Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:32 PM JST

PDB ID	:	6J0G
Title	:	Crystal structure of intracellular B30.2 domain of BTN3A3 mutant in complex with HMBPP
Authors	:	Yang, Y.Y.; Liu, W.D.; Cai, N.N.; Chen, C.C.; Guo, R.T.; Zhang, Y.H.
Deposited on	:	2018-12-24
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

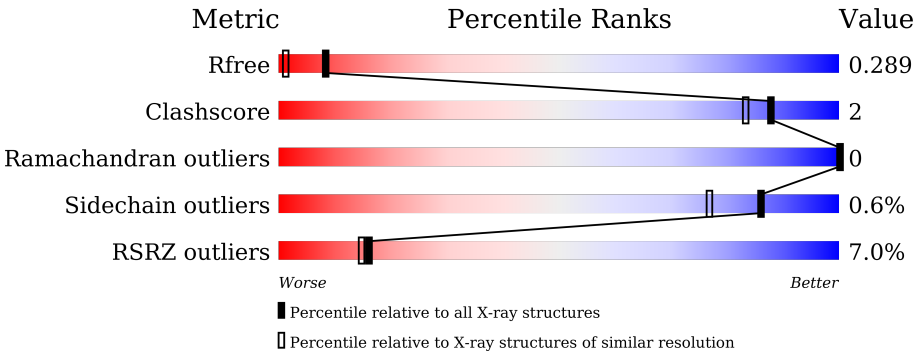
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	221	5% 83% • 14%
1	B	221	5% 77% 9% 14%
1	C	221	7% 81% 5% 14%
1	D	221	7% 83% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7091 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 Butyrophilin subfamily 3 member A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	3	0
			1562	1004	263	287	8			
1	B	190	Total	C	N	O	S	0	2	0
			1557	1000	263	287	7			
1	C	189	Total	C	N	O	S	0	0	0
			1539	987	260	285	7			
1	D	189	Total	C	N	O	S	0	1	0
			1543	990	260	286	7			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	MET	-	initiating methionine	UNP O00478
A	266	GLY	-	expression tag	UNP O00478
A	267	SER	-	expression tag	UNP O00478
A	268	SER	-	expression tag	UNP O00478
A	269	HIS	-	expression tag	UNP O00478
A	270	HIS	-	expression tag	UNP O00478
A	271	HIS	-	expression tag	UNP O00478
A	272	HIS	-	expression tag	UNP O00478
A	273	HIS	-	expression tag	UNP O00478
A	274	HIS	-	expression tag	UNP O00478
A	275	SER	-	expression tag	UNP O00478
A	276	SER	-	expression tag	UNP O00478
A	277	GLY	-	expression tag	UNP O00478
A	278	LEU	-	expression tag	UNP O00478
A	279	VAL	-	expression tag	UNP O00478
A	280	PRO	-	expression tag	UNP O00478
A	281	ARG	-	expression tag	UNP O00478
A	282	GLY	-	expression tag	UNP O00478
A	283	SER	-	expression tag	UNP O00478
A	284	HIS	-	expression tag	UNP O00478
A	285	MET	-	expression tag	UNP O00478

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Chain	Residue	Modelled	Actual	Comment	Reference
A	286	GLU	-	expression tag	UNP O00478
A	287	ASN	-	expression tag	UNP O00478
A	288	LEU	-	expression tag	UNP O00478
A	289	TYR	-	expression tag	UNP O00478
A	290	PHE	-	expression tag	UNP O00478
A	291	GLN	-	expression tag	UNP O00478
A	292	GLY	-	expression tag	UNP O00478
A	293	ALA	-	expression tag	UNP O00478
A	294	GLY	-	expression tag	UNP O00478
A	295	ALA	-	expression tag	UNP O00478
A	296	GLY	-	expression tag	UNP O00478
A	297	ALA	-	expression tag	UNP O00478
A	351	HIS	ARG	engineered mutation	UNP O00478
B	265	MET	-	initiating methionine	UNP O00478
B	266	GLY	-	expression tag	UNP O00478
B	267	SER	-	expression tag	UNP O00478
B	268	SER	-	expression tag	UNP O00478
B	269	HIS	-	expression tag	UNP O00478
B	270	HIS	-	expression tag	UNP O00478
B	271	HIS	-	expression tag	UNP O00478
B	272	HIS	-	expression tag	UNP O00478
B	273	HIS	-	expression tag	UNP O00478
B	274	HIS	-	expression tag	UNP O00478
B	275	SER	-	expression tag	UNP O00478
B	276	SER	-	expression tag	UNP O00478
B	277	GLY	-	expression tag	UNP O00478
B	278	LEU	-	expression tag	UNP O00478
B	279	VAL	-	expression tag	UNP O00478
B	280	PRO	-	expression tag	UNP O00478
B	281	ARG	-	expression tag	UNP O00478
B	282	GLY	-	expression tag	UNP O00478
B	283	SER	-	expression tag	UNP O00478
B	284	HIS	-	expression tag	UNP O00478
B	285	MET	-	expression tag	UNP O00478
B	286	GLU	-	expression tag	UNP O00478
B	287	ASN	-	expression tag	UNP O00478
B	288	LEU	-	expression tag	UNP O00478
B	289	TYR	-	expression tag	UNP O00478
B	290	PHE	-	expression tag	UNP O00478
B	291	GLN	-	expression tag	UNP O00478
B	292	GLY	-	expression tag	UNP O00478
B	293	ALA	-	expression tag	UNP O00478

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Chain	Residue	Modelled	Actual	Comment	Reference
B	294	GLY	-	expression tag	UNP O00478
B	295	ALA	-	expression tag	UNP O00478
B	296	GLY	-	expression tag	UNP O00478
B	297	ALA	-	expression tag	UNP O00478
B	351	HIS	ARG	engineered mutation	UNP O00478
C	265	MET	-	initiating methionine	UNP O00478
C	266	GLY	-	expression tag	UNP O00478
C	267	SER	-	expression tag	UNP O00478
C	268	SER	-	expression tag	UNP O00478
C	269	HIS	-	expression tag	UNP O00478
C	270	HIS	-	expression tag	UNP O00478
C	271	HIS	-	expression tag	UNP O00478
C	272	HIS	-	expression tag	UNP O00478
C	273	HIS	-	expression tag	UNP O00478
C	274	HIS	-	expression tag	UNP O00478
C	275	SER	-	expression tag	UNP O00478
C	276	SER	-	expression tag	UNP O00478
C	277	GLY	-	expression tag	UNP O00478
C	278	LEU	-	expression tag	UNP O00478
C	279	VAL	-	expression tag	UNP O00478
C	280	PRO	-	expression tag	UNP O00478
C	281	ARG	-	expression tag	UNP O00478
C	282	GLY	-	expression tag	UNP O00478
C	283	SER	-	expression tag	UNP O00478
C	284	HIS	-	expression tag	UNP O00478
C	285	MET	-	expression tag	UNP O00478
C	286	GLU	-	expression tag	UNP O00478
C	287	ASN	-	expression tag	UNP O00478
C	288	LEU	-	expression tag	UNP O00478
C	289	TYR	-	expression tag	UNP O00478
C	290	PHE	-	expression tag	UNP O00478
C	291	GLN	-	expression tag	UNP O00478
C	292	GLY	-	expression tag	UNP O00478
C	293	ALA	-	expression tag	UNP O00478
C	294	GLY	-	expression tag	UNP O00478
C	295	ALA	-	expression tag	UNP O00478
C	296	GLY	-	expression tag	UNP O00478
C	297	ALA	-	expression tag	UNP O00478
C	351	HIS	ARG	engineered mutation	UNP O00478
D	265	MET	-	initiating methionine	UNP O00478
D	266	GLY	-	expression tag	UNP O00478
D	267	SER	-	expression tag	UNP O00478

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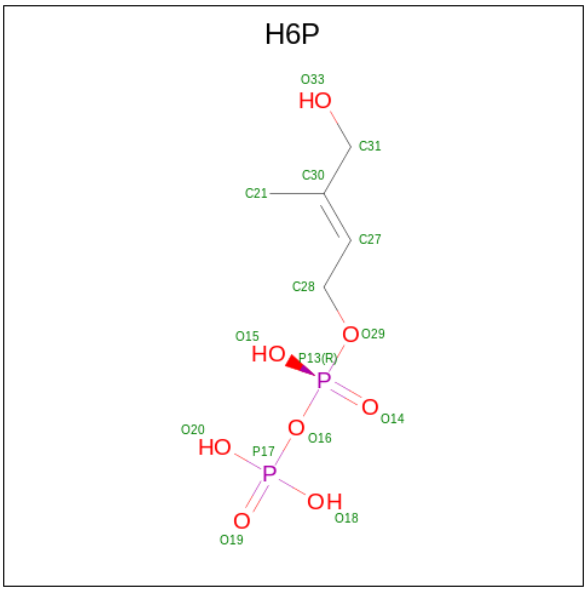
Chain	Residue	Modelled	Actual	Comment	Reference
D	268	SER	-	expression tag	UNP O00478
D	269	HIS	-	expression tag	UNP O00478
D	270	HIS	-	expression tag	UNP O00478
D	271	HIS	-	expression tag	UNP O00478
D	272	HIS	-	expression tag	UNP O00478
D	273	HIS	-	expression tag	UNP O00478
D	274	HIS	-	expression tag	UNP O00478
D	275	SER	-	expression tag	UNP O00478
D	276	SER	-	expression tag	UNP O00478
D	277	GLY	-	expression tag	UNP O00478
D	278	LEU	-	expression tag	UNP O00478
D	279	VAL	-	expression tag	UNP O00478
D	280	PRO	-	expression tag	UNP O00478
D	281	ARG	-	expression tag	UNP O00478
D	282	GLY	-	expression tag	UNP O00478
D	283	SER	-	expression tag	UNP O00478
D	284	HIS	-	expression tag	UNP O00478
D	285	MET	-	expression tag	UNP O00478
D	286	GLU	-	expression tag	UNP O00478
D	287	ASN	-	expression tag	UNP O00478
D	288	LEU	-	expression tag	UNP O00478
D	289	TYR	-	expression tag	UNP O00478
D	290	PHE	-	expression tag	UNP O00478
D	291	GLN	-	expression tag	UNP O00478
D	292	GLY	-	expression tag	UNP O00478
D	293	ALA	-	expression tag	UNP O00478
D	294	GLY	-	expression tag	UNP O00478
D	295	ALA	-	expression tag	UNP O00478
D	296	GLY	-	expression tag	UNP O00478
D	297	ALA	-	expression tag	UNP O00478
D	351	HIS	ARG	engineered mutation	UNP O00478

- Molecule 2 is (2E)-4-hydroxy-3-methylbut-2-en-1-yl trihydrogen diphosphate (three-letter code: H6P) (formula: $C_5H_{12}O_8P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 15 5 8 2	0	0
2	B	1	Total C O P 15 5 8 2	0	0
2	C	1	Total C O P 15 5 8 2	0	0
2	D	1	Total C O P 15 5 8 2	0	0

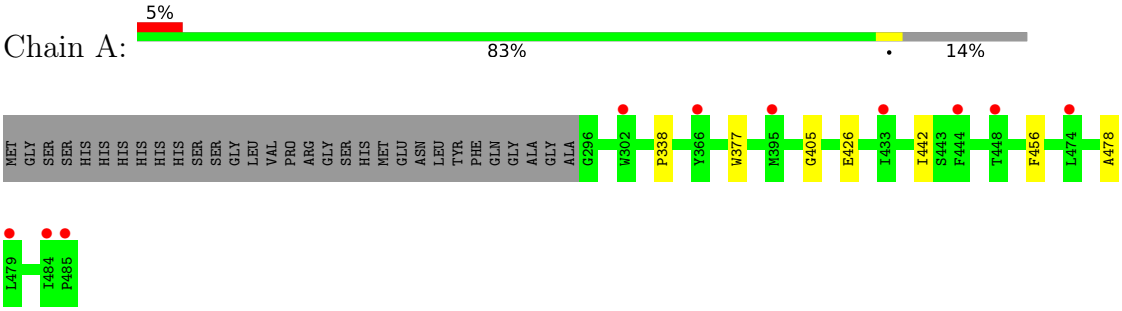
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	193	Total O 193 193	0	0
3	B	211	Total O 211 211	0	0
3	C	211	Total O 211 211	0	0
3	D	215	Total O 215 215	0	0

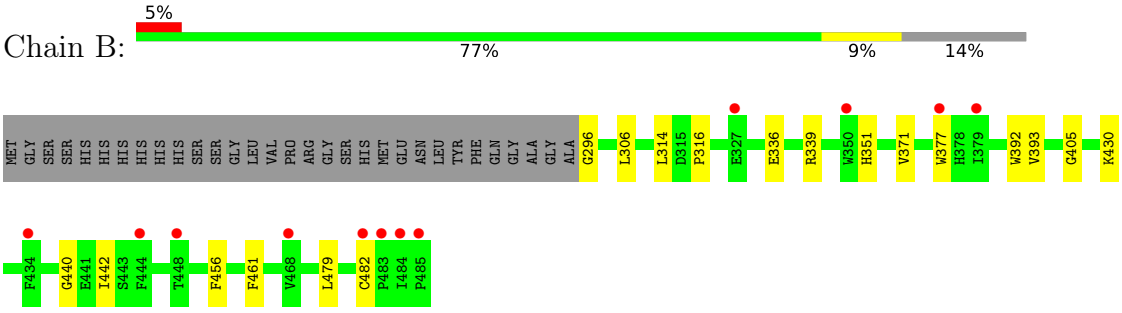
3 Residue-property plots (i)

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.

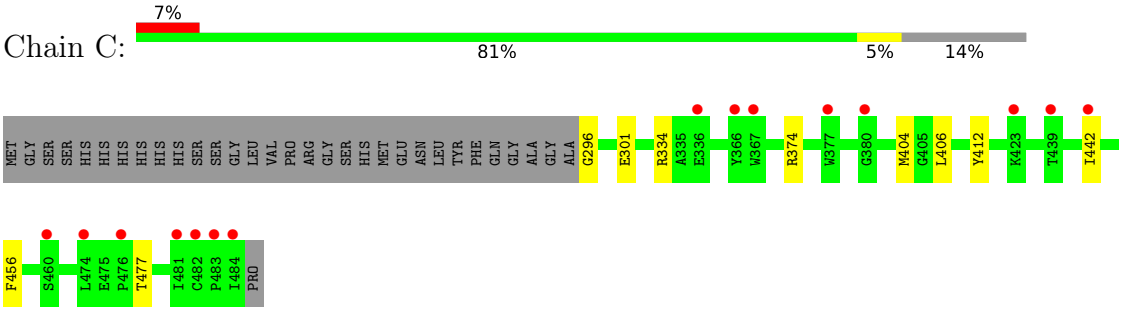
• Molecule 1: Butyrophilin subfamily 3 member A3



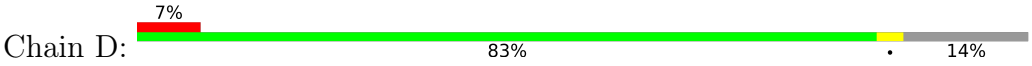
• Molecule 1: Butyrophilin subfamily 3 member A3

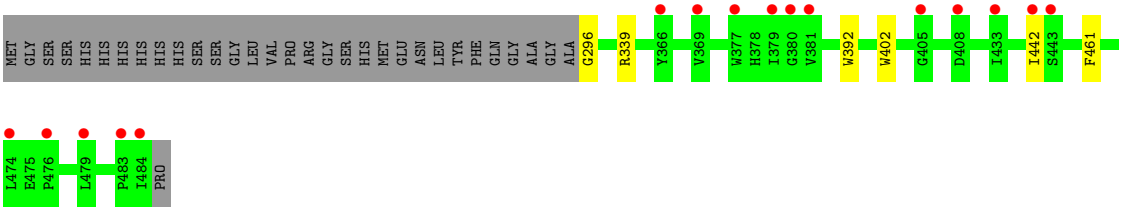


• Molecule 1: Butyrophilin subfamily 3 member A3



• Molecule 1: Butyrophilin subfamily 3 member A3




MET
GLY
SER
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SER
GLY
LEU
VAL
PRO
ARG
GLY
SER
HIS
MET
GLU
ASN
LEU
TYR
PHE
GLN
GLY
ALA
GLY
ALA
G296
R339
Y366
V369
W377
H378
I379
G380
V381
W392
W402
G405
D408
I433
I442
S443
F461
L474
E475
P476
L479
P483
I484
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	39.11Å 67.11Å 75.44Å 85.78° 86.88° 86.90°	Depositor
Resolution (Å)	24.68 – 1.60 24.77 – 1.59	Depositor EDS
% Data completeness (in resolution range)	95.4 (24.68-1.60) 95.7 (24.77-1.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.59Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.242 , 0.289 0.243 , 0.289	Depositor DCC
R_{free} test set	4898 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7091	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7001e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H6P

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	0.35	0/1622	0.57	0/2211
1	B	0.36	0/1614	0.58	0/2201
1	C	0.38	0/1588	0.57	0/2164
1	D	0.35	0/1595	0.58	0/2174
All	All	0.36	0/6419	0.57	0/8750

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1562	0	1506	4	0
1	B	1557	0	1497	12	0
1	C	1539	0	1476	5	0
1	D	1543	0	1483	6	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
3	A	193	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	211	0	0	3	1
3	C	211	0	0	2	0
3	D	215	0	0	1	0
All	All	7091	0	5998	25	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (25) 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:C:374:ARG:NH1	1:C:477:THR:O	2.24	0.71
1:B:392:TRP:O	3:B:601:HOH:O	2.11	0.68
1:B:339:ARG:NH2	3:B:604:HOH:O	2.30	0.64
1:C:301:GLU:OE1	3:C:601:HOH:O	2.15	0.64
1:D:442:ILE:HD11	1:D:461:PHE:HZ	1.65	0.59
1:B:296:GLY:N	3:B:607:HOH:O	2.36	0.58
1:C:296:GLY:N	3:C:607:HOH:O	2.39	0.55
1:B:351[A]:HIS:HE1	1:B:393:VAL:O	1.89	0.55
1:D:442:ILE:HD11	1:D:461:PHE:CZ	2.44	0.52
1:B:336:GLU:OE1	1:D:339:ARG:NH2	2.43	0.47
1:B:442:ILE:HG23	1:B:456:PHE:HB2	1.97	0.47
1:B:440:GLY:HA2	1:B:461:PHE:CE2	2.50	0.46
1:B:371:VAL:HG12	1:B:479:LEU:HD11	1.96	0.46
1:B:377:TRP:CZ3	1:B:405:GLY:HA2	2.52	0.45
1:D:402:TRP:CD1	1:D:442:ILE:HD13	2.51	0.45
1:B:430:LYS:HE2	1:B:482:CYS:SG	2.57	0.44
1:B:314:LEU:O	1:B:316:PRO:HD3	2.18	0.43
1:C:442:ILE:HG23	1:C:456:PHE:HB2	2.00	0.43
1:C:406:LEU:HD13	1:C:412:TYR:CZ	2.54	0.42
1:A:478:ALA:O	3:A:601:HOH:O	2.21	0.42
1:B:479:LEU:HD12	1:B:479:LEU:HA	1.84	0.42
1:A:442:ILE:HG23	1:A:456:PHE:HB2	2.02	0.42
1:A:377:TRP:CZ3	1:A:405:GLY:HA2	2.55	0.41
1:D:296:GLY:O	3:D:601:HOH:O	2.21	0.41
1:A:338:PRO:HG3	1:D:392:TRP:CE3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:743:HOH:O	3:B:773:HOH:O[1_655]	2.18	0.02

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	191/221 (86%)	190 (100%)	1 (0%)	0	100	100
1	B	190/221 (86%)	189 (100%)	1 (0%)	0	100	100
1	C	187/221 (85%)	186 (100%)	1 (0%)	0	100	100
1	D	188/221 (85%)	187 (100%)	1 (0%)	0	100	100
All	All	756/884 (86%)	752 (100%)	4 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	170/191 (89%)	169 (99%)	1 (1%)	86	77
1	B	169/191 (88%)	168 (99%)	1 (1%)	86	77
1	C	166/191 (87%)	164 (99%)	2 (1%)	71	54
1	D	167/191 (87%)	167 (100%)	0	100	100
All	All	672/764 (88%)	668 (99%)	4 (1%)	86	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	426	GLU
1	B	306	LEU
1	C	334	ARG
1	C	404	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	H6P	C	501	-	11,14,14	1.13	1 (9%)	13,20,20	1.19	2 (15%)
2	H6P	B	501	-	11,14,14	1.04	0	13,20,20	0.73	0
2	H6P	A	501	-	11,14,14	0.96	0	13,20,20	0.85	0
2	H6P	D	501	-	11,14,14	1.15	1 (9%)	13,20,20	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H6P	C	501	-	-	3/15/15/15	-
2	H6P	B	501	-	-	4/15/15/15	-
2	H6P	A	501	-	-	3/15/15/15	-
2	H6P	D	501	-	-	4/15/15/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	H6P	O29-C28	-2.25	1.40	1.43
2	D	501	H6P	O29-C28	-2.13	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	H6P	O18-P17-O16	2.76	113.89	104.64
2	C	501	H6P	C28-C27-C30	-2.18	122.27	126.04

There are no chirality outliers.

All (14) torsion outliers are listed below:

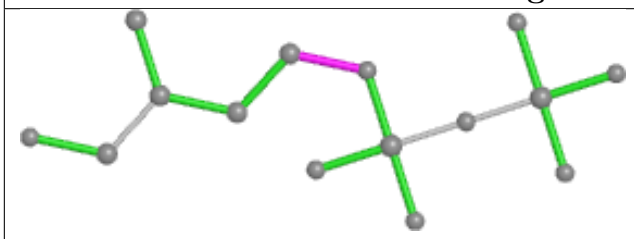
Mol	Chain	Res	Type	Atoms
2	C	501	H6P	P17-O16-P13-O29
2	C	501	H6P	P13-O16-P17-O18
2	D	501	H6P	P13-O16-P17-O18
2	A	501	H6P	P17-O16-P13-O29
2	B	501	H6P	P17-O16-P13-O29
2	D	501	H6P	P17-O16-P13-O29
2	B	501	H6P	P13-O16-P17-O19
2	A	501	H6P	P13-O16-P17-O18
2	A	501	H6P	P13-O16-P17-O20
2	B	501	H6P	P13-O16-P17-O18
2	B	501	H6P	P13-O16-P17-O20
2	C	501	H6P	P13-O16-P17-O20
2	D	501	H6P	P13-O16-P17-O20
2	D	501	H6P	P13-O16-P17-O19

There are no ring outliers.

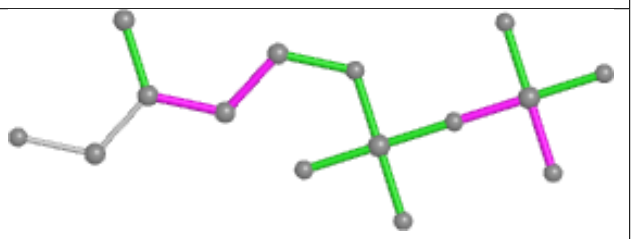
No monomer is involved in short contacts.

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.

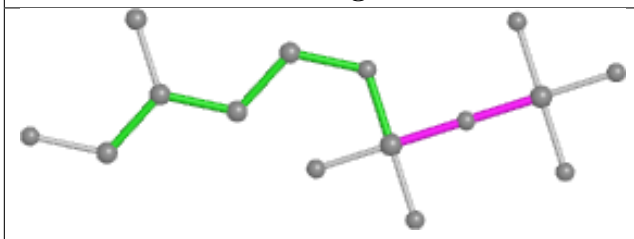
Ligand H6P C 501



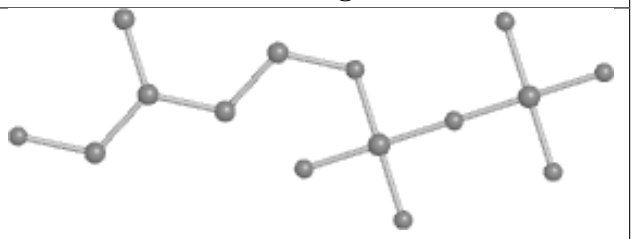
Bond lengths



Bond angles

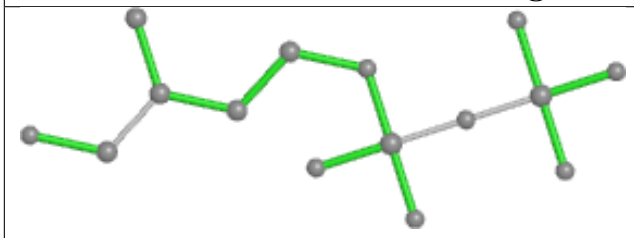


Torsions

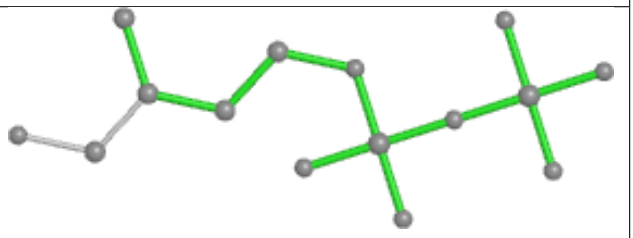


Rings

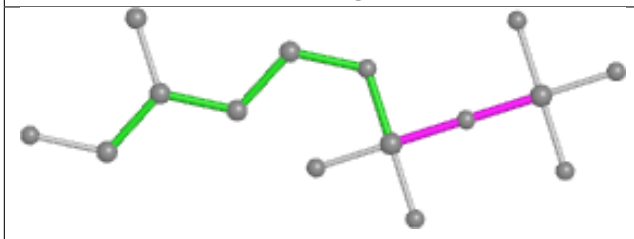
Ligand H6P B 501



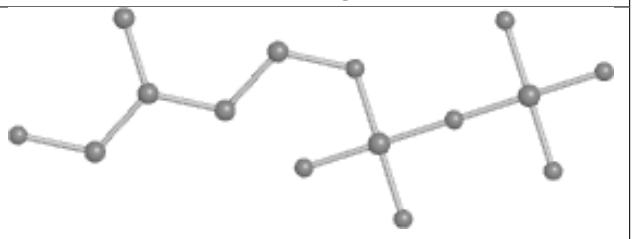
Bond lengths



Bond angles

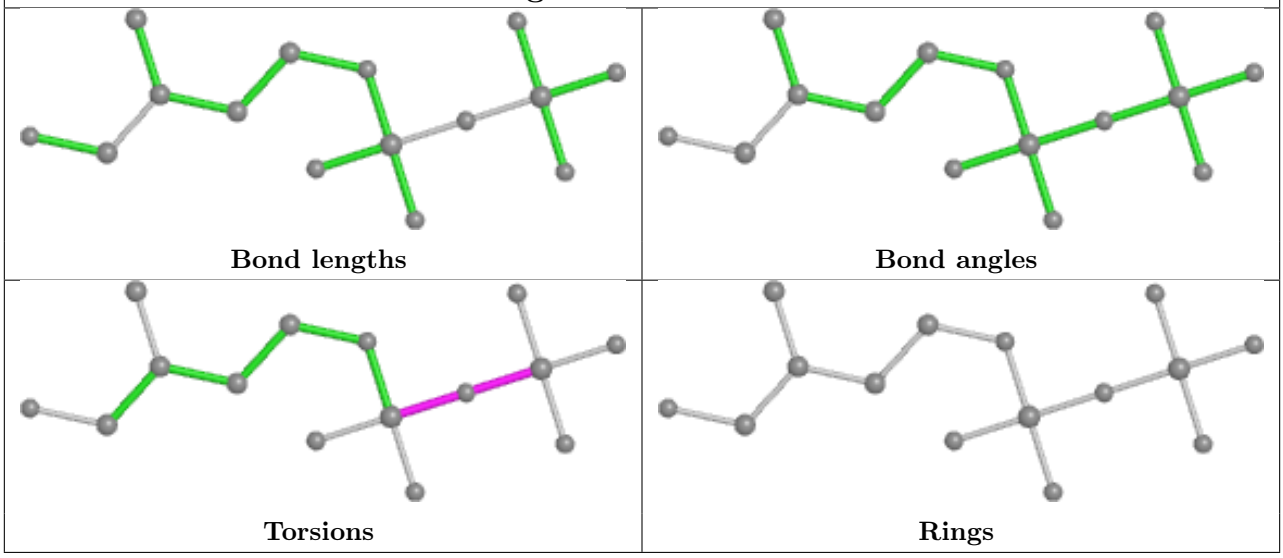


Torsions

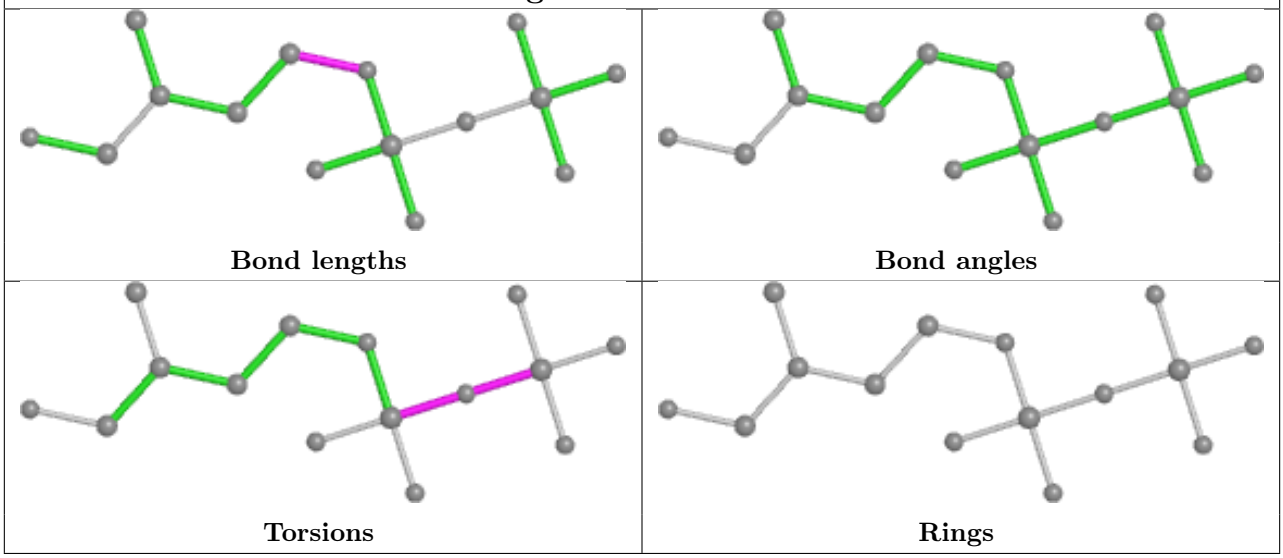


Rings

Ligand H6P A 501



Ligand H6P D 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	190/221 (85%)	0.63	10 (5%)	26	24	14, 23, 33, 60	0
1	B	190/221 (85%)	0.57	12 (6%)	20	18	13, 22, 32, 55	0
1	C	189/221 (85%)	0.79	15 (7%)	12	11	14, 23, 34, 43	0
1	D	189/221 (85%)	0.76	16 (8%)	10	9	14, 22, 33, 43	0
All	All	758/884 (85%)	0.69	53 (6%)	16	15	13, 23, 33, 60	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	PRO	5.3
1	B	485	PRO	5.1
1	C	484	ILE	4.3
1	B	484	ILE	4.3
1	B	448	THR	4.0
1	C	366	TYR	3.4
1	D	369	VAL	3.3
1	D	484	ILE	3.3
1	D	474	LEU	3.1
1	D	442	ILE	3.0
1	C	482	CYS	2.9
1	A	484	ILE	2.8
1	C	423	LYS	2.8
1	B	468	VAL	2.8
1	B	482	CYS	2.8
1	D	377	TRP	2.7
1	C	483	PRO	2.7
1	D	476	PRO	2.7
1	A	302	TRP	2.6
1	D	433	ILE	2.6
1	A	474	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	483	PRO	2.6
1	D	379	ILE	2.6
1	A	444	PHE	2.5
1	B	444	PHE	2.5
1	D	381	VAL	2.4
1	A	433	ILE	2.3
1	B	379	ILE	2.3
1	A	366	TYR	2.3
1	C	442	ILE	2.3
1	B	350	TRP	2.3
1	D	479	LEU	2.3
1	B	434	PHE	2.3
1	D	408	ASP	2.3
1	C	377	TRP	2.2
1	C	481	ILE	2.2
1	D	366	TYR	2.2
1	B	483	PRO	2.2
1	A	479	LEU	2.2
1	A	395[A]	MET	2.2
1	C	336	GLU	2.2
1	C	476	PRO	2.2
1	D	380	GLY	2.2
1	C	439	THR	2.2
1	B	327	GLU	2.1
1	C	367	TRP	2.1
1	C	380	GLY	2.1
1	A	448	THR	2.1
1	D	443	SER	2.1
1	C	460	SER	2.0
1	C	474	LEU	2.0
1	B	377	TRP	2.0
1	D	405	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

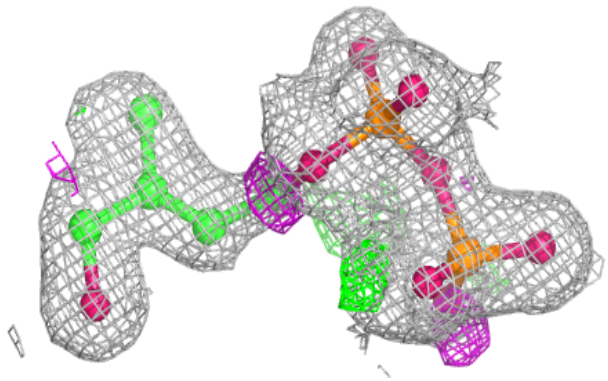
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

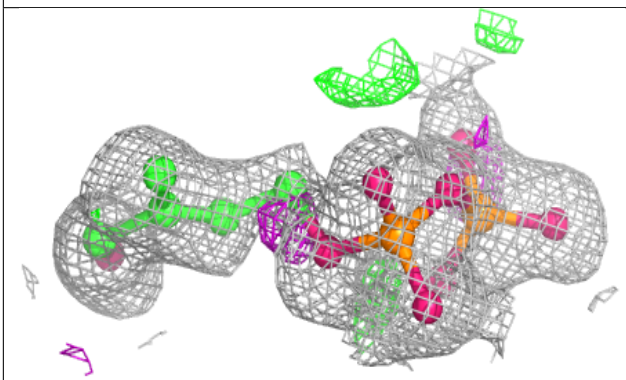
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	H6P	A	501	15/15	0.94	0.09	17,21,24,28	0
2	H6P	C	501	15/15	0.94	0.10	15,20,25,26	0
2	H6P	B	501	15/15	0.95	0.09	17,21,23,24	0
2	H6P	D	501	15/15	0.95	0.11	16,19,24,29	0

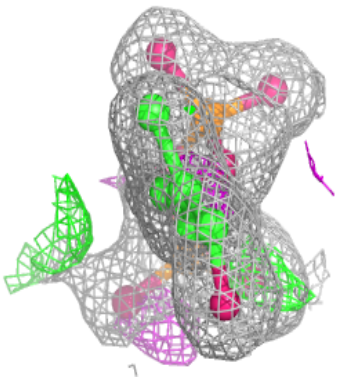
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H6P 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)

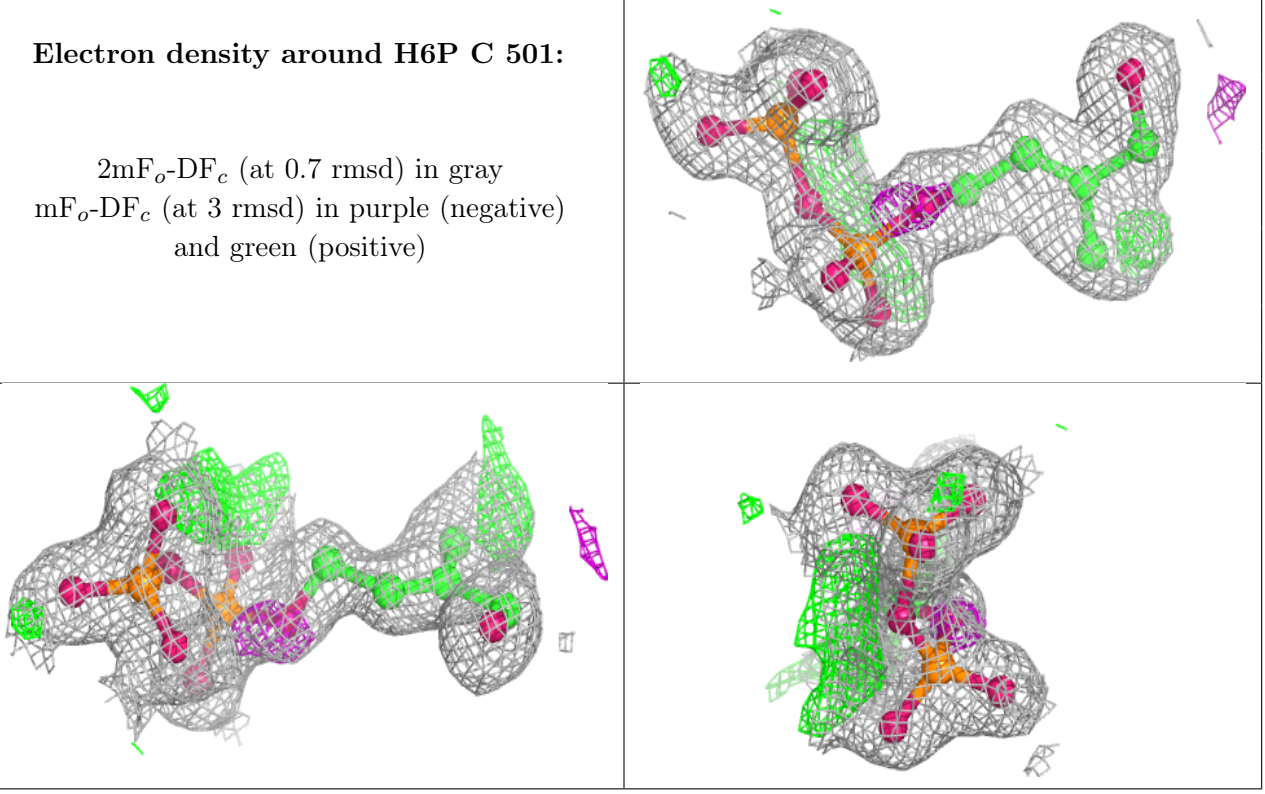






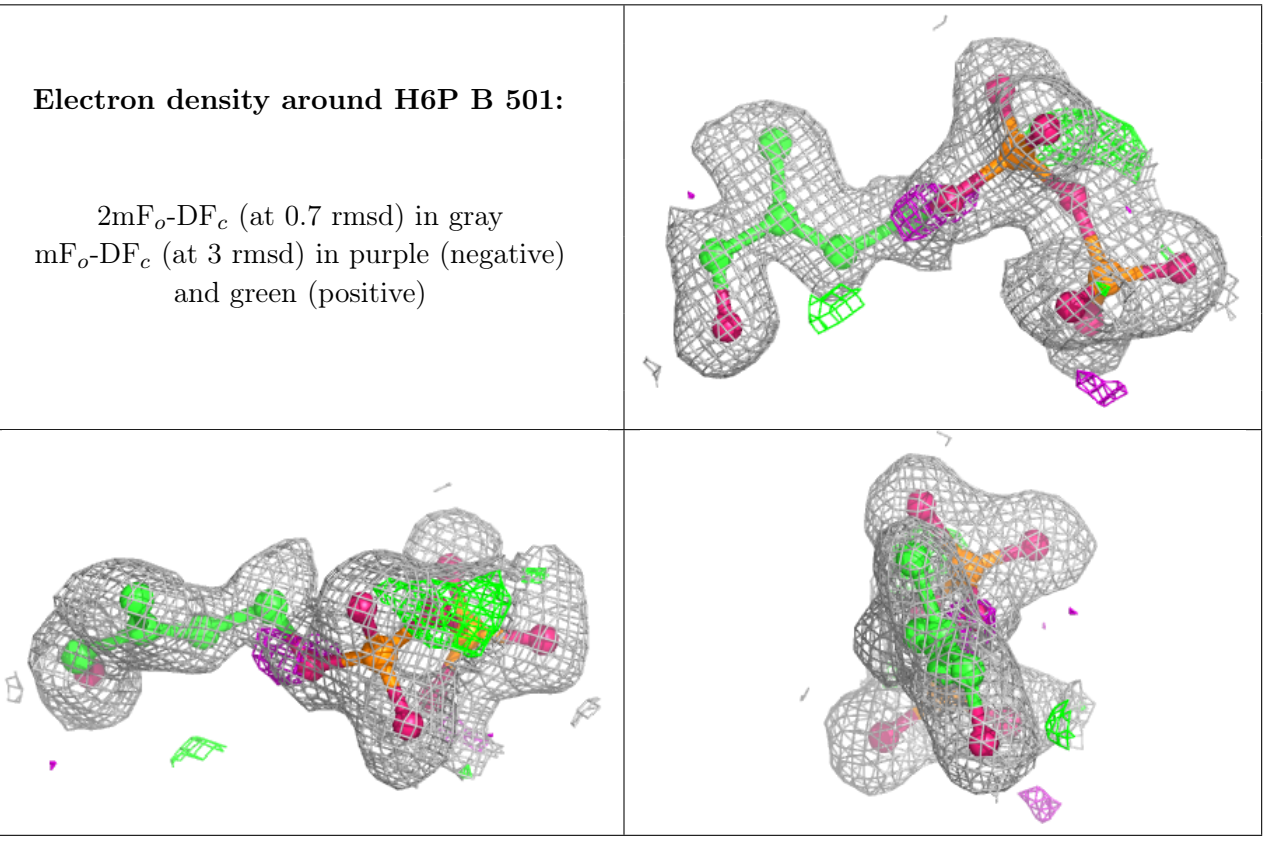
Electron density around H6P C 501:

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



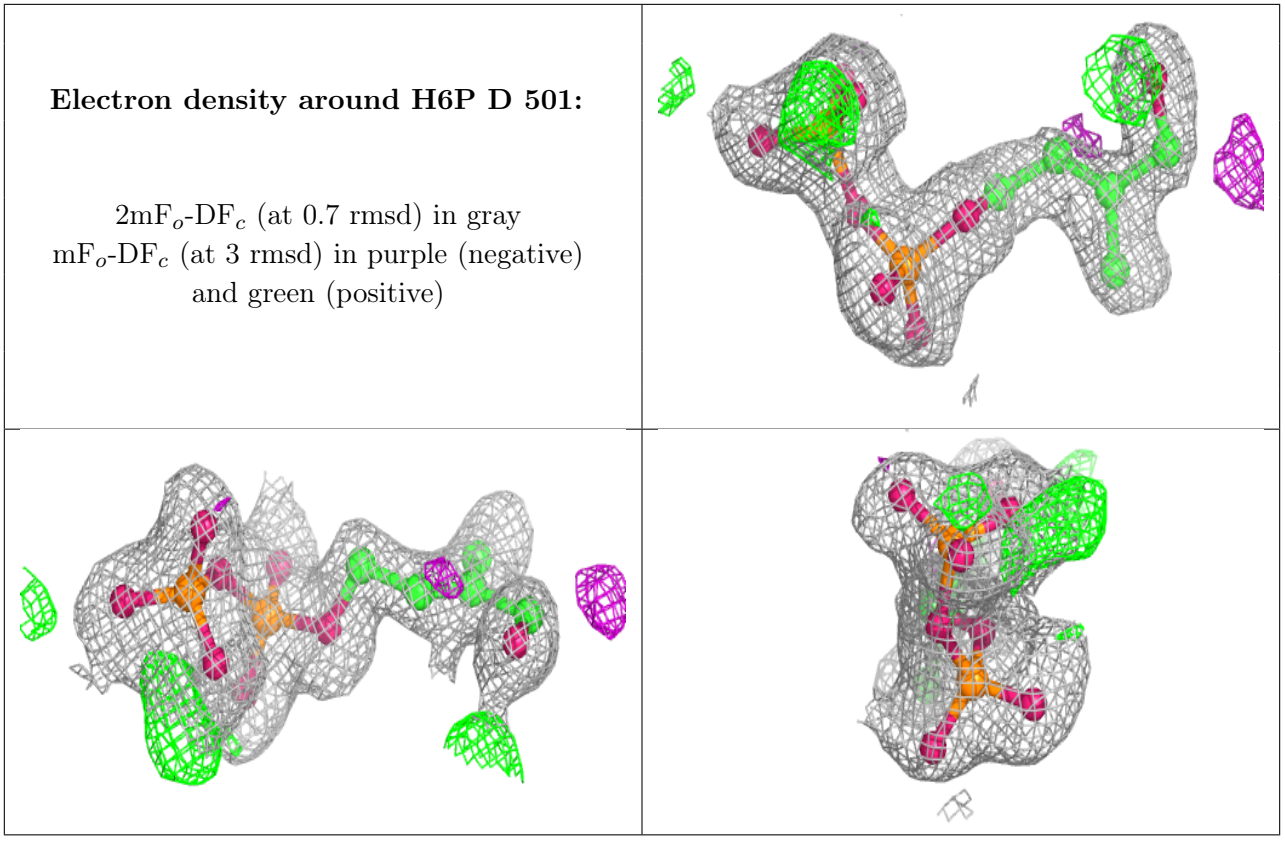
Electron density around H6P B 501:

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



Electron density around H6P 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)



6.5 Other polymers (i)

There are no such residues in this entry.