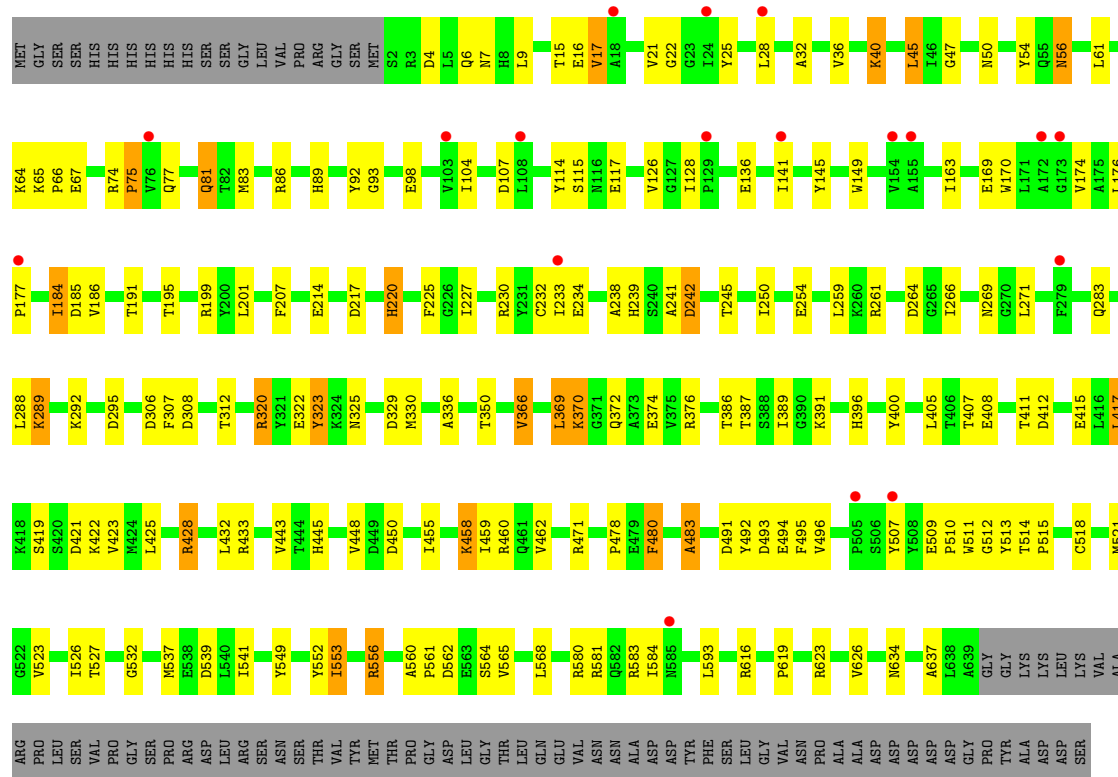


• Molecule 1: Gsy2p





• Molecule 1: Gsy2p



• Molecule 1: Gsy2p



SER	G532	N446	F315	L213	Q77
PRO	F533	M447	F316	E214	H78
ASP	I541	D450	I317	D217	A79
LEU	Y552	L454	E322	V218	S85
ARG			K326	E221	G93
SER	R556	Q463			
ASN		L464	E333	R224	V103
SER	L568	F465	A334	I104	I103
THR		N466	L335	I227	L105
VAL	Y571	S467	A336	C232	V111
MET	M572	R471	R337	I233	
THR		V472	L338	V243	D121
PRO	T584	K473			
GLY	R587	M474	K348	A252	L125
ASP			K349		
LEU	T590	P478	T350	K260	I128
GLY	E591		I355		P129
THR		L481	V356	P263	I141
LEU	S594	N482		D264	
GLN	D595	A483	E367	G265	G144
VAL	L596	N484	A368		
ASN	L597	N485	L369	P268	
ASN	D598	P486	K370		F150
ALA	M599	A487	G371	L271	L157
ASP	K600	L488			D158
ASP	R601		A373	I274	
TYR	M602	D491	E374		A162
PHE		Y492		H280	I163
SER	V607	D493	L378	E281	H166
LEU		E494	E379	F282	F167
GLY	L612			Q283	H168
VAL	A613	C499	I389	N284	V174
ASN		H500	G390	L285	A175
PRO	F622	L501	K391	H286	
ALA		G502		A287	
ALA	N631	V503	N403	L288	L178
ASP		F504	L409	K289	C179
ASP	M635	P505			
ASP	D636	S506	D412	I293	R182
ASP	A637	Y507		N294	
ASP	L638		L416	D295	V186
GLY	A639	F510	L417	F296	V187
PRO		G511		V297	T188
TYR	GLY	G512	L425		I189
ALA	LYS	Y513	K426	H302	L196
ASP	LYS	T514	R427	G303	
ASP	LEU		R428	C304	
SER	LYS	E517			
	VAL	C518	L429	F307	Y200
	ALA			D308	
	ARG	V523	L430	L309	G205
	PRO	F524	L432	D310	SER
	LEU	S525	R433	N311	PHE
	SER	I526	R434	T312	D208
	VAL	T527	P435	L313	
	PRO	T528	H445	Y314	C212
	GLY				

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	193.49Å 203.98Å 206.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 2.95 48.46 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.46-2.95) 99.7 (48.46-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.224 , 0.271 0.223 , 0.274	Depositor DCC
R_{free} test set	4240 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20806	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: 1S3, U5P, PEG, G6P, BA

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	0.47	0/5270	0.90	4/7141 (0.1%)
1	B	0.60	1/5298 (0.0%)	0.96	7/7180 (0.1%)
1	C	0.47	0/5279	0.86	2/7153 (0.0%)
1	D	0.57	3/5269 (0.1%)	0.93	3/7138 (0.0%)
All	All	0.53	4/21116 (0.0%)	0.91	16/28612 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	GLY	C-O	6.42	1.32	1.23
1	D	431	ALA	N-CA	5.40	1.53	1.46
1	B	296	PHE	CA-CB	5.35	1.61	1.53
1	D	485	ASN	CA-C	5.22	1.59	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	VAL	N-CA-C	-7.63	105.72	111.90
1	A	485	ASN	CA-C-N	7.21	126.92	119.56
1	A	485	ASN	C-N-CA	7.21	126.92	119.56
1	D	487	ILE	N-CA-C	7.20	118.00	111.81
1	B	517	GLU	N-CA-C	-6.26	104.37	111.07

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	5145	0	5054	98	0
1	B	5163	0	5075	115	0
1	C	5154	0	5061	112	0
1	D	5146	0	5051	125	0
2	A	21	0	11	0	0
2	B	21	0	11	0	0
2	C	21	0	11	0	0
2	D	21	0	11	0	0
3	A	16	0	11	2	0
3	B	16	0	11	1	0
3	C	16	0	11	3	0
3	D	16	0	11	1	0
4	A	7	0	10	0	0
4	B	7	0	10	0	0
4	C	7	0	10	3	0
4	D	7	0	10	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	C	15	0	11	1	0
All	All	20806	0	20380	438	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 438 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:336:ALA:HB2	1:A:462:VAL:HG11	1.32	1.08
1:D:428:ARG:HH11	1:D:428:ARG:HG2	0.86	1.00
1:A:336:ALA:HB2	1:A:462:VAL:CG1	1.92	0.98
1:D:428:ARG:HH11	1:D:428:ARG:CG	1.78	0.96
1:D:428:ARG:HG2	1:D:428:ARG:NH1	1.65	0.95

There are no symmetry-related clashes.

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%)	574 (90%)	53 (8%)	9 (1%)	9	24
1	B	639/724 (88%)	569 (89%)	59 (9%)	11 (2%)	7	20
1	C	637/724 (88%)	576 (90%)	52 (8%)	9 (1%)	9	24
1	D	634/724 (88%)	567 (89%)	57 (9%)	10 (2%)	7	21
All	All	2546/2896 (88%)	2286 (90%)	221 (9%)	39 (2%)	8	23

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	441	PRO
1	B	111	VAL
1	B	304	CYS
1	B	367	GLU

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	551/622 (89%)	517 (94%)	34 (6%)	16	39
1	B	554/622 (89%)	511 (92%)	43 (8%)	11	30
1	C	552/622 (89%)	506 (92%)	46 (8%)	10	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	551/622 (89%)	502 (91%)	49 (9%)	9	24
All	All	2208/2488 (89%)	2036 (92%)	172 (8%)	11	30

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	513	TYR
1	D	337	ARG
1	C	541	ILE
1	D	125	LEU
1	D	372[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	19	ASN
1	D	461	GLN
1	D	168	HIS
1	D	280	HIS
1	D	621	GLN

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](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 for Mogul analysis.

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	U5P	D	801	-	22,22,22	1.10	2 (9%)	32,33,33	1.77	5 (15%)
6	1S3	C	801	-	14,16,16	0.59	0	19,25,25	1.28	4 (21%)
3	G6P	D	802	-	16,16,16	0.48	0	23,24,24	0.98	2 (8%)
3	G6P	A	802	-	16,16,16	0.58	0	23,24,24	1.09	2 (8%)
4	PEG	D	803	-	6,6,6	0.42	0	5,5,5	0.41	0
3	G6P	C	803	-	16,16,16	0.57	0	23,24,24	0.81	0
3	G6P	B	802	-	16,16,16	0.46	0	23,24,24	1.08	1 (4%)
4	PEG	C	804	-	6,6,6	0.50	0	5,5,5	0.26	0
2	U5P	B	801	-	22,22,22	1.12	3 (13%)	32,33,33	1.89	5 (15%)
2	U5P	C	802	-	22,22,22	1.11	2 (9%)	32,33,33	1.80	7 (21%)
2	U5P	A	801	-	22,22,22	1.16	3 (13%)	32,33,33	1.78	7 (21%)
4	PEG	A	803	-	6,6,6	0.60	0	5,5,5	0.33	0
4	PEG	B	803	-	6,6,6	0.46	0	5,5,5	0.43	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	U5P	D	801	-	-	3/10/26/26	0/2/2/2
6	1S3	C	801	-	-	0/2/32/32	0/2/2/2
3	G6P	D	802	-	-	3/6/26/26	0/1/1/1
3	G6P	A	802	-	-	3/6/26/26	0/1/1/1
4	PEG	D	803	-	-	3/4/4/4	-
3	G6P	C	803	-	-	1/6/26/26	0/1/1/1
3	G6P	B	802	-	-	2/6/26/26	0/1/1/1
4	PEG	C	804	-	-	3/4/4/4	-
2	U5P	B	801	-	-	3/10/26/26	0/2/2/2
2	U5P	C	802	-	-	1/10/26/26	0/2/2/2
2	U5P	A	801	-	-	5/10/26/26	0/2/2/2
4	PEG	A	803	-	-	3/4/4/4	-
4	PEG	B	803	-	-	2/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	802	U5P	C2-N1	2.61	1.42	1.38
2	A	801	U5P	C4-N3	-2.58	1.34	1.38
2	B	801	U5P	C6-C5	2.35	1.40	1.35
2	B	801	U5P	C4-N3	-2.30	1.34	1.38
2	B	801	U5P	C2-N1	2.29	1.42	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	U5P	N3-C2-N1	5.26	121.74	114.89
2	B	801	U5P	C4-N3-C2	-5.26	120.08	126.61
2	A	801	U5P	C4-N3-C2	-5.04	120.36	126.61
2	D	801	U5P	C4-N3-C2	-5.02	120.38	126.61
2	D	801	U5P	N3-C2-N1	4.84	121.19	114.89

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	U5P	C5'-O5'-P-O2P
2	B	801	U5P	C5'-O5'-P-O3P
3	A	802	G6P	C6-O6-P-O3P
3	B	802	G6P	C4-C5-C6-O6
3	B	802	G6P	O5-C5-C6-O6

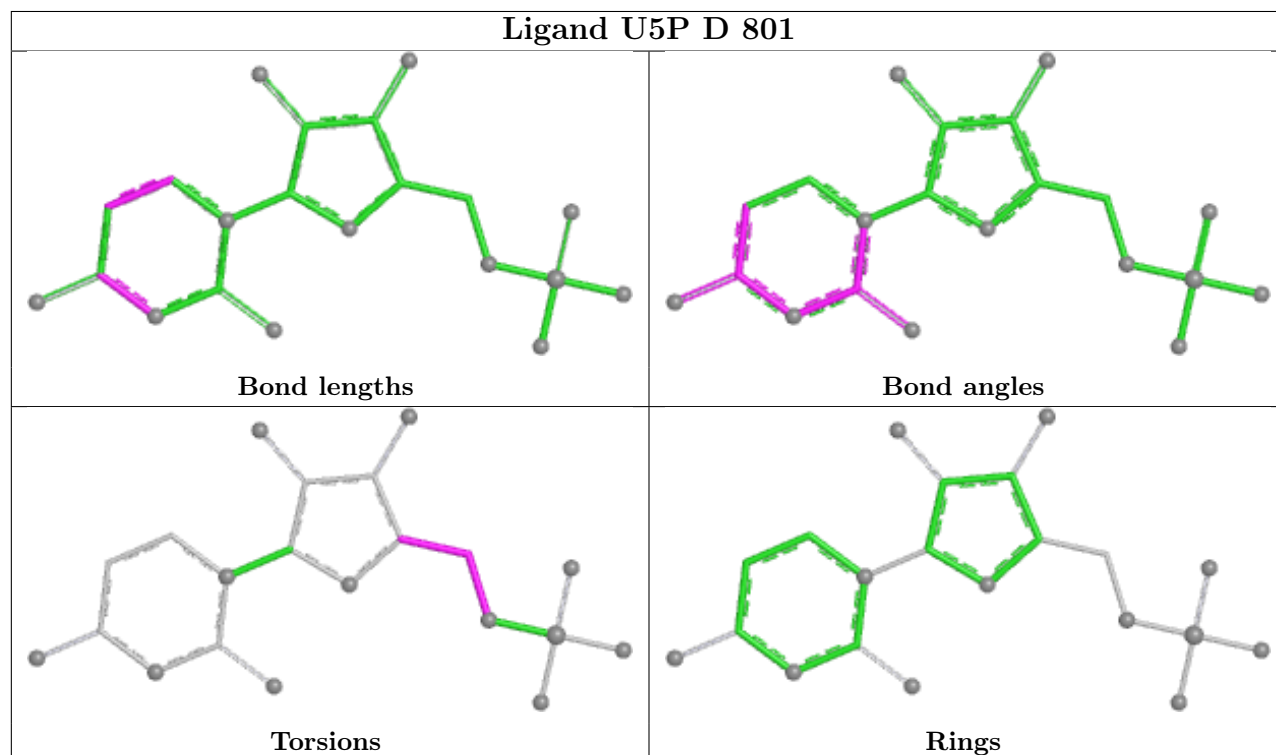
There are no ring outliers.

6 monomers are involved in 11 short contacts:

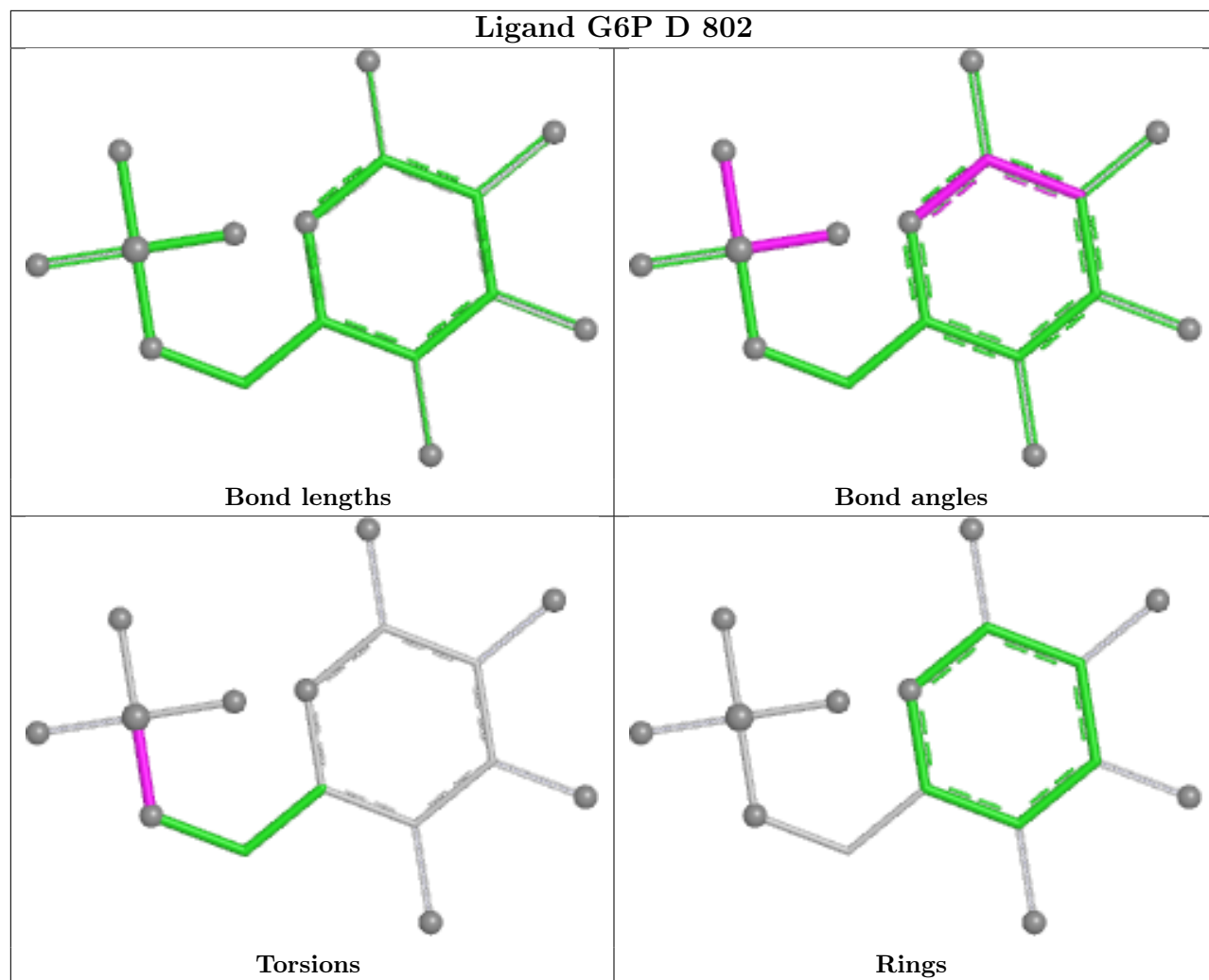
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	801	1S3	1	0
3	D	802	G6P	1	0
3	A	802	G6P	2	0
3	C	803	G6P	3	0
3	B	802	G6P	1	0
4	C	804	PEG	3	0

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.

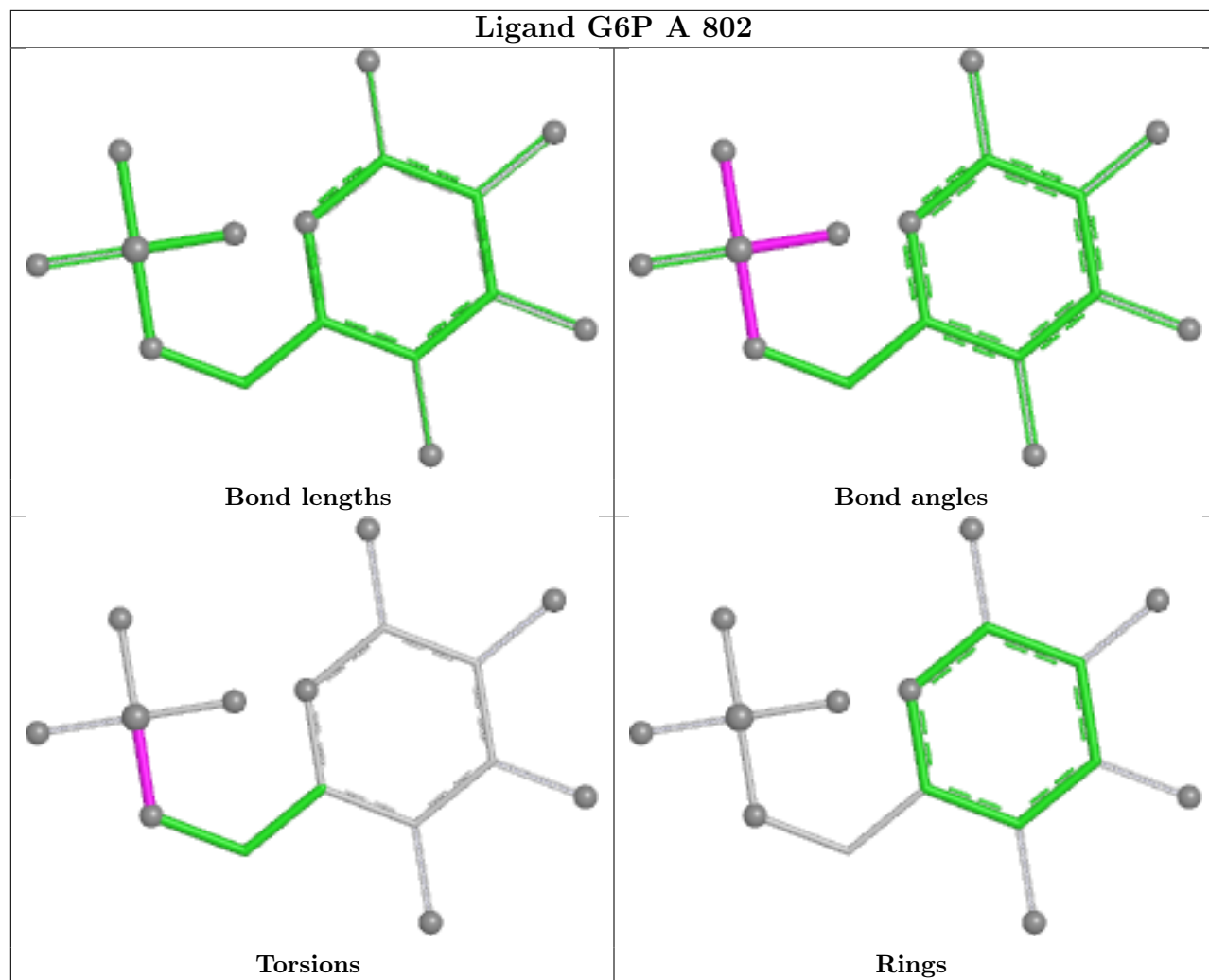
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



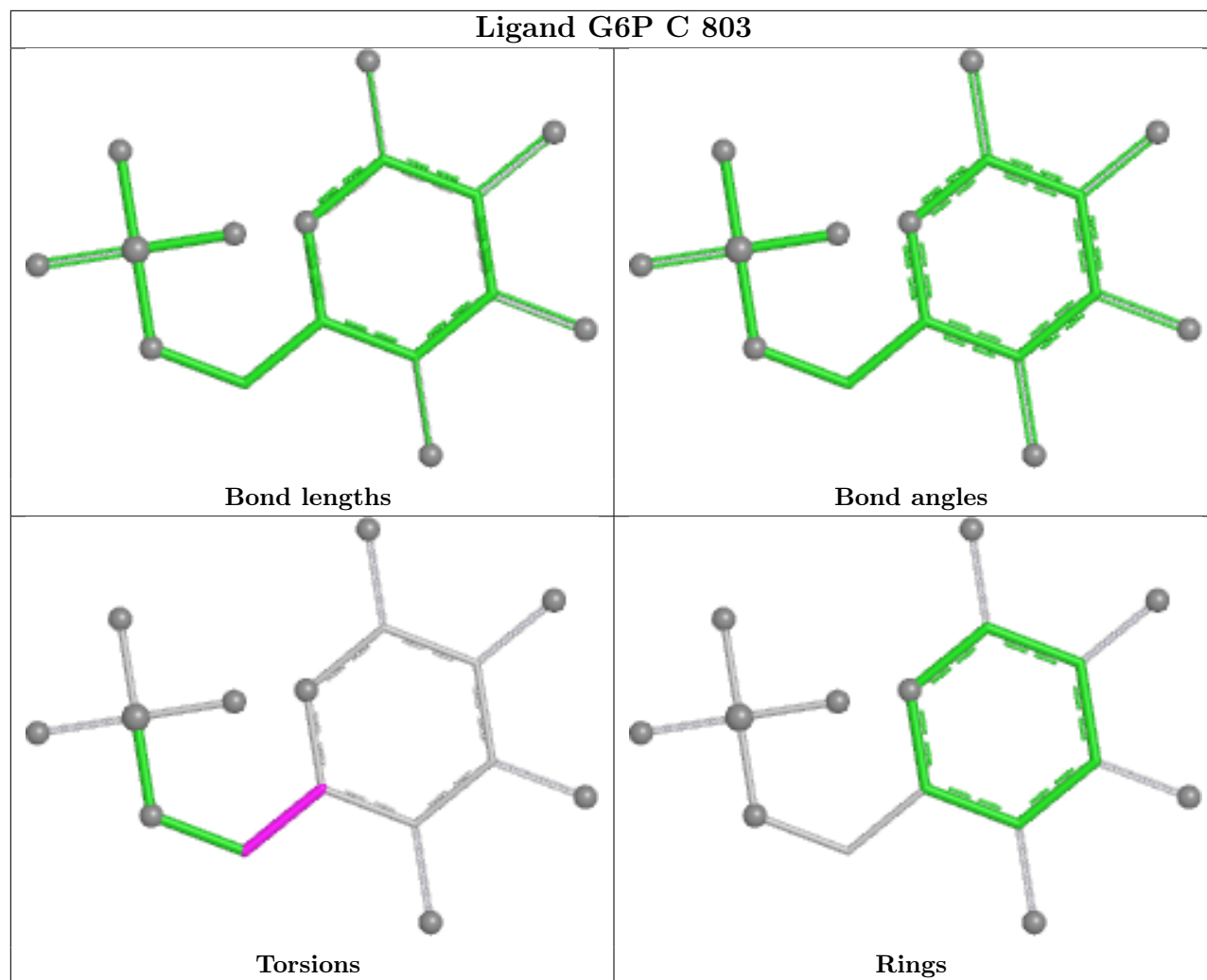
Ligand G6P D 802



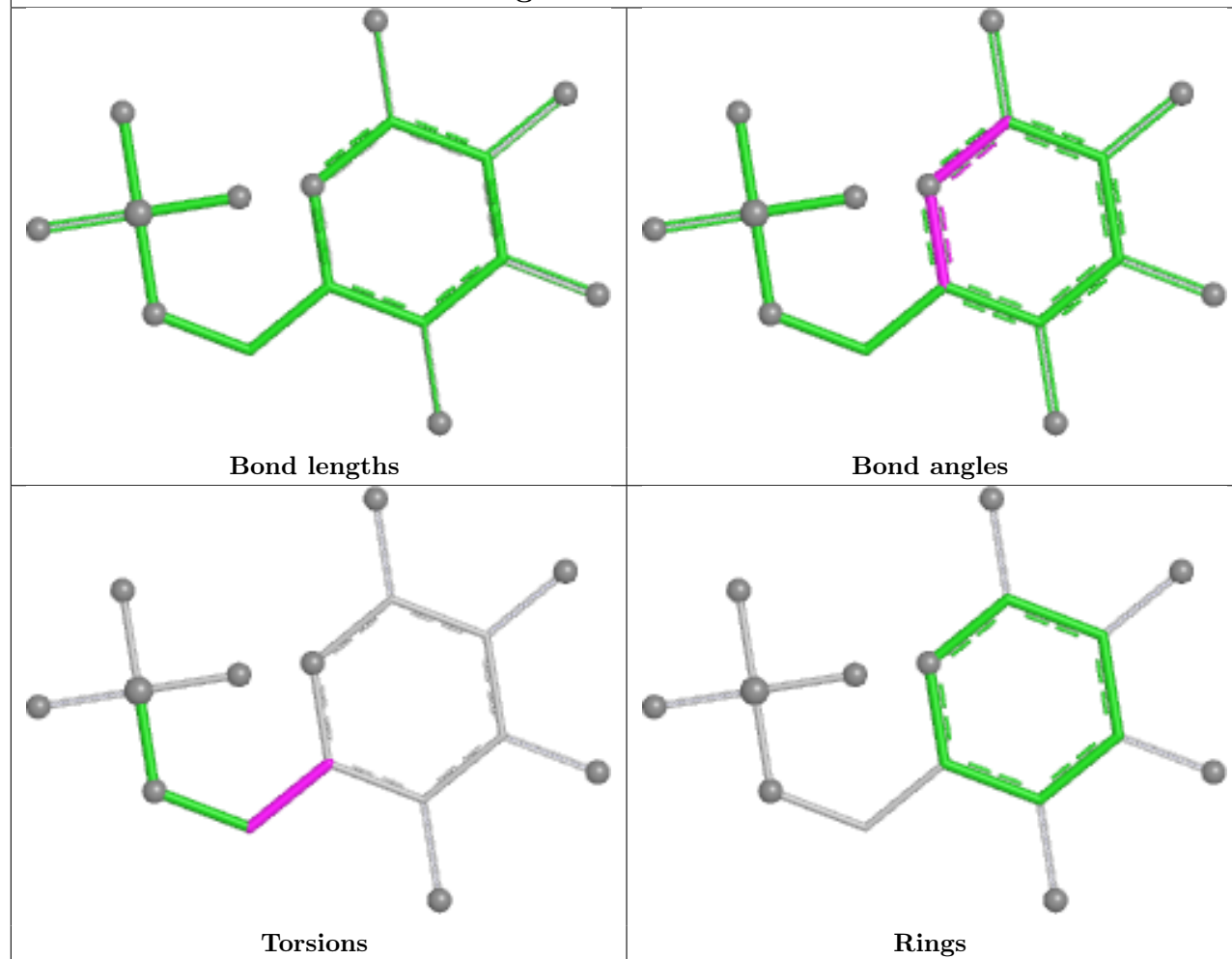
Ligand G6P A 802



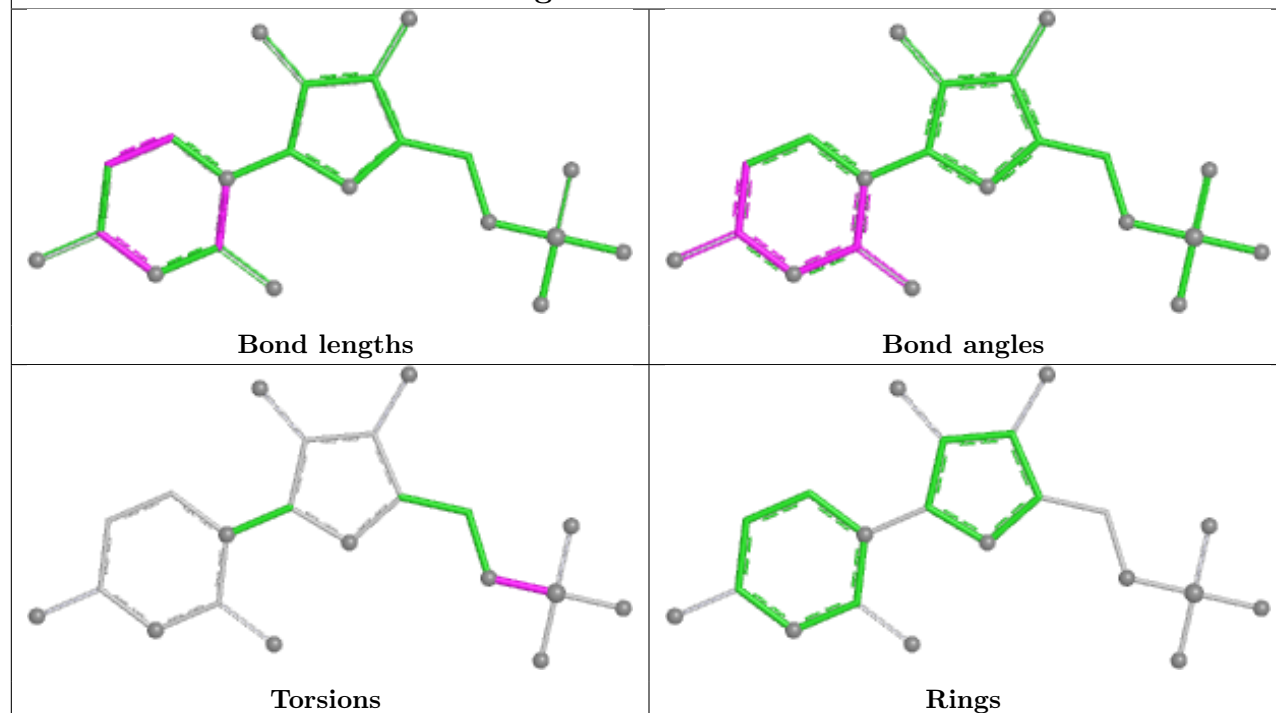
Ligand G6P C 803

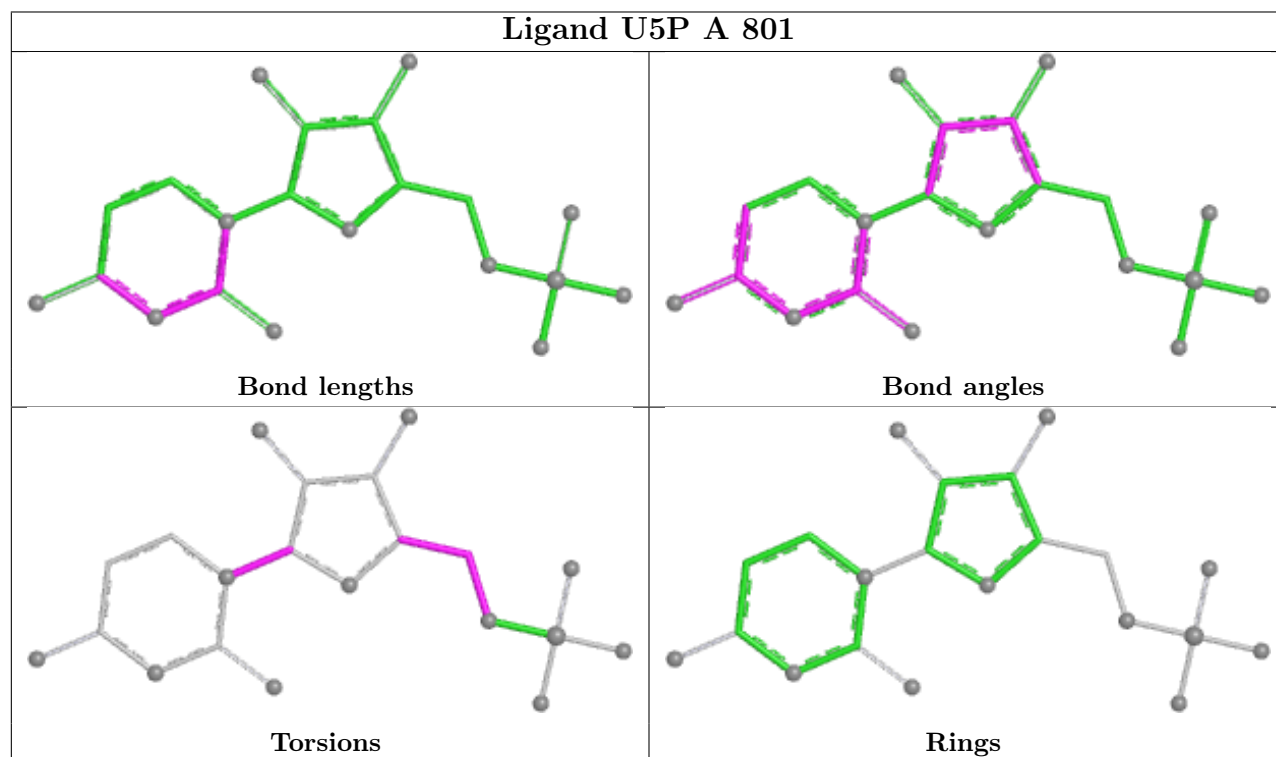
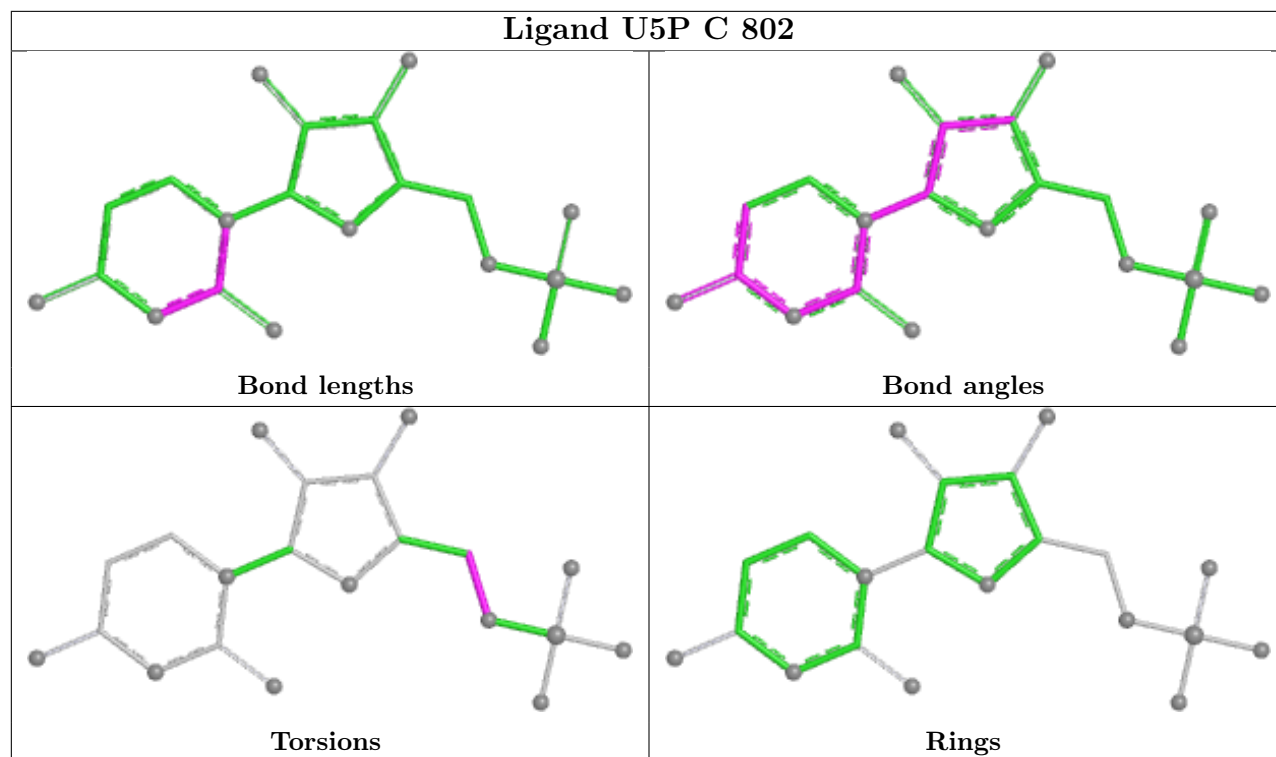


Ligand G6P B 802



Ligand U5P B 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	638/724 (88%)	0.06	15 (2%) 59 51	53, 103, 165, 226	0
1	B	638/724 (88%)	-0.10	6 (0%) 81 76	22, 86, 150, 198	3 (0%)
1	C	638/724 (88%)	0.27	18 (2%) 55 47	43, 108, 183, 247	1 (0%)
1	D	636/724 (87%)	0.03	7 (1%) 78 73	18, 104, 190, 223	2 (0%)
All	All	2550/2896 (88%)	0.07	46 (1%) 67 59	18, 101, 179, 247	6 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	PRO	3.4
1	C	173	GLY	3.3
1	A	305	PHE	3.3
1	D	205	GLY	3.2
1	C	279	PHE	3.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

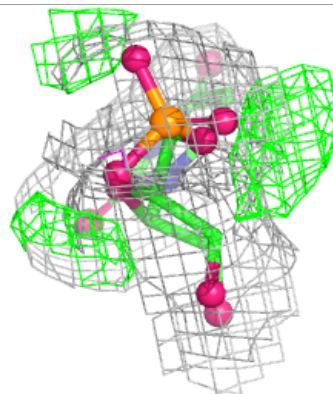
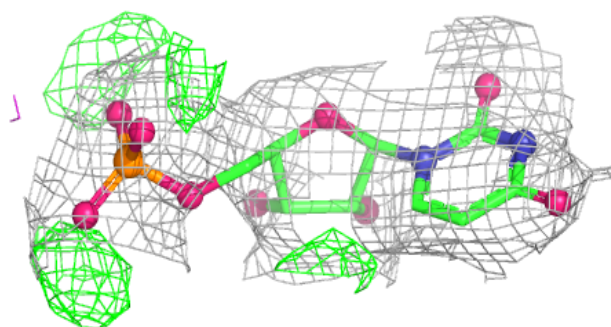
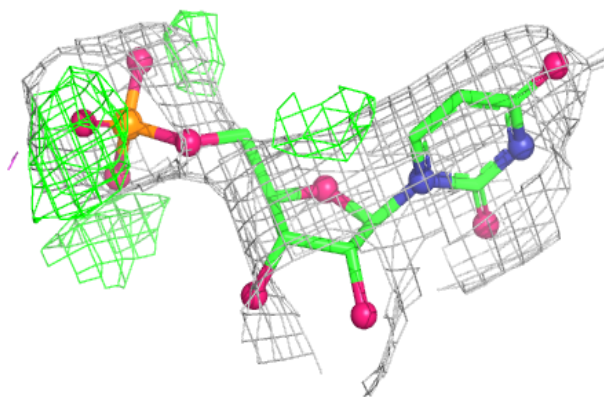
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	BA	B	805	1/1	0.81	0.08	245,245,245,245	0
2	U5P	C	802	21/21	0.83	0.13	95,123,162,163	0
6	1S3	C	801	15/15	0.84	0.11	107,130,156,156	0
4	PEG	D	803	7/7	0.89	0.19	90,90,95,96	0
4	PEG	B	803	7/7	0.90	0.16	98,103,115,115	0
5	BA	D	805	1/1	0.91	0.08	227,227,227,227	0
2	U5P	D	801	21/21	0.91	0.08	93,105,112,127	0
2	U5P	A	801	21/21	0.92	0.09	89,103,120,123	0
4	PEG	A	803	7/7	0.93	0.11	71,74,82,85	0
2	U5P	B	801	21/21	0.93	0.07	82,91,100,105	0
5	BA	D	804	1/1	0.94	0.09	159,159,159,159	0
5	BA	B	804	1/1	0.94	0.13	149,149,149,149	0
5	BA	A	805	1/1	0.94	0.04	212,212,212,212	0
3	G6P	A	802	16/16	0.95	0.08	80,92,98,102	0
3	G6P	C	803	16/16	0.96	0.06	66,77,83,84	0
3	G6P	D	802	16/16	0.97	0.07	55,67,75,78	0
4	PEG	C	804	7/7	0.97	0.10	88,89,96,96	0
3	G6P	B	802	16/16	0.97	0.07	56,74,80,80	0
5	BA	A	804	1/1	0.98	0.06	135,135,135,135	0
5	BA	C	805	1/1	0.99	0.07	145,145,145,145	0

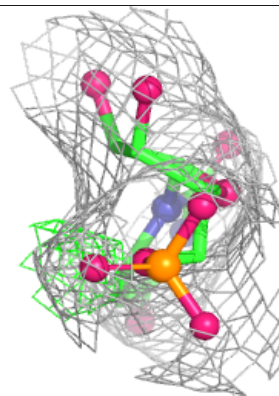
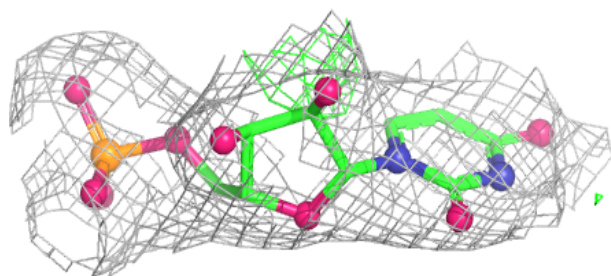
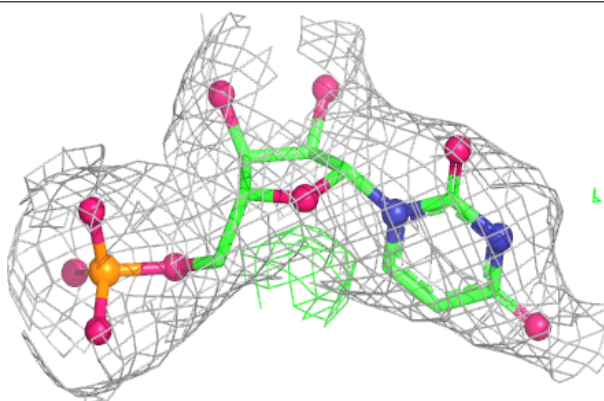
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U5P C 802:

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

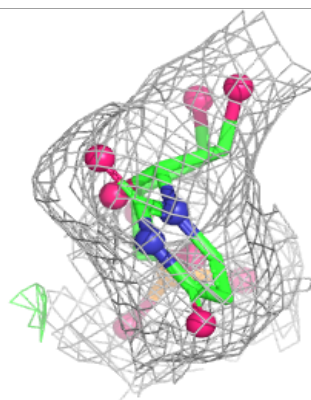
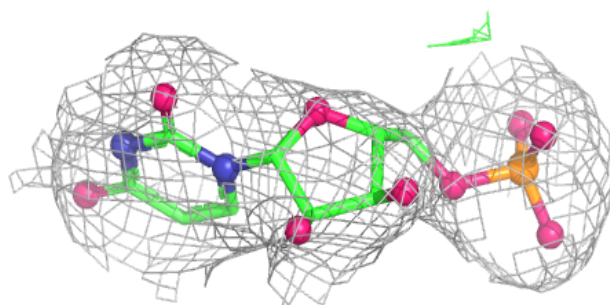
**Electron density around U5P D 801:**

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

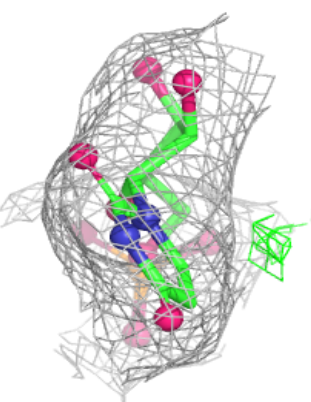
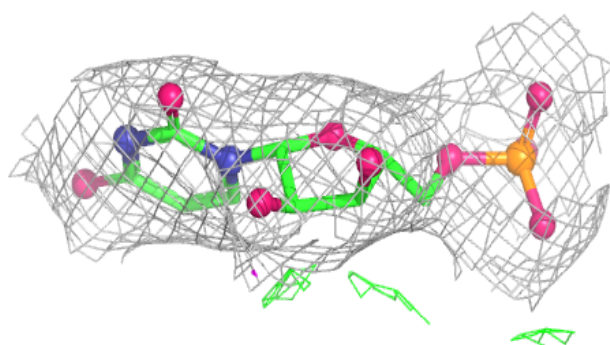
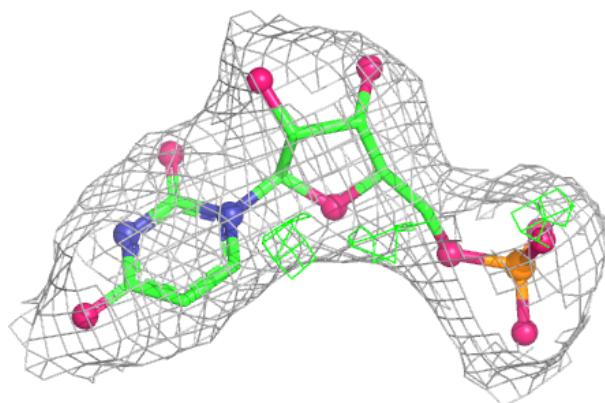


Electron density around U5P A 801:

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

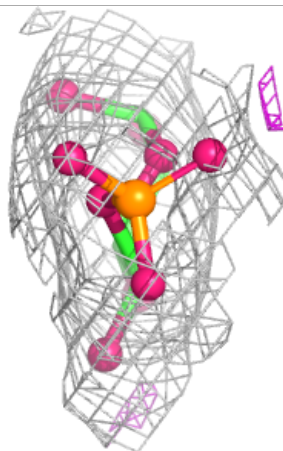
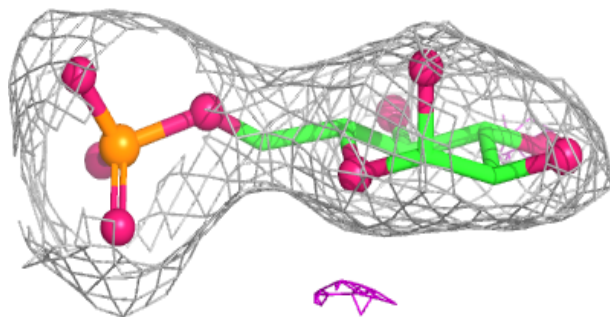
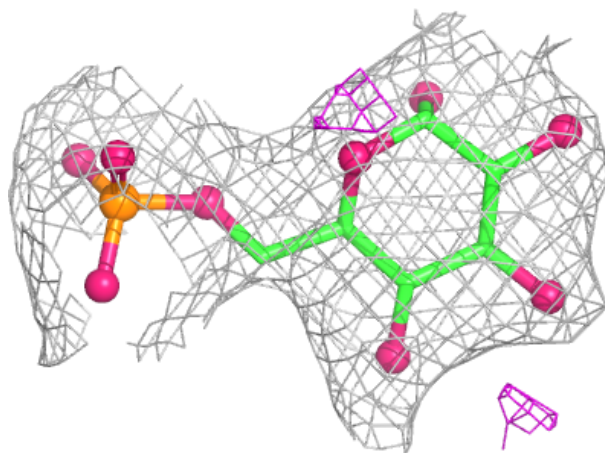
**Electron density around U5P B 801:**

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



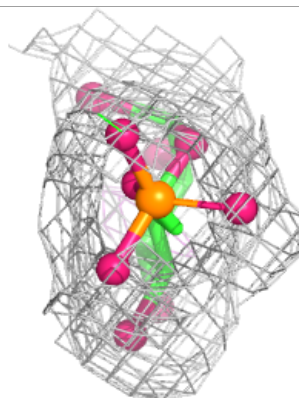
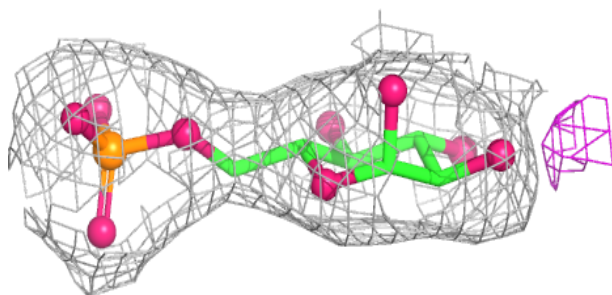
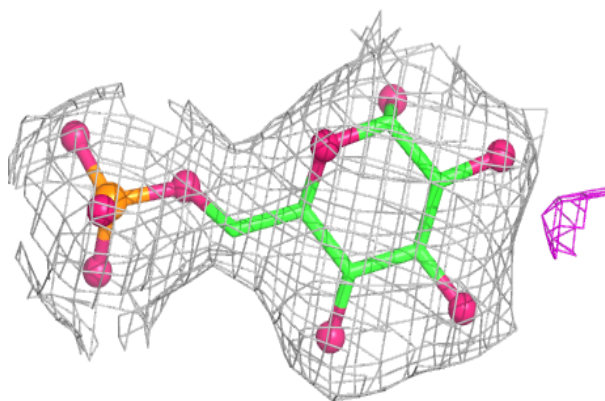
Electron density around G6P A 802:

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

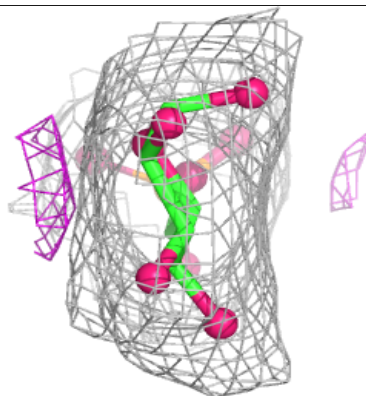
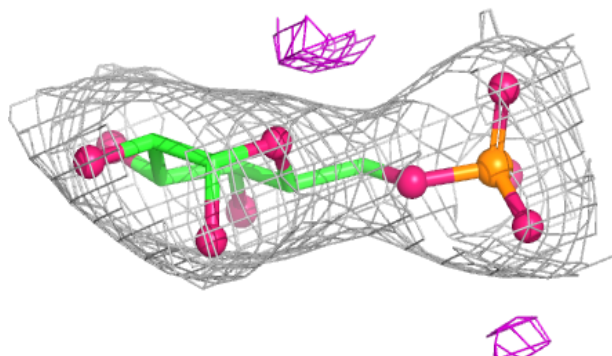
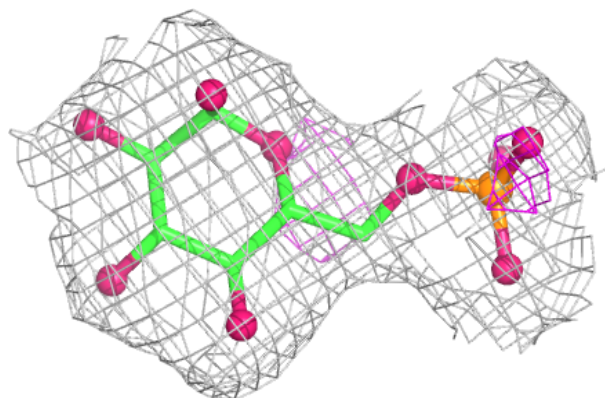


Electron density around G6P C 803:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

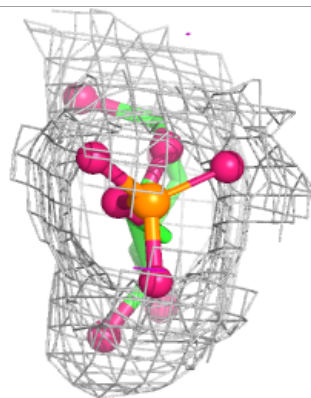
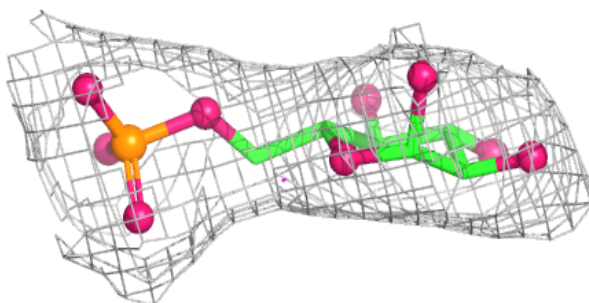
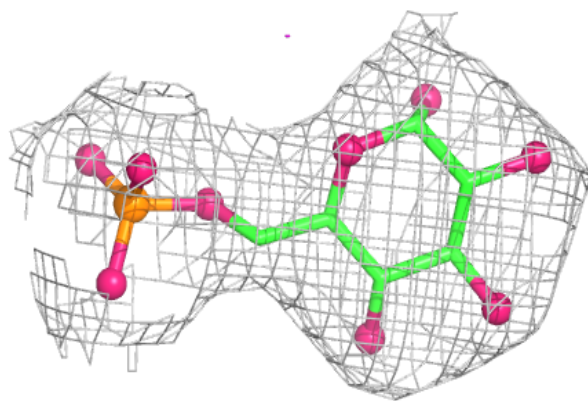
**Electron density around G6P D 802:**

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



Electron density around G6P 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.