Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 09:09 PM EDT

PDB ID	:	4KQ2
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 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 (i) 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 (i)) were used in the production of this report:

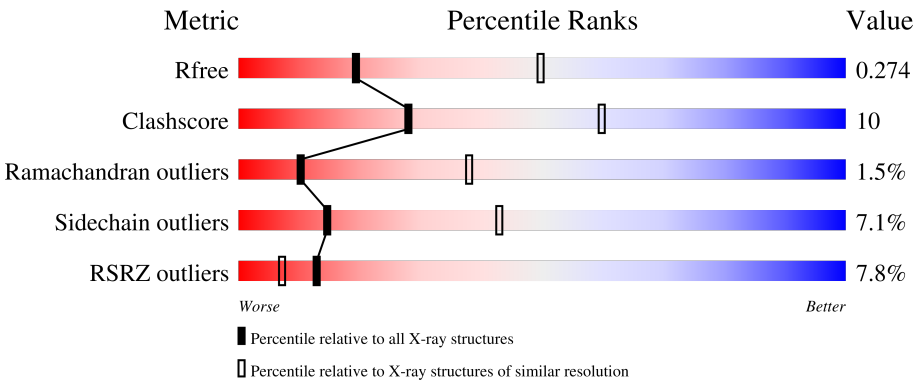
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	7%, 66%, 20%, •, 12%
1	B	724	3%, 67%, 18%, •, 12%
1	C	724	11%, 64%, 21%, •, 12%
1	D	724	7%, 64%, 22%, •, 12%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	638	5145	3286	896	944	19	0	0	0
1	B	638	5163	3298	900	946	19	0	3	0
1	C	638	5154	3291	898	946	19	0	1	0
1	D	636	5146	3284	897	946	19	0	2	0

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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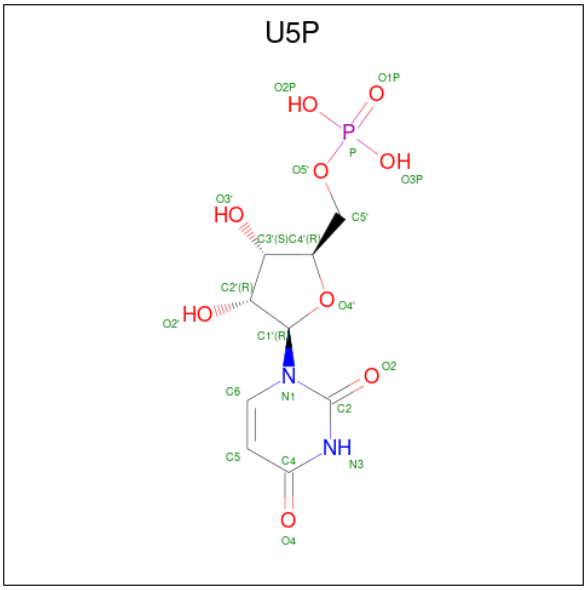
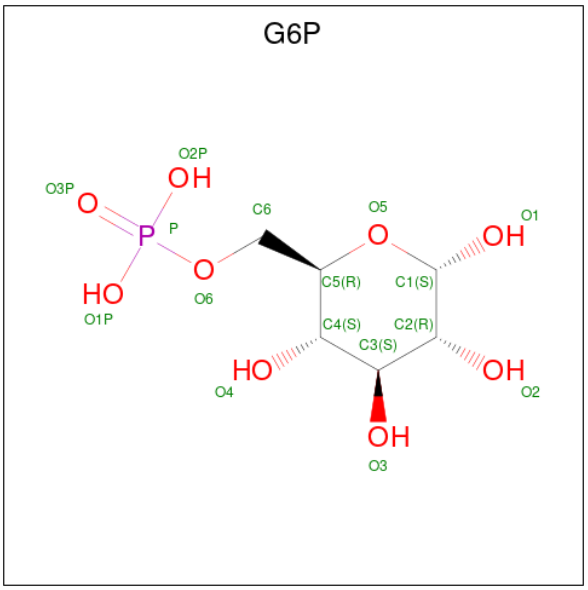
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP E7NKU1
D	-17	GLY	-	expression tag	UNP E7NKU1
D	-16	SER	-	expression tag	UNP E7NKU1
D	-15	SER	-	expression tag	UNP E7NKU1
D	-14	HIS	-	expression tag	UNP E7NKU1
D	-13	HIS	-	expression tag	UNP E7NKU1
D	-12	HIS	-	expression 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 (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



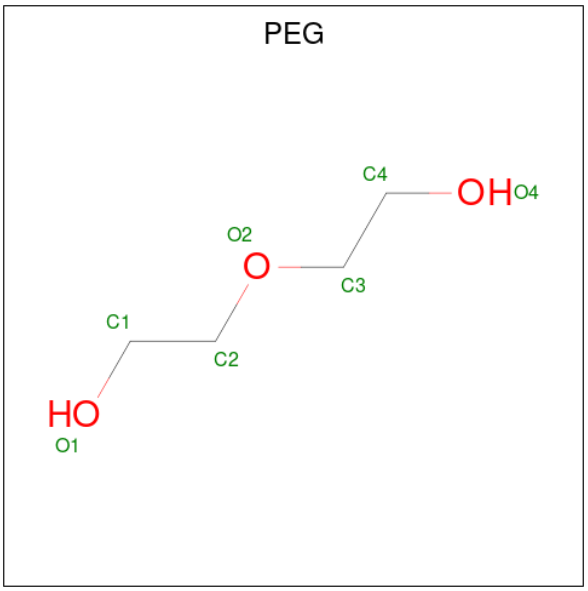
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	21	9	2	9	1	0	0
2	B	1	21	9	2	9	1	0	0
2	C	1	21	9	2	9	1	0	0
2	D	1	21	9	2	9	1	0	0

- 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
			Total	C	O	P			
3	A	1	16	6	9	1		0	0
3	B	1	16	6	9	1		0	0
3	C	1	16	6	9	1		0	0
3	D	1	16	6	9	1		0	0

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

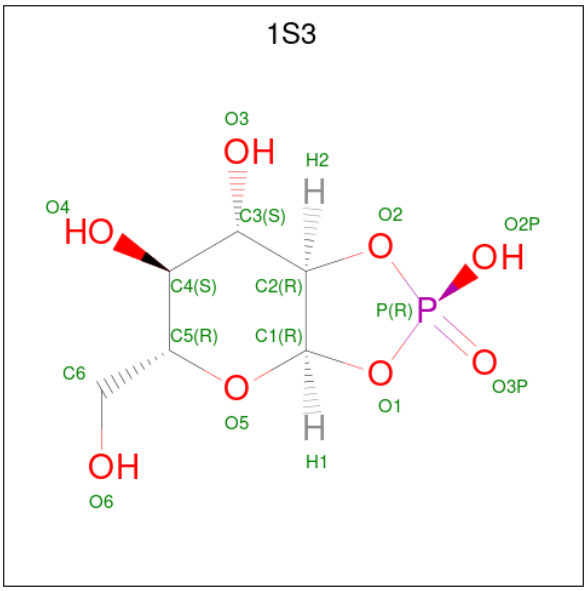


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0
4	B	1	7	4	3	0	0
4	C	1	7	4	3	0	0
4	D	1	7	4	3	0	0

- Molecule 5 is BARIUM ION (three-letter code: BA) (formula: Ba).

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

- 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 (three-letter code: 1S3) (formula: $C_6H_{11}O_8P$).



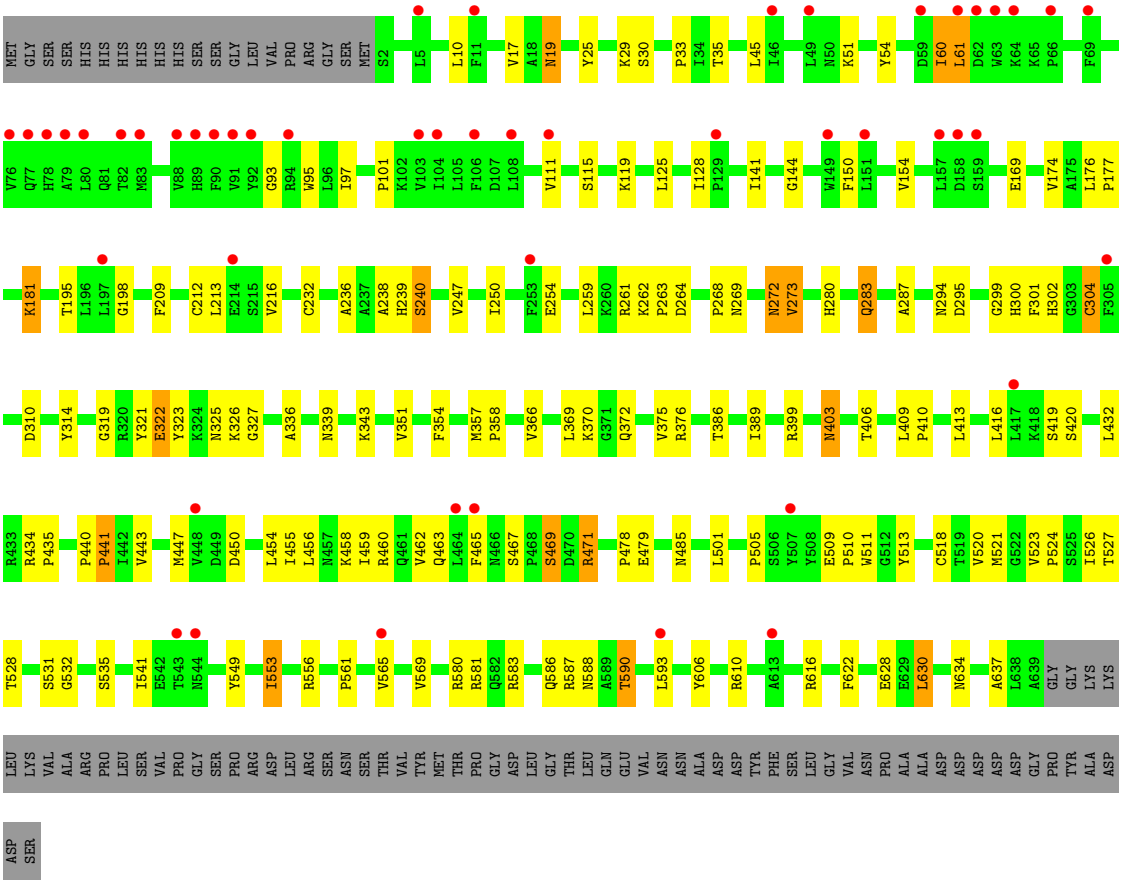
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
6	C	1	15	6	8	1	0	0

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.

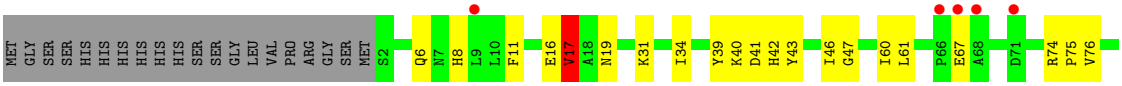
• Molecule 1: Gsy2p

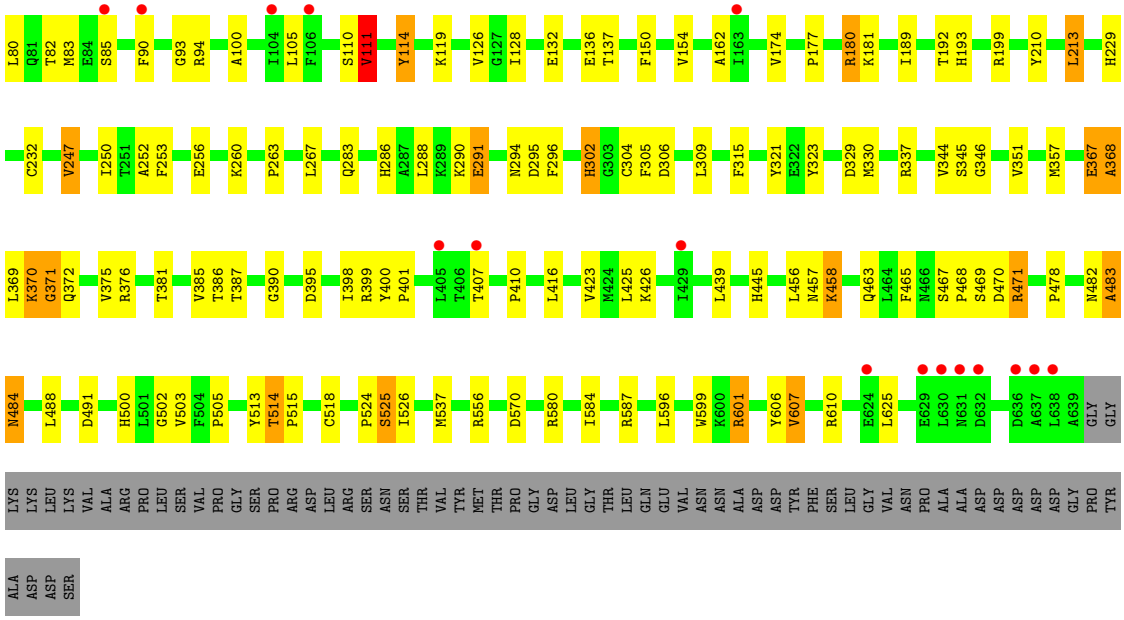
Chain A:



• Molecule 1: Gsy2p

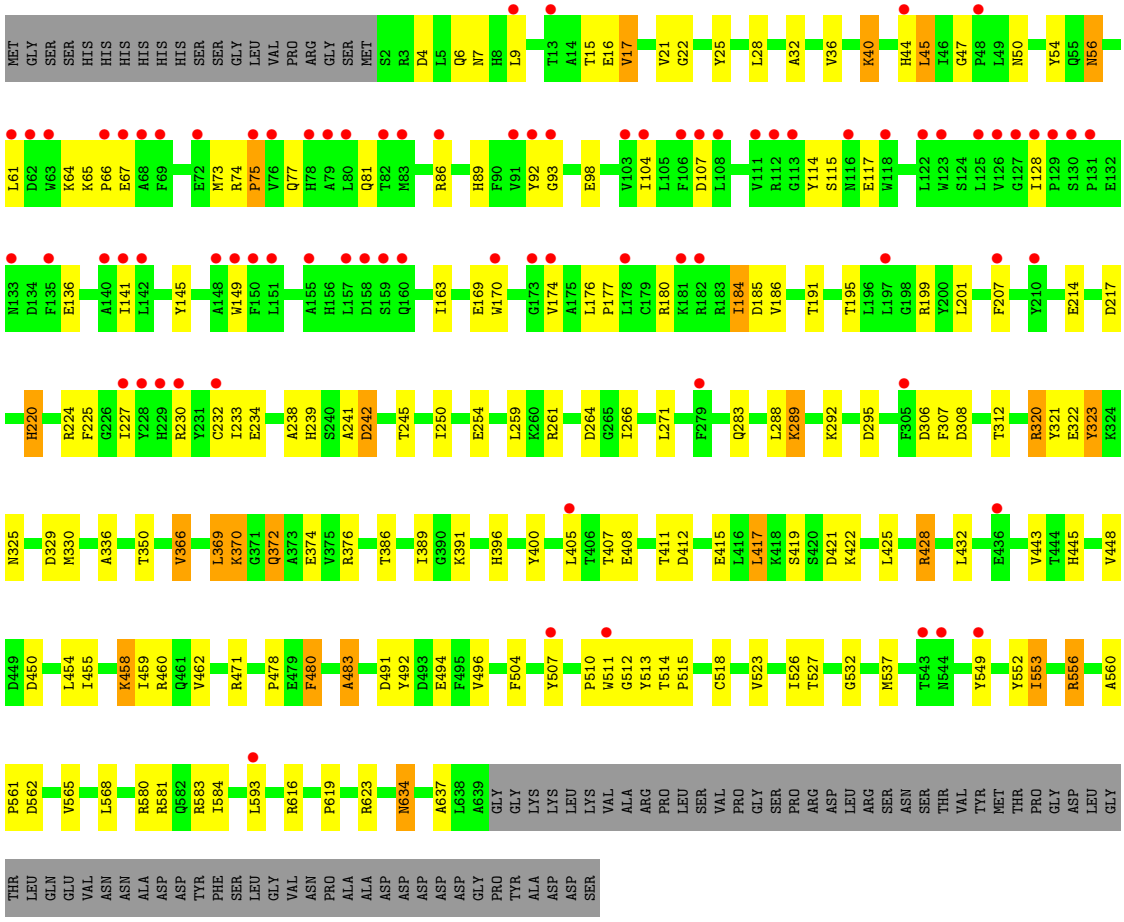
Chain B:





- Molecule 1: Gsy2p

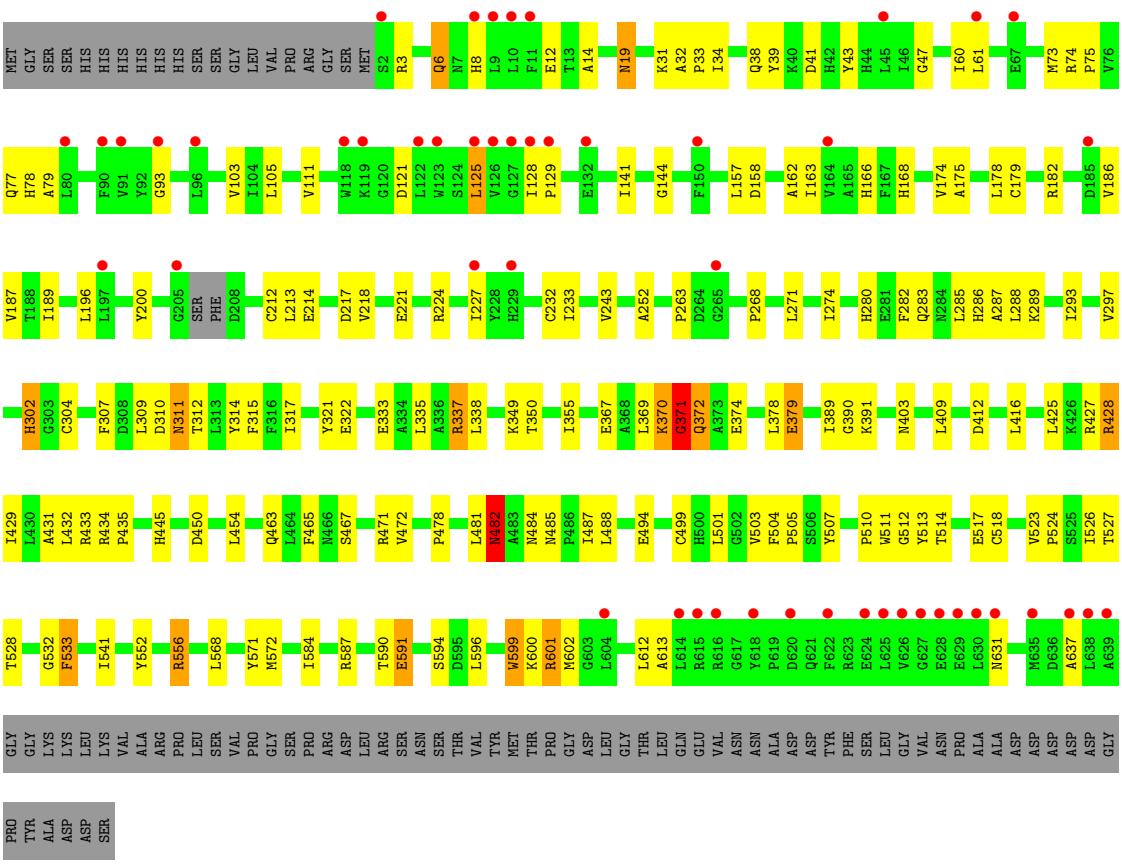
Chain C:



- Molecule 1: Gsy2p

Chain D:

7%
64%
22%
12%


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER MET S2 R3 Q6 N7 H8 L9 L10 F11 E12 T13 A14 N19 K31 A32 P33 I34 Q38 Y39 K40 D41 H42 Y43 H44 L45 I46 G47 I60 L61 E67 M73 R74 P75 V76
Q77 H78 A79 L80 F90 V91 Y92 G93 L96 V103 I104 L105 V111 W118 K119 G120 D121 L122 W123 S124 L125 V126 G127 I128 P129 E132 I141 G144 F150 L157 D158 A162 I163 V164 A165 H166 F167 H168 V174 A175 L178 C179 R182 D185 V186
V187 T188 I189 L196 L197 Y200 G205 SER PHE D208 C212 L213 E214 D217 V218 E221 R224 I227 Y228 H229 C232 I233 V243 A252 P263 D264 G265 P268 L271 I274 H280 E281 F282 Q283 N284 L285 H286 A287 L288 K289 I293 V297
H302 G303 C304 F307 D308 L309 D310 N311 T312 L313 Y314 F315 F316 I317 Y321 E322 E333 A334 L335 A336 R337 L338 K349 T350 I355 E367 A368 L369 K370 G371 Q372 A373 E374 L378 E379 I389 G390 K391 N403 L409 D412 L416 L425 K426 R427 R428
I429 L430 A431 L432 R433 R434 P435 H445 D450 L454 Q463 L464 F465 N466 S467 R471 V472 P478 L481 N482 A483 N484 N485 P486 I487 L488 E494 C499 H500 L501 G502 V503 F504 P505 S506 Y507 P510 W511 G512 Y513 T514 E517 C518 V523 P524 S525 I526 T527
T528 G532 F533 I541 Y552 R556 L568 Y571 M572 I584 R587 T590 E591 S594 D595 L596 W599 K600 R601 M602 G603 L604 L612 A613 L614 R615 R616 G617 Y618 P619 D620 Q621 F622 R623 E624 L625 V626 G627 E628 E629 L630 N631 M635 D636 A637 L638 A639
GLY GLY LYS LYS LEU LYS VAL ALA ARG PRO LEU SER VAL PRO GLY SER PRO ARG ASP LEU ARG SER ASN SER THR VAL TYR MET THR PRO GLY ASP LEU GLY THR LEU GLN GLU VAL ASN ASN ALA ASP ASP TYR PHE SER LEU GLY VAL ASN PRO ALA ASP ASP ASP ASP GLY
PRO TYR ALA ASP ASP SER

4 Data and refinement statistics (i)

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 48.41 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.46-2.95) 99.8 (48.41-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.96%)	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)	0.29 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, G6P, 1S3, BA, U5P

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	0.36	0/5270	0.56	0/7141
1	B	0.44	0/5298	0.63	0/7180
1	C	0.35	0/5279	0.56	0/7153
1	D	0.42	1/5269 (0.0%)	0.62	2/7138 (0.0%)
All	All	0.39	1/21116 (0.0%)	0.60	2/28612 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	GLY	C-O	5.58	1.32	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	372[A]	GLN	CA-CB-CG	5.01	124.43	113.40
1	D	372[B]	GLN	CA-CB-CG	5.01	124.43	113.40

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	5145	0	5054	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5163	0	5075	101	0
1	C	5154	0	5061	105	0
1	D	5146	0	5051	117	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	0	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	407	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 10.

All (407) 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
1:B:471:ARG:HH11	1:B:471:ARG:HG2	1.30	0.93
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.07	0.90
1:C:336:ALA:HB2	1:C:462:VAL:HG11	1.54	0.88
1:A:336:ALA:CB	1:A:462:VAL:CG1	2.56	0.83
1:B:439:LEU:HD22	1:B:467:SER:HA	1.60	0.83
1:B:445[B]:HIS:ND1	1:B:478:PRO:HD2	1.93	0.83
1:B:445[A]:HIS:ND1	1:B:478:PRO:HD2	1.93	0.82
1:D:482:ASN:HD22	1:D:484:ASN:H	1.24	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:HG2	1:D:280:HIS:HE1	1.42	0.82
1:C:312:THR:HG22	1:C:350:THR:HB	1.59	0.81
1:A:323:TYR:OH	1:A:458:LYS:HG3	1.83	0.79
1:B:180:ARG:HG3	1:B:180:ARG:HH11	1.48	0.78
1:D:3:ARG:NH2	1:D:158:ASP:O	2.17	0.77
1:C:330:MET:HG3	1:C:565:VAL:HG22	1.65	0.76
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.21	0.76
1:B:503:VAL:HG22	1:B:526:ILE:HD12	1.67	0.75
1:C:336:ALA:HB2	1:C:462:VAL:CG1	2.16	0.75
1:D:429:ILE:HA	1:D:432:LEU:HD12	1.67	0.75
1:D:74:ARG:N	1:D:75:PRO:HD2	2.01	0.74
1:D:482:ASN:ND2	1:D:484:ASN:H	1.86	0.72
1:A:299:GLY:HA2	1:A:375:VAL:HG21	1.69	0.72
1:A:369:LEU:HB3	1:C:369:LEU:HD22	1.72	0.72
1:A:501:LEU:HD21	1:A:526:ILE:HD12	1.71	0.71
1:A:177:PRO:HA	1:A:240:SER:OG	1.90	0.70
1:D:221:GLU:OE2	1:D:224:ARG:NH1	2.24	0.70
1:C:32:ALA:O	1:C:36:VAL:HG23	1.90	0.70
1:A:510:PRO:O	1:A:532:GLY:HA3	1.91	0.70
1:B:74:ARG:N	1:B:75:PRO:HD2	2.07	0.69
1:C:307:PHE:HD2	1:C:312:THR:HG21	1.56	0.69
1:D:471:ARG:HA	1:D:471:ARG:NE	2.06	0.69
1:C:391:LYS:HZ3	4:C:804:PEG:H22	1.57	0.69
1:B:367:GLU:O	1:B:369:LEU:N	2.24	0.69
1:D:471:ARG:HA	1:D:471:ARG:HE	1.59	0.68
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.76	0.68
1:D:526:ILE:HG21	1:D:568:LEU:HD13	1.76	0.68
1:B:193:HIS:HD2	1:B:247:VAL:HG11	1.59	0.67
1:B:463:GLN:CG	1:B:465:PHE:HE2	2.07	0.67
1:D:481:LEU:O	1:D:482:ASN:HB2	1.94	0.67
1:B:514:THR:HB	1:B:515:PRO:CD	2.25	0.67
1:A:283:GLN:HG3	3:A:802:G6P:O1	1.95	0.66
1:D:511:TRP:HA	1:D:532:GLY:HA3	1.78	0.66
1:B:463:GLN:HG2	1:B:465:PHE:HE2	1.61	0.66
1:C:583:ARG:NH1	3:C:803:G6P:O1P	2.29	0.65
1:A:463:GLN:HG2	1:A:465:PHE:HE1	1.62	0.65
1:C:50:ASN:O	1:C:54:TYR:HB3	1.96	0.65
1:B:471:ARG:HG2	1:B:471:ARG:NH1	2.04	0.65
1:B:8:HIS:HB2	1:B:162:ALA:O	1.98	0.64
1:D:283:GLN:HG3	3:D:802:G6P:O1	1.97	0.64
1:D:485:ASN:OD1	1:D:488:LEU:N	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:THR:O	1:C:553:ILE:HA	1.98	0.64
1:B:180:ARG:HG3	1:B:180:ARG:NH1	2.05	0.63
1:C:217:ASP:HB3	1:C:220:HIS:HB2	1.78	0.63
1:D:463:GLN:HA	1:D:465:PHE:CE2	2.32	0.63
1:B:330:MET:HE2	1:B:505:PRO:HB2	1.81	0.63
1:C:336:ALA:CB	1:C:462:VAL:CG1	2.76	0.63
1:B:180:ARG:HH11	1:B:180:ARG:CG	2.12	0.62
1:B:580:ARG:O	1:B:584:ILE:HG13	1.99	0.62
1:D:309:LEU:C	1:D:311:ASN:H	2.03	0.62
1:A:580:ARG:HA	1:A:583:ARG:NH1	2.14	0.62
1:C:510:PRO:O	1:C:532:GLY:HA3	1.99	0.62
1:A:586:GLN:O	1:A:590:THR:HG22	2.00	0.62
1:B:482:ASN:O	1:B:484:ASN:N	2.30	0.61
1:C:307:PHE:CD2	1:C:312:THR:HG21	2.35	0.61
1:D:378:LEU:HA	1:D:428:ARG:HG3	1.81	0.61
1:C:16:GLU:HG2	1:C:22:GLY:H	1.65	0.61
1:A:357:MET:O	1:A:478:PRO:HA	1.99	0.61
1:B:6:GLN:HE21	1:B:625:LEU:HD23	1.66	0.61
1:C:458:LYS:O	1:C:462:VAL:HG23	2.01	0.60
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.81	0.60
1:B:128:ILE:HG12	1:B:232:CYS:HB3	1.82	0.60
1:C:201:LEU:HB3	1:C:207:PHE:HE1	1.67	0.60
1:A:372:GLN:HE21	1:A:376:ARG:HH21	1.49	0.60
1:C:391:LYS:NZ	4:C:804:PEG:H22	2.17	0.60
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.84	0.60
1:A:264:ASP:OD1	1:A:616:ARG:NH1	2.34	0.59
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.01	0.59
1:B:370:LYS:O	1:B:371:GLY:C	2.39	0.59
1:A:587:ARG:HA	1:A:590:THR:HG23	1.84	0.59
1:D:485:ASN:OD1	1:D:487:ILE:N	2.36	0.58
1:A:443:VAL:HG13	1:A:456:LEU:HD21	1.85	0.58
1:D:507:TYR:HB2	1:D:556:ARG:NH2	2.19	0.58
1:C:396:HIS:NE2	1:C:405:LEU:HD12	2.19	0.58
1:D:599:TRP:HA	1:D:599:TRP:CE3	2.38	0.58
1:C:61:LEU:HB2	1:C:93:GLY:HA2	1.85	0.58
1:B:213:LEU:HD21	1:B:253:PHE:CE1	2.39	0.58
1:C:322:GLU:HB3	1:C:325:ASN:HB2	1.86	0.57
1:D:335:LEU:HD22	1:D:472:VAL:HG11	1.87	0.57
1:A:283:GLN:NE2	1:A:588:ASN:OD1	2.38	0.57
1:A:336:ALA:CB	1:A:462:VAL:HG11	2.16	0.57
1:C:400:TYR:CD2	1:C:408:GLU:HA	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:O	1:A:343:LYS:HG3	2.04	0.57
1:D:14:ALA:HB2	1:D:168:HIS:HB2	1.87	0.57
1:C:264:ASP:O	1:C:634:ASN:HB2	2.03	0.57
1:B:110:SER:O	1:B:111:VAL:HG13	2.05	0.57
1:B:502:GLY:O	1:B:525:SER:HA	2.05	0.57
1:C:619:PRO:O	1:C:623:ARG:HB2	2.05	0.57
1:A:319:GLY:HA3	1:A:326:LYS:HE3	1.87	0.56
1:B:193:HIS:HD2	1:B:247:VAL:CG1	2.17	0.56
1:A:505:PRO:HA	1:A:528:THR:HG23	1.87	0.56
1:B:302:HIS:HD1	1:B:302:HIS:C	2.08	0.56
1:B:193:HIS:CD2	1:B:247:VAL:HG11	2.40	0.56
1:B:467:SER:O	1:B:470:ASP:HB2	2.05	0.56
1:C:238:ALA:O	1:C:261:ARG:NH1	2.37	0.56
1:D:307:PHE:H	1:D:307:PHE:HD1	1.53	0.56
1:C:445:HIS:ND1	1:C:478:PRO:HD2	2.21	0.56
1:D:349:LYS:O	1:D:471:ARG:HD3	2.06	0.56
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.88	0.56
1:C:4:ASP:OD2	1:C:7:ASN:HB3	2.06	0.55
1:A:336:ALA:CB	1:A:462:VAL:HG13	2.36	0.55
1:D:428:ARG:CG	1:D:428:ARG:NH1	2.49	0.55
1:B:395:ASP:O	1:B:398:ILE:HG22	2.07	0.55
1:C:239:HIS:NE2	1:C:259:LEU:O	2.38	0.55
1:C:239:HIS:CE1	1:C:261:ARG:HB2	2.42	0.55
1:B:213:LEU:HD21	1:B:253:PHE:HE1	1.72	0.55
1:A:236:ALA:O	1:A:240:SER:HB2	2.07	0.55
1:B:357:MET:O	1:B:478:PRO:HA	2.06	0.55
1:B:482:ASN:C	1:B:484:ASN:H	2.10	0.54
1:D:503:VAL:O	1:D:505:PRO:HD3	2.07	0.54
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.37	0.54
1:D:631:ASN:HB3	1:D:637:ALA:HB1	1.89	0.54
1:A:587:ARG:HA	1:A:590:THR:CG2	2.38	0.54
1:D:61:LEU:HB2	1:D:93:GLY:HA2	1.90	0.54
1:C:308:ASP:O	1:C:312:THR:HG23	2.08	0.54
1:C:443:VAL:HG22	1:C:445:HIS:H	1.73	0.54
1:D:314:TYR:O	1:D:315:PHE:HD1	1.91	0.54
1:D:599:TRP:C	1:D:601:ARG:H	2.11	0.53
1:A:327:GLY:HA3	1:A:505:PRO:O	2.08	0.53
1:C:396:HIS:CD2	1:C:405:LEU:HD12	2.44	0.53
1:D:315:PHE:HE2	1:D:572:MET:HG2	1.74	0.53
1:D:283:GLN:HE21	1:D:584:ILE:HG23	1.72	0.53
1:C:225:PHE:O	1:C:227:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLU:OE2	1:D:337:ARG:NH1	2.39	0.53
4:C:804:PEG:H31	1:D:379:GLU:HG3	1.90	0.53
1:C:526:ILE:HG12	1:C:552:TYR:HB2	1.91	0.53
1:A:300:HIS:HD2	1:A:301:PHE:CE1	2.27	0.53
1:D:217:ASP:O	1:D:221:GLU:HG2	2.08	0.53
1:D:187:VAL:HG11	1:D:613:ALA:O	2.08	0.52
1:D:309:LEU:O	1:D:311:ASN:N	2.39	0.52
1:D:591:GLU:O	1:D:594:SER:HB3	2.09	0.52
1:A:565:VAL:O	1:A:569:VAL:HG23	2.08	0.52
1:B:385:VAL:HG21	1:B:425:LEU:HD11	1.92	0.52
1:C:336:ALA:CB	1:C:462:VAL:HG13	2.38	0.52
1:D:74:ARG:N	1:D:75:PRO:CD	2.72	0.52
1:A:95:TRP:HB3	1:A:101:PRO:HD2	1.91	0.52
1:B:39:TYR:HB2	1:B:43:TYR:HB2	1.92	0.52
1:C:141:ILE:HA	1:C:174:VAL:HG11	1.92	0.52
1:B:295:ASP:OD1	1:B:295:ASP:C	2.48	0.52
1:B:607:VAL:HG23	1:B:610:ARG:HH21	1.75	0.52
1:B:80:LEU:HD22	1:B:90:PHE:CE2	2.45	0.51
1:A:141:ILE:HA	1:A:174:VAL:HG11	1.92	0.51
1:C:201:LEU:HB3	1:C:207:PHE:CE1	2.44	0.51
1:D:482:ASN:HD22	1:D:484:ASN:N	2.01	0.51
1:A:366:VAL:O	1:A:370:LYS:HB2	2.11	0.51
1:B:456:LEU:O	1:B:458:LYS:N	2.43	0.51
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.45	0.51
1:D:282:PHE:CD2	1:D:591:GLU:HG3	2.46	0.51
1:B:31:LYS:HE2	1:B:606:TYR:CE2	2.45	0.51
1:B:367:GLU:O	1:B:368:ALA:C	2.48	0.51
1:C:283:GLN:HB3	3:C:803:G6P:O1	2.11	0.51
1:A:304:CYS:HB2	1:A:434:ARG:HD3	1.93	0.51
1:A:239:HIS:CE1	1:A:259:LEU:O	2.64	0.51
1:A:29:LYS:HG3	1:A:97:ILE:HD13	1.93	0.51
1:A:302:HIS:HB2	1:A:432:LEU:HD22	1.92	0.50
1:B:290:LYS:O	1:B:290:LYS:HG2	2.10	0.50
1:C:176:LEU:HB2	1:C:177:PRO:HD3	1.93	0.50
1:D:289:LYS:HE3	1:D:494:GLU:HG2	1.93	0.50
1:A:19:ASN:H	1:A:19:ASN:HD22	1.60	0.50
1:A:509:GLU:OE2	1:A:531:SER:HB2	2.11	0.50
1:B:513:TYR:CD1	1:B:513:TYR:N	2.79	0.50
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.46	0.50
1:B:286:HIS:HD2	1:B:587:ARG:NH2	2.10	0.50
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ARG:HD3	1:B:100:ALA:HB1	1.94	0.49
1:D:374[B]:GLU:O	1:D:374[B]:GLU:CD	2.51	0.49
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.93	0.49
1:D:282:PHE:CE2	1:D:591:GLU:HG3	2.47	0.49
1:B:315:PHE:CD2	1:B:351:VAL:HG11	2.46	0.49
1:C:512:GLY:O	1:C:515:PRO:HD2	2.12	0.49
1:B:193:HIS:CD2	1:B:247:VAL:CG1	2.96	0.49
1:D:302:HIS:O	1:D:434:ARG:HD2	2.12	0.49
1:D:19:ASN:HD22	1:D:19:ASN:N	2.11	0.49
1:C:16:GLU:HB3	1:C:25:TYR:HB2	1.95	0.49
1:A:128:ILE:HG12	1:A:232:CYS:HB3	1.93	0.49
1:A:283:GLN:CG	1:D:280:HIS:CE1	2.89	0.49
1:A:399:ARG:HD3	1:A:403:ASN:OD1	2.13	0.49
1:C:128:ILE:HG12	1:C:232:CYS:HB3	1.95	0.49
1:D:309:LEU:HA	1:D:312:THR:OG1	2.12	0.49
1:B:513:TYR:H	1:B:513:TYR:HD1	1.61	0.49
1:C:56:ASN:H	1:C:56:ASN:ND2	2.10	0.49
1:D:178:LEU:O	1:D:182:ARG:HB2	2.12	0.49
1:A:314:TYR:CD1	1:A:354:PHE:HE2	2.31	0.49
1:C:264:ASP:CG	1:C:616:ARG:HH12	2.15	0.49
1:D:315:PHE:CE2	1:D:572:MET:HG2	2.48	0.49
1:B:500:HIS:O	1:B:524:PRO:HD2	2.12	0.48
1:C:580:ARG:NE	3:C:803:G6P:O1P	2.40	0.48
1:D:513:TYR:CD1	1:D:513:TYR:N	2.81	0.48
1:D:596:LEU:HA	1:D:601:ARG:HD3	1.95	0.48
1:A:518:CYS:SG	1:A:523:VAL:HB	2.53	0.48
1:D:121:ASP:O	1:D:125:LEU:HB2	2.13	0.48
1:D:144:GLY:HA3	1:D:174:VAL:HB	1.95	0.48
1:A:403:ASN:N	1:A:403:ASN:ND2	2.60	0.48
1:D:31:LYS:O	1:D:34:ILE:HG22	2.14	0.48
1:D:587:ARG:HA	1:D:590:THR:HG22	1.95	0.48
1:C:560:ALA:C	1:C:562:ASP:H	2.15	0.48
1:A:61:LEU:HB2	1:A:93:GLY:HA2	1.95	0.48
1:A:628:GLU:HG3	1:A:630:LEU:HD23	1.95	0.48
1:B:344:VAL:C	1:B:346:GLY:H	2.16	0.48
1:C:65:LYS:HE2	1:C:67:GLU:HB3	1.96	0.48
1:D:612:LEU:HG	1:D:612:LEU:O	2.13	0.48
1:D:283:GLN:NE2	1:D:584:ILE:HG23	2.29	0.48
1:A:264:ASP:CG	1:A:616:ARG:HH12	2.18	0.47
1:B:150:PHE:O	1:B:154:VAL:HG23	2.14	0.47
1:B:514:THR:HB	1:B:515:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLU:HG3	1:C:21:VAL:HB	1.96	0.47
1:A:440:PRO:O	1:A:441:PRO:O	2.32	0.47
1:B:11:PHE:HD1	1:B:46:ILE:HD11	1.79	0.47
1:D:370:LYS:O	1:D:371:GLY:C	2.53	0.47
1:D:374[A]:GLU:HG2	1:D:431:ALA:HB1	1.95	0.47
1:D:425:LEU:O	1:D:429:ILE:HG13	2.14	0.47
1:B:463:GLN:CG	1:B:465:PHE:CE2	2.94	0.47
1:B:306:ASP:OD2	1:B:468:PRO:HB3	2.15	0.47
1:D:39:TYR:HB2	1:D:43:TYR:HB2	1.95	0.47
1:D:268:PRO:HB2	1:D:602:MET:CE	2.45	0.47
1:B:82:THR:O	1:B:85:SER:HB2	2.15	0.47
1:C:74:ARG:N	1:C:75:PRO:HD2	2.29	0.47
1:C:145:TYR:O	1:C:149:TRP:HB2	2.15	0.47
1:C:374:GLU:HB3	1:C:432:LEU:HD23	1.97	0.47
1:D:12:GLU:HG3	1:D:166:HIS:HB3	1.97	0.47
1:D:510:PRO:O	1:D:532:GLY:HA3	2.15	0.47
1:C:306:ASP:HA	1:D:403:ASN:HD21	1.80	0.47
1:D:513:TYR:O	1:D:517:GLU:HG3	2.15	0.47
1:A:287:ALA:HB2	3:A:802:G6P:H2	1.97	0.47
1:C:336:ALA:HB1	1:C:462:VAL:HG13	1.96	0.46
1:C:458:LYS:HE2	1:C:462:VAL:CG2	2.44	0.46
1:C:28:LEU:HD22	1:C:45:LEU:HD21	1.98	0.46
1:C:184:ILE:HG22	1:C:185:ASP:H	1.81	0.46
1:D:79:ALA:HB2	1:D:157:LEU:HD12	1.98	0.46
1:A:409:LEU:HD12	1:B:426:LYS:HE3	1.97	0.46
1:B:302:HIS:C	1:B:302:HIS:ND1	2.69	0.46
1:B:385:VAL:O	1:B:387:THR:N	2.49	0.46
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.51	0.46
1:C:176:LEU:HD22	1:C:241:ALA:HB2	1.98	0.46
1:C:483:ALA:N	1:C:491:ASP:OD1	2.38	0.46
1:A:150:PHE:O	1:A:154:VAL:HG23	2.16	0.46
1:D:428:ARG:HA	1:D:428:ARG:HD3	1.57	0.46
1:A:60:ILE:HD12	1:A:60:ILE:H	1.81	0.46
1:B:286:HIS:CD2	1:B:587:ARG:CZ	2.99	0.46
1:B:39:TYR:HB3	1:B:42:HIS:HB2	1.98	0.45
1:C:170:TRP:HB3	1:C:234:GLU:HG3	1.96	0.45
1:C:307:PHE:HD2	1:C:312:THR:CG2	2.26	0.45
1:D:463:GLN:HA	1:D:465:PHE:HE2	1.79	0.45
1:D:501:LEU:HD21	1:D:526:ILE:CD1	2.46	0.45
1:D:528:THR:HG21	1:D:556:ARG:HG3	1.96	0.45
1:D:47:GLY:O	1:D:105:LEU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:ARG:HE	1:D:471:ARG:CA	2.29	0.45
1:D:227:ILE:O	1:D:227:ILE:HG22	2.16	0.45
1:A:195:THR:OG1	1:A:254:GLU:OE1	2.34	0.45
1:D:501:LEU:HD21	1:D:526:ILE:HD12	1.99	0.45
1:D:599:TRP:HA	1:D:599:TRP:HE3	1.79	0.45
1:A:213:LEU:O	1:A:216:VAL:HG22	2.17	0.45
1:A:471:ARG:NE	1:A:471:ARG:HA	2.30	0.45
1:B:11:PHE:CD1	1:B:46:ILE:HD11	2.51	0.45
1:C:320:ARG:NH2	1:C:322:GLU:OE1	2.49	0.45
1:B:210:TYR:CE1	1:B:250:ILE:HD11	2.51	0.45
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.82	0.45
1:C:560:ALA:O	1:C:562:ASP:N	2.49	0.45
1:A:302:HIS:CG	1:A:302:HIS:O	2.70	0.45
1:B:267:LEU:HB3	1:B:606:TYR:CE1	2.51	0.45
1:D:523:VAL:HA	1:D:524:PRO:HD3	1.81	0.45
1:B:47:GLY:O	1:B:105:LEU:HA	2.17	0.45
1:B:410:PRO:HG2	1:B:416:LEU:HD21	1.99	0.45
1:C:17:VAL:HG13	1:C:45:LEU:HD22	1.99	0.45
1:C:417:LEU:HD22	1:C:422:LYS:HG3	1.99	0.45
1:D:41:ASP:OD2	1:D:73:MET:HG3	2.17	0.45
1:C:386:THR:HG21	1:D:390:GLY:CA	2.47	0.44
1:C:634:ASN:ND2	1:C:637:ALA:H	2.15	0.44
1:A:386:THR:HG21	1:B:390:GLY:CA	2.47	0.44
1:C:191:THR:HA	1:C:245:THR:O	2.17	0.44
1:D:482:ASN:ND2	1:D:484:ASN:HB2	2.32	0.44
1:A:450:ASP:CG	1:A:460:ARG:HH22	2.20	0.44
1:B:491:ASP:OD1	1:D:427:ARG:NH2	2.33	0.44
1:C:65:LYS:HA	1:C:66:PRO:HD3	1.88	0.44
1:C:366:VAL:O	1:C:370:LYS:HB2	2.17	0.44
1:B:17:VAL:C	1:B:19:ASN:H	2.21	0.44
1:D:286:HIS:O	1:D:287:ALA:C	2.55	0.44
1:A:25:TYR:CE2	1:A:95:TRP:HZ2	2.35	0.44
1:A:386:THR:HA	1:A:389:ILE:HD12	1.99	0.44
1:B:286:HIS:CD2	1:B:587:ARG:NH2	2.86	0.44
1:A:51:LYS:HA	1:A:54:TYR:CD1	2.53	0.44
1:A:176:LEU:HB2	1:A:177:PRO:HD3	1.99	0.44
1:A:447:MET:HB2	1:A:450:ASP:HB2	2.00	0.44
1:C:114:TYR:O	1:C:117:GLU:HG2	2.18	0.44
1:C:396:HIS:HE1	1:C:407:THR:O	2.01	0.44
1:A:322:GLU:HG2	1:A:325:ASN:HB2	1.99	0.44
1:D:144:GLY:O	1:D:175:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:ARG:HB2	1:D:435:PRO:HD2	2.00	0.44
1:D:285:LEU:HD23	1:D:285:LEU:HA	1.78	0.44
1:C:518:CYS:SG	1:C:523:VAL:HB	2.58	0.43
1:A:294:ASN:O	1:A:295:ASP:C	2.56	0.43
1:A:527:THR:O	1:A:553:ILE:HA	2.18	0.43
1:A:386:THR:HG21	1:B:390:GLY:HA2	2.00	0.43
1:A:549:TYR:HD2	1:A:593:LEU:HG	1.82	0.43
1:B:80:LEU:HB3	1:B:90:PHE:CZ	2.53	0.43
1:C:511:TRP:HB3	6:C:801:1S3:O4	2.18	0.43
1:D:32:ALA:HB3	1:D:33:PRO:HD3	2.01	0.43
1:D:367:GLU:OE1	1:D:367:GLU:HA	2.18	0.43
1:A:410:PRO:HG2	1:A:416:LEU:HD21	1.99	0.43
1:B:114:TYR:N	1:B:114:TYR:CD1	2.85	0.43
1:B:302:HIS:CD2	1:B:371:GLY:HA2	2.53	0.43
1:B:283:GLN:O	1:B:286:HIS:HB3	2.19	0.43
1:D:293:ILE:O	1:D:297:VAL:HG23	2.19	0.43
1:D:309:LEU:C	1:D:311:ASN:N	2.70	0.43
1:D:317:ILE:HG22	1:D:355:ILE:HA	1.99	0.43
1:B:76:VAL:O	1:B:80:LEU:HG	2.18	0.43
1:C:372[A]:GLN:HE21	1:C:372[A]:GLN:HB3	1.67	0.43
1:A:634:ASN:HB2	1:A:637:ALA:H	1.84	0.43
1:B:256:GLU:O	1:B:260:LYS:HA	2.17	0.43
1:C:507:TYR:HB2	1:C:556:ARG:NH2	2.34	0.43
1:D:445:HIS:ND1	1:D:478:PRO:HD2	2.33	0.43
1:B:596:LEU:HA	1:B:601:ARG:HD3	2.00	0.42
1:C:17:VAL:HG21	1:C:47:GLY:HA3	2.01	0.42
1:D:338:LEU:HD22	1:D:572:MET:HB3	2.00	0.42
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.51	0.42
1:D:189:ILE:HG23	1:D:243:VAL:HB	2.01	0.42
1:C:455:ILE:O	1:C:459:ILE:HG13	2.19	0.42
1:C:526:ILE:HG12	1:C:552:TYR:CB	2.49	0.42
1:C:580:ARG:O	1:C:584:ILE:HG13	2.19	0.42
1:A:467:SER:O	1:A:469:SER:N	2.53	0.42
1:C:44:HIS:HE1	1:C:73:MET:HE1	1.84	0.42
1:C:227:ILE:HG23	1:C:230:ARG:HD2	2.00	0.42
1:D:335:LEU:HD22	1:D:472:VAL:CG1	2.47	0.42
1:B:291:GLU:O	1:B:294:ASN:HB2	2.19	0.42
1:C:492:TYR:O	1:C:496:VAL:HG23	2.19	0.42
1:D:389:ILE:HG23	1:D:416:LEU:HD13	2.02	0.42
1:A:273:VAL:HG13	1:A:520:VAL:HG13	2.01	0.42
1:B:39:TYR:O	1:B:41:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:HIS:O	1:C:107:ASP:HB3	2.20	0.42
1:C:242:ASP:OD1	1:C:242:ASP:N	2.53	0.42
1:A:250:ILE:HD12	1:A:250:ILE:HA	1.80	0.42
1:B:514:THR:HB	1:B:515:PRO:HD3	2.00	0.42
1:C:174:VAL:HG22	1:C:233:ILE:HG21	2.01	0.42
1:C:289:LYS:HG3	1:C:494:GLU:HB3	2.01	0.42
1:C:396:HIS:HD2	1:C:415:GLU:OE2	2.02	0.42
1:C:549:TYR:HD2	1:C:593:LEU:HD21	1.84	0.42
1:D:252:ALA:HB1	1:D:263:PRO:HG2	2.01	0.42
1:D:552:TYR:HB3	1:D:571:TYR:CD2	2.55	0.42
1:A:463:GLN:HA	1:A:465:PHE:CE1	2.55	0.42
1:C:195:THR:OG1	1:C:254:GLU:OE2	2.30	0.42
1:A:198:GLY:HA2	1:A:209:PHE:CE2	2.54	0.42
1:A:262:LYS:HA	1:A:263:PRO:HD3	1.88	0.42
1:B:119:LYS:HE2	1:B:132:GLU:OE2	2.20	0.42
1:B:296:PHE:HA	1:B:372[B]:GLN:NE2	2.35	0.42
1:D:75:PRO:CB	1:D:158:ASP:HB2	2.50	0.42
1:A:351:VAL:O	1:A:351:VAL:HG12	2.20	0.42
1:A:523:VAL:HA	1:A:524:PRO:HD3	1.93	0.42
1:C:417:LEU:HD23	1:C:421:ASP:HB2	2.01	0.42
1:B:61:LEU:HB2	1:B:93:GLY:HA2	2.01	0.41
1:B:599:TRP:HA	1:B:599:TRP:CE3	2.55	0.41
1:C:526:ILE:HG21	1:C:568:LEU:CD1	2.51	0.41
1:A:19:ASN:H	1:A:19:ASN:ND2	2.19	0.41
1:B:252:ALA:HA	1:B:263:PRO:HG2	2.02	0.41
1:B:400:TYR:CD2	1:B:401:PRO:HA	2.55	0.41
1:C:580:ARG:O	1:C:581:ARG:C	2.59	0.41
1:D:78:HIS:HB2	1:D:157:LEU:HD13	2.02	0.41
1:A:238:ALA:O	1:A:261:ARG:NH1	2.52	0.41
1:A:403:ASN:N	1:A:403:ASN:HD22	2.17	0.41
1:C:428:ARG:HA	1:C:428:ARG:HD3	1.70	0.41
1:A:247:VAL:O	1:A:268:PRO:HA	2.21	0.41
1:B:114:TYR:N	1:B:114:TYR:HD1	2.18	0.41
1:D:369:LEU:HD23	1:D:487:ILE:HG23	2.03	0.41
1:B:375:VAL:O	1:B:375:VAL:CG1	2.69	0.41
1:C:92:TYR:HD1	1:C:104:ILE:HG12	1.85	0.41
1:C:480:PHE:HD1	1:C:480:PHE:HA	1.80	0.41
1:D:533:PHE:CD1	1:D:533:PHE:C	2.94	0.41
1:A:115:SER:O	1:A:119:LYS:HG3	2.20	0.41
1:A:455:ILE:O	1:A:459:ILE:HG13	2.20	0.41
1:B:337:ARG:HH11	1:B:337:ARG:HD2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:THR:OG1	1:D:528:THR:N	2.54	0.41
1:A:10:LEU:HD13	1:A:610:ARG:HD3	2.02	0.41
1:A:125:LEU:HD22	1:A:181:LYS:HG2	2.03	0.41
1:D:128:ILE:HA	1:D:129:PRO:HD2	1.98	0.41
1:D:174:VAL:HG22	1:D:233:ILE:HG21	2.03	0.41
1:A:30:SER:O	1:A:272:ASN:ND2	2.54	0.41
1:B:323:TYR:OH	1:B:458:LYS:HG2	2.20	0.41
1:B:483:ALA:HB2	1:B:491:ASP:N	2.36	0.41
1:D:196:LEU:O	1:D:200:TYR:HD2	2.04	0.41
1:A:357:MET:HA	1:A:358:PRO:HD3	1.93	0.40
1:B:74:ARG:N	1:B:75:PRO:CD	2.79	0.40
1:B:471:ARG:NH1	1:B:471:ARG:CG	2.75	0.40
1:D:38:GLN:HB3	1:D:39:TYR:CD1	2.57	0.40
1:A:269:ASN:HB2	1:A:511:TRP:CD1	2.57	0.40
1:B:439:LEU:HD22	1:B:467:SER:CA	2.40	0.40
1:C:74:ARG:NH1	1:C:77:GLN:OE1	2.54	0.40
1:C:425:LEU:HB3	1:D:409:LEU:HD21	2.04	0.40
1:A:606:TYR:HB3	1:A:610:ARG:NH2	2.37	0.40
1:B:137:THR:HG21	1:B:229:HIS:HD2	1.86	0.40
1:C:386:THR:HA	1:C:389:ILE:HD12	2.02	0.40
1:B:174:VAL:O	1:B:177:PRO:HD2	2.22	0.40
1:D:8:HIS:HB2	1:D:162:ALA:O	2.21	0.40
1:A:314:TYR:HD1	1:A:354:PHE:HE2	1.69	0.40
1:C:64:LYS:HG2	1:C:81:GLN:NE2	2.35	0.40
1:C:289:LYS:O	1:C:292:LYS:HB2	2.21	0.40

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%)	11 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	639/724 (88%)	569 (89%)	59 (9%)	11 (2%)	9	34
1	C	637/724 (88%)	576 (90%)	52 (8%)	9 (1%)	11	39
1	D	634/724 (88%)	567 (89%)	57 (9%)	10 (2%)	9	36
All	All	2546/2896 (88%)	2286 (90%)	221 (9%)	39 (2%)	10	38

All (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
1	B	368	ALA
1	B	457	ASN
1	B	483	ALA
1	D	111	VAL
1	D	482	ASN
1	D	600	LYS
1	B	17	VAL
1	B	371	GLY
1	B	386	THR
1	C	6	GLN
1	C	17	VAL
1	D	310	ASP
1	D	311	ASN
1	D	601	ARG
1	A	419	SER
1	A	435	PRO
1	B	40	LYS
1	C	40	LYS
1	C	169	GLU
1	C	561	PRO
1	B	345	SER
1	C	115	SER
1	A	169	GLU
1	A	413	LEU
1	A	561	PRO
1	C	323	TYR
1	C	483	ALA
1	D	6	GLN

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Mol	Chain	Res	Type
1	D	499	CYS
1	C	75	PRO
1	A	273	VAL
1	D	512	GLY
1	A	33	PRO
1	D	371	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	551/622 (89%)	518 (94%)	33 (6%)	19	50
1	B	554/622 (89%)	515 (93%)	39 (7%)	15	43
1	C	552/622 (89%)	506 (92%)	46 (8%)	11	35
1	D	551/622 (89%)	511 (93%)	40 (7%)	14	41
All	All	2208/2488 (89%)	2050 (93%)	158 (7%)	14	42

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	35	THR
1	A	45	LEU
1	A	60	ILE
1	A	61	LEU
1	A	111	VAL
1	A	181	LYS
1	A	212	CYS
1	A	240	SER
1	A	272	ASN
1	A	283	GLN
1	A	304	CYS
1	A	310	ASP
1	A	321	TYR
1	A	322	GLU

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Mol	Chain	Res	Type
1	A	403	ASN
1	A	406	THR
1	A	420	SER
1	A	454	LEU
1	A	469	SER
1	A	471	ARG
1	A	479	GLU
1	A	485	ASN
1	A	513	TYR
1	A	521	MET
1	A	535	SER
1	A	541	ILE
1	A	553	ILE
1	A	556	ARG
1	A	581	ARG
1	A	590	THR
1	A	622	PHE
1	A	630	LEU
1	B	16	GLU
1	B	17	VAL
1	B	34	ILE
1	B	60	ILE
1	B	67	GLU
1	B	83	MET
1	B	111	VAL
1	B	114	TYR
1	B	126	VAL
1	B	136	GLU
1	B	180	ARG
1	B	181	LYS
1	B	192	THR
1	B	199	ARG
1	B	213	LEU
1	B	247	VAL
1	B	288	LEU
1	B	291	GLU
1	B	302	HIS
1	B	321	TYR
1	B	370	LYS
1	B	376	ARG
1	B	381	THR
1	B	399	ARG

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Mol	Chain	Res	Type
1	B	407	THR
1	B	423	VAL
1	B	458	LYS
1	B	469	SER
1	B	471	ARG
1	B	484	ASN
1	B	488	LEU
1	B	514	THR
1	B	518	CYS
1	B	525	SER
1	B	537	MET
1	B	556	ARG
1	B	570	ASP
1	B	601	ARG
1	B	607	VAL
1	C	9	LEU
1	C	15	THR
1	C	40	LYS
1	C	45	LEU
1	C	56	ASN
1	C	86	ARG
1	C	98	GLU
1	C	136	GLU
1	C	180	ARG
1	C	184	ILE
1	C	199	ARG
1	C	214	GLU
1	C	220	HIS
1	C	224	ARG
1	C	242	ASP
1	C	250	ILE
1	C	266	ILE
1	C	271	LEU
1	C	288	LEU
1	C	289	LYS
1	C	295	ASP
1	C	320	ARG
1	C	321	TYR
1	C	366	VAL
1	C	369	LEU
1	C	370	LYS
1	C	372[A]	GLN

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Mol	Chain	Res	Type
1	C	372[B]	GLN
1	C	376	ARG
1	C	411	THR
1	C	412	ASP
1	C	417	LEU
1	C	419	SER
1	C	428	ARG
1	C	448	VAL
1	C	454	LEU
1	C	458	LYS
1	C	471	ARG
1	C	480	PHE
1	C	504	PHE
1	C	513	TYR
1	C	514	THR
1	C	537	MET
1	C	553	ILE
1	C	556	ARG
1	C	634	ASN
1	D	6	GLN
1	D	19	ASN
1	D	60	ILE
1	D	77	GLN
1	D	103	VAL
1	D	125	LEU
1	D	179	CYS
1	D	212	CYS
1	D	213	LEU
1	D	214	GLU
1	D	218	VAL
1	D	271	LEU
1	D	274	ILE
1	D	288	LEU
1	D	302	HIS
1	D	304	CYS
1	D	321	TYR
1	D	322	GLU
1	D	337	ARG
1	D	350	THR
1	D	370	LYS
1	D	372[A]	GLN
1	D	372[B]	GLN

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Mol	Chain	Res	Type
1	D	379	GLU
1	D	391	LYS
1	D	412	ASP
1	D	428	ARG
1	D	433	ARG
1	D	450	ASP
1	D	454	LEU
1	D	467	SER
1	D	482	ASN
1	D	504	PHE
1	D	514	THR
1	D	518	CYS
1	D	533	PHE
1	D	541	ILE
1	D	556	ARG
1	D	591	GLU
1	D	599	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	272	ASN
1	A	300	HIS
1	A	372	GLN
1	A	477	HIS
1	A	585	ASN
1	A	586	GLN
1	B	6	GLN
1	B	193	HIS
1	B	286	HIS
1	B	403	ASN
1	B	621	GLN
1	C	6	GLN
1	C	44	HIS
1	C	56	ASN
1	C	362	ASN
1	C	396	HIS
1	C	621	GLN
1	C	634	ASN
1	D	19	ASN
1	D	168	HIS

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Mol	Chain	Res	Type
1	D	211	ASN
1	D	280	HIS
1	D	403	ASN
1	D	482	ASN
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 monosaccharides 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	$\#\|Z\| > 2$
4	PEG	D	803	-	6,6,6	0.42	0	5,5,5	0.41	0
4	PEG	A	803	-	6,6,6	0.60	0	5,5,5	0.34	0
3	G6P	C	803	-	16,16,16	0.56	0	24,24,24	0.80	0
2	U5P	B	801	-	22,22,22	1.10	3 (13%)	33,33,33	1.80	5 (15%)
3	G6P	D	802	-	16,16,16	0.47	0	24,24,24	0.97	2 (8%)
6	1S3	C	801	-	14,16,16	0.63	0	19,25,25	1.31	4 (21%)
4	PEG	B	803	-	6,6,6	0.45	0	5,5,5	0.44	0
2	U5P	D	801	-	22,22,22	1.08	2 (9%)	33,33,33	1.69	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	U5P	A	801	-	22,22,22	1.13	2 (9%)	33,33,33	1.71	6 (18%)
3	G6P	A	802	-	16,16,16	0.58	0	24,24,24	1.10	2 (8%)
2	U5P	C	802	-	22,22,22	1.09	1 (4%)	33,33,33	1.74	7 (21%)
3	G6P	B	802	-	16,16,16	0.46	0	24,24,24	1.07	1 (4%)
4	PEG	C	804	-	6,6,6	0.49	0	5,5,5	0.27	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
4	PEG	D	803	-	-	3/4/4/4	-
4	PEG	A	803	-	-	3/4/4/4	-
3	G6P	C	803	-	-	2/6/26/26	0/1/1/1
2	U5P	B	801	-	-	3/10/26/26	0/2/2/2
3	G6P	D	802	-	-	3/6/26/26	0/1/1/1
6	1S3	C	801	-	-	0/2/32/32	0/2/2/2
4	PEG	B	803	-	-	2/4/4/4	-
2	U5P	D	801	-	-	3/10/26/26	0/2/2/2
2	U5P	A	801	-	-	5/10/26/26	0/2/2/2
3	G6P	A	802	-	-	3/6/26/26	0/1/1/1
2	U5P	C	802	-	-	2/10/26/26	0/2/2/2
3	G6P	B	802	-	-	2/6/26/26	0/1/1/1
4	PEG	C	804	-	-	3/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	802	U5P	C2-N1	2.56	1.42	1.38
2	A	801	U5P	C4-N3	-2.44	1.34	1.38
2	B	801	U5P	C6-C5	2.37	1.40	1.35
2	D	801	U5P	C6-C5	2.29	1.40	1.35
2	B	801	U5P	C2-N1	2.25	1.42	1.38
2	B	801	U5P	C4-N3	-2.17	1.34	1.38
2	D	801	U5P	C4-N3	-2.11	1.34	1.38
2	A	801	U5P	C2-N3	-2.06	1.34	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	U5P	N3-C2-N1	5.16	121.74	114.89
2	B	801	U5P	C4-N3-C2	-4.92	120.08	126.58
2	D	801	U5P	N3-C2-N1	4.74	121.19	114.89
2	A	801	U5P	C4-N3-C2	-4.72	120.36	126.58
2	D	801	U5P	C4-N3-C2	-4.70	120.38	126.58
2	C	802	U5P	C4-N3-C2	-4.27	120.94	126.58
2	A	801	U5P	N3-C2-N1	4.24	120.52	114.89
2	C	802	U5P	N3-C2-N1	3.90	120.07	114.89
2	A	801	U5P	C5-C4-N3	3.83	120.57	114.84
2	C	802	U5P	C5-C4-N3	3.64	120.29	114.84
2	B	801	U5P	C5-C4-N3	3.23	119.67	114.84
2	D	801	U5P	C5-C4-N3	3.16	119.57	114.84
2	C	802	U5P	O4-C4-C5	-3.13	119.66	125.16
3	A	802	G6P	O2P-P-O1P	2.88	118.66	107.64
2	D	801	U5P	O2-C2-N1	-2.85	118.99	122.79
2	A	801	U5P	O4-C4-C5	-2.78	120.27	125.16
3	B	802	G6P	C1-O5-C5	2.77	118.89	113.66
2	B	801	U5P	O2-C2-N1	-2.75	119.14	122.79
2	D	801	U5P	O4-C4-C5	-2.63	120.53	125.16
2	C	802	U5P	C3'-C2'-C1'	2.62	106.41	101.43
6	C	801	1S3	O5-C1-O1	2.54	113.93	109.34
2	B	801	U5P	O4-C4-C5	-2.40	120.94	125.16
2	A	801	U5P	C3'-C2'-C1'	2.29	105.77	101.43
3	D	802	G6P	O2P-P-O1P	2.22	116.14	107.64
6	C	801	1S3	P-O1-C1	-2.20	106.80	111.26
3	A	802	G6P	O2P-P-O6	-2.20	100.89	106.73
6	C	801	1S3	O2-P-O3P	-2.15	110.08	115.76
2	C	802	U5P	C2'-C1'-N1	-2.09	107.29	113.22
6	C	801	1S3	O1-P-O3P	-2.07	110.31	115.76
3	D	802	G6P	O5-C1-C2	-2.06	106.62	110.28
2	A	801	U5P	O2-C2-N1	-2.04	120.07	122.79
2	C	802	U5P	C1'-N1-C2	2.02	121.22	117.57

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	U5P	O4'-C4'-C5'-O5'
2	B	801	U5P	C5'-O5'-P-O2P
2	B	801	U5P	C5'-O5'-P-O3P
2	D	801	U5P	O4'-C4'-C5'-O5'
3	A	802	G6P	C6-O6-P-O3P
3	B	802	G6P	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	802	G6P	O5-C5-C6-O6
3	C	803	G6P	C4-C5-C6-O6
3	D	802	G6P	C6-O6-P-O2P
4	D	803	PEG	O1-C1-C2-O2
4	A	803	PEG	O1-C1-C2-O2
4	B	803	PEG	O2-C3-C4-O4
4	C	804	PEG	O2-C3-C4-O4
2	B	801	U5P	C5'-O5'-P-O1P
3	D	802	G6P	C6-O6-P-O3P
3	C	803	G6P	O5-C5-C6-O6
2	D	801	U5P	C4'-C5'-O5'-P
4	A	803	PEG	O2-C3-C4-O4
3	D	802	G6P	C6-O6-P-O1P
4	A	803	PEG	C1-C2-O2-C3
4	D	803	PEG	C1-C2-O2-C3
4	D	803	PEG	C4-C3-O2-C2
2	D	801	U5P	C3'-C4'-C5'-O5'
2	C	802	U5P	C4'-C5'-O5'-P
2	A	801	U5P	C3'-C4'-C5'-O5'
2	A	801	U5P	O4'-C1'-N1-C6
2	A	801	U5P	C2'-C1'-N1-C6
4	C	804	PEG	C4-C3-O2-C2
3	A	802	G6P	C6-O6-P-O1P
3	A	802	G6P	C6-O6-P-O2P
2	C	802	U5P	O4'-C4'-C5'-O5'
4	B	803	PEG	O1-C1-C2-O2
4	C	804	PEG	C1-C2-O2-C3
2	A	801	U5P	C4'-C5'-O5'-P

There are no ring outliers.

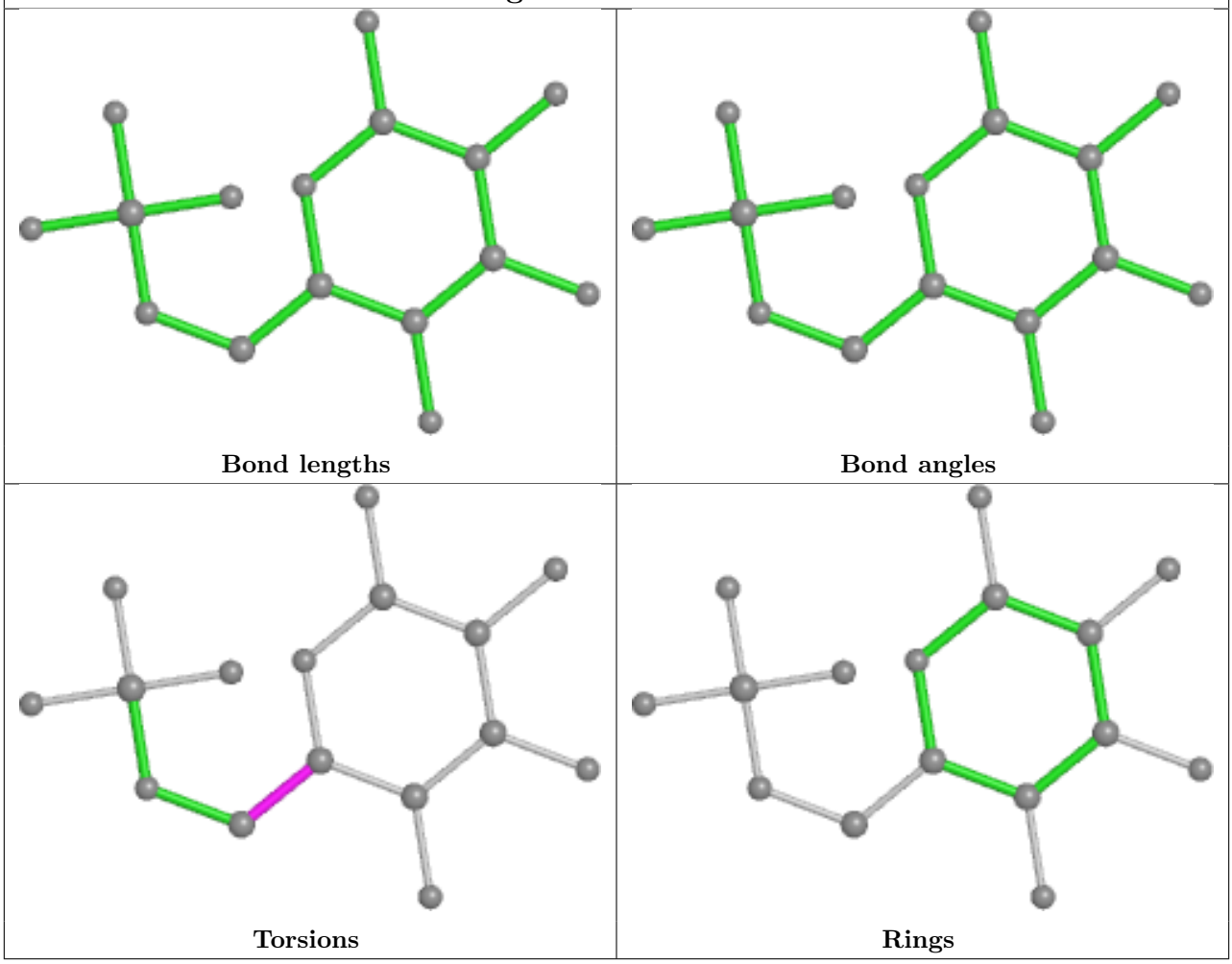
5 monomers are involved in 10 short contacts:

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

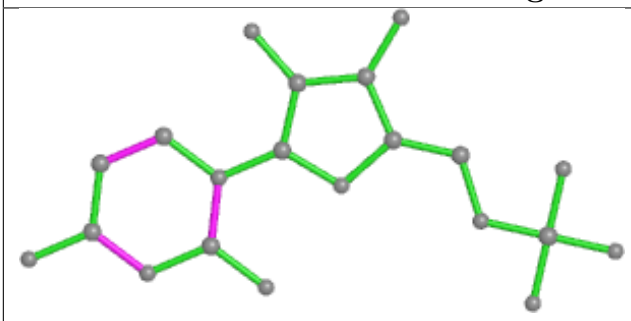
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

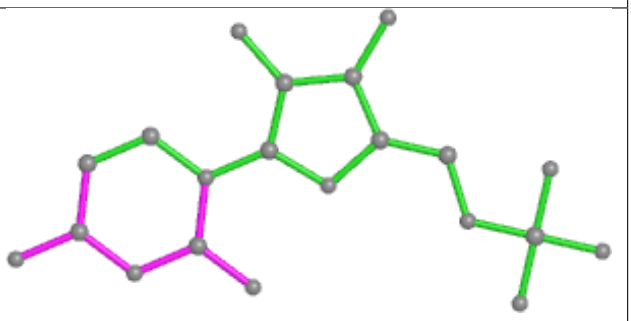
Ligand G6P C 803



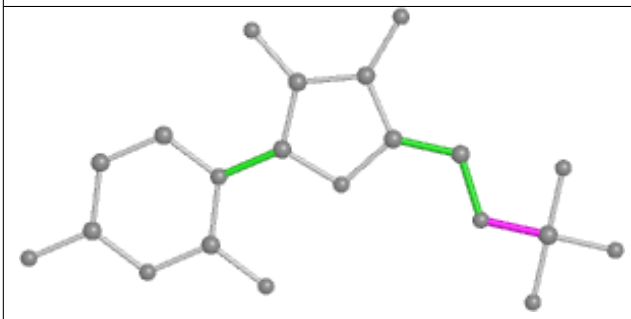
Ligand U5P B 801



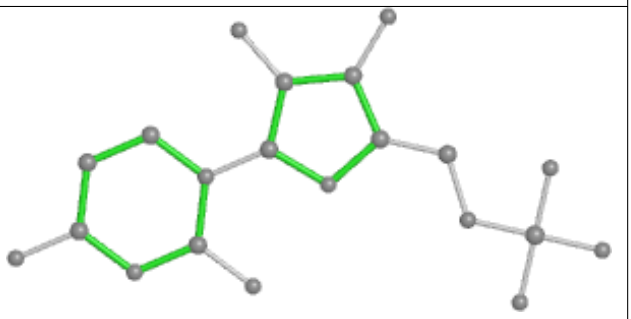
Bond lengths



Bond angles

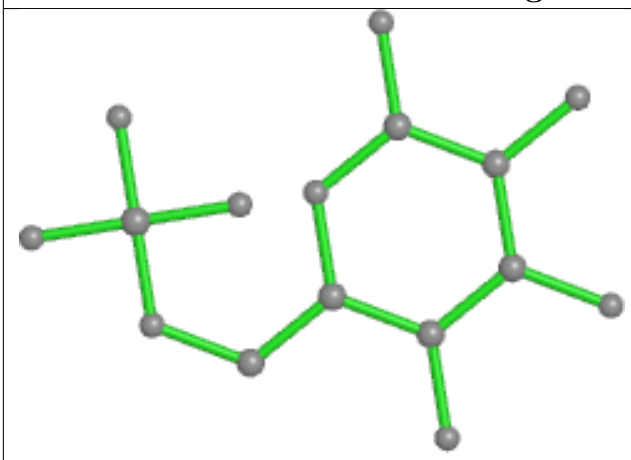


Torsions



Rings

Ligand G6P D 802



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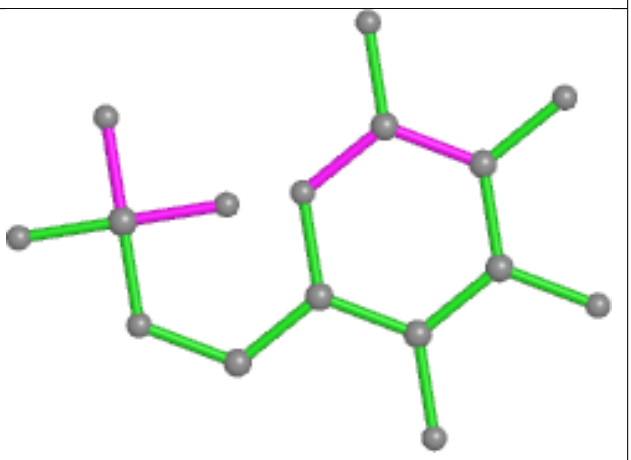
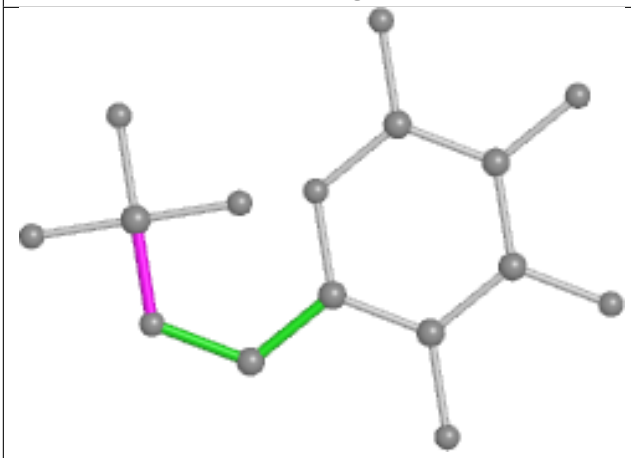
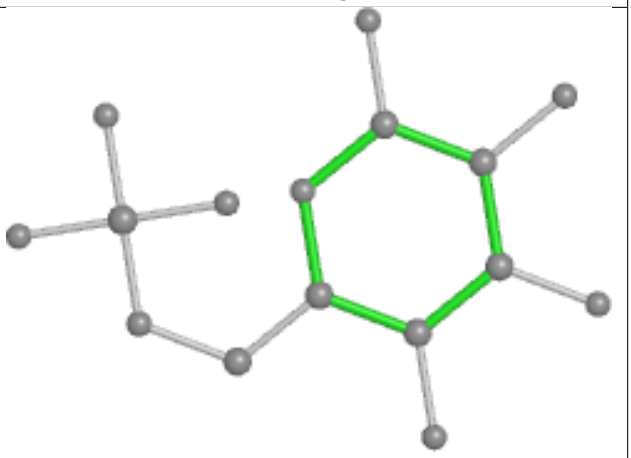


Bond angles

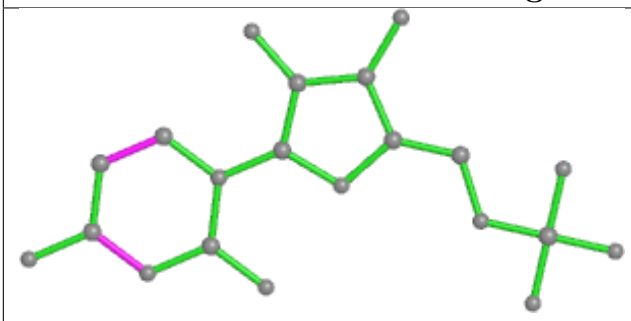


Torsions

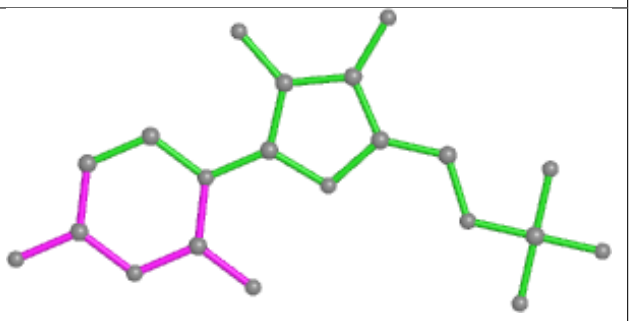


Rings

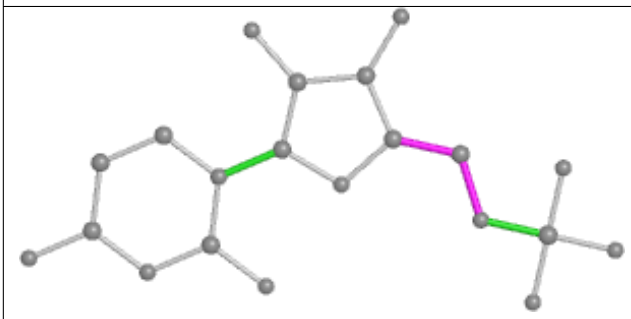
Ligand U5P D 801



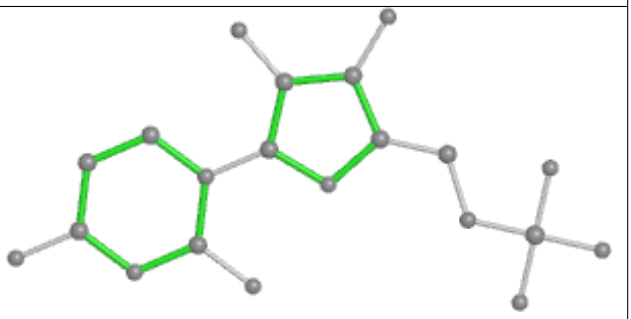
Bond lengths



Bond angles

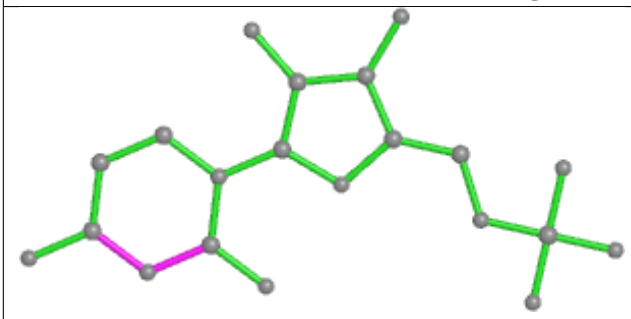


Torsions



Rings

Ligand U5P A 801



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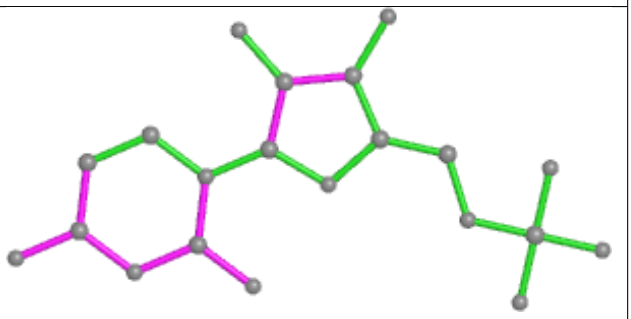
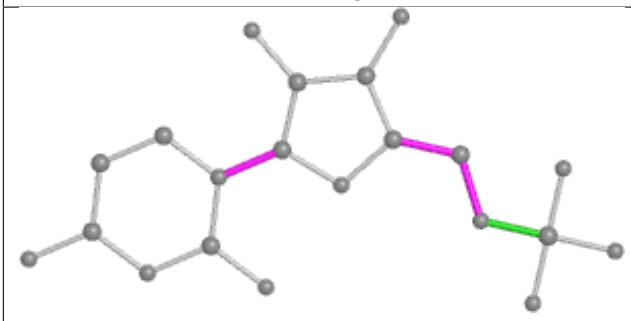
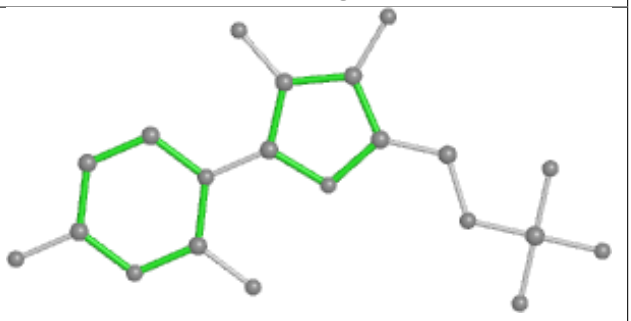


Bond angles

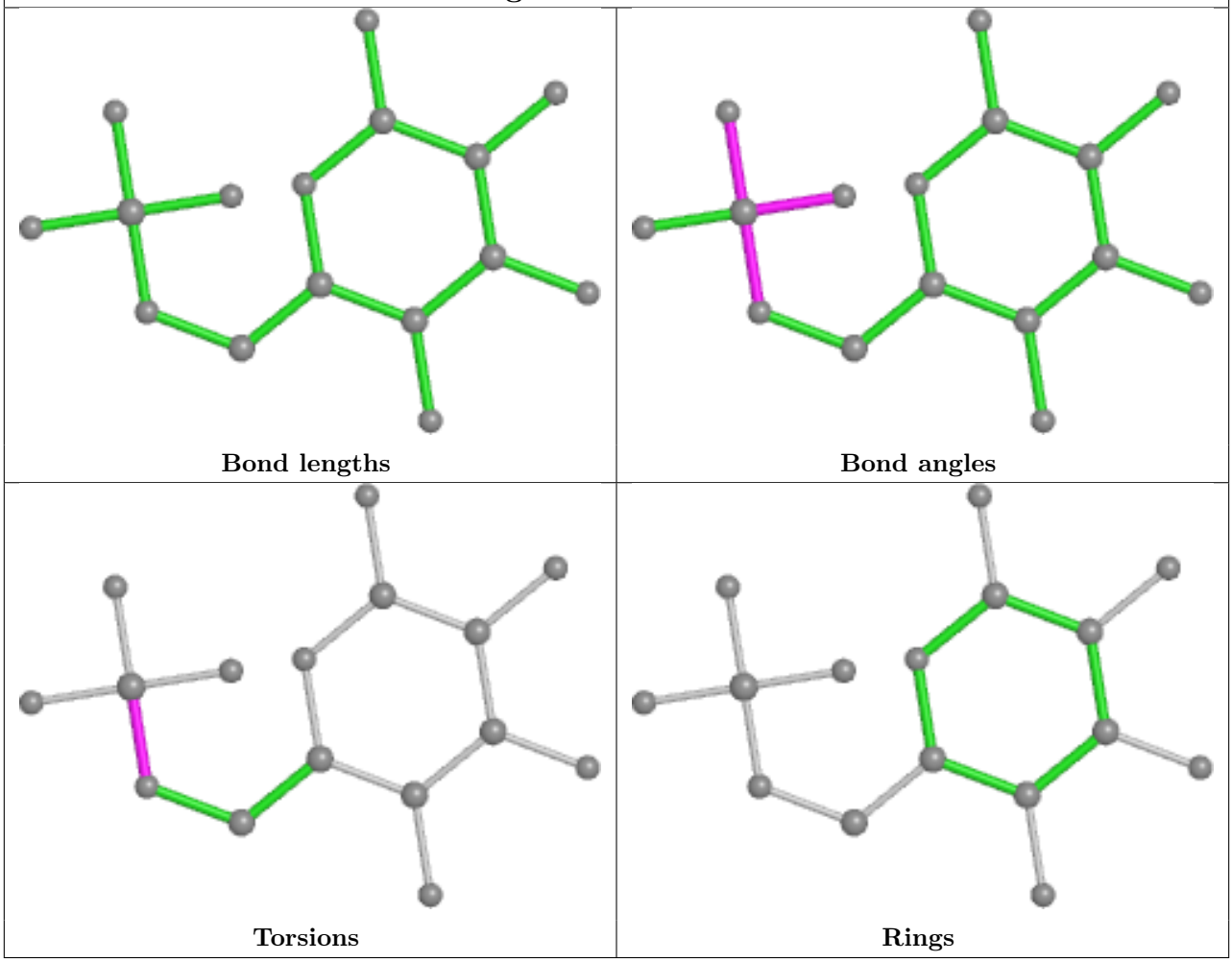


Torsions

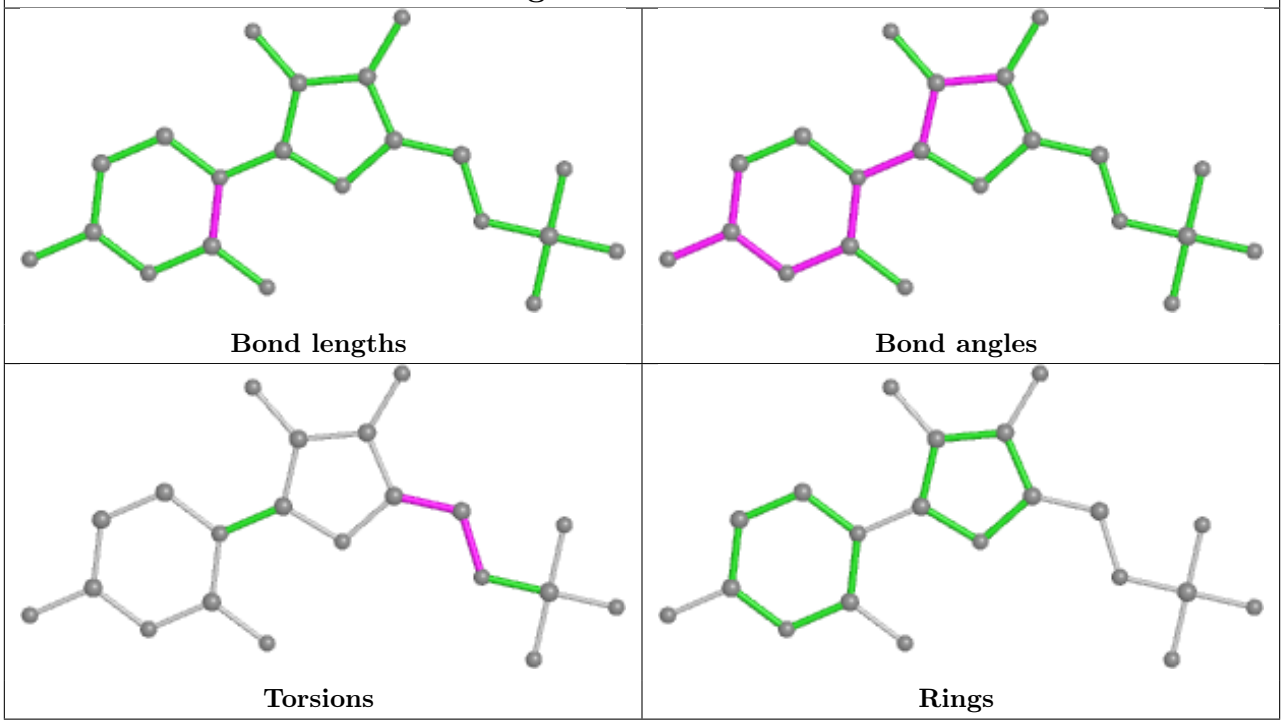


Rings

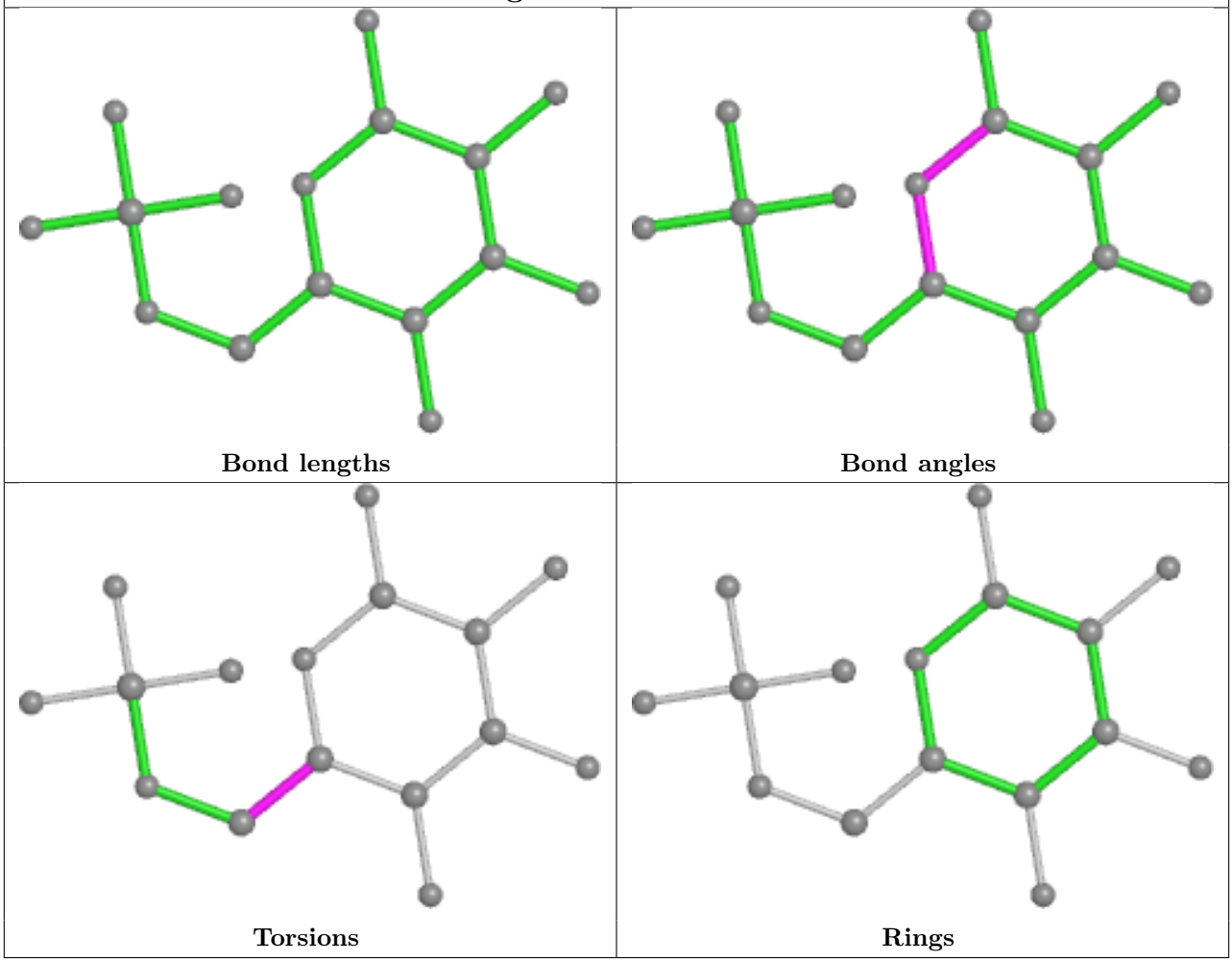
Ligand G6P A 802



Ligand U5P C 802



Ligand G6P B 802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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%)	0.41	49 (7%)	13	7	53, 103, 165, 226	0
1	B	638/724 (88%)	0.17	21 (3%)	46	30	24, 86, 150, 198	0
1	C	638/724 (88%)	0.70	80 (12%)	3	2	45, 108, 183, 247	0
1	D	636/724 (87%)	0.45	50 (7%)	12	7	30, 104, 190, 223	0
All	All	2550/2896 (88%)	0.43	200 (7%)	13	7	24, 101, 179, 247	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	638	LEU	9.9
1	C	141	ILE	8.3
1	C	111	VAL	7.6
1	C	63	TRP	7.2
1	B	630	LEU	7.1
1	C	108	LEU	7.0
1	C	91	VAL	7.0
1	D	630	LEU	6.8
1	D	125	LEU	6.6
1	C	127	GLY	6.4
1	A	91	VAL	6.2
1	C	103	VAL	6.1
1	C	106	PHE	6.1
1	C	155	ALA	5.9
1	D	626	VAL	5.7
1	C	129	PRO	5.6
1	C	131	PRO	5.5
1	D	627	GLY	5.3
1	A	77	GLN	5.3
1	B	624	GLU	5.2
1	C	128	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	63	TRP	5.0
1	C	92	TYR	5.0
1	C	83	MET	5.0
1	A	61	LEU	4.9
1	D	622	PHE	4.8
1	A	92	TYR	4.8
1	C	181	LYS	4.7
1	D	639	ALA	4.4
1	C	76	VAL	4.4
1	D	631	ASN	4.4
1	C	126	VAL	4.3
1	D	129	PRO	4.3
1	A	80	LEU	4.3
1	D	122	LEU	4.2
1	A	104	ILE	4.2
1	C	68	ALA	4.2
1	D	123	TRP	4.2
1	D	126	VAL	4.2
1	D	618	TYR	4.2
1	D	635	MET	4.1
1	D	2	SER	4.1
1	D	10	LEU	4.1
1	D	629	GLU	4.1
1	C	157	LEU	4.1
1	C	107	ASP	4.0
1	D	205	GLY	4.0
1	D	614	LEU	4.0
1	D	628	GLU	4.0
1	D	625	LEU	4.0
1	C	170	TRP	3.9
1	D	637	ALA	3.9
1	A	76	VAL	3.8
1	A	305	PHE	3.8
1	C	544	ASN	3.7
1	C	279	PHE	3.7
1	D	91	VAL	3.6
1	B	67	GLU	3.6
1	A	90	PHE	3.6
1	D	604	LEU	3.5
1	C	142	LEU	3.4
1	A	197	LEU	3.4
1	A	64	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	624	GLU	3.4
1	A	5	LEU	3.4
1	A	78	HIS	3.4
1	C	118	TRP	3.4
1	C	123	TRP	3.3
1	D	45	LEU	3.3
1	C	86	ARG	3.3
1	D	127	GLY	3.3
1	A	106	PHE	3.3
1	C	149	TRP	3.3
1	D	128	ILE	3.2
1	C	62	ASP	3.2
1	D	229	HIS	3.2
1	C	133	ASN	3.2
1	B	632	ASP	3.2
1	D	61	LEU	3.1
1	A	79	ALA	3.1
1	C	80	LEU	3.1
1	B	405	LEU	3.1
1	C	79	ALA	3.1
1	B	629	GLU	3.1
1	C	78	HIS	3.1
1	D	67	GLU	3.1
1	D	132	GLU	3.0
1	C	125	LEU	3.0
1	C	227	ILE	3.0
1	A	88	VAL	3.0
1	D	150	PHE	3.0
1	C	549	TYR	2.9
1	B	106	PHE	2.9
1	C	66	PRO	2.9
1	D	265	GLY	2.9
1	C	69	PHE	2.9
1	C	173	GLY	2.9
1	C	67	GLU	2.9
1	C	229	HIS	2.9
1	C	116	ASN	2.9
1	A	507	TYR	2.8
1	C	104	ILE	2.8
1	C	210	TYR	2.8
1	D	9	LEU	2.8
1	C	151	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	140	ALA	2.8
1	C	543	THR	2.8
1	A	89	HIS	2.8
1	B	71	ASP	2.8
1	D	616	ARG	2.7
1	A	214	GLU	2.7
1	C	135	PHE	2.7
1	C	228	TYR	2.7
1	A	543	THR	2.7
1	A	62	ASP	2.6
1	D	620	ASP	2.6
1	B	163	ILE	2.6
1	A	158	ASP	2.6
1	A	83	MET	2.6
1	A	151	LEU	2.6
1	A	464	LEU	2.6
1	C	174	VAL	2.6
1	C	48	PRO	2.6
1	C	178	LEU	2.6
1	B	631	ASN	2.6
1	A	108	LEU	2.6
1	B	638	LEU	2.5
1	D	164	VAL	2.5
1	C	207	PHE	2.5
1	A	129	PRO	2.5
1	D	118	TRP	2.5
1	C	112	ARG	2.5
1	A	103	VAL	2.5
1	C	182	ARG	2.5
1	C	93	GLY	2.5
1	A	149	TRP	2.5
1	B	85	SER	2.4
1	B	637	ALA	2.4
1	B	636	ASP	2.4
1	C	230	ARG	2.4
1	B	9	LEU	2.4
1	A	565	VAL	2.4
1	C	44	HIS	2.4
1	A	448	VAL	2.4
1	D	615	ARG	2.4
1	A	66	PRO	2.4
1	C	61	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	130	SER	2.3
1	D	8	HIS	2.3
1	A	544	ASN	2.3
1	C	305	PHE	2.3
1	C	160	GLN	2.3
1	C	197	LEU	2.3
1	D	227	ILE	2.3
1	C	113	GLY	2.3
1	D	93	GLY	2.3
1	D	185	ASP	2.3
1	A	157	LEU	2.3
1	A	69	PHE	2.3
1	C	82	THR	2.3
1	C	593	LEU	2.3
1	D	197	LEU	2.2
1	A	465	PHE	2.2
1	B	407	THR	2.2
1	D	90	PHE	2.2
1	B	68	ALA	2.2
1	C	507	TYR	2.2
1	A	417	LEU	2.2
1	A	593	LEU	2.2
1	A	46	ILE	2.2
1	C	148	ALA	2.2
1	D	80	LEU	2.2
1	C	159	SER	2.2
1	C	158	ASP	2.2
1	C	122	LEU	2.2
1	B	429	ILE	2.2
1	A	82	THR	2.2
1	A	11	PHE	2.1
1	A	253	PHE	2.1
1	D	96	LEU	2.1
1	C	13	THR	2.1
1	A	613	ALA	2.1
1	B	90	PHE	2.1
1	C	75	PRO	2.1
1	C	232	CYS	2.1
1	C	72	GLU	2.1
1	A	49	LEU	2.0
1	D	11	PHE	2.1
1	A	59	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	159	SER	2.0
1	A	111	VAL	2.0
1	A	94	ARG	2.0
1	C	511	TRP	2.0
1	C	436	GLU	2.0
1	C	9	LEU	2.0
1	C	150	PHE	2.0
1	B	104	ILE	2.0
1	D	119	LYS	2.0
1	B	66	PRO	2.0
1	C	405	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BA	B	805	1/1	0.64	0.06	245,245,245,245	0
5	BA	D	805	1/1	0.78	0.07	227,227,227,227	0
6	1S3	C	801	15/15	0.82	0.21	107,130,156,156	0
4	PEG	C	804	7/7	0.84	0.34	88,89,96,96	0
4	PEG	B	803	7/7	0.85	0.25	98,103,115,115	0
2	U5P	C	802	21/21	0.87	0.26	95,123,162,163	0
5	BA	A	805	1/1	0.88	0.17	212,212,212,212	0
4	PEG	D	803	7/7	0.92	0.23	90,90,95,96	0
4	PEG	A	803	7/7	0.92	0.19	71,74,82,85	0
5	BA	B	804	1/1	0.92	0.26	149,149,149,149	0
2	U5P	A	801	21/21	0.93	0.23	89,103,120,123	0
5	BA	D	804	1/1	0.93	0.22	159,159,159,159	0

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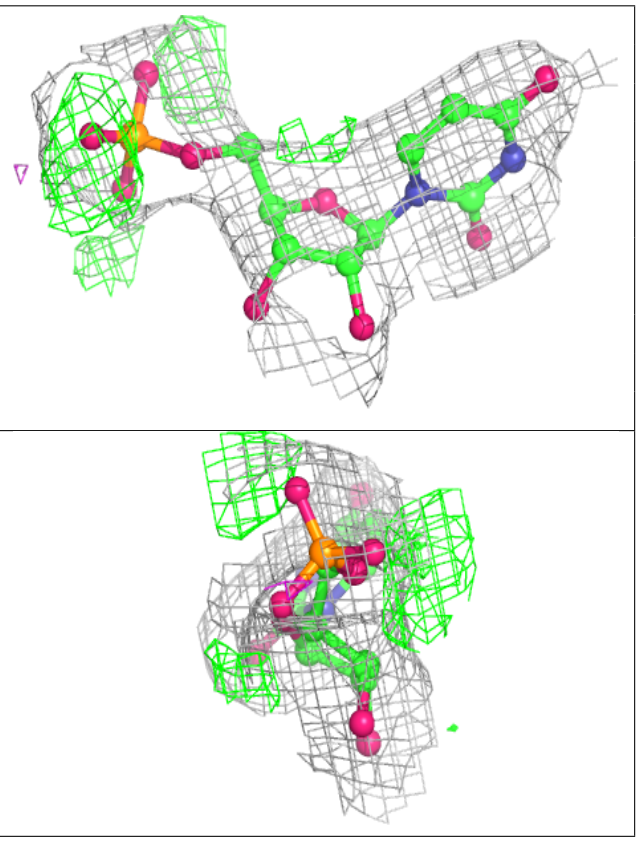
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	U5P	D	801	21/21	0.94	0.15	93,105,112,127	0
2	U5P	B	801	21/21	0.96	0.15	82,91,100,105	0
3	G6P	B	802	16/16	0.98	0.19	56,74,80,80	0
3	G6P	C	803	16/16	0.98	0.15	66,77,83,84	0
3	G6P	D	802	16/16	0.98	0.16	55,67,75,78	0
5	BA	A	804	1/1	0.98	0.22	135,135,135,135	0
3	G6P	A	802	16/16	0.98	0.16	80,92,98,102	0
5	BA	C	805	1/1	0.99	0.23	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.

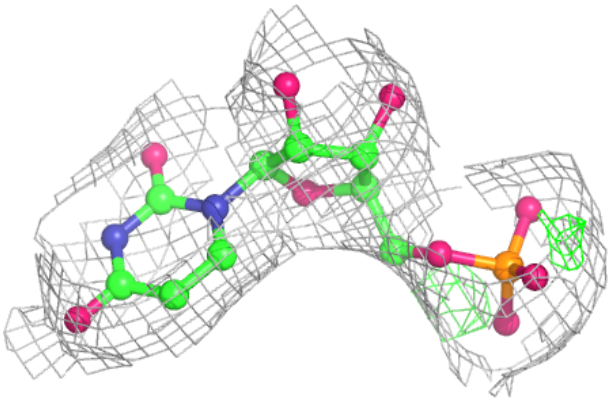
Electron density around U5P C 802:

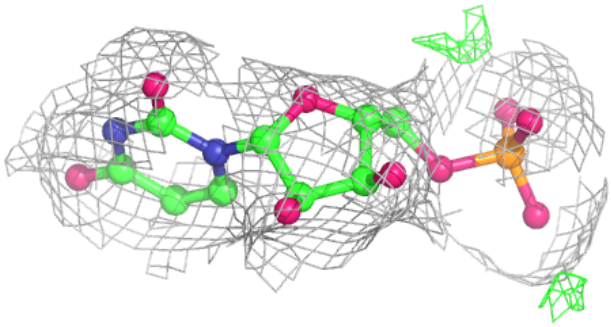
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

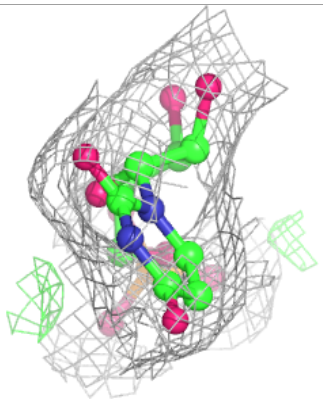


Electron density around U5P A 801:

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

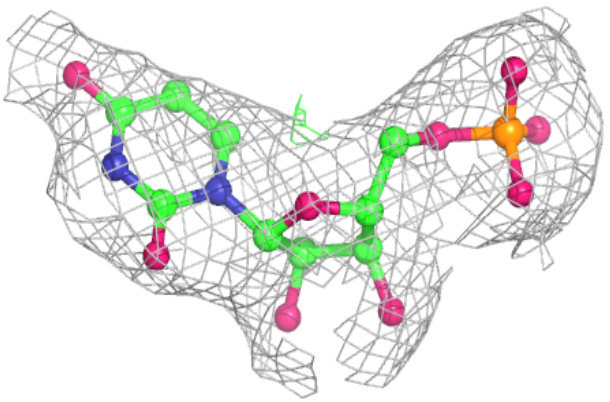


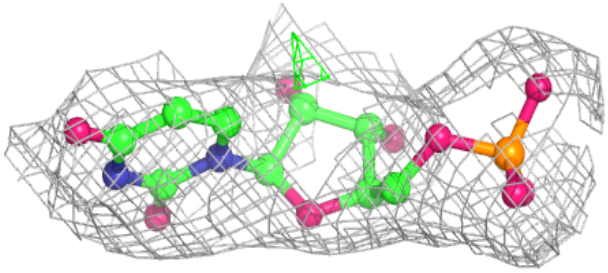


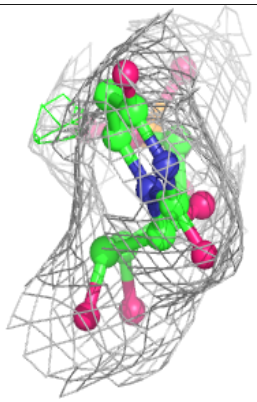


Electron density around U5P D 801:

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

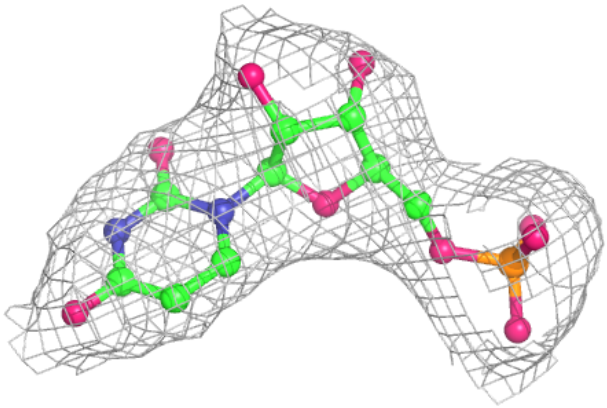


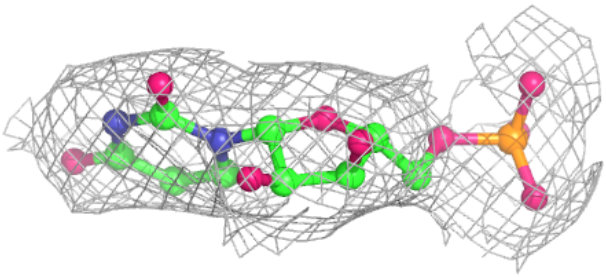


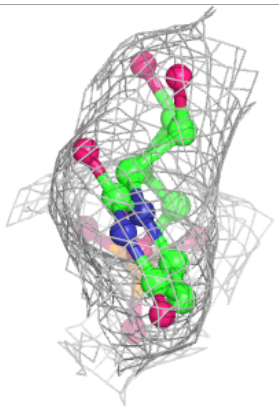


Electron density around U5P B 801:

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

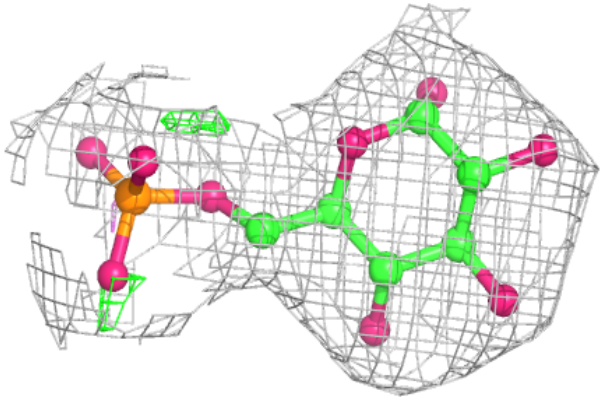


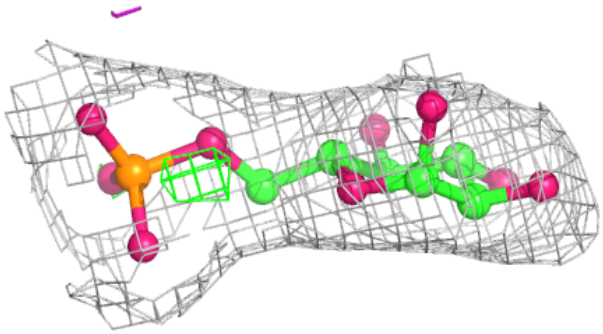


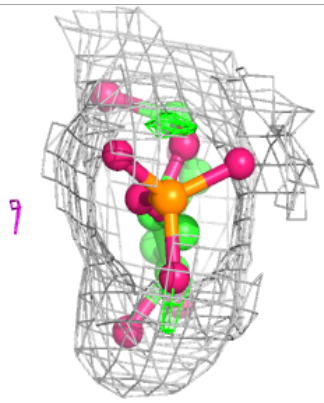


Electron density around G6P B 802:

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

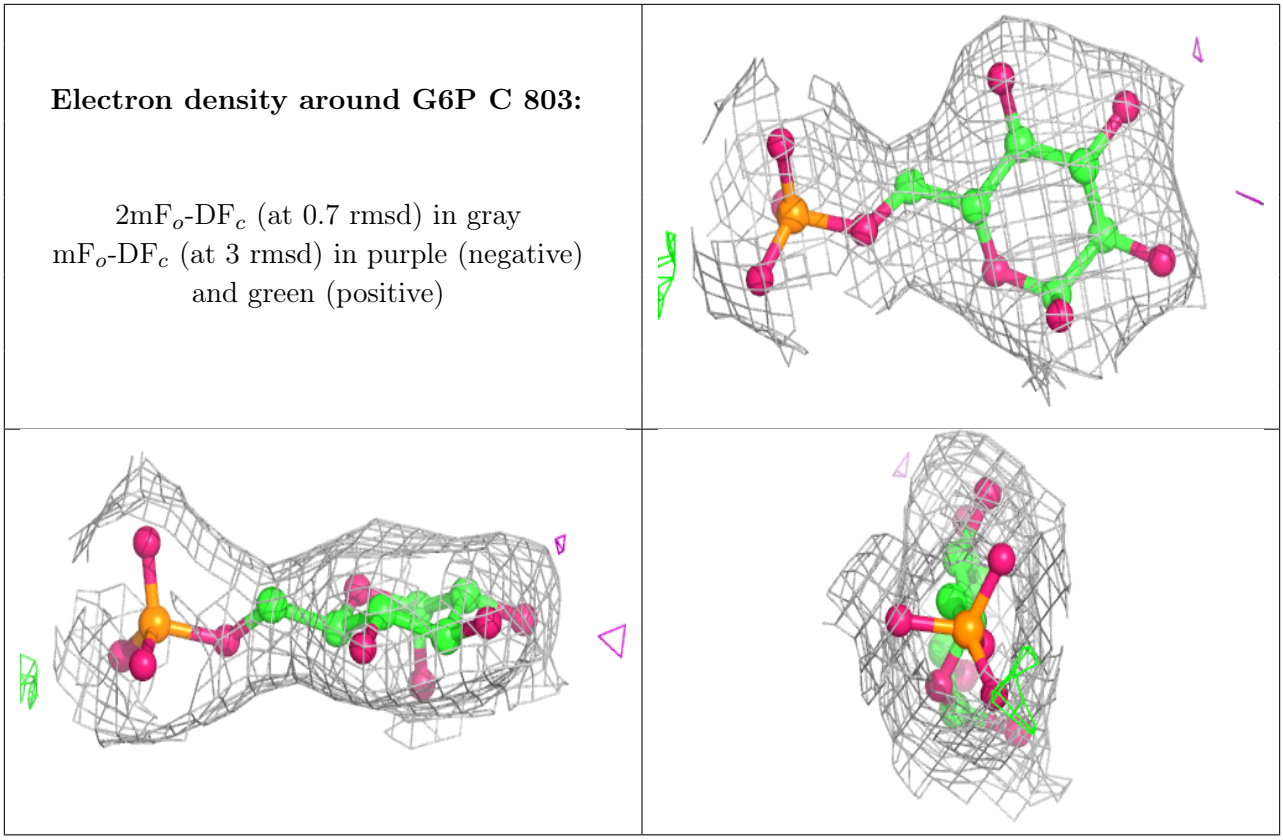






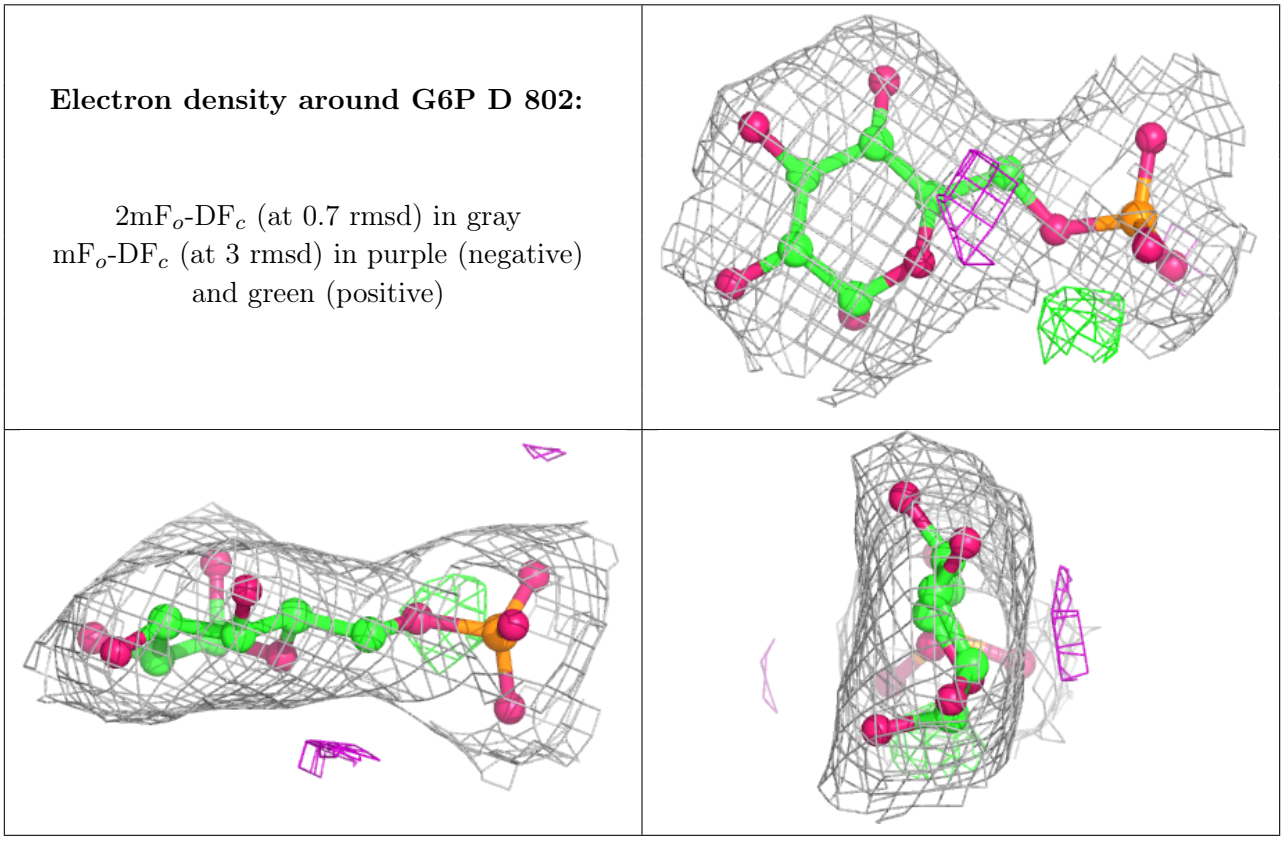
Electron density around G6P C 803:

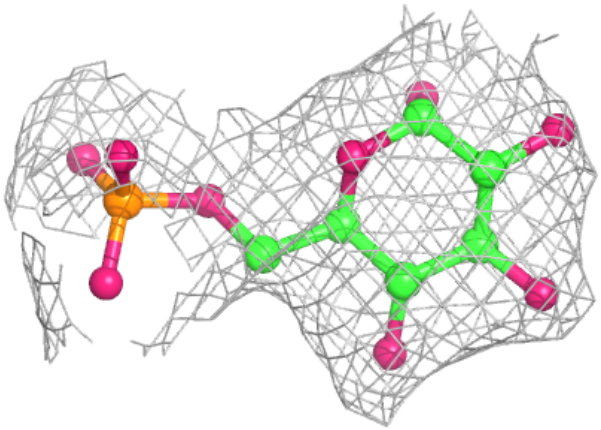
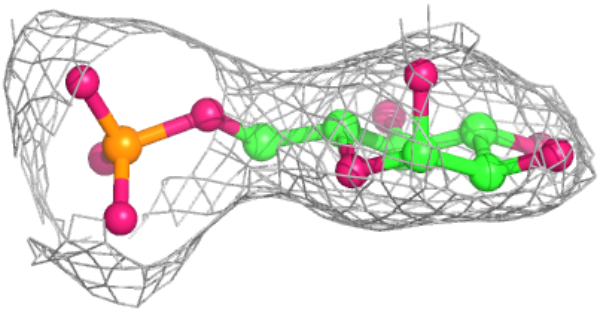
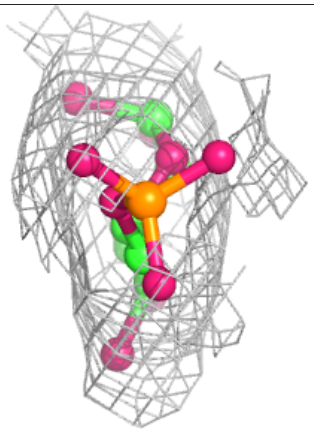
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G6P D 802:

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



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.