Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 04:12 PM EDT

PDB ID	:	5V0T
Title	:	Crystal structure of an alpha,alpha-trehalose-phosphate synthase (UDP-forming) from Burkholderia xenovorans in complex with glucose-6-phosphate
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2017-02-28
Resolution	:	1.95 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:

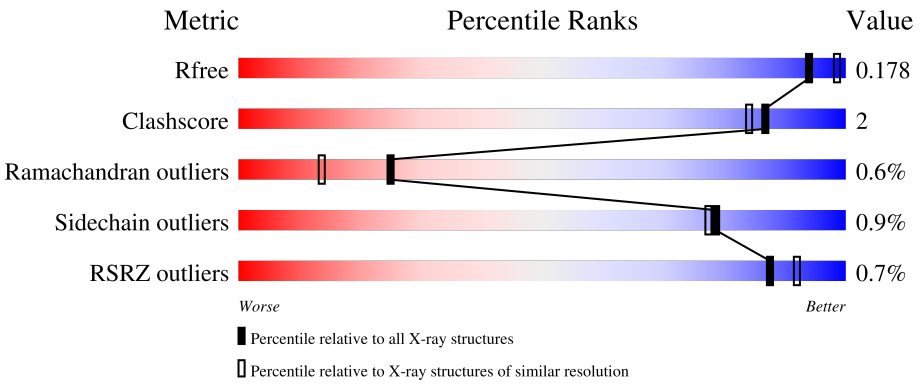
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	494	86% 5% 8%
1	B	494	85% 7% 8%
1	C	494	87% • 9%
1	D	494	87% 5% 9%
1	E	494	% 86% 6% 7%

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Mol	Chain	Length	Quality of chain
1	F	494	% 87% 5% 8%
1	G	494	% 86% 5% • 8%
1	H	494	% 86% 5% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	D	506	-	-	X	-
6	OXD	C	506	-	X	-	-
6	OXD	F	506	-	X	-	-
8	TAR	E	503	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 32349 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 Alpha,alpha-trehalose-phosphate synthase (UDP-forming).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3619	2309	651	646	13	0	9	0
1	B	453	3669	2341	659	656	13	0	17	0
1	C	452	3588	2292	645	638	13	0	3	0
1	D	452	3626	2317	657	639	13	0	8	0
1	E	457	3664	2338	658	655	13	0	12	0
1	F	455	3637	2321	658	645	13	0	9	0
1	G	454	3567	2281	638	635	13	0	12	0
1	H	451	3538	2261	632	632	13	0	10	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13W28
A	2	ALA	-	expression tag	UNP Q13W28
A	3	HIS	-	expression tag	UNP Q13W28
A	4	HIS	-	expression tag	UNP Q13W28
A	5	HIS	-	expression tag	UNP Q13W28
A	6	HIS	-	expression tag	UNP Q13W28
A	7	HIS	-	expression tag	UNP Q13W28
A	8	HIS	-	expression tag	UNP Q13W28
B	1	MET	-	initiating methionine	UNP Q13W28
B	2	ALA	-	expression tag	UNP Q13W28
B	3	HIS	-	expression tag	UNP Q13W28
B	4	HIS	-	expression tag	UNP Q13W28
B	5	HIS	-	expression tag	UNP Q13W28

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP Q13W28
B	7	HIS	-	expression tag	UNP Q13W28
B	8	HIS	-	expression tag	UNP Q13W28
C	1	MET	-	initiating methionine	UNP Q13W28
C	2	ALA	-	expression tag	UNP Q13W28
C	3	HIS	-	expression tag	UNP Q13W28
C	4	HIS	-	expression tag	UNP Q13W28
C	5	HIS	-	expression tag	UNP Q13W28
C	6	HIS	-	expression tag	UNP Q13W28
C	7	HIS	-	expression tag	UNP Q13W28
C	8	HIS	-	expression tag	UNP Q13W28
D	1	MET	-	initiating methionine	UNP Q13W28
D	2	ALA	-	expression tag	UNP Q13W28
D	3	HIS	-	expression tag	UNP Q13W28
D	4	HIS	-	expression tag	UNP Q13W28
D	5	HIS	-	expression tag	UNP Q13W28
D	6	HIS	-	expression tag	UNP Q13W28
D	7	HIS	-	expression tag	UNP Q13W28
D	8	HIS	-	expression tag	UNP Q13W28
E	1	MET	-	initiating methionine	UNP Q13W28
E	2	ALA	-	expression tag	UNP Q13W28
E	3	HIS	-	expression tag	UNP Q13W28
E	4	HIS	-	expression tag	UNP Q13W28
E	5	HIS	-	expression tag	UNP Q13W28
E	6	HIS	-	expression tag	UNP Q13W28
E	7	HIS	-	expression tag	UNP Q13W28
E	8	HIS	-	expression tag	UNP Q13W28
F	1	MET	-	initiating methionine	UNP Q13W28
F	2	ALA	-	expression tag	UNP Q13W28
F	3	HIS	-	expression tag	UNP Q13W28
F	4	HIS	-	expression tag	UNP Q13W28
F	5	HIS	-	expression tag	UNP Q13W28
F	6	HIS	-	expression tag	UNP Q13W28
F	7	HIS	-	expression tag	UNP Q13W28
F	8	HIS	-	expression tag	UNP Q13W28
G	1	MET	-	initiating methionine	UNP Q13W28
G	2	ALA	-	expression tag	UNP Q13W28
G	3	HIS	-	expression tag	UNP Q13W28
G	4	HIS	-	expression tag	UNP Q13W28
G	5	HIS	-	expression tag	UNP Q13W28
G	6	HIS	-	expression tag	UNP Q13W28
G	7	HIS	-	expression tag	UNP Q13W28

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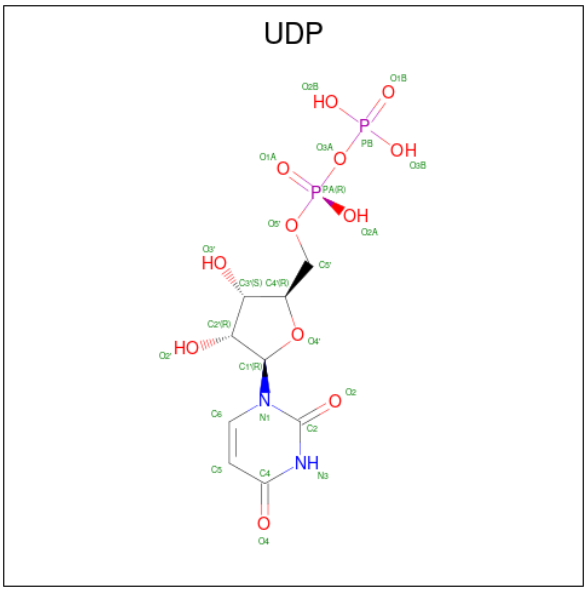
Chain	Residue	Modelled	Actual	Comment	Reference
G	8	HIS	-	expression tag	UNP Q13W28
H	1	MET	-	initiating methionine	UNP Q13W28
H	2	ALA	-	expression tag	UNP Q13W28
H	3	HIS	-	expression tag	UNP Q13W28
H	4	HIS	-	expression tag	UNP Q13W28
H	5	HIS	-	expression tag	UNP Q13W28
H	6	HIS	-	expression tag	UNP Q13W28
H	7	HIS	-	expression tag	UNP Q13W28
H	8	HIS	-	expression tag	UNP Q13W28

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



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

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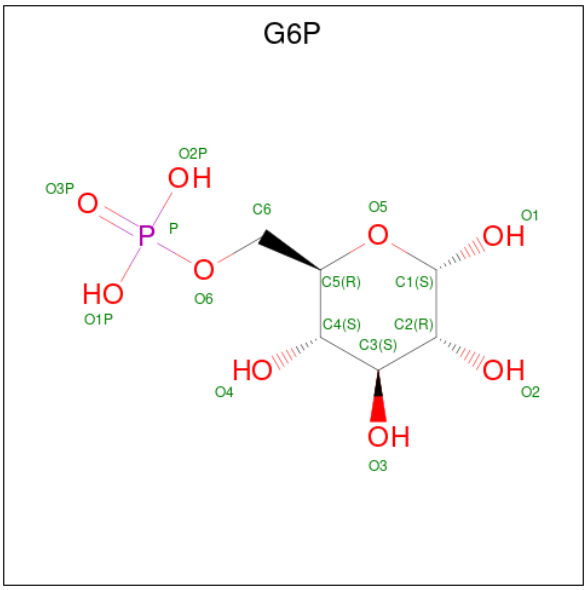
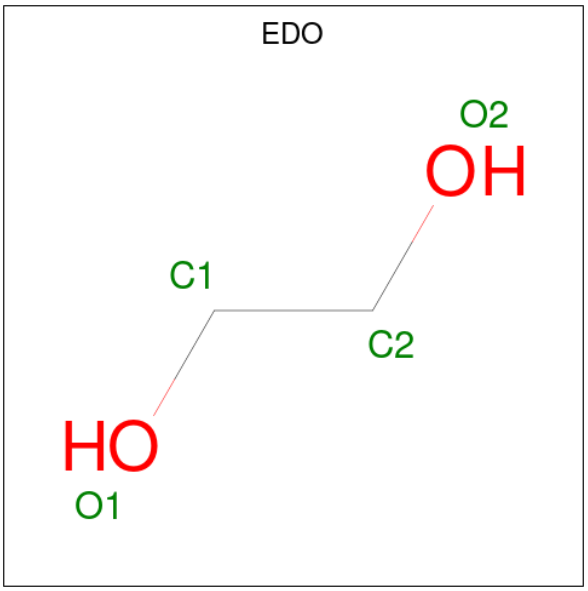
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	H	1	25	9	2	12	2	0	0

- 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
			Total	C	O	P		
3	B	1	16	6	9	1	0	0
			Total	C	O	P		
3	C	1	16	6	9	1	0	0
			Total	C	O	P		
3	D	1	16	6	9	1	0	0
			Total	C	O	P		
3	E	1	16	6	9	1	0	0
			Total	C	O	P		
3	F	1	16	6	9	1	0	0
			Total	C	O	P		
3	G	1	16	6	9	1	0	0
			Total	C	O	P		
3	H	1	16	6	9	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	E	1	4	2	2	0	0
			Total	C	O		
4	E	1	4	2	2	0	0
			Total	C	O		
4	F	1	4	2	2	0	0
			Total	C	O		
4	G	1	4	2	2	0	0
			Total	C	O		
4	H	1	4	2	2	0	0

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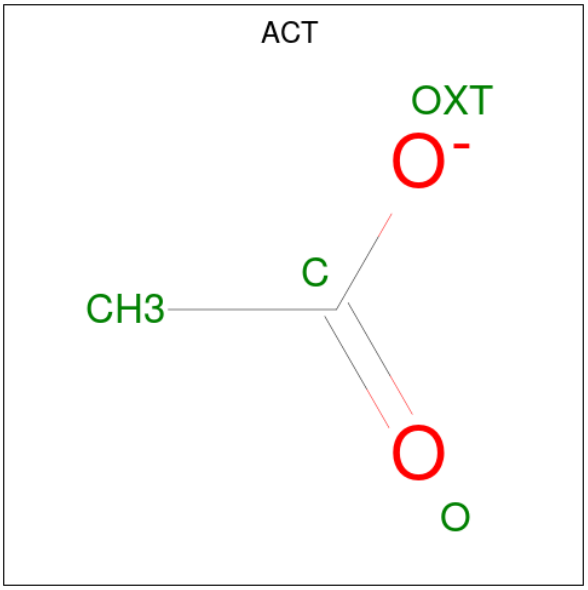
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	H	1	4	2	2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	D	1	4	2	2	0	0
5	D	1	4	2	2	0	0

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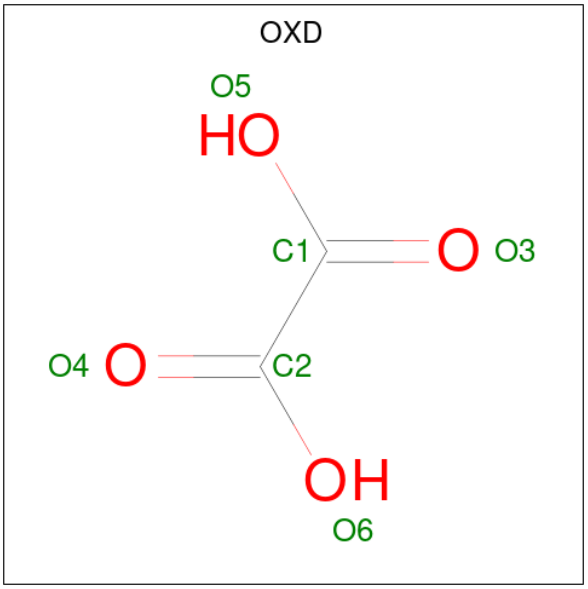
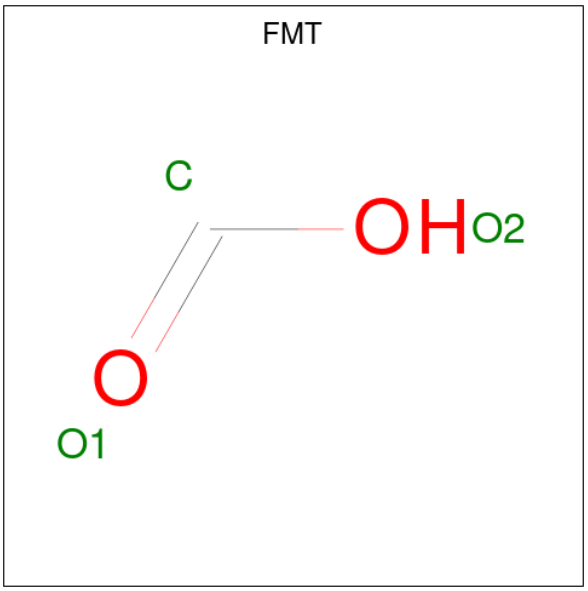
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	E	1	4	2	2		0	0
5	F	1	4	2	2		0	0
5	F	1	4	2	2		0	0
5	G	1	4	2	2		0	0
5	H	1	4	2	2		0	0

- Molecule 6 is OXALIC ACID (three-letter code: OXD) (formula: $C_2H_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	6	2	4		0	0
6	B	1	6	2	4		0	0
6	C	1	6	2	4		0	0
6	E	1	12	4	8		0	1
6	F	1	6	2	4		0	0

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	3	1	2	0	0
			Total	C	O		
7	A	1	3	1	2	0	0
			Total	C	O		
7	A	1	3	1	2	0	0
			Total	C	O		
7	A	1	3	1	2	0	0
			Total	C	O		
7	A	1	3	1	2	0	0
			Total	C	O		
7	A	1	3	1	2	0	0
			Total	C	O		
7	B	1	3	1	2	0	0
			Total	C	O		
7	B	1	3	1	2	0	0
			Total	C	O		
7	B	1	3	1	2	0	0
			Total	C	O		
7	B	1	3	1	2	0	0
			Total	C	O		
7	B	1	3	1	2	0	0
			Total	C	O		
7	B	1	3	1	2	0	0
			Total	C	O		
7	C	1	3	1	2	0	0
			Total	C	O		
7	C	1	3	1	2	0	0

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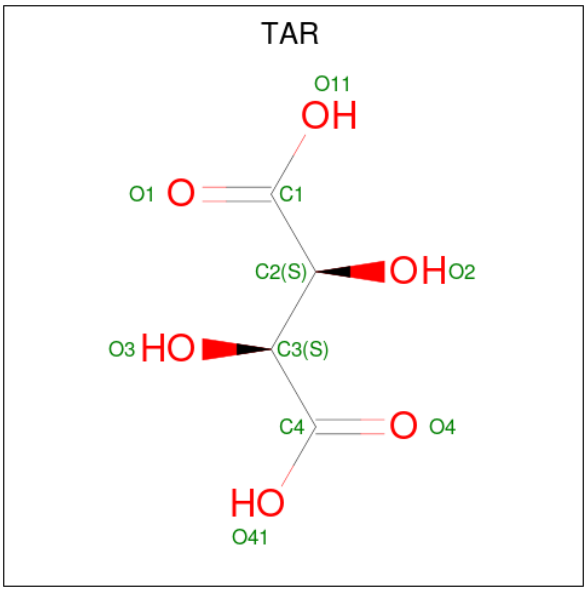
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	D	1	3	1	2		0	0
			Total	C	O			
7	D	1	3	1	2		0	0
			Total	C	O			
7	D	1	3	1	2		0	0
			Total	C	O			
7	D	1	3	1	2		0	0
			Total	C	O			
7	E	1	3	1	2		0	0
			Total	C	O			
7	E	1	3	1	2		0	0
			Total	C	O			
7	E	1	3	1	2		0	0
			Total	C	O			
7	E	1	3	1	2		0	0
			Total	C	O			
7	F	1	3	1	2		0	0
			Total	C	O			
7	F	1	3	1	2		0	0
			Total	C	O			
7	F	1	3	1	2		0	0
			Total	C	O			
7	H	1	3	1	2		0	0
			Total	C	O			
7	H	1	3	1	2		0	0

- Molecule 8 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	E	1	10	4	6	0	0

- Molecule 9 is water.

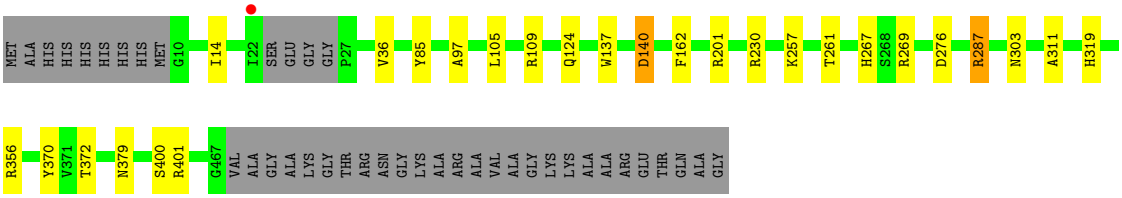
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	423	425	425	0	2
9	B	401	404	404	0	4
9	C	413	415	415	0	2
9	D	395	397	397	0	2
9	E	383	385	385	0	2
9	F	368	370	370	0	2
9	G	253	255	255	0	2
9	H	214	215	215	0	1

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.

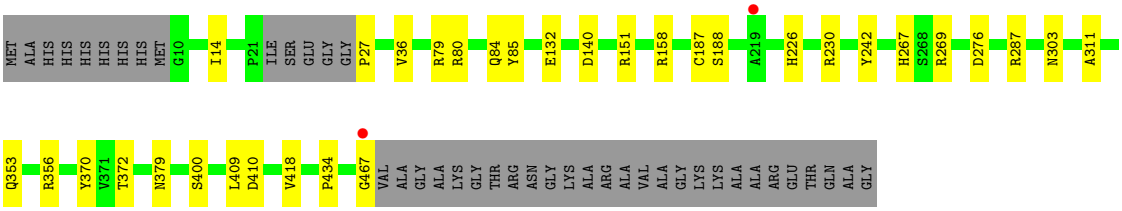
• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain A:



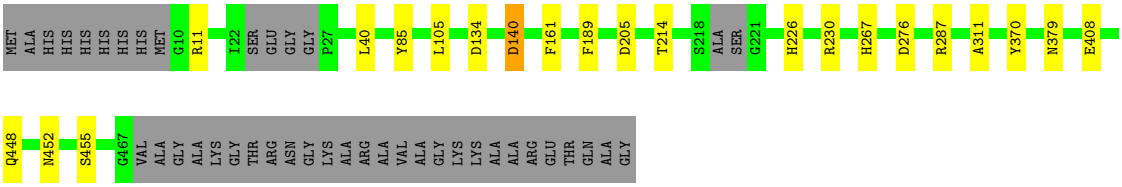
• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain B:



• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain C:

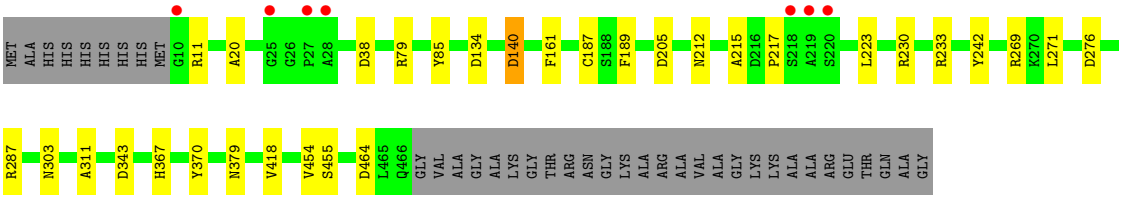


• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain D:

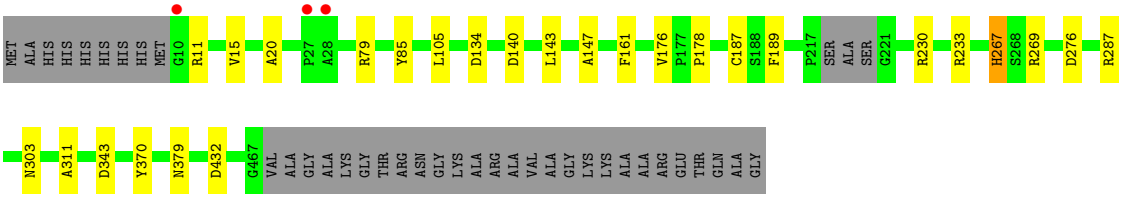
• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain E:



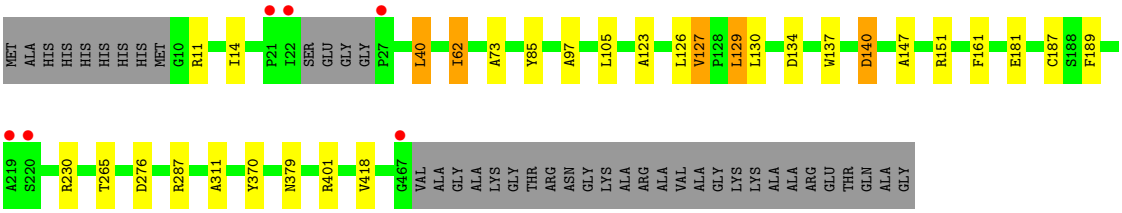
• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain F:



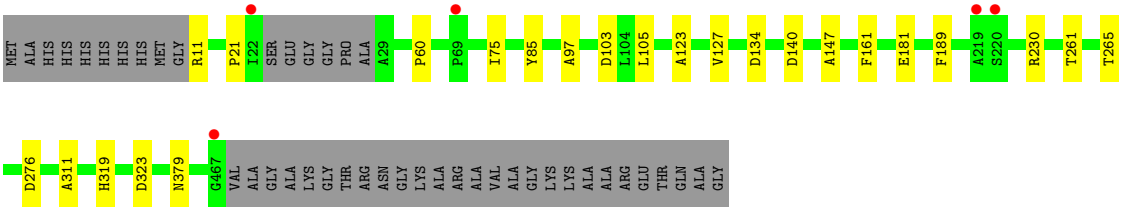
• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain G:



• Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.92Å 105.95Å 135.71Å 91.36° 90.37° 89.97°	Depositor
Resolution (Å)	50.00 – 1.95 47.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-1.95) 94.0 (47.88-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.155 , 0.178 0.156 , 0.178	Depositor DCC
R_{free} test set	1982 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l 0.016 for -h,k,-l 0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	32349	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: TAR, EDO, ACT, UDP, OXD, G6P, FMT

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	0.39	0/3735	0.56	1/5076 (0.0%)
1	B	0.38	0/3797	0.58	2/5156 (0.0%)
1	C	0.38	0/3685	0.55	1/5005 (0.0%)
1	D	0.37	0/3739	0.54	1/5075 (0.0%)
1	E	0.38	0/3790	0.55	0/5149
1	F	0.37	0/3751	0.54	0/5094
1	G	0.34	0/3690	0.52	0/5022
1	H	0.33	0/3655	0.50	0/4977
All	All	0.37	0/29842	0.54	5/40554 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	410[A]	ASP	C-N-CA	8.36	139.86	122.30
1	B	410[B]	ASP	C-N-CA	8.36	139.86	122.30
1	C	40	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	287	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	D	40	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	409	LEU	Peptide

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	3619	0	3568	15	0
1	B	3669	0	3627	20	0
1	C	3588	0	3542	10	0
1	D	3626	0	3598	14	0
1	E	3664	0	3629	18	0
1	F	3637	0	3593	17	0
1	G	3567	0	3482	21	0
1	H	3538	0	3422	14	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
2	E	25	0	11	0	0
2	F	25	0	11	0	0
2	G	25	0	11	0	0
2	H	25	0	11	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
3	E	16	0	11	0	0
3	F	16	0	11	0	0
3	G	16	0	11	0	0
3	H	16	0	11	0	0
4	A	8	0	12	0	0
4	B	12	0	18	0	0
4	C	8	0	12	0	0
4	D	8	0	12	1	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	8	0	12	0	0
5	A	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	0	15	0	0
5	C	4	0	3	0	0
5	D	8	0	6	2	0
5	E	4	0	3	0	0
5	F	8	0	6	0	0
5	G	4	0	3	0	0
5	H	4	0	3	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
6	C	6	0	0	0	0
6	E	12	0	0	0	0
6	F	6	0	0	1	0
7	A	18	0	6	1	0
7	B	18	0	6	2	0
7	C	6	0	2	0	0
7	D	12	0	4	0	0
7	E	12	0	4	1	0
7	F	9	0	3	0	0
7	H	6	0	2	0	0
8	E	10	0	4	1	0
9	A	425	0	0	4	0
9	B	404	0	0	4	0
9	C	415	0	0	1	0
9	D	397	0	0	6	0
9	E	385	0	0	3	0
9	F	370	0	0	4	0
9	G	255	0	0	1	0
9	H	215	0	0	0	0
All	All	32349	0	28803	124	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 2.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PRO:O	1:B:353:GLN:NE2	2.10	0.84
1:B:356:ARG:NH2	9:B:601:HOH:O	2.05	0.82
1:B:230[A]:ARG:NH1	9:B:603:HOH:O	2.18	0.75
1:E:343:ASP:HA	1:H:265[B]:THR:HG21	1.69	0.74
1:A:356:ARG:NH2	9:A:601:HOH:O	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ILE:HD11	1:G:73:ALA:HB1	1.72	0.71
1:E:212[A]:ASN:ND2	9:E:603:HOH:O	2.26	0.69
1:D:230:ARG:NH1	9:D:602:HOH:O	2.25	0.68
1:A:230:ARG:NH1	9:A:602:HOH:O	2.28	0.67
1:F:267:HIS:O	1:F:267:HIS:ND1	2.31	0.64
1:F:343:ASP:HA	1:G:265[B]:THR:HG21	1.78	0.64
1:B:353:GLN:OE1	9:B:602:HOH:O	2.16	0.62
1:D:425:GLU:OE1	9:D:601:HOH:O	2.16	0.61
1:D:325:ARG:HH22	5:D:506:ACT:H2	1.65	0.60
1:H:60:PRO:HB2	1:H:75:ILE:HG12	1.84	0.60
1:F:432:ASP:OD2	9:F:601:HOH:O	2.17	0.59
1:C:105:LEU:HD22	1:G:418:VAL:HG11	1.83	0.59
1:A:105:LEU:HD22	1:E:418:VAL:HG11	1.85	0.59
1:E:187:CYS:O	1:E:230:ARG:HD3	2.04	0.58
1:E:233:ARG:NH1	1:E:464:ASP:O	2.38	0.57
1:H:276:ASP:O	1:H:311:ALA:HA	2.05	0.57
1:E:242:TYR:HH	1:E:455[A]:SER:HG	1.53	0.56
1:G:127:VAL:HA	1:G:130:LEU:HD12	1.87	0.56
1:G:276:ASP:O	1:G:311:ALA:HA	2.06	0.55
1:G:401[B]:ARG:HH21	1:G:401[B]:ARG:HG3	1.72	0.55
1:D:263:LYS:NZ	9:D:849[B]:HOH:O	2.37	0.54
6:F:506:OXD:O4	9:F:602:HOH:O	2.18	0.54
1:A:401:ARG:NH2	9:A:607:HOH:O	2.42	0.52
1:C:230:ARG:NH1	9:C:601:HOH:O	2.18	0.51
1:H:11:ARG:HB3	1:H:134:ASP:OD1	2.11	0.51
1:D:287:ARG:HG3	1:D:370:TYR:CE2	2.45	0.51
1:H:97:ALA:HB2	1:H:105:LEU:HD12	1.91	0.51
1:C:276:ASP:O	1:C:311:ALA:HA	2.11	0.51
1:G:14:ILE:HD13	1:G:137:TRP:HB3	1.93	0.51
1:G:181:GLU:OE1	1:G:181:GLU:N	2.39	0.51
1:E:79:ARG:NH1	9:E:605:HOH:O	2.38	0.50
1:A:97:ALA:HB2	1:A:105:LEU:HD12	1.93	0.50
1:D:79:ARG:NH1	9:D:604:HOH:O	2.29	0.50
1:A:319:HIS:H	7:A:508:FMT:C	2.24	0.50
1:D:276:ASP:O	1:D:311:ALA:HA	2.12	0.50
4:D:504:EDO:H21	1:H:103:ASP:HA	1.93	0.49
1:E:11:ARG:HB3	1:E:134:ASP:OD1	2.12	0.49
1:G:187:CYS:O	1:G:230:ARG:HD3	2.12	0.49
1:F:276:ASP:O	1:F:311:ALA:HA	2.13	0.49
1:F:11:ARG:HB3	1:F:134:ASP:OD1	2.13	0.48
1:F:187:CYS:O	1:F:230:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ASP:O	1:E:311:ALA:HA	2.14	0.48
1:G:147:ALA:HB2	1:G:189:PHE:CE1	2.48	0.48
5:D:506:ACT:H1	9:D:946:HOH:O	2.13	0.48
1:G:147:ALA:O	1:G:151:ARG:HG2	2.13	0.48
1:B:434:PRO:HG2	1:D:425:GLU:HG2	1.96	0.47
1:B:226:HIS:HD2	9:B:638:HOH:O	1.97	0.47
1:G:161:PHE:HB2	1:G:189:PHE:CE1	2.49	0.47
1:C:214:THR:OG1	1:C:226:HIS:HB2	2.14	0.47
1:F:161:PHE:HB2	1:F:189:PHE:CE1	2.50	0.47
1:H:261:THR:O	1:H:265[B]:THR:HG23	2.15	0.47
1:B:269:ARG:NH2	1:B:303:ASN:OD1	2.48	0.47
1:B:276:ASP:O	1:B:311:ALA:HA	2.15	0.47
1:G:97:ALA:HB2	1:G:105:LEU:HD12	1.95	0.47
1:C:287:ARG:HG3	1:C:370:TYR:CZ	2.51	0.46
1:H:147:ALA:HB2	1:H:189:PHE:CE1	2.49	0.46
1:A:276:ASP:O	1:A:311:ALA:HA	2.15	0.46
1:B:158:ARG:NH2	1:B:467:GLY:O	2.49	0.46
8:E:503:TAR:O11	8:E:503:TAR:O3	2.29	0.46
1:G:11:ARG:HB3	1:G:134:ASP:OD1	2.15	0.45
1:F:176:VAL:HG12	1:F:178:PRO:HD2	1.97	0.45
1:A:201[B]:ARG:NH2	7:E:509:FMT:H	2.32	0.45
1:C:161:PHE:HB2	1:C:189:PHE:CE1	2.52	0.45
1:E:205[B]:ASP:OD1	9:E:601:HOH:O	2.21	0.45
1:E:271:LEU:H	1:E:367:HIS:HD1	1.64	0.45
1:B:418[A]:VAL:HG11	1:F:105:LEU:HD22	1.97	0.45
1:A:257:LYS:O	1:A:261:THR:HG23	2.18	0.44
1:D:11:ARG:HB3	1:D:134:ASP:OD1	2.17	0.44
1:H:161:PHE:HB2	1:H:189:PHE:CE1	2.52	0.44
1:H:319:HIS:NE2	1:H:323:ASP:OD2	2.50	0.44
1:B:79:ARG:NH1	7:B:513:FMT:O1	2.47	0.44
1:C:408:GLU:OE1	1:C:448:GLN:NE2	2.50	0.44
1:H:181:GLU:OE1	1:H:181:GLU:N	2.46	0.44
1:A:287:ARG:HG3	1:A:370:TYR:CZ	2.53	0.44
1:C:448:GLN:NE2	1:C:452:ASN:OD1	2.51	0.44
1:B:14:ILE:HG21	1:B:36:VAL:HG11	1.99	0.43
1:G:401[A]:ARG:NH2	9:G:606:HOH:O	2.51	0.43
1:A:124:GLN:HG2	9:A:638:HOH:O	2.18	0.43
1:D:97:ALA:HB2	1:D:105:LEU:HD12	1.99	0.43
1:A:14:ILE:HG21	1:A:36:VAL:HG11	2.00	0.43
1:C:287:ARG:HG3	1:C:370:TYR:CE2	2.53	0.43
1:E:217:PRO:HA	1:E:223:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:ASP:CA	1:H:265[B]:THR:HG21	2.45	0.43
1:F:15:VAL:HG12	1:F:143:LEU:HD13	2.01	0.43
1:F:343:ASP:CA	1:G:265[B]:THR:HG21	2.48	0.43
1:H:147:ALA:HB2	1:H:189:PHE:CD1	2.54	0.43
1:F:79:ARG:NH1	9:F:608:HOH:O	2.41	0.43
1:A:269:ARG:NH1	1:A:303:ASN:OD1	2.52	0.42
1:E:287:ARG:HG3	1:E:370:TYR:CZ	2.53	0.42
1:B:287:ARG:HG3	1:B:370:TYR:CE2	2.53	0.42
1:F:269:ARG:NH2	1:F:303:ASN:OD1	2.49	0.42
1:G:40:LEU:HD12	1:G:40:LEU:HA	1.84	0.42
1:B:242:TYR:CZ	7:B:516:FMT:H	2.55	0.42
1:E:215:ALA:O	1:E:217:PRO:HD3	2.19	0.42
1:F:287:ARG:HG3	1:F:370:TYR:CZ	2.54	0.42
1:D:452:ASN:ND2	9:D:623:HOH:O	2.52	0.42
1:D:287:ARG:HG3	1:D:370:TYR:CZ	2.55	0.42
1:E:269:ARG:NH2	1:E:303:ASN:OD1	2.52	0.42
1:D:147:ALA:HB2	1:D:189:PHE:CE1	2.56	0.41
1:G:161:PHE:HB2	1:G:189:PHE:CD1	2.56	0.41
1:B:80:ARG:HE	1:B:84:GLN:HE22	1.67	0.41
1:A:372:THR:HA	1:A:400:SER:HB2	2.02	0.41
1:D:161:PHE:HB2	1:D:189:PHE:CE1	2.56	0.41
1:G:126:LEU:HA	1:G:129:LEU:HD12	2.01	0.41
1:B:372:THR:HA	1:B:400:SER:HB2	2.03	0.41
1:B:187:CYS:O	1:B:230[B]:ARG:NE	2.54	0.41
1:B:287:ARG:HG3	1:B:370:TYR:CZ	2.55	0.41
1:F:233:ARG:NH2	9:F:620:HOH:O	2.53	0.41
1:G:287:ARG:HG3	1:G:370:TYR:CZ	2.56	0.41
1:A:137:TRP:HE1	1:A:162:PHE:HB2	1.86	0.41
1:B:230[B]:ARG:HE	1:B:230[B]:ARG:HB3	1.46	0.41
1:C:11:ARG:HB3	1:C:134:ASP:OD1	2.21	0.41
1:F:287:ARG:HG3	1:F:370:TYR:CE2	2.56	0.41
1:G:123:ALA:O	1:G:127:VAL:HG12	2.20	0.41
1:H:123:ALA:O	1:H:127:VAL:HG23	2.21	0.41
1:E:161:PHE:HB2	1:E:189:PHE:CE1	2.56	0.41
1:E:38:ASP:HB3	1:E:454[A]:VAL:HG11	2.03	0.40
1:B:151[B]:ARG:NH1	1:B:188:SER:O	2.55	0.40
1:F:147:ALA:HB2	1:F:189:PHE:CE1	2.57	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	460/494 (93%)	443 (96%)	14 (3%)	3 (1%)	22	11
1	B	466/494 (94%)	450 (97%)	13 (3%)	3 (1%)	25	14
1	C	449/494 (91%)	434 (97%)	12 (3%)	3 (1%)	22	11
1	D	454/494 (92%)	438 (96%)	14 (3%)	2 (0%)	34	22
1	E	467/494 (94%)	447 (96%)	17 (4%)	3 (1%)	25	14
1	F	460/494 (93%)	444 (96%)	12 (3%)	4 (1%)	17	8
1	G	462/494 (94%)	447 (97%)	13 (3%)	2 (0%)	34	22
1	H	457/494 (92%)	445 (97%)	10 (2%)	2 (0%)	34	22
All	All	3675/3952 (93%)	3548 (96%)	105 (3%)	22 (1%)	25	14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	21	PRO
1	A	379	ASN
1	B	267	HIS
1	B	379	ASN
1	C	267	HIS
1	C	379	ASN
1	D	379	ASN
1	E	379	ASN
1	F	379	ASN
1	G	379	ASN
1	H	379	ASN
1	A	140	ASP
1	A	267	HIS
1	B	140	ASP
1	F	140	ASP
1	C	140	ASP
1	E	140	ASP

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Mol	Chain	Res	Type
1	F	267	HIS
1	D	140	ASP
1	E	20	ALA
1	F	20	ALA
1	G	140	ASP

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	370/393 (94%)	367 (99%)	3 (1%)	81	80
1	B	377/393 (96%)	375 (100%)	2 (0%)	88	88
1	C	366/393 (93%)	362 (99%)	4 (1%)	73	71
1	D	371/393 (94%)	366 (99%)	5 (1%)	69	65
1	E	377/393 (96%)	375 (100%)	2 (0%)	88	88
1	F	371/393 (94%)	370 (100%)	1 (0%)	92	92
1	G	356/393 (91%)	350 (98%)	6 (2%)	60	55
1	H	350/393 (89%)	347 (99%)	3 (1%)	78	77
All	All	2938/3144 (93%)	2912 (99%)	26 (1%)	78	77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	109	ARG
1	A	140	ASP
1	B	85	TYR
1	B	132	GLU
1	C	85	TYR
1	C	140	ASP
1	C	205	ASP
1	C	455	SER
1	D	62	ILE

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Mol	Chain	Res	Type
1	D	85	TYR
1	D	140	ASP
1	D	205	ASP
1	D	455	SER
1	E	85	TYR
1	E	140	ASP
1	F	85	TYR
1	G	40	LEU
1	G	62	ILE
1	G	85	TYR
1	G	127	VAL
1	G	129	LEU
1	G	140	ASP
1	H	85	TYR
1	H	140	ASP
1	H	230	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	319	HIS
1	B	353	GLN
1	C	17	ASN
1	C	267	HIS
1	C	319	HIS
1	C	448	GLN
1	D	91	ASN
1	F	91	ASN
1	F	297	HIS
1	H	91	ASN
1	H	448	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)

80 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	FMT	B	516	-	2,2,2	0.66	0	1,1,1	0.21	0
4	EDO	C	504	-	3,3,3	0.55	0	2,2,2	0.22	0
4	EDO	D	504	-	3,3,3	0.50	0	2,2,2	0.33	0
3	G6P	H	502	-	16,16,16	0.61	0	24,24,24	0.92	1 (4%)
4	EDO	B	503	-	3,3,3	0.48	0	2,2,2	0.29	0
7	FMT	B	514	-	2,2,2	0.68	0	1,1,1	0.20	0
7	FMT	F	507	-	2,2,2	0.68	0	1,1,1	0.20	0
6	OXD	E	506[B]	-	5,5,5	1.82	1 (20%)	6,6,6	1.17	0
8	TAR	E	503	-	9,9,9	1.09	0	12,12,12	1.23	2 (16%)
5	ACT	D	506	-	3,3,3	1.17	0	3,3,3	1.43	0
7	FMT	D	510	-	2,2,2	0.63	0	1,1,1	0.11	0
5	ACT	B	505	-	3,3,3	1.32	0	3,3,3	1.58	1 (33%)
2	UDP	A	501	-	24,26,26	0.53	0	37,40,40	0.60	1 (2%)
3	G6P	E	502	-	16,16,16	0.61	0	24,24,24	0.72	0
6	OXD	B	510	-	5,5,5	1.82	1 (20%)	6,6,6	1.23	0
7	FMT	E	507	-	2,2,2	0.69	0	1,1,1	0.21	0
7	FMT	C	507	-	2,2,2	0.68	0	1,1,1	0.31	0
7	FMT	A	513	-	2,2,2	0.63	0	1,1,1	0.15	0
4	EDO	E	511	-	3,3,3	0.50	0	2,2,2	0.44	0
7	FMT	E	509	-	2,2,2	0.67	0	1,1,1	0.20	0
4	EDO	H	504	-	3,3,3	0.57	0	2,2,2	0.14	0
5	ACT	B	506	-	3,3,3	1.46	1 (33%)	3,3,3	1.53	0
7	FMT	B	511	-	2,2,2	0.69	0	1,1,1	0.33	0
3	G6P	B	502	-	16,16,16	0.59	0	24,24,24	0.67	0
7	FMT	E	508	-	2,2,2	0.70	0	1,1,1	0.23	0
7	FMT	A	509	-	2,2,2	0.67	0	1,1,1	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	F	503	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	B	504	-	3,3,3	0.52	0	2,2,2	0.19	0
7	FMT	F	508	-	2,2,2	0.70	0	1,1,1	0.28	0
7	FMT	B	512	-	2,2,2	0.68	0	1,1,1	0.11	0
5	ACT	F	505	-	3,3,3	1.32	0	3,3,3	1.42	0
2	UDP	E	501	-	24,26,26	0.44	0	37,40,40	0.62	1 (2%)
7	FMT	C	508	-	2,2,2	0.63	0	1,1,1	0.10	0
6	OXD	A	507	-	5,5,5	1.84	1 (20%)	6,6,6	1.20	0
5	ACT	E	505	-	3,3,3	1.40	1 (33%)	3,3,3	1.40	0
2	UDP	F	501	-	24,26,26	0.36	0	37,40,40	0.34	0
7	FMT	A	508	-	2,2,2	0.67	0	1,1,1	0.21	0
7	FMT	A	511	-	2,2,2	0.70	0	1,1,1	0.26	0
4	EDO	A	503	-	3,3,3	0.51	0	2,2,2	0.38	0
2	UDP	G	501	-	24,26,26	0.52	0	37,40,40	0.61	1 (2%)
7	FMT	A	510	-	2,2,2	0.70	0	1,1,1	0.22	0
4	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.29	0
7	FMT	H	507	-	2,2,2	0.66	0	1,1,1	0.24	0
4	EDO	E	504	-	3,3,3	0.44	0	2,2,2	0.41	0
5	ACT	A	505	-	3,3,3	1.33	0	3,3,3	1.49	0
7	FMT	B	515	-	2,2,2	0.71	0	1,1,1	0.24	0
7	FMT	F	509	-	2,2,2	0.67	0	1,1,1	0.26	0
4	EDO	B	517	-	3,3,3	0.51	0	2,2,2	0.23	0
3	G6P	D	502	-	16,16,16	0.60	0	24,24,24	1.11	2 (8%)
7	FMT	E	510	-	2,2,2	0.66	0	1,1,1	0.21	0
7	FMT	H	506	-	2,2,2	0.69	0	1,1,1	0.15	0
6	OXD	F	506	-	5,5,5	1.82	1 (20%)	6,6,6	1.25	1 (16%)
5	ACT	F	504	-	3,3,3	1.48	1 (33%)	3,3,3	1.45	0
2	UDP	C	501	-	24,26,26	0.41	0	37,40,40	0.67	1 (2%)
5	ACT	H	505	-	3,3,3	1.33	1 (33%)	3,3,3	1.58	1 (33%)
2	UDP	D	501	-	24,26,26	0.42	0	37,40,40	0.47	0
4	EDO	G	503	-	3,3,3	0.49	0	2,2,2	0.25	0
5	ACT	G	504	-	3,3,3	1.51	1 (33%)	3,3,3	1.24	0
5	ACT	B	509	-	3,3,3	1.40	1 (33%)	3,3,3	1.34	0
6	OXD	E	506[A]	-	5,5,5	1.85	1 (20%)	6,6,6	1.18	0
3	G6P	F	502	-	16,16,16	0.52	0	24,24,24	0.68	0
5	ACT	B	508	-	3,3,3	1.60	1 (33%)	3,3,3	1.52	0
7	FMT	D	507	-	2,2,2	0.69	0	1,1,1	0.22	0
3	G6P	G	502	-	16,16,16	0.61	0	24,24,24	0.87	1 (4%)
7	FMT	D	509	-	2,2,2	0.64	0	1,1,1	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ACT	B	507	-	3,3,3	1.40	1 (33%)	3,3,3	1.52	0
4	EDO	H	503	-	3,3,3	0.48	0	2,2,2	0.28	0
7	FMT	A	512	-	2,2,2	0.64	0	1,1,1	0.24	0
3	G6P	C	502	-	16,16,16	0.69	0	24,24,24	1.03	1 (4%)
6	OXD	C	506	-	5,5,5	1.70	1 (20%)	6,6,6	1.44	2 (33%)
4	EDO	A	504	-	3,3,3	0.59	0	2,2,2	0.12	0
3	G6P	A	502	-	16,16,16	0.59	0	24,24,24	0.83	1 (4%)
5	ACT	A	506	-	3,3,3	1.33	0	3,3,3	1.37	0
4	EDO	C	503	-	3,3,3	0.49	0	2,2,2	0.28	0
2	UDP	H	501	-	24,26,26	0.60	0	37,40,40	0.66	1 (2%)
7	FMT	D	508	-	2,2,2	0.69	0	1,1,1	0.27	0
5	ACT	D	505	-	3,3,3	1.25	0	3,3,3	1.45	0
5	ACT	C	505	-	3,3,3	1.38	0	3,3,3	1.44	0
7	FMT	B	513	-	2,2,2	0.68	0	1,1,1	0.22	0
2	UDP	B	501	-	24,26,26	0.43	0	37,40,40	0.62	1 (2%)

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	EDO	E	504	-	-	0/1/1/1	-
3	G6P	C	502	-	-	0/6/26/26	0/1/1/1
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	D	504	-	-	1/1/1/1	-
6	OXD	C	506	-	-	4/4/4/4	-
4	EDO	B	517	-	-	0/1/1/1	-
3	G6P	D	502	-	-	0/6/26/26	0/1/1/1
4	EDO	H	503	-	-	0/1/1/1	-
3	G6P	H	502	-	-	1/6/26/26	0/1/1/1
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
3	G6P	A	502	-	-	0/6/26/26	0/1/1/1
6	OXD	F	506	-	-	4/4/4/4	-
2	UDP	E	501	-	-	3/16/32/32	0/2/2/2
2	UDP	C	501	-	-	4/16/32/32	0/2/2/2
2	UDP	D	501	-	-	3/16/32/32	0/2/2/2
6	OXD	E	506[B]	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TAR	E	503	-	-	12/12/12/12	-
6	OXD	A	507	-	-	4/4/4/4	-
4	EDO	G	503	-	-	0/1/1/1	-
2	UDP	A	501	-	-	3/16/32/32	0/2/2/2
3	G6P	E	502	-	-	1/6/26/26	0/1/1/1
4	EDO	C	503	-	-	0/1/1/1	-
2	UDP	F	501	-	-	3/16/32/32	0/2/2/2
2	UDP	H	501	-	-	4/16/32/32	0/2/2/2
6	OXD	E	506[A]	-	-	4/4/4/4	-
6	OXD	B	510	-	-	4/4/4/4	-
4	EDO	E	511	-	-	1/1/1/1	-
3	G6P	F	502	-	-	2/6/26/26	0/1/1/1
4	EDO	H	504	-	-	1/1/1/1	-
3	G6P	B	502	-	-	0/6/26/26	0/1/1/1
2	UDP	B	501	-	-	4/16/32/32	0/2/2/2
4	EDO	A	503	-	-	0/1/1/1	-
3	G6P	G	502	-	-	2/6/26/26	0/1/1/1
2	UDP	G	501	-	-	3/16/32/32	0/2/2/2
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	F	503	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	506[A]	OXD	C2-C1	-2.91	1.46	1.54
6	E	506[B]	OXD	C2-C1	-2.85	1.46	1.54
6	A	507	OXD	C2-C1	-2.83	1.46	1.54
6	B	510	OXD	C2-C1	-2.81	1.46	1.54
6	F	506	OXD	C2-C1	-2.71	1.46	1.54
6	C	506	OXD	C2-C1	-2.56	1.47	1.54
5	B	508	ACT	CH3-C	2.51	1.59	1.49
5	G	504	ACT	CH3-C	2.17	1.58	1.49
5	F	504	ACT	CH3-C	2.16	1.58	1.49
5	B	509	ACT	CH3-C	2.13	1.58	1.49
5	H	505	ACT	CH3-C	2.07	1.57	1.49
5	E	505	ACT	CH3-C	2.05	1.57	1.49
5	B	507	ACT	CH3-C	2.04	1.57	1.49
5	B	506	ACT	CH3-C	2.03	1.57	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	G6P	O5-C5-C6	2.90	112.51	106.67
3	D	502	G6P	O5-C5-C6	2.66	112.04	106.67
3	H	502	G6P	O5-C5-C6	2.52	111.76	106.67
3	A	502	G6P	O5-C5-C6	2.51	111.73	106.67
3	G	502	G6P	O5-C5-C6	2.49	111.69	106.67
2	G	501	UDP	O3B-PB-O3A	2.43	112.77	104.64
8	E	503	TAR	O41-C4-C3	2.37	119.67	113.27
3	D	502	G6P	O1P-P-O6	-2.36	100.46	106.73
2	H	501	UDP	O3B-PB-O3A	2.32	112.42	104.64
2	B	501	UDP	O3B-PB-O3A	2.24	112.15	104.64
6	C	506	OXD	O5-C1-C2	2.24	119.81	113.16
2	E	501	UDP	O3B-PB-O3A	2.19	111.98	104.64
2	C	501	UDP	O3B-PB-O3A	2.19	111.98	104.64
6	C	506	OXD	O6-C2-C1	2.14	119.52	113.16
2	A	501	UDP	O3B-PB-O3A	2.12	111.74	104.64
8	E	503	TAR	O11-C1-C2	2.07	118.85	113.27
5	H	505	ACT	O-C-CH3	-2.05	114.37	122.33
6	F	506	OXD	O5-C1-C2	2.03	119.20	113.16
5	B	505	ACT	O-C-CH3	-2.01	114.50	122.33

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	501	UDP	O4'-C4'-C5'-O5'
6	A	507	OXD	O3-C1-C2-O4
6	A	507	OXD	O3-C1-C2-O6
6	A	507	OXD	O5-C1-C2-O4
6	A	507	OXD	O5-C1-C2-O6
8	E	503	TAR	O2-C2-C3-O3
8	E	503	TAR	C1-C2-C3-C4
8	E	503	TAR	O2-C2-C3-C4
8	E	503	TAR	C2-C3-C4-O41
8	E	503	TAR	C1-C2-C3-O3
2	A	501	UDP	O4'-C4'-C5'-O5'
2	E	501	UDP	O4'-C4'-C5'-O5'
2	F	501	UDP	O4'-C4'-C5'-O5'
2	H	501	UDP	O4'-C4'-C5'-O5'
8	E	503	TAR	C2-C3-C4-O4
6	E	506[B]	OXD	O3-C1-C2-O4
6	E	506[B]	OXD	O5-C1-C2-O6
8	E	503	TAR	O3-C3-C4-O41
8	E	503	TAR	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
8	E	503	TAR	O11-C1-C2-C3
6	E	506[B]	OXD	O3-C1-C2-O6
6	E	506[B]	OXD	O5-C1-C2-O4
2	G	501	UDP	C3'-C4'-C5'-O5'
6	F	506	OXD	O3-C1-C2-O4
6	F	506	OXD	O3-C1-C2-O6
6	F	506	OXD	O5-C1-C2-O4
4	A	504	EDO	O1-C1-C2-O2
4	C	504	EDO	O1-C1-C2-O2
4	E	511	EDO	O1-C1-C2-O2
4	H	504	EDO	O1-C1-C2-O2
6	C	506	OXD	O3-C1-C2-O4
6	C	506	OXD	O5-C1-C2-O6
8	E	503	TAR	O1-C1-C2-C3
2	F	501	UDP	C3'-C4'-C5'-O5'
6	C	506	OXD	O3-C1-C2-O6
6	C	506	OXD	O5-C1-C2-O4
2	C	501	UDP	O4'-C4'-C5'-O5'
6	E	506[A]	OXD	O3-C1-C2-O4
2	B	501	UDP	O4'-C4'-C5'-O5'
2	D	501	UDP	O4'-C4'-C5'-O5'
6	F	506	OXD	O5-C1-C2-O6
2	H	501	UDP	C3'-C4'-C5'-O5'
2	A	501	UDP	PB-O3A-PA-O5'
2	B	501	UDP	PB-O3A-PA-O5'
2	C	501	UDP	PB-O3A-PA-O5'
2	D	501	UDP	PB-O3A-PA-O5'
2	E	501	UDP	PB-O3A-PA-O5'
2	F	501	UDP	PB-O3A-PA-O5'
2	G	501	UDP	PB-O3A-PA-O5'
2	H	501	UDP	PB-O3A-PA-O5'
2	B	501	UDP	PA-O3A-PB-O1B
6	B	510	OXD	O5-C1-C2-O6
6	E	506[A]	OXD	O5-C1-C2-O6
6	E	506[A]	OXD	O3-C1-C2-O6
2	A	501	UDP	C3'-C4'-C5'-O5'
2	E	501	UDP	C3'-C4'-C5'-O5'
6	E	506[A]	OXD	O5-C1-C2-O4
6	B	510	OXD	O3-C1-C2-O4
8	E	503	TAR	O1-C1-C2-O2
3	F	502	G6P	C6-O6-P-O3P
8	E	503	TAR	O11-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	H	502	G6P	C5-C6-O6-P
2	B	501	UDP	C3'-C4'-C5'-O5'
3	G	502	G6P	C6-O6-P-O2P
2	C	501	UDP	PA-O3A-PB-O1B
2	H	501	UDP	PA-O3A-PB-O1B
6	B	510	OXD	O3-C1-C2-O6
6	B	510	OXD	O5-C1-C2-O4
4	D	504	EDO	O1-C1-C2-O2
2	C	501	UDP	C3'-C4'-C5'-O5'
2	D	501	UDP	C3'-C4'-C5'-O5'
3	E	502	G6P	C5-C6-O6-P
3	F	502	G6P	C5-C6-O6-P
3	G	502	G6P	C5-C6-O6-P

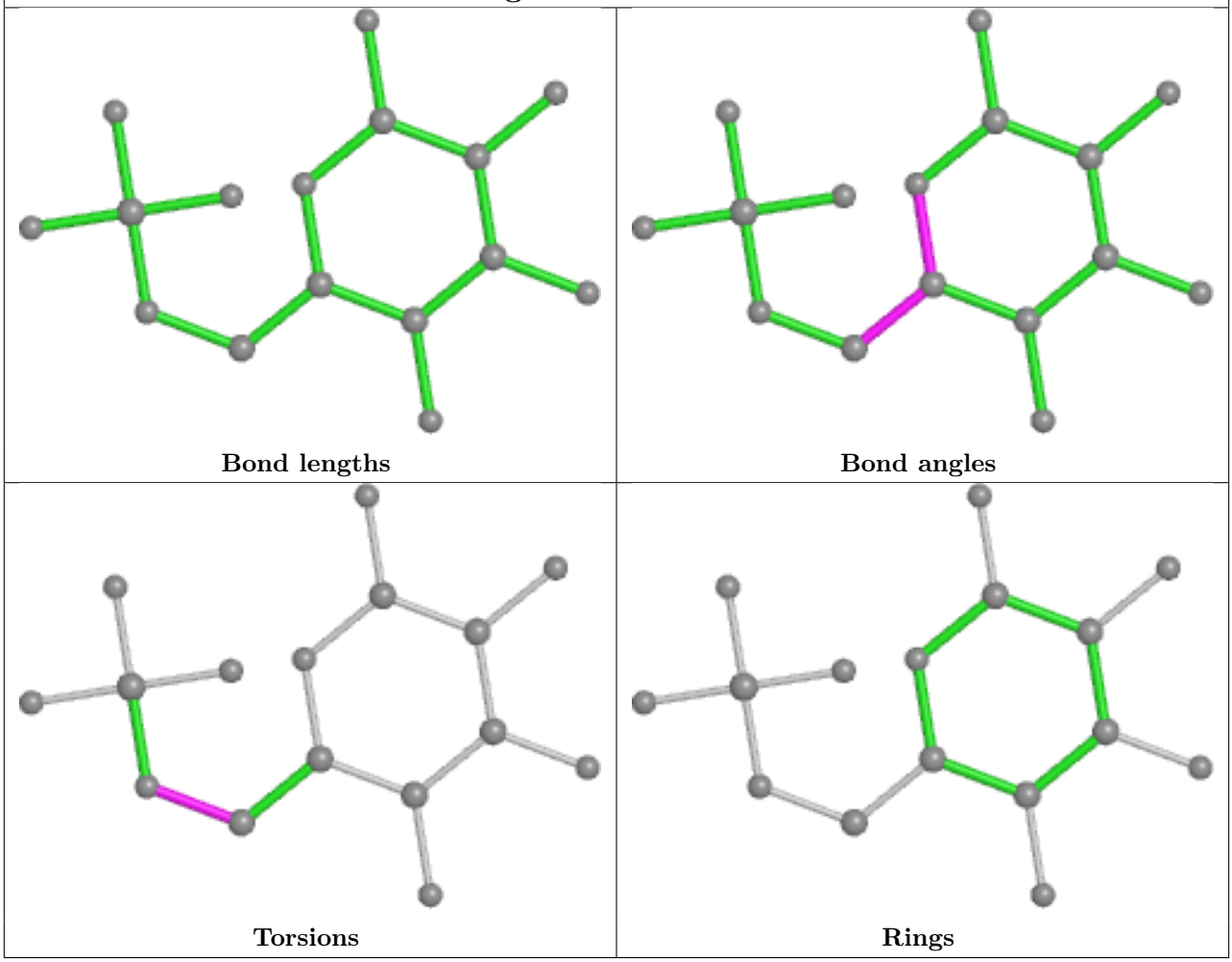
There are no ring outliers.

8 monomers are involved in 9 short contacts:

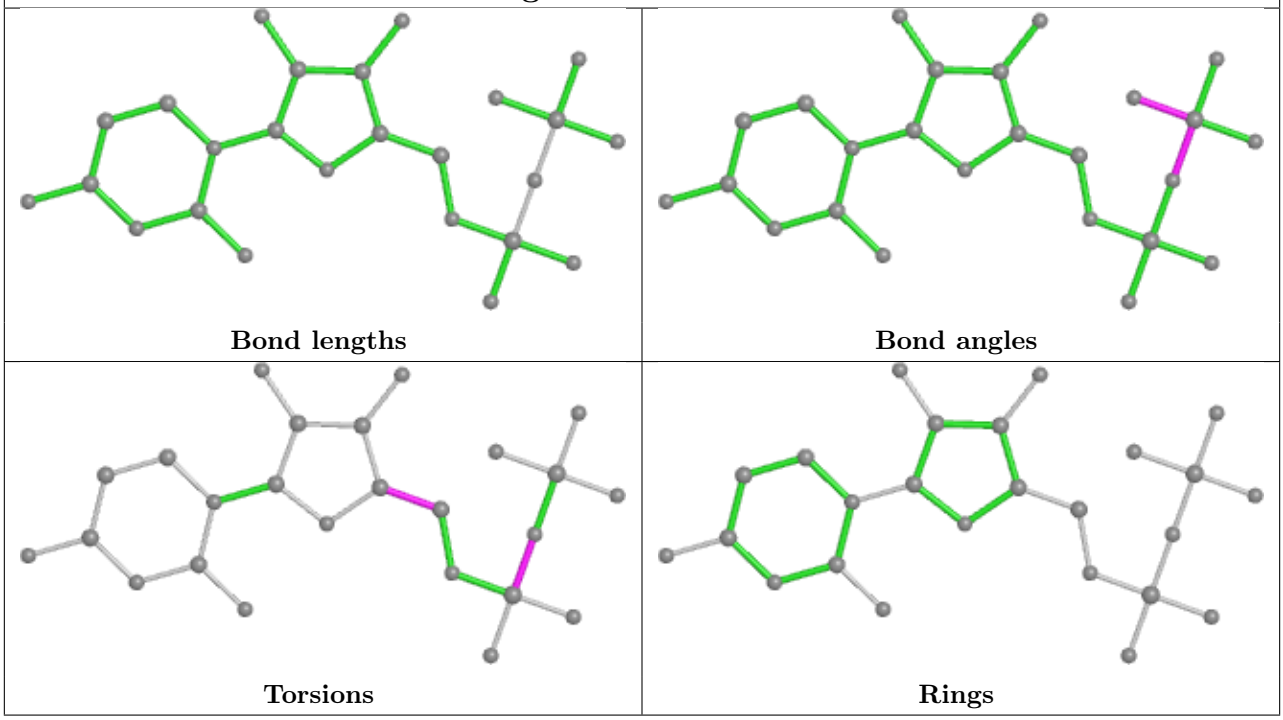
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	516	FMT	1	0
4	D	504	EDO	1	0
8	E	503	TAR	1	0
5	D	506	ACT	2	0
7	E	509	FMT	1	0
7	A	508	FMT	1	0
6	F	506	OXD	1	0
7	B	513	FMT	1	0

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

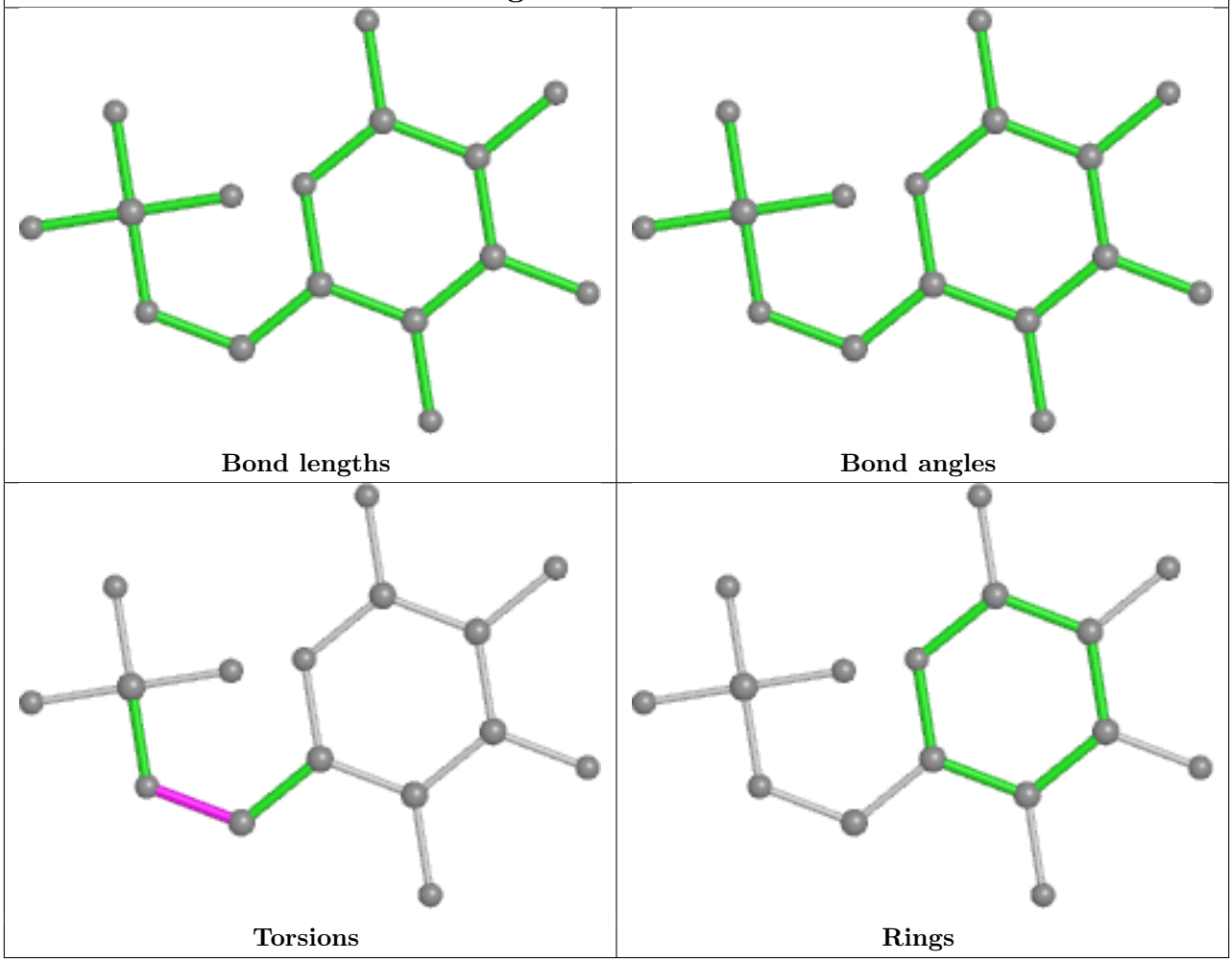
Ligand G6P H 502



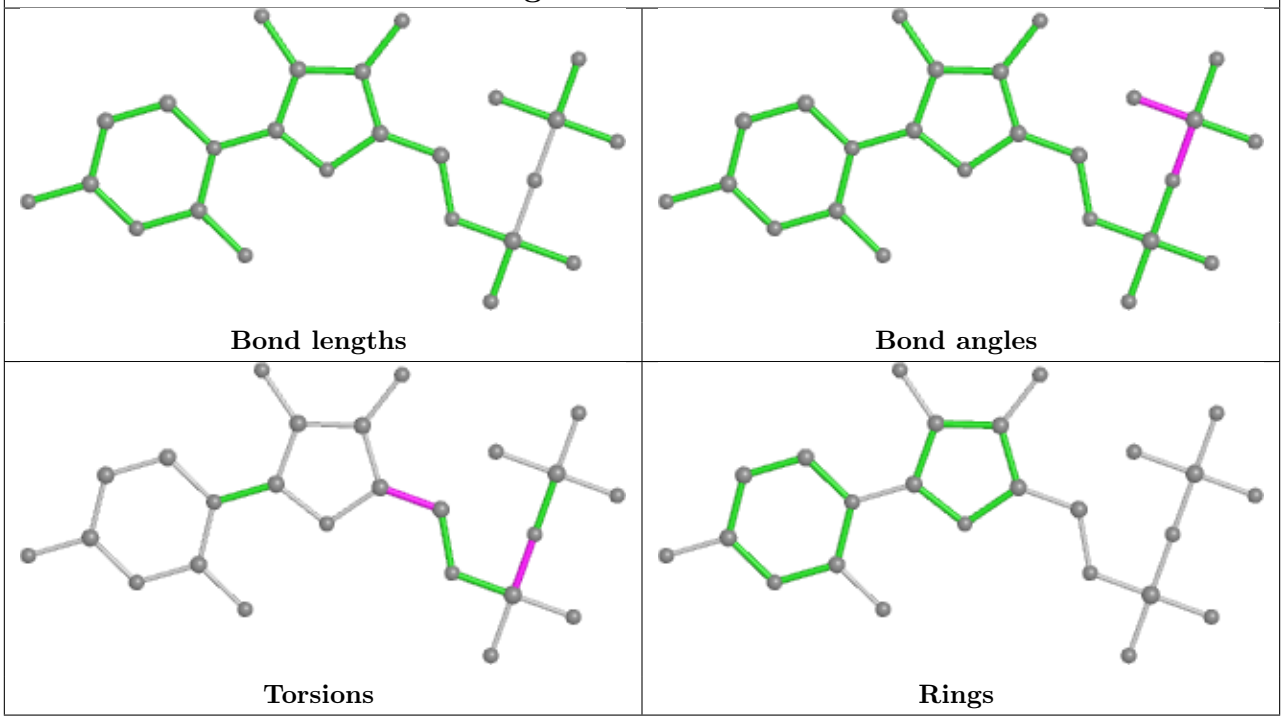
Ligand UDP A 501



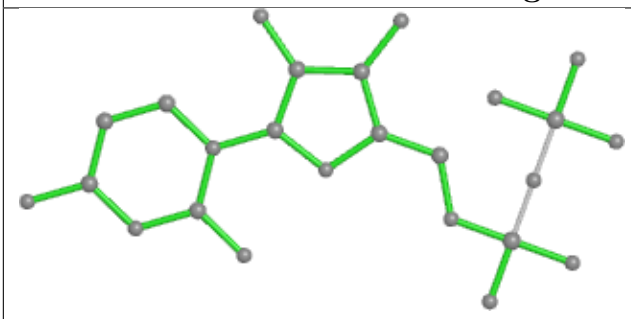
Ligand G6P E 502



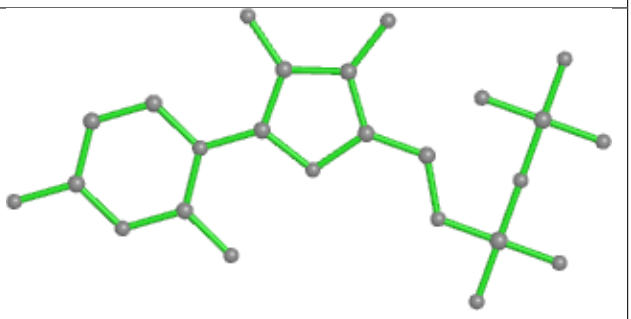
Ligand UDP E 501



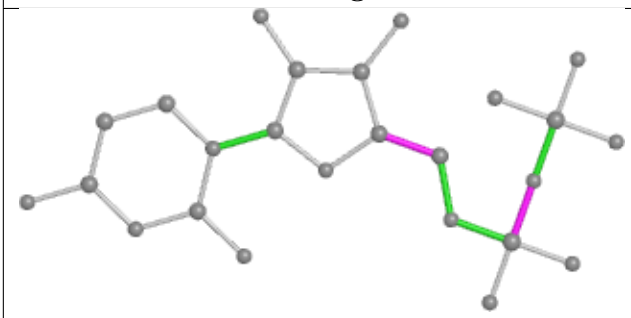
Ligand UDP F 501



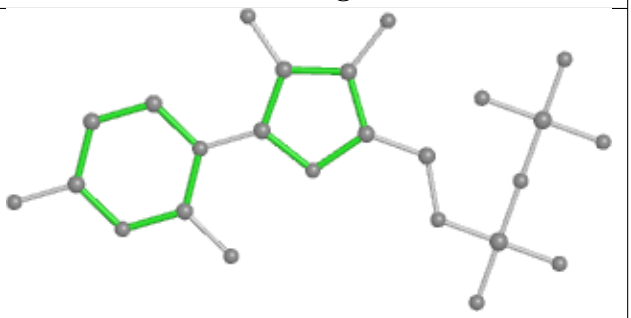
Bond lengths



Bond angles

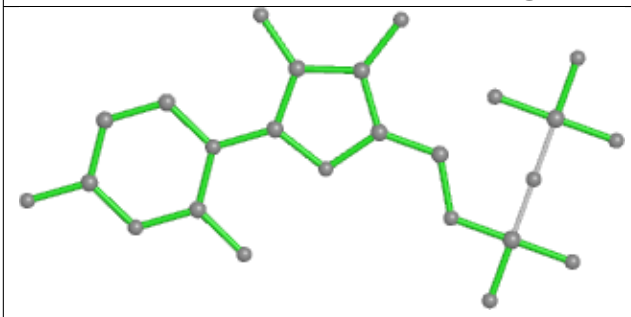


Torsions

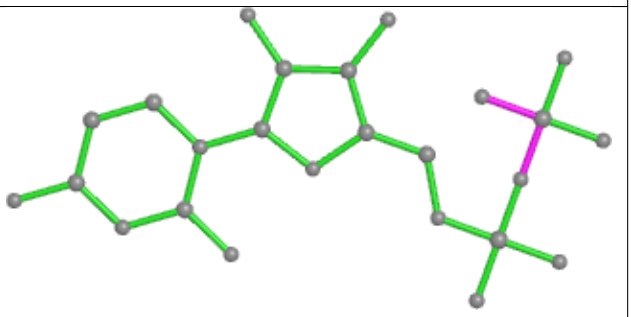


Rings

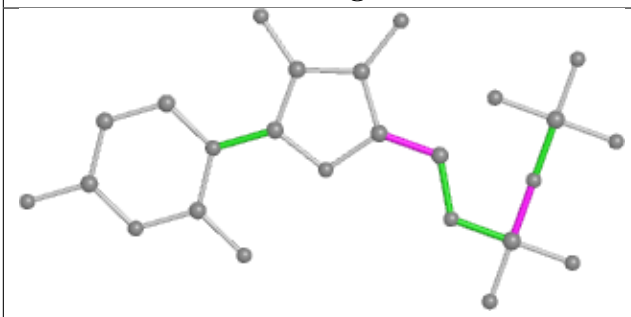
Ligand UDP G 501



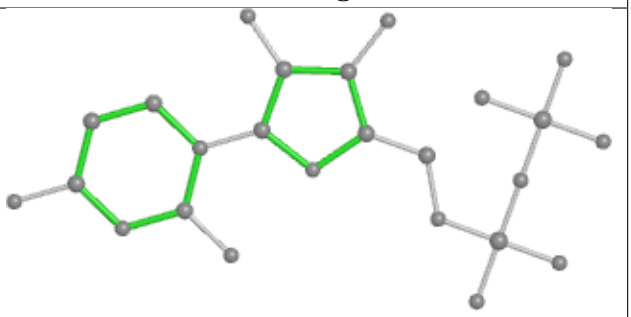
Bond lengths



Bond angles

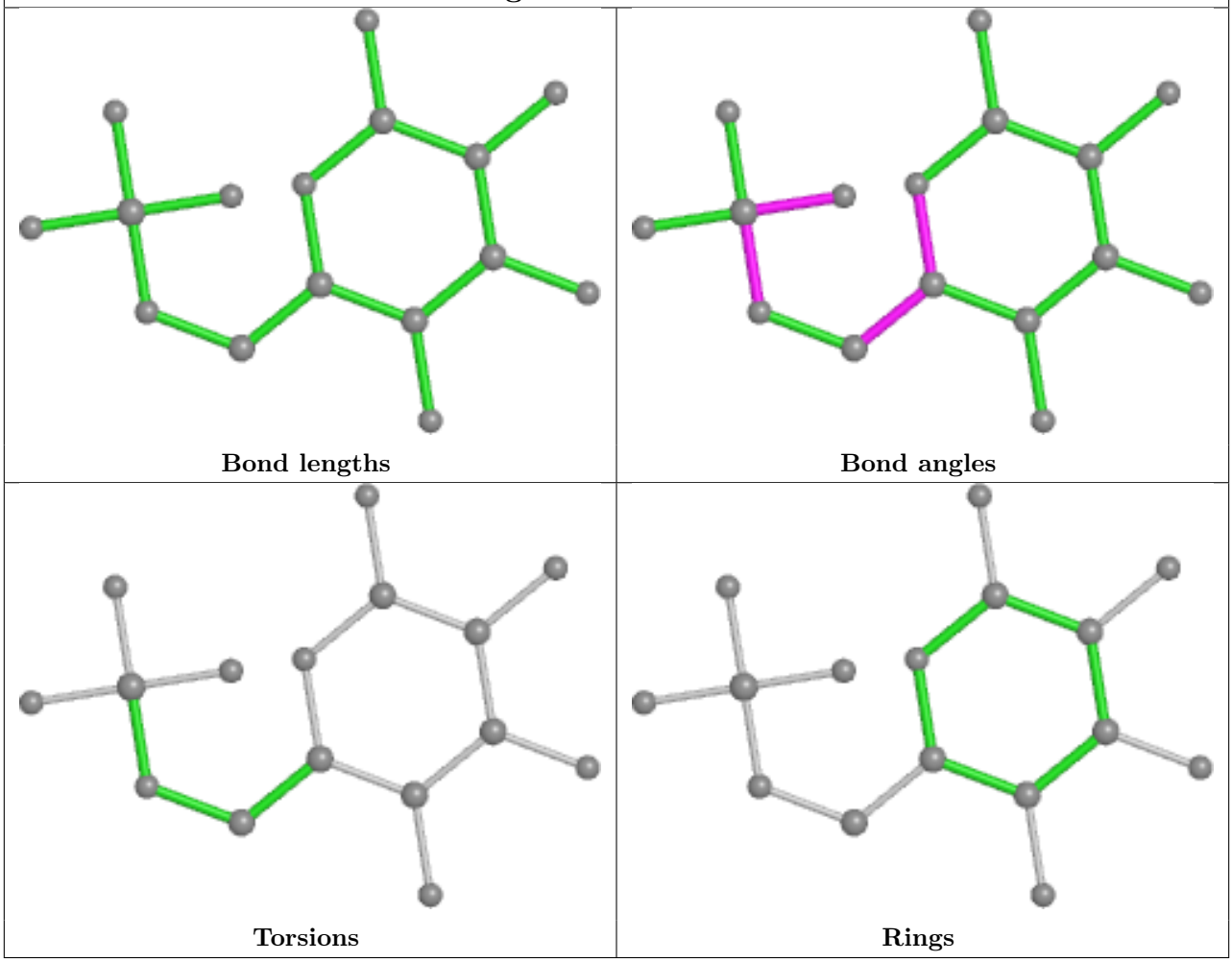


Torsions

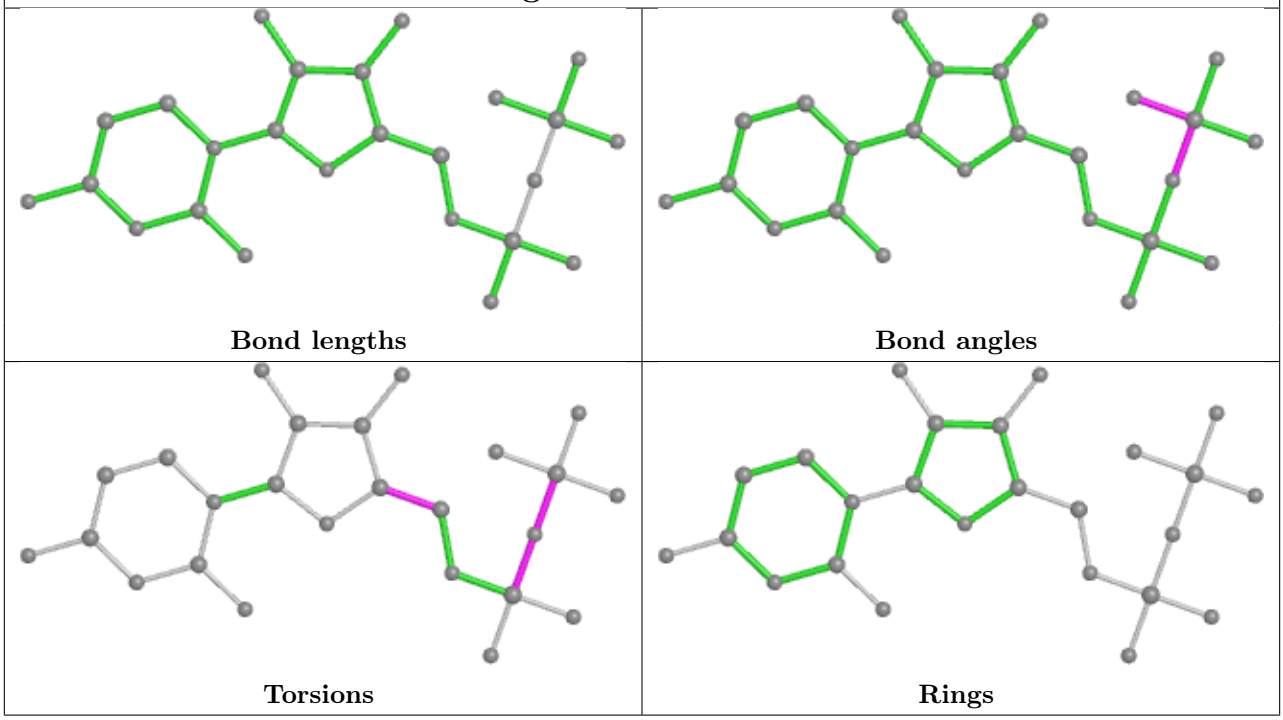


Rings

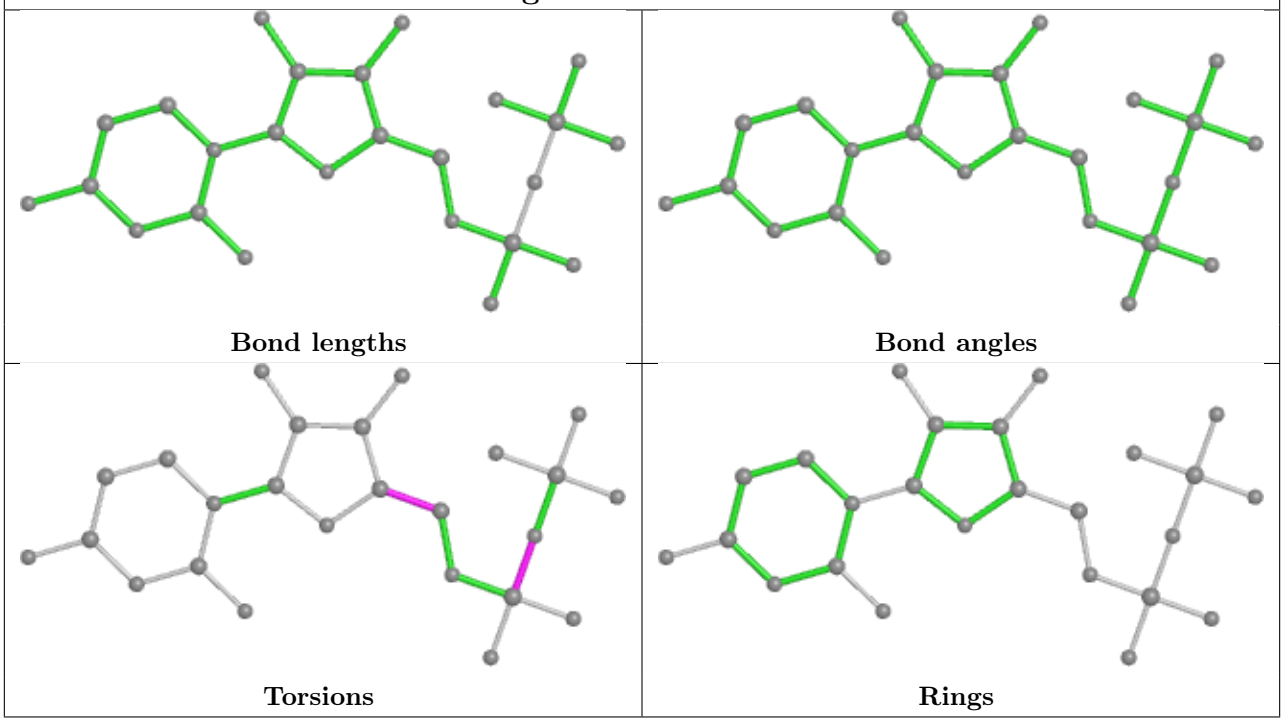
Ligand G6P D 502



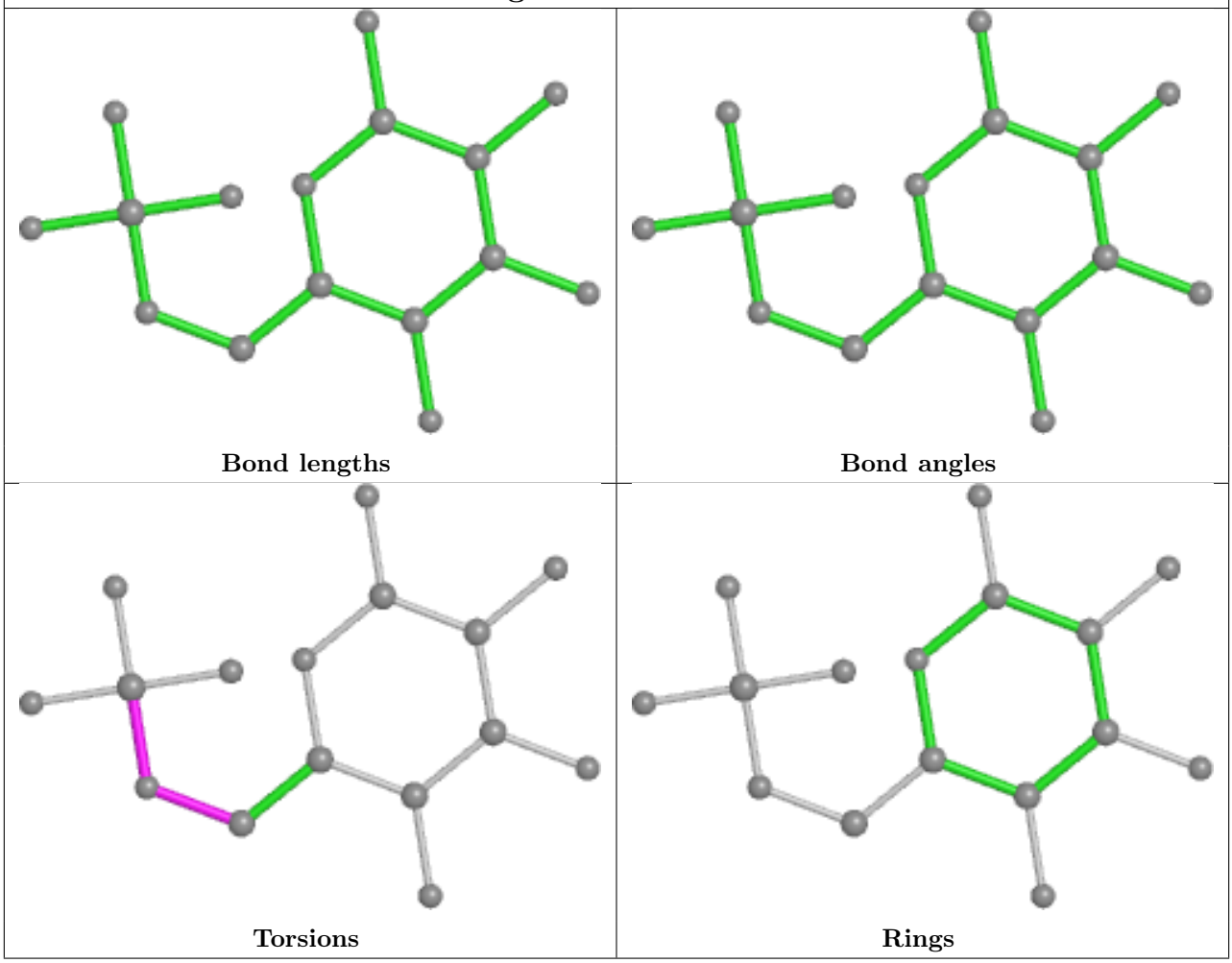
Ligand UDP C 501



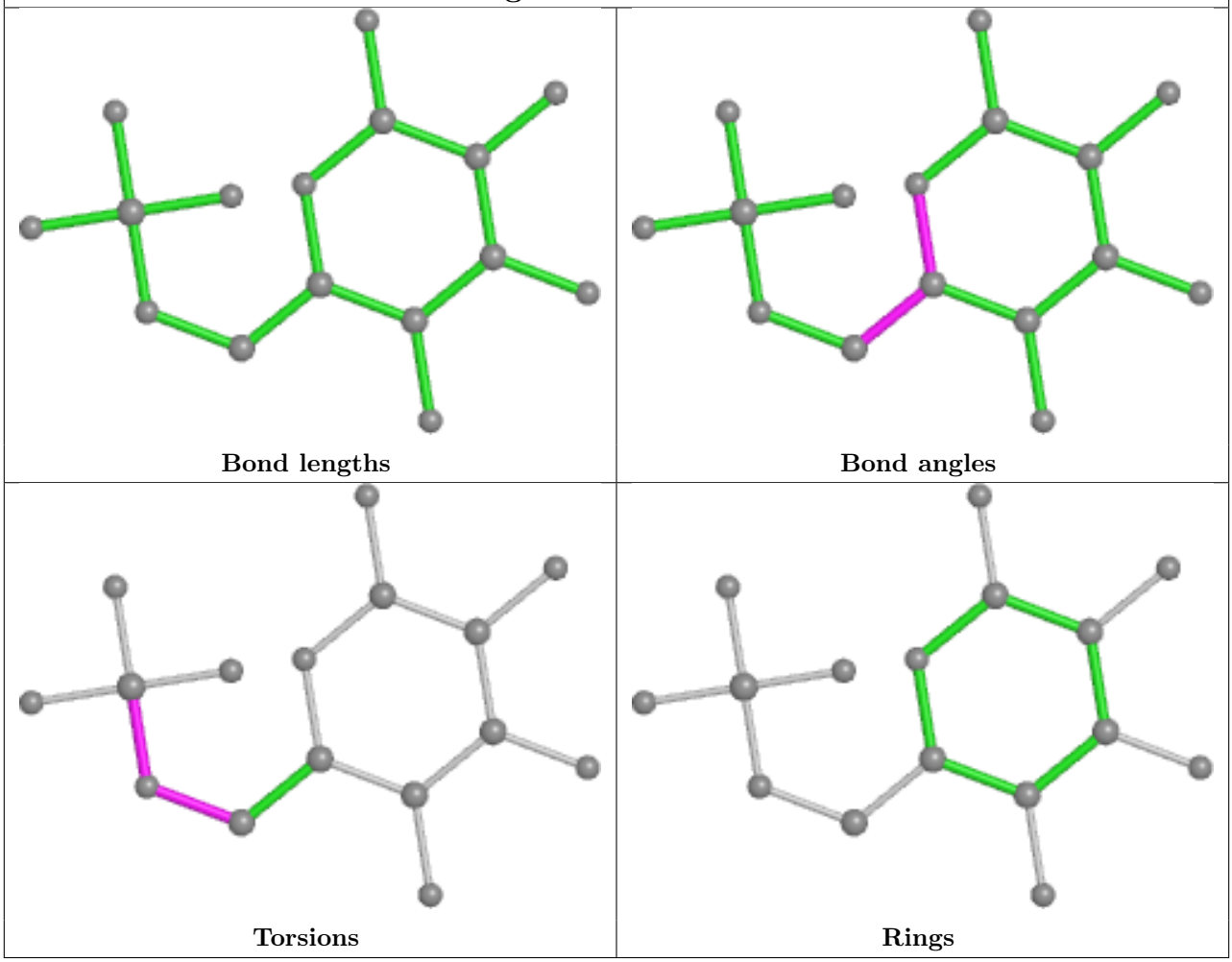
Ligand UDP D 501



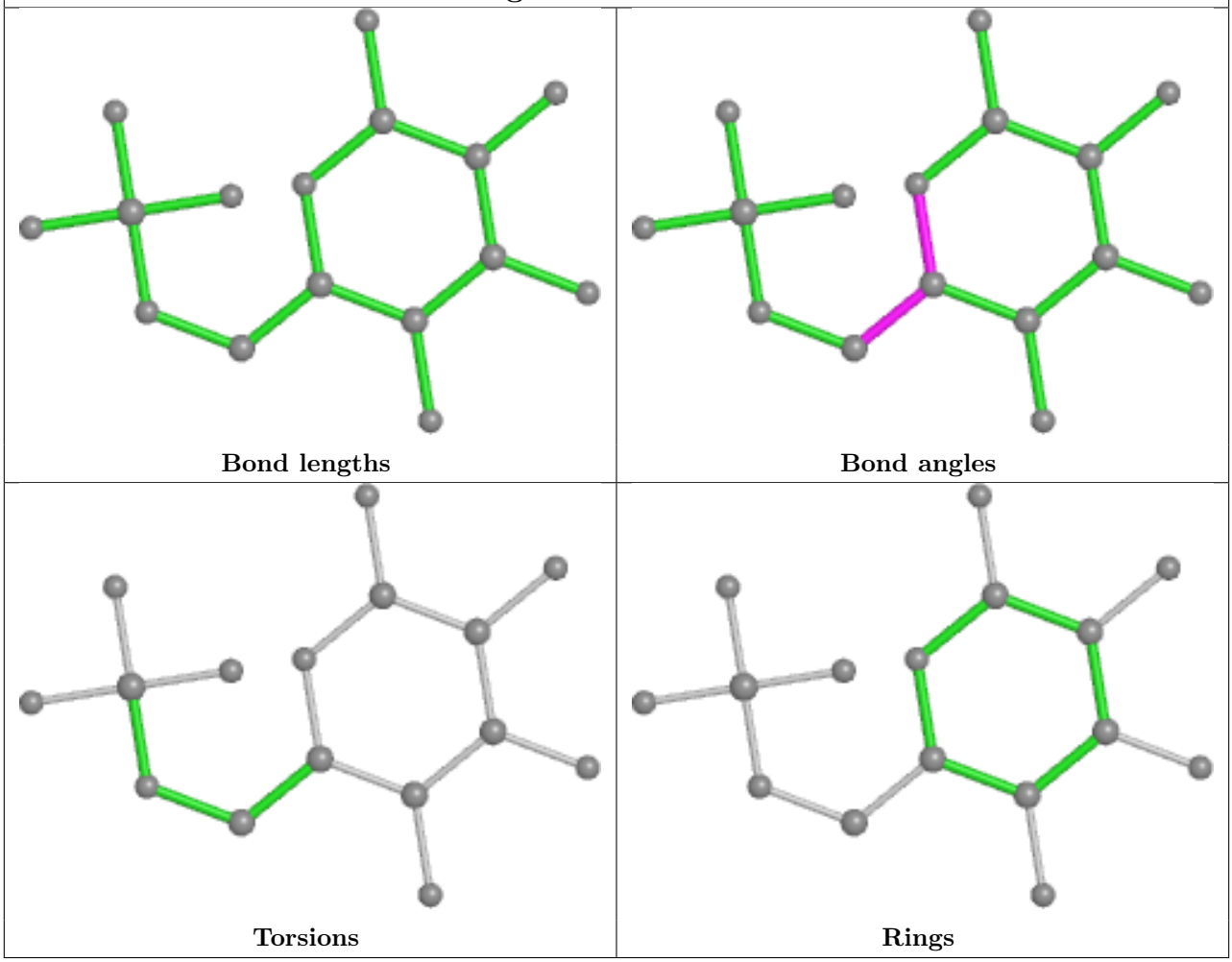
Ligand G6P F 502



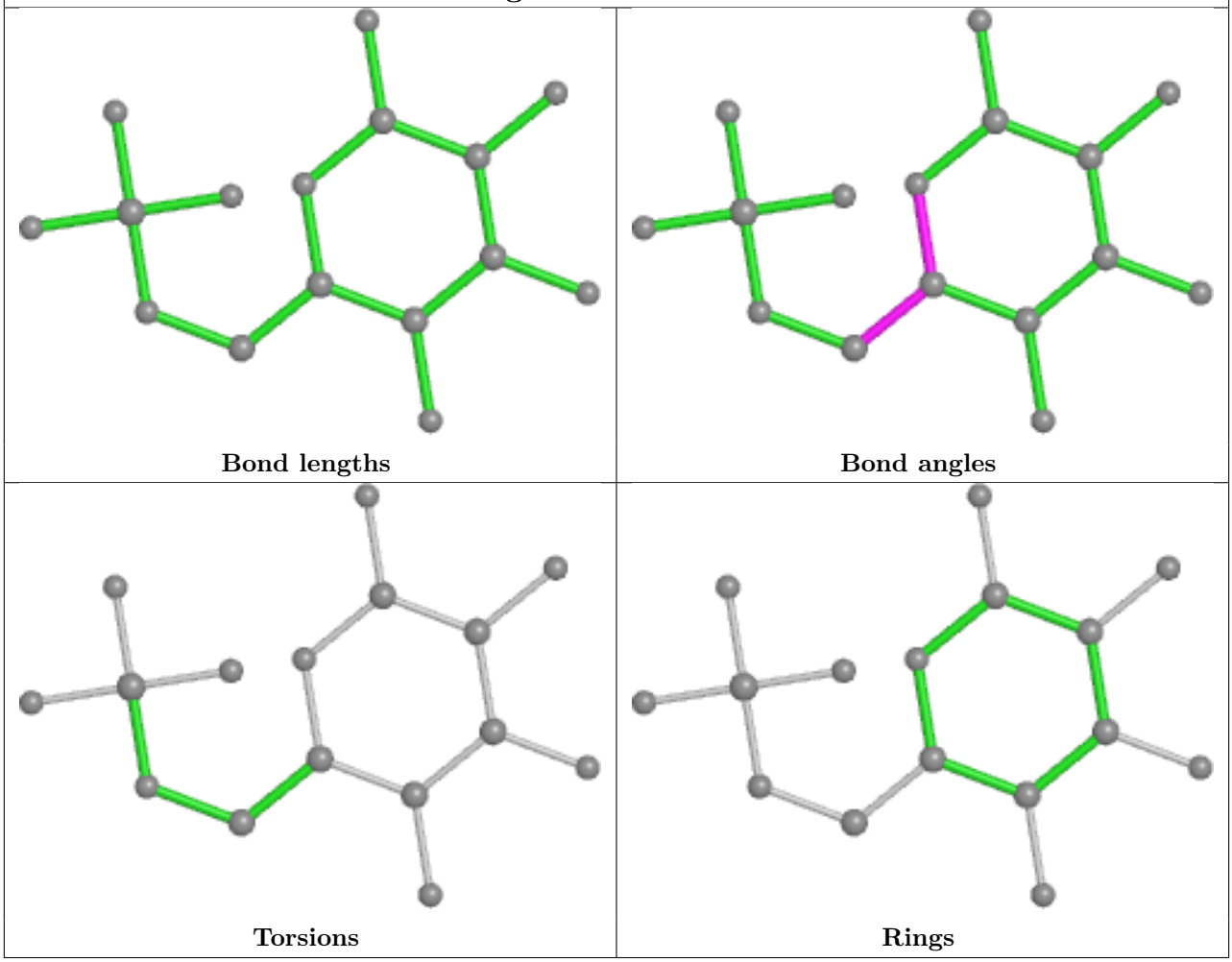
Ligand G6P G 502



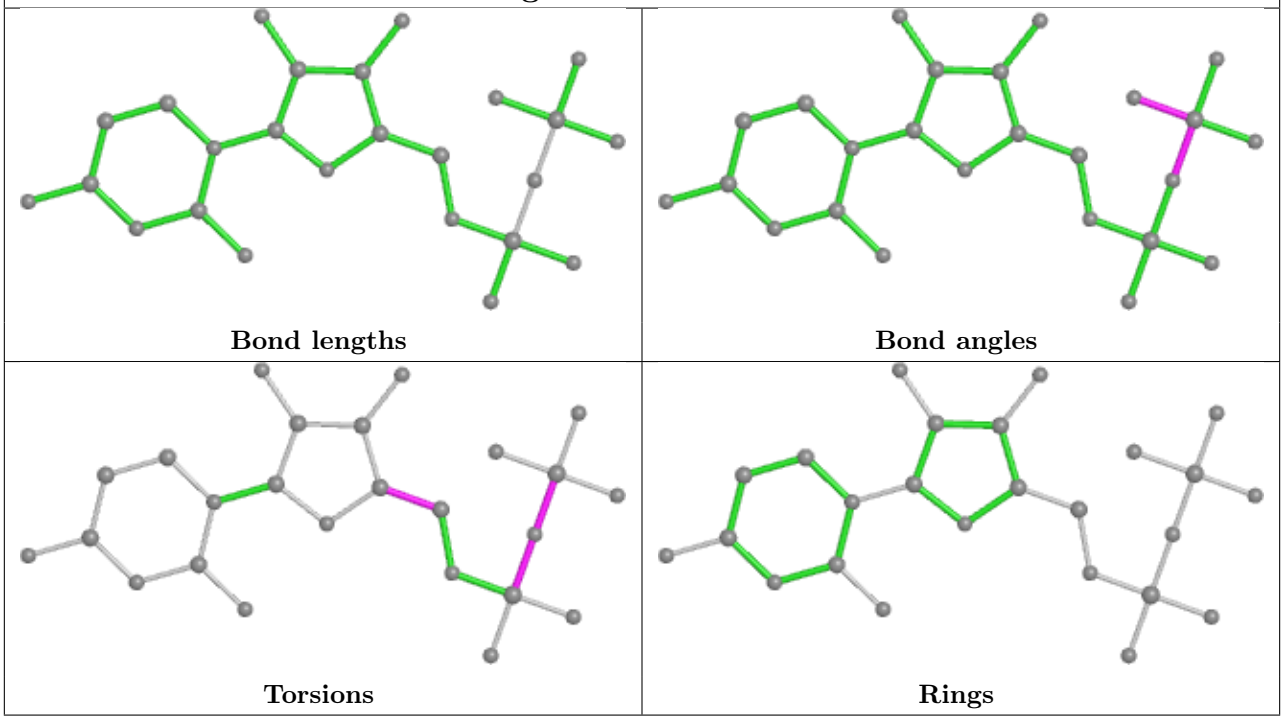
Ligand G6P C 502



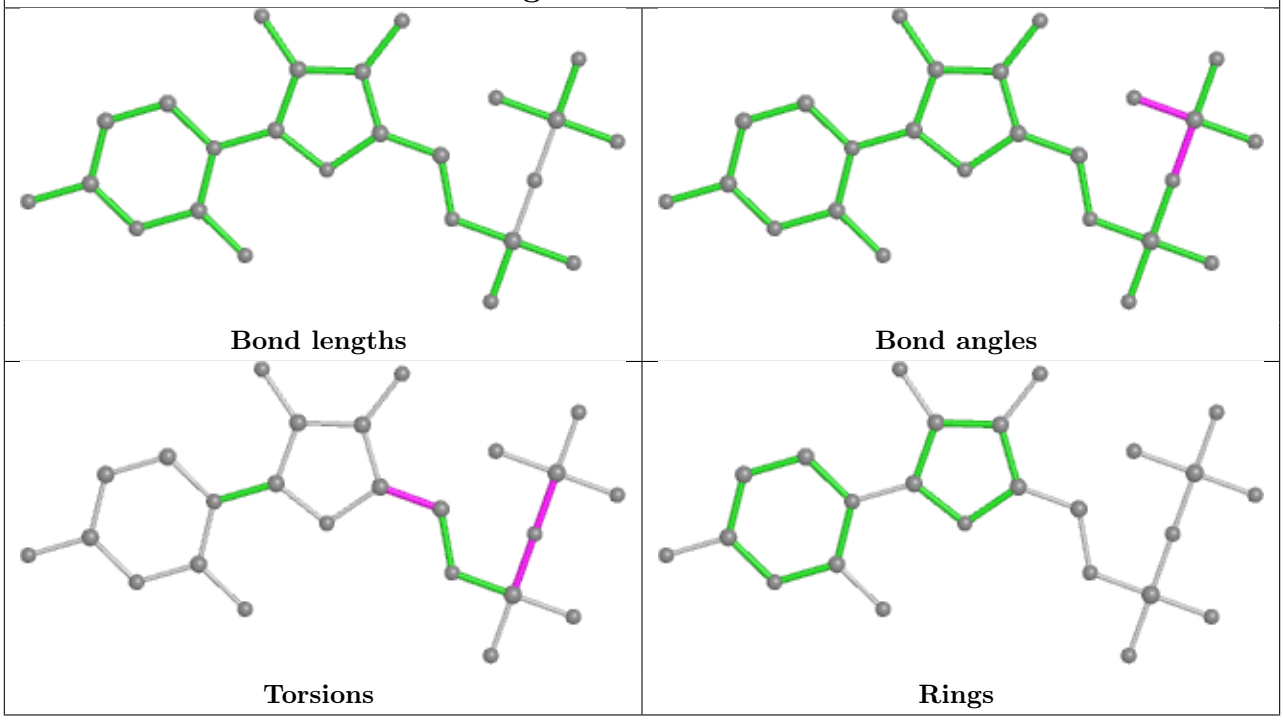
Ligand G6P A 502



Ligand UDP H 501



Ligand UDP B 501



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	454/494 (91%)	-0.63	1 (0%)	95	97	15, 24, 46, 76	0
1	B	453/494 (91%)	-0.65	2 (0%)	92	95	16, 25, 46, 82	0
1	C	452/494 (91%)	-0.61	0	100	100	16, 26, 47, 91	0
1	D	452/494 (91%)	-0.61	0	100	100	16, 27, 48, 95	0
1	E	457/494 (92%)	-0.51	7 (1%)	73	81	16, 27, 56, 95	0
1	F	455/494 (92%)	-0.49	3 (0%)	87	92	17, 28, 56, 76	0
1	G	454/494 (91%)	-0.32	6 (1%)	77	83	19, 39, 72, 106	0
1	H	451/494 (91%)	-0.25	5 (1%)	80	85	18, 41, 76, 97	0
All	All	3628/3952 (91%)	-0.51	24 (0%)	87	92	15, 29, 61, 106	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	219	ALA	5.3
1	E	10	GLY	4.4
1	B	219	ALA	3.5
1	H	22	ILE	3.4
1	H	219	ALA	3.2
1	F	10	GLY	3.2
1	G	21	PRO	3.2
1	E	27	PRO	3.1
1	E	28	ALA	3.0
1	G	22	ILE	2.8
1	F	27	PRO	2.8
1	G	467	GLY	2.8
1	H	220	SER	2.7
1	E	219	ALA	2.7
1	G	27	PRO	2.5
1	H	69	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	22	ILE	2.4
1	H	467	GLY	2.4
1	E	25	GLY	2.2
1	E	220	SER	2.2
1	G	220	SER	2.1
1	F	28	ALA	2.1
1	B	467	GLY	2.0
1	E	218	SER	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
8	TAR	E	503	10/10	0.63	0.33	71,75,81,84	0
7	FMT	D	509	3/3	0.69	0.16	46,46,51,54	0
5	ACT	E	505	4/4	0.71	0.22	68,68,68,71	0
7	FMT	F	509	3/3	0.74	0.21	79,79,79,81	0
5	ACT	B	507	4/4	0.75	0.26	62,71,72,74	0
7	FMT	A	513	3/3	0.76	0.21	45,45,54,56	0
5	ACT	B	506	4/4	0.76	0.17	48,48,58,59	0
5	ACT	D	506	4/4	0.77	0.16	28,54,60,62	0
4	EDO	H	504	4/4	0.77	0.26	48,49,50,51	0
5	ACT	B	508	4/4	0.77	0.21	51,57,61,64	0
5	ACT	B	509	4/4	0.79	0.19	66,68,70,70	0
7	FMT	H	506	3/3	0.81	0.25	49,49,49,51	0
7	FMT	E	508	3/3	0.81	0.16	69,69,70,71	0
7	FMT	B	516	3/3	0.82	0.14	73,73,73,75	0
7	FMT	A	512	3/3	0.82	0.16	58,58,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	FMT	B	514	3/3	0.82	0.39	64,64,65,69	0
7	FMT	E	509	3/3	0.83	0.18	63,63,65,67	0
4	EDO	D	504	4/4	0.83	0.20	51,55,55,59	0
7	FMT	E	510	3/3	0.84	0.11	64,64,66,68	0
7	FMT	D	510	3/3	0.84	0.12	55,55,55,60	0
6	OXD	B	510	6/6	0.84	0.21	71,71,74,78	0
5	ACT	A	506	4/4	0.84	0.15	57,65,67,69	0
7	FMT	B	512	3/3	0.85	0.36	53,53,57,59	0
5	ACT	D	505	4/4	0.86	0.10	35,40,43,45	0
5	ACT	H	505	4/4	0.86	0.13	38,49,51,53	0
7	FMT	F	507	3/3	0.87	0.18	54,54,58,59	0
7	FMT	D	507	3/3	0.87	0.15	61,61,62,64	0
7	FMT	B	515	3/3	0.87	0.17	70,70,70,71	0
7	FMT	C	508	3/3	0.87	0.26	38,38,44,47	0
6	OXD	C	506	6/6	0.89	0.24	70,75,76,77	0
7	FMT	B	513	3/3	0.89	0.16	48,48,55,56	0
4	EDO	E	511	4/4	0.90	0.12	59,59,61,62	0
4	EDO	A	504	4/4	0.90	0.14	48,49,50,51	0
5	ACT	F	504	4/4	0.90	0.12	40,44,50,53	0
7	FMT	E	507	3/3	0.91	0.23	67,67,68,69	0
7	FMT	A	509	3/3	0.91	0.21	52,52,54,58	0
5	ACT	B	505	4/4	0.92	0.13	37,45,51,52	0
5	ACT	F	505	4/4	0.92	0.25	58,59,61,61	0
5	ACT	G	504	4/4	0.92	0.10	36,47,49,49	0
7	FMT	A	510	3/3	0.92	0.14	63,63,65,67	0
7	FMT	A	511	3/3	0.92	0.27	73,73,73,75	0
4	EDO	B	517	4/4	0.92	0.15	40,55,62,63	0
4	EDO	B	504	4/4	0.93	0.15	49,50,50,52	0
5	ACT	A	505	4/4	0.93	0.12	39,51,53,53	0
7	FMT	A	508	3/3	0.93	0.08	45,45,45,46	0
4	EDO	H	503	4/4	0.93	0.18	34,42,49,51	0
7	FMT	H	507	3/3	0.93	0.12	66,66,66,68	0
6	OXD	A	507	6/6	0.93	0.14	63,64,70,74	0
4	EDO	G	503	4/4	0.94	0.12	34,37,47,51	0
6	OXD	E	506[A]	6/6	0.94	0.21	57,57,58,58	6
6	OXD	E	506[B]	6/6	0.94	0.21	56,57,58,59	6
6	OXD	F	506	6/6	0.94	0.14	67,68,70,71	0
7	FMT	D	508	3/3	0.95	0.09	47,47,49,50	0
4	EDO	C	504	4/4	0.95	0.20	42,44,45,45	0
7	FMT	B	511	3/3	0.95	0.08	40,40,43,43	0
5	ACT	C	505	4/4	0.95	0.10	35,39,45,45	0
7	FMT	C	507	3/3	0.96	0.10	43,43,47,48	0

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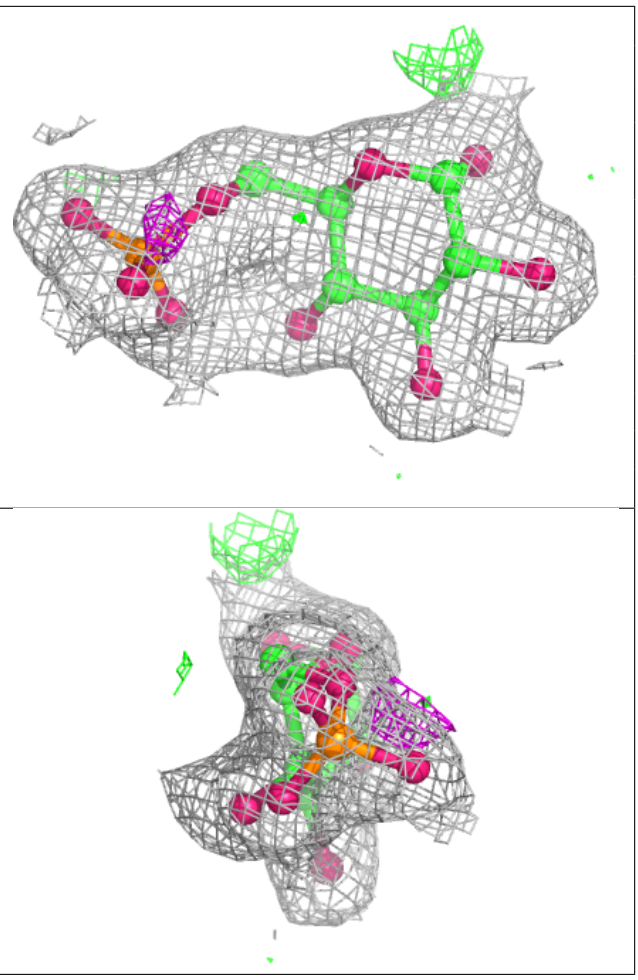
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	E	504	4/4	0.96	0.11	33,34,37,38	0
4	EDO	F	503	4/4	0.96	0.14	36,38,41,41	0
4	EDO	C	503	4/4	0.97	0.12	29,37,38,43	0
3	G6P	G	502	16/16	0.97	0.08	28,32,35,36	0
4	EDO	D	503	4/4	0.97	0.12	27,30,33,36	0
7	FMT	F	508	3/3	0.97	0.08	47,47,49,52	0
4	EDO	A	503	4/4	0.98	0.07	30,35,38,38	0
2	UDP	G	501	25/25	0.98	0.07	22,27,32,34	0
4	EDO	B	503	4/4	0.98	0.07	27,32,35,41	0
3	G6P	H	502	16/16	0.98	0.07	31,34,41,43	0
2	UDP	C	501	25/25	0.99	0.07	14,18,21,21	0
2	UDP	D	501	25/25	0.99	0.08	15,18,21,22	0
2	UDP	E	501	25/25	0.99	0.07	15,19,21,23	0
2	UDP	F	501	25/25	0.99	0.06	16,21,23,24	0
2	UDP	A	501	25/25	0.99	0.07	14,18,23,23	0
2	UDP	H	501	25/25	0.99	0.08	23,29,33,37	0
3	G6P	A	502	16/16	0.99	0.08	13,18,19,21	0
3	G6P	B	502	16/16	0.99	0.07	13,19,21,23	0
3	G6P	C	502	16/16	0.99	0.08	15,19,21,21	0
3	G6P	D	502	16/16	0.99	0.08	14,19,22,25	0
3	G6P	E	502	16/16	0.99	0.06	19,23,25,26	0
3	G6P	F	502	16/16	0.99	0.06	19,24,30,30	0
2	UDP	B	501	25/25	0.99	0.07	15,18,22,25	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.

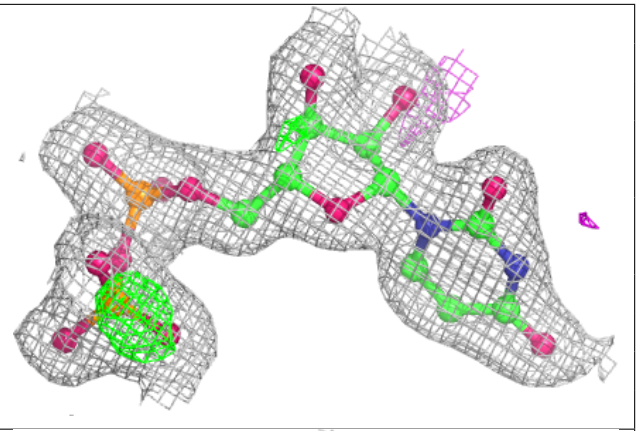
Electron density around G6P G 502:

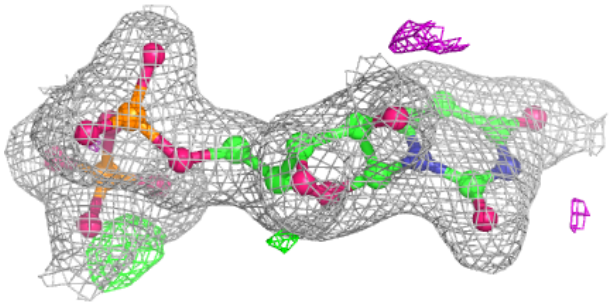
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

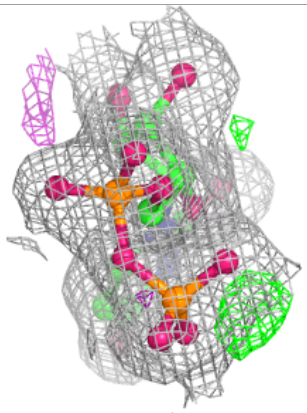


Electron density around UDP G 501:

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

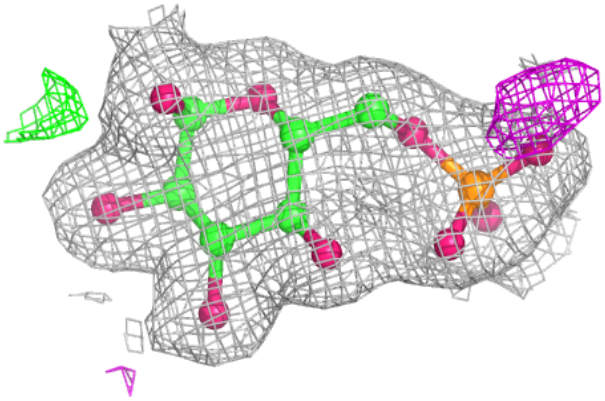


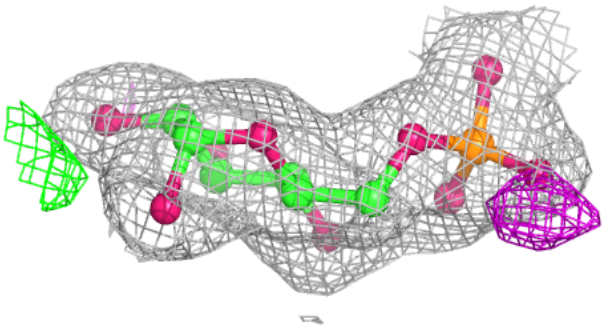


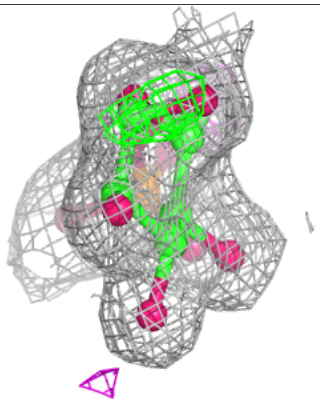


Electron density around G6P H 502:

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

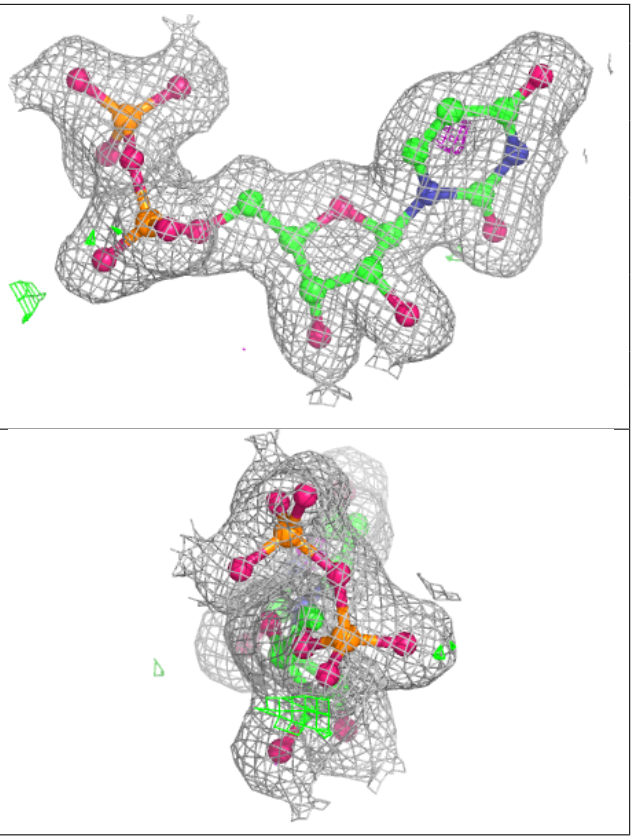






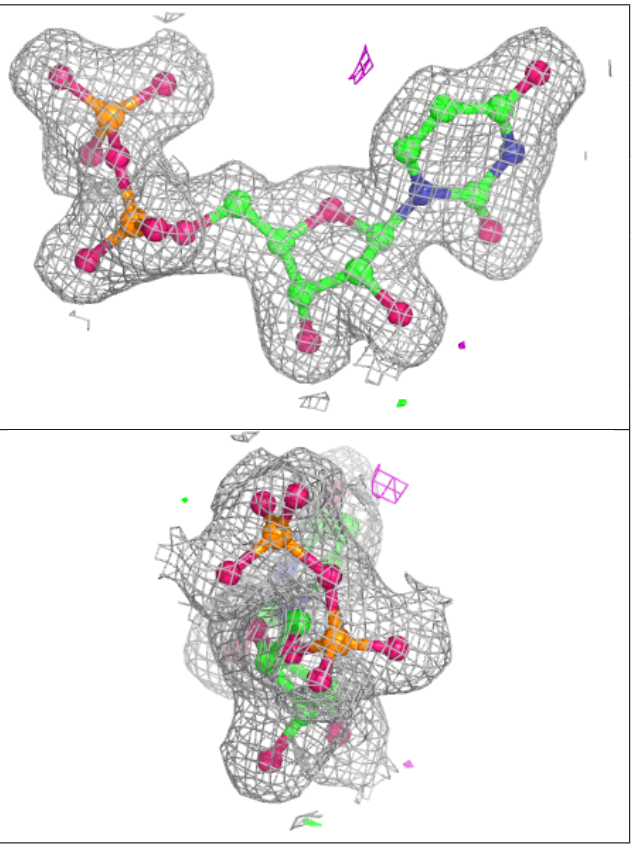
Electron density around UDP C 501:

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



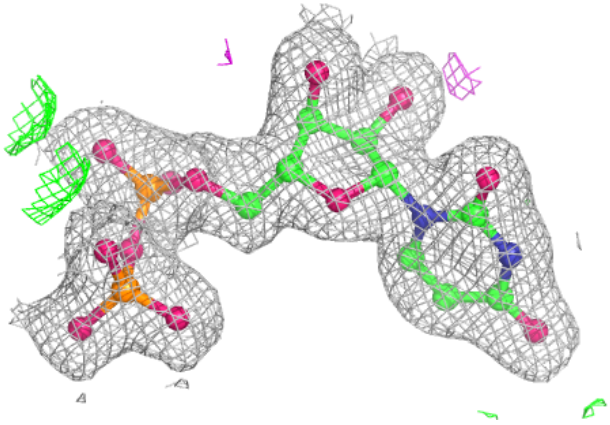
Electron density around UDP D 501:

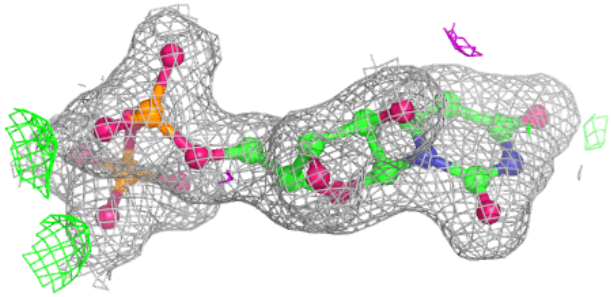
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

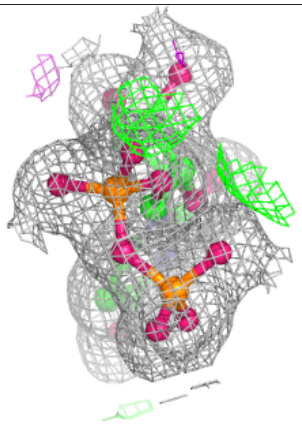


Electron density around UDP E 501:

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

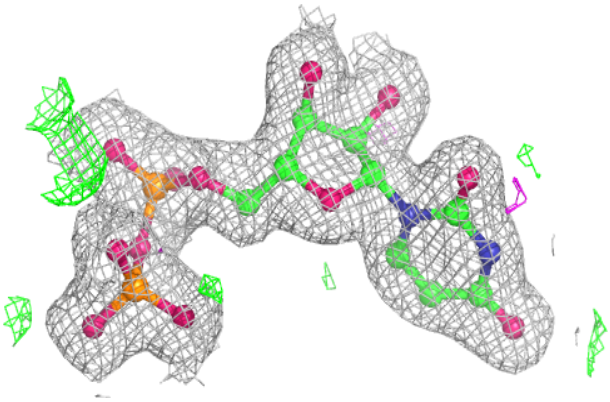


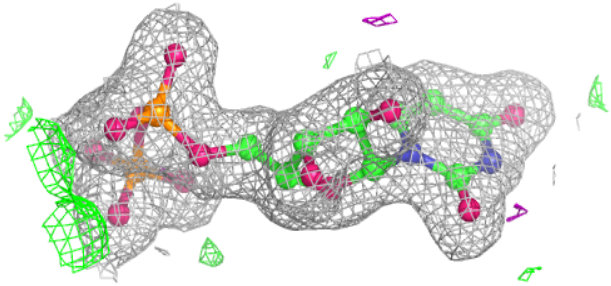


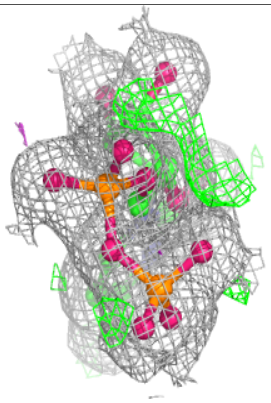


Electron density around UDP F 501:

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

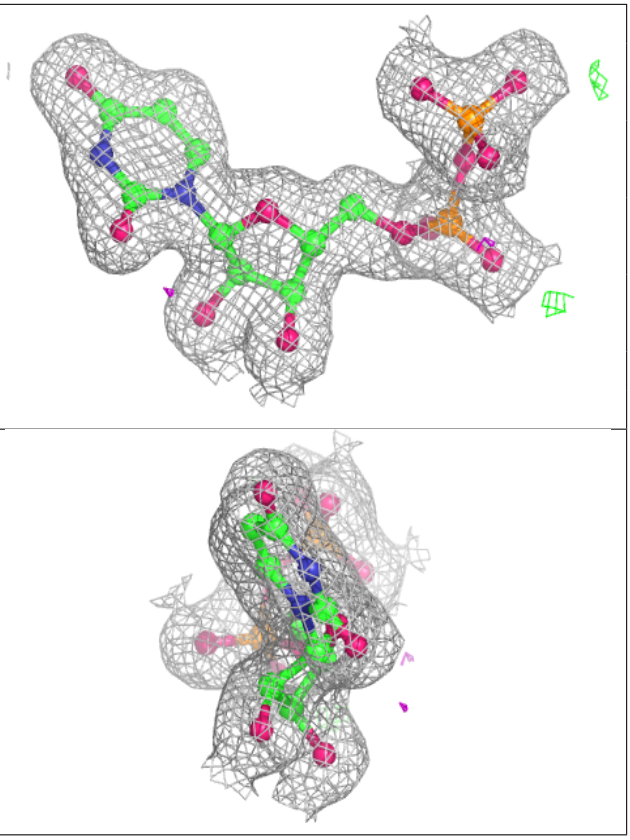






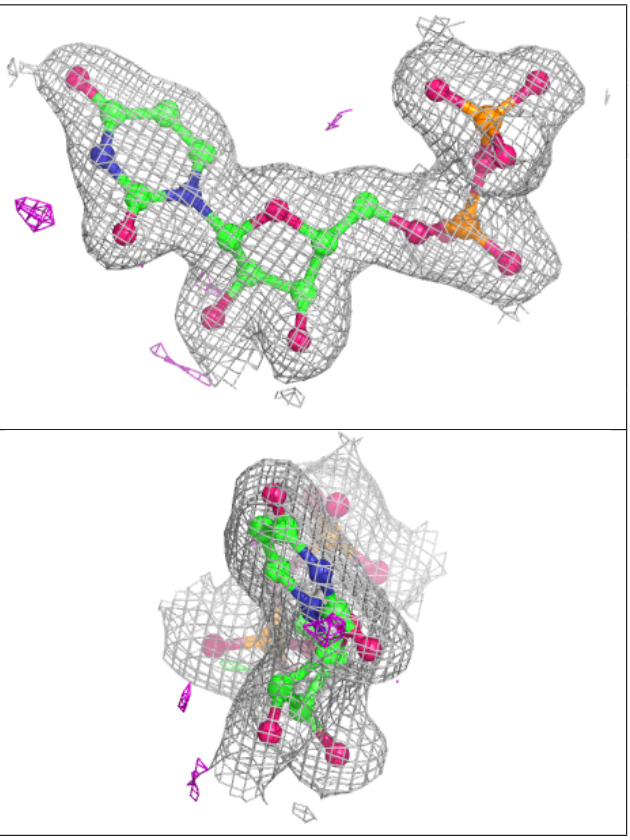
Electron density around UDP A 501:

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



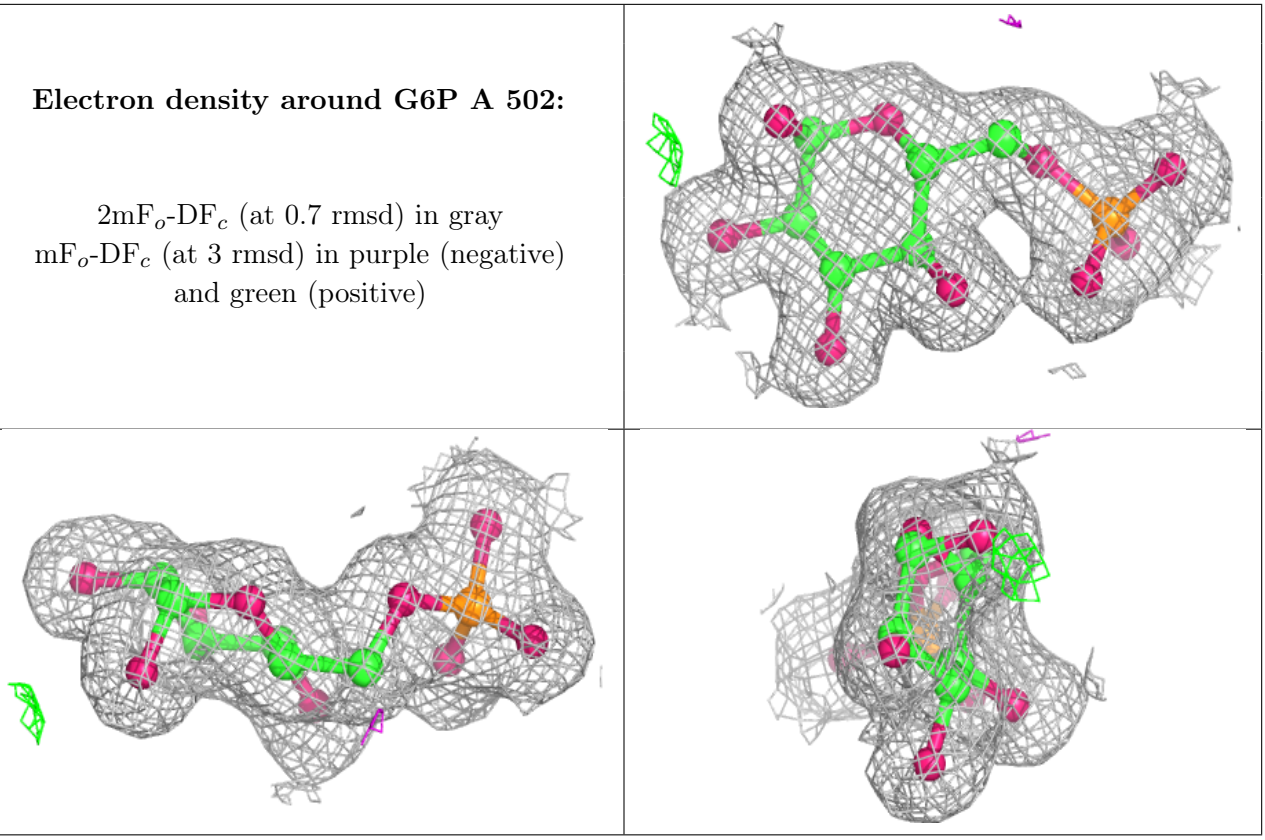
Electron density around UDP H 501:

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



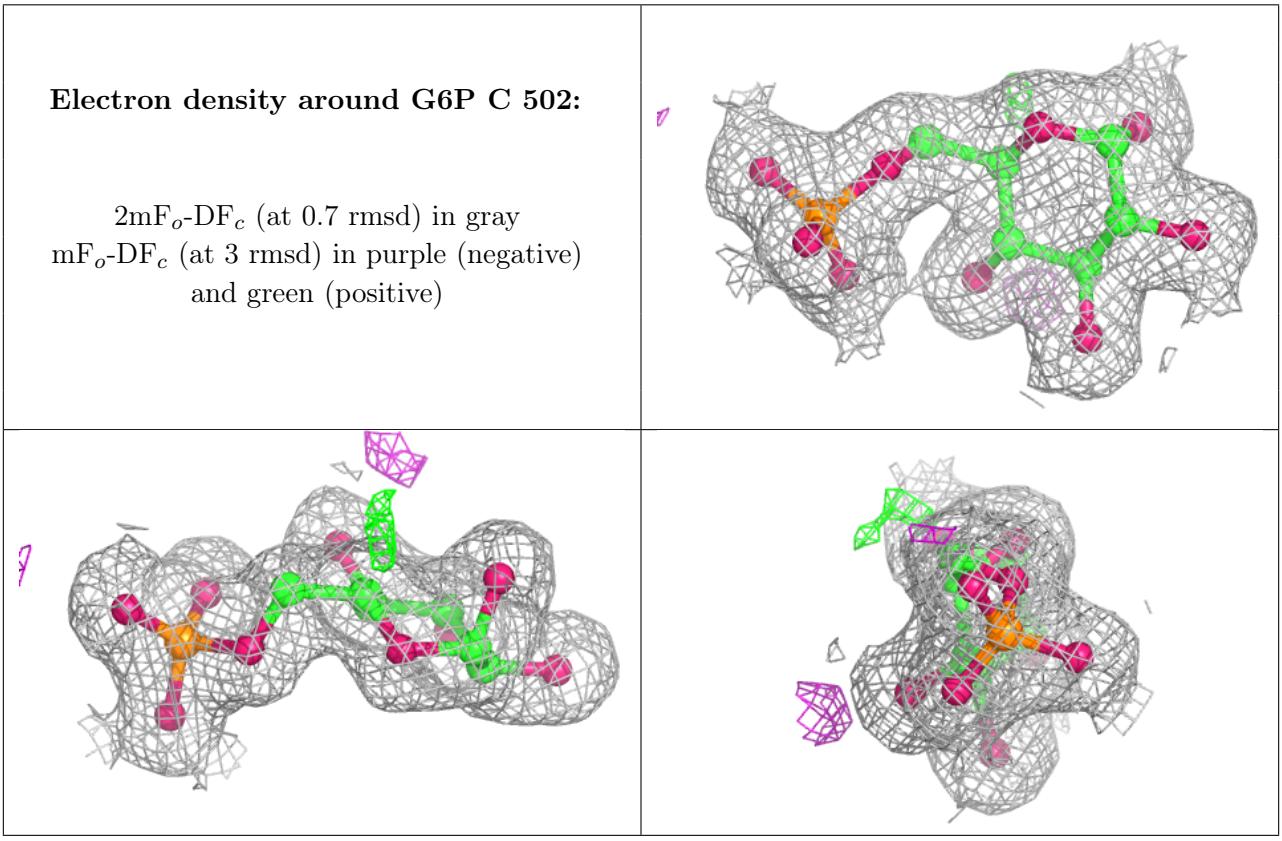
Electron density around G6P A 502:

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



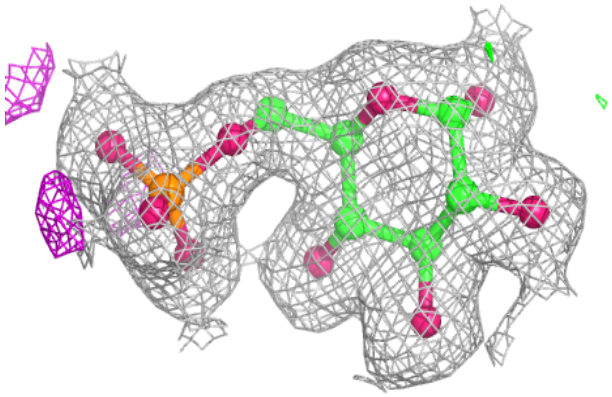
Electron density around G6P C 502:

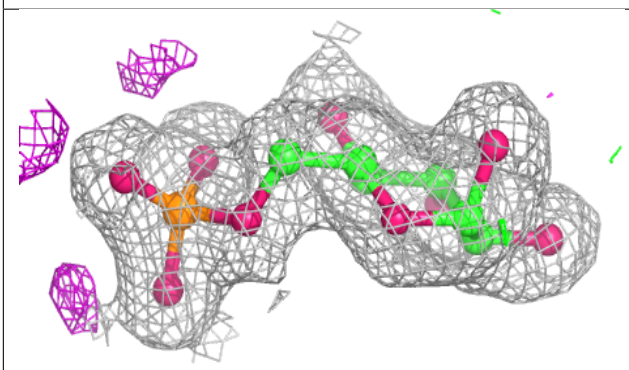
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

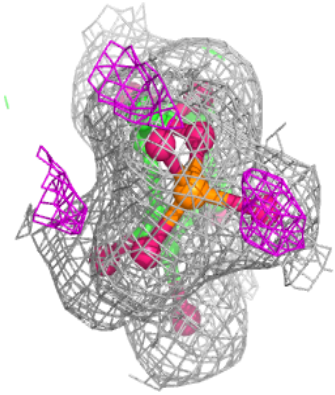


Electron density around G6P D 502:

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

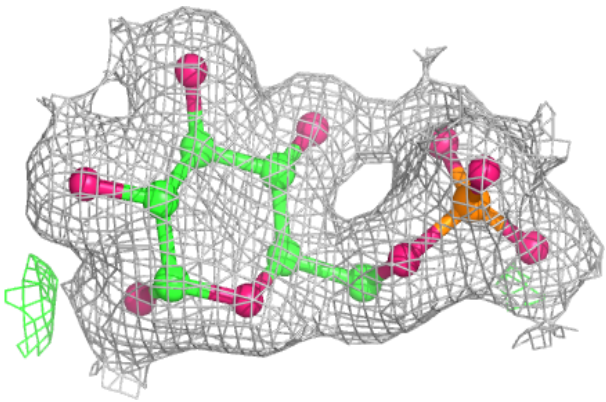


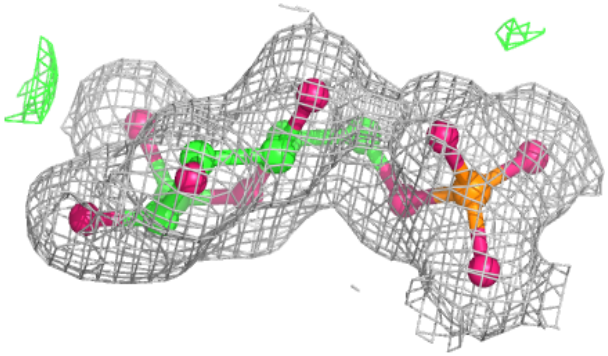


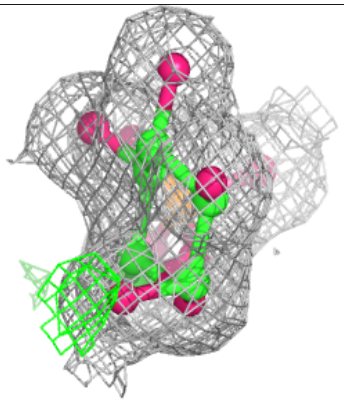


Electron density around G6P E 502:

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

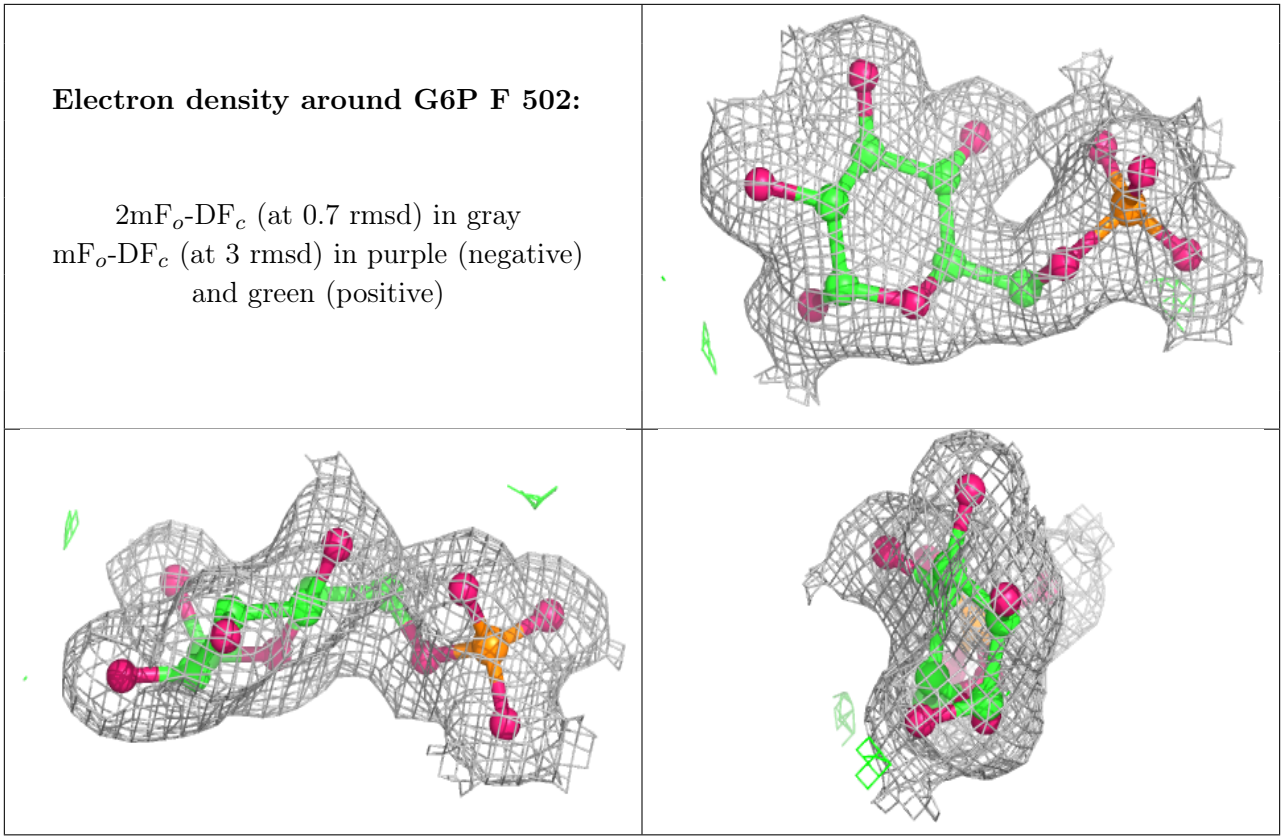






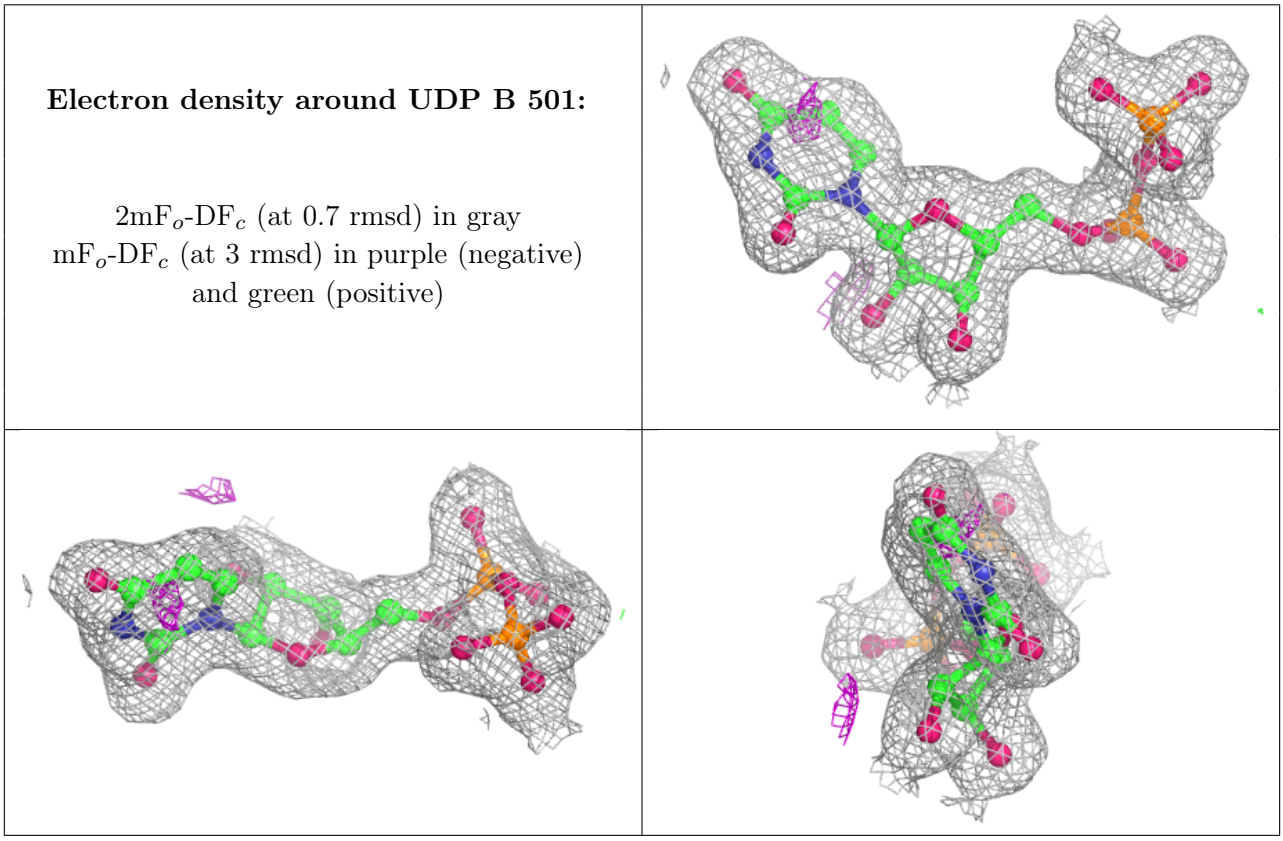
Electron density around G6P F 502:

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



Electron density around UDP B 501:

$2mF_o$-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.