



Full wwPDB X-ray Structure Validation Report

Jan 4, 2024 – 09:34 am GMT

PDB ID : 5IN3
Title : Crystal structure of glucose-1-phosphate bound nucleotidylated human galactose-1-phosphate uridylyltransferase
Authors : Kopec, J.; McCorvie, T.; Tallant, C.; Velupillai, S.; Shrestha, L.; Fitzpatrick, F.; Patel, D.; Chalk, R.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Yue, W.W.
Deposited on : 2016-03-07
Resolution : 1.73 Å(reported)

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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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (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

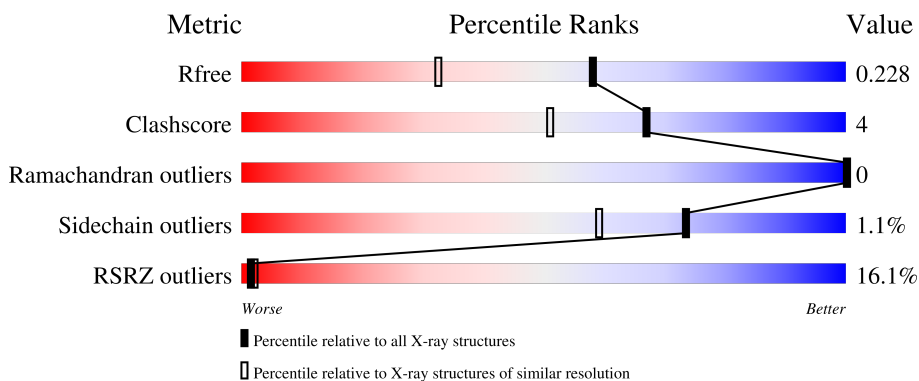
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	 10% 75% 6% 9%
1	B	401	 16% 75% 7% 18%

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
4	EDO	B	404	-	-	-	X
4	EDO	B	408	-	-	-	X
4	EDO	B	411	-	-	-	X
4	EDO	B	412	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11316 atoms, of which 5356 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 Galactose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	330	5281	1720	2588	477	482	14	0	5	0
1	A	324	5213	1699	2556	467	476	15	0	6	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP P07902
B	-20	HIS	-	expression tag	UNP P07902
B	-19	HIS	-	expression tag	UNP P07902
B	-18	HIS	-	expression tag	UNP P07902
B	-17	HIS	-	expression tag	UNP P07902
B	-16	HIS	-	expression tag	UNP P07902
B	-15	HIS	-	expression tag	UNP P07902
B	-14	SER	-	expression tag	UNP P07902
B	-13	SER	-	expression tag	UNP P07902
B	-12	GLY	-	expression tag	UNP P07902
B	-11	VAL	-	expression tag	UNP P07902
B	-10	ASP	-	expression tag	UNP P07902
B	-9	LEU	-	expression tag	UNP P07902
B	-8	GLY	-	expression tag	UNP P07902
B	-7	THR	-	expression tag	UNP P07902
B	-6	GLU	-	expression tag	UNP P07902
B	-5	ASN	-	expression tag	UNP P07902
B	-4	LEU	-	expression tag	UNP P07902
B	-3	TYR	-	expression tag	UNP P07902
B	-2	PHE	-	expression tag	UNP P07902
B	-1	GLN	-	expression tag	UNP P07902
B	0	SER	-	expression tag	UNP P07902
A	-21	MET	-	initiating methionine	UNP P07902
A	-20	HIS	-	expression tag	UNP P07902
A	-19	HIS	-	expression tag	UNP P07902

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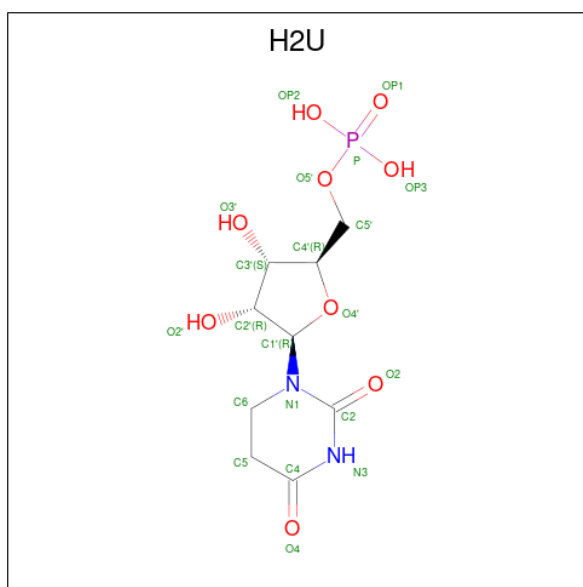
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	HIS	-	expression tag	UNP P07902
A	-17	HIS	-	expression tag	UNP P07902
A	-16	HIS	-	expression tag	UNP P07902
A	-15	HIS	-	expression tag	UNP P07902
A	-14	SER	-	expression tag	UNP P07902
A	-13	SER	-	expression tag	UNP P07902
A	-12	GLY	-	expression tag	UNP P07902
A	-11	VAL	-	expression tag	UNP P07902
A	-10	ASP	-	expression tag	UNP P07902
A	-9	LEU	-	expression tag	UNP P07902
A	-8	GLY	-	expression tag	UNP P07902
A	-7	THR	-	expression tag	UNP P07902
A	-6	GLU	-	expression tag	UNP P07902
A	-5	ASN	-	expression tag	UNP P07902
A	-4	LEU	-	expression tag	UNP P07902
A	-3	TYR	-	expression tag	UNP P07902
A	-2	PHE	-	expression tag	UNP P07902
A	-1	GLN	-	expression tag	UNP P07902
A	0	SER	-	expression tag	UNP P07902

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5,6-DIHYDROURIDINE-5'-MONOPHOSPHATE (three-letter code: H2U) (formula: C₉H₁₅N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
3	B	1	31	9	11	2	8	1	0	0
3	A	1	31	9	11	2	8	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	H			O
4	B	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0

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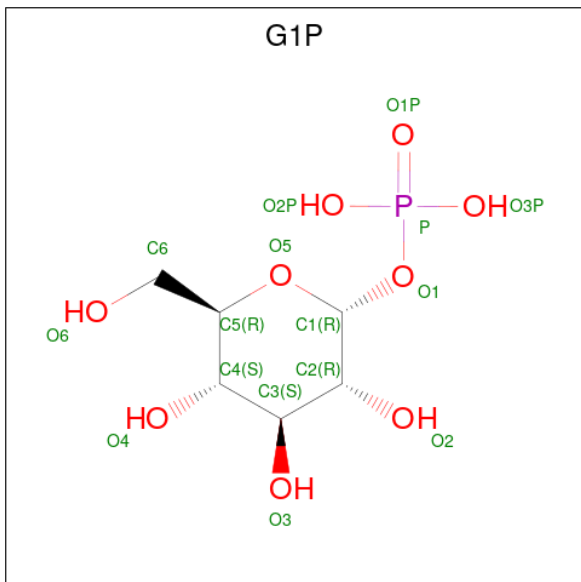
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is 1-O-phosphono-alpha-D-glucopyranose (three-letter code: G1P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
5	A	1	Total	C	H	O	P	0	0
			27	6	11	9	1		

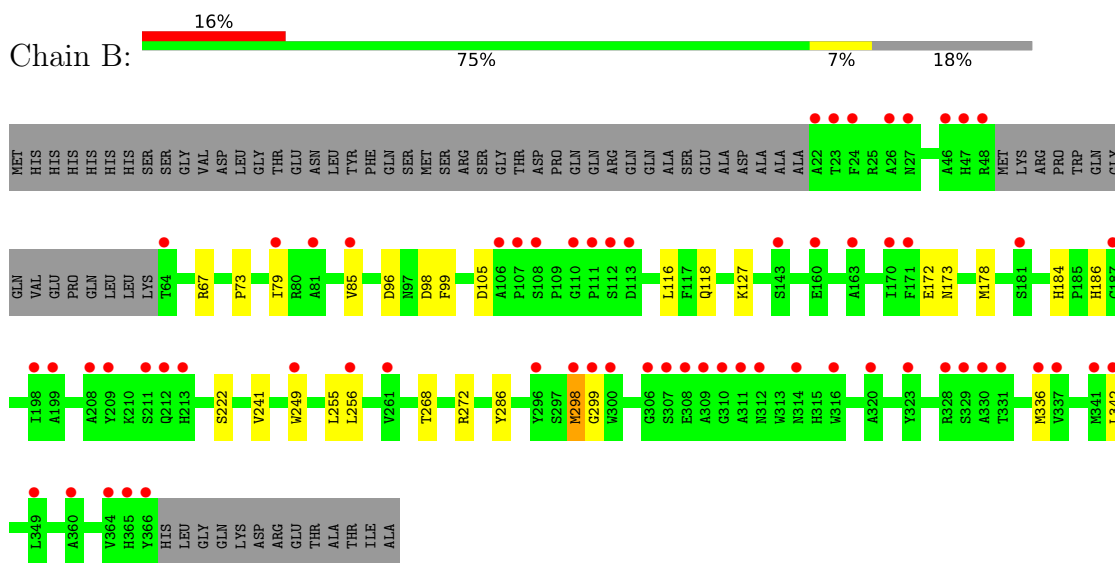
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	188	Total	O	0	0
			188	188		
6	A	236	Total	O	0	0
			236	236		

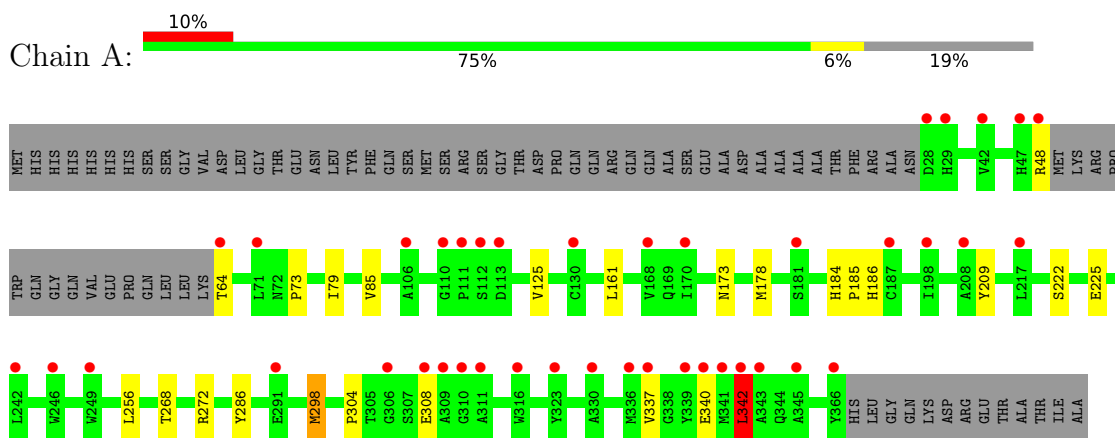
3 Residue-property plots [i](#)

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: Galactose-1-phosphate uridylyltransferase



- Molecule 1: Galactose-1-phosphate uridylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.76Å 107.99Å 126.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.29 – 1.73 40.29 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.29-1.73) 100.0 (40.29-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.73Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.228 0.198 , 0.228	Depositor DCC
R_{free} test set	4231 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtrriage
Anisotropy	0.676	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11316	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G1P, EDO, ZN, H2U

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	0.49	0/2766	0.64	1/3779 (0.0%)
1	B	0.44	0/2805	0.60	0/3832
All	All	0.46	0/5571	0.62	1/7611 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	LEU	CA-CB-CG	-5.21	103.31	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2657	2556	2546	21	1
1	B	2693	2588	2567	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	11	13	3	0
3	B	20	11	12	4	0
4	A	52	78	78	0	2
4	B	60	90	90	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	16	11	11	0	0
5	B	16	11	11	0	0
6	A	236	0	0	2	2
6	B	188	0	0	4	3
All	All	5960	5356	5328	42	4

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 4.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:MET:SD	6:A:682:HOH:O	1.95	1.20
1:A:186:HIS:NE2	3:A:402:H2U:P	2.25	1.09
1:B:186:HIS:NE2	3:B:402:H2U:P	2.29	1.05
1:A:304:PRO:O	6:A:501:HOH:O	1.85	0.94
1:B:118:GLN:OE1	4:B:407:EDO:O2	1.96	0.83
1:A:79:ILE:HD12	1:A:85:VAL:HG22	1.64	0.78
1:B:299:GLY:HA3	1:A:342:LEU:HD22	1.68	0.73
1:A:79:ILE:CD1	1:A:85:VAL:HG22	2.21	0.70
1:B:173[B]:ASN:ND2	1:B:178:MET:O	2.25	0.69
1:B:105:ASP:OD1	6:B:502:HOH:O	2.11	0.69
4:B:407:EDO:O1	6:B:501:HOH:O	2.09	0.69
1:A:173[B]:ASN:ND2	1:A:178:MET:O	2.24	0.67
1:B:172:GLU:H	1:B:298:MET:HE3	1.60	0.66
1:A:222:SER:OG	1:A:256:LEU:HD11	1.97	0.65
1:B:222:SER:OG	1:B:256:LEU:HD11	1.98	0.63
1:B:172:GLU:N	1:B:298:MET:HE3	2.15	0.60
1:B:79:ILE:HG12	1:B:85:VAL:HG22	1.85	0.58
1:A:184:HIS:O	1:A:186:HIS:ND1	2.32	0.58
1:A:298:MET:O	1:A:298:MET:HE3	2.04	0.56
1:B:73:PRO:CG	3:B:402:H2U:H51	2.35	0.56
1:B:184:HIS:O	1:B:186:HIS:ND1	2.34	0.55
1:B:116:LEU:HD21	1:A:209:TYR:CE2	2.43	0.54
1:B:186:HIS:CD2	3:B:402:H2U:P	3.01	0.54
1:B:299:GLY:CA	1:A:342:LEU:HD22	2.38	0.53
1:A:73:PRO:CG	3:A:402:H2U:H51	2.39	0.52
1:B:73:PRO:HG3	3:B:402:H2U:H51	1.93	0.51
1:A:337:VAL:O	1:A:340[A]:GLU:OE1	2.28	0.51
1:A:186:HIS:CD2	3:A:402:H2U:P	3.04	0.47
1:B:96:ASP:OD1	1:B:127:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:HH11	4:B:417:EDO:H11	1.81	0.44
1:B:241:VAL:HG22	1:B:255:LEU:HD13	1.99	0.44
1:A:64:THR:HG23	1:A:64:THR:O	2.18	0.44
1:B:67:ARG:HH11	4:B:417:EDO:H22	1.83	0.43
1:A:125:VAL:HG21	1:A:161:LEU:HD22	2.01	0.43
1:A:184:HIS:CG	1:A:185:PRO:HD2	2.54	0.43
1:A:268:THR:O	1:A:272:ARG:HG3	2.19	0.42
1:B:249:TRP:CZ2	1:B:336:MET:HG3	2.53	0.42
1:B:98:ASP:OD1	6:B:503:HOH:O	2.21	0.42
1:B:268:THR:O	1:B:272:ARG:HG3	2.20	0.41
1:B:99:PHE:O	1:A:48:ARG:NH2	2.50	0.41
1:A:225:GLU:HA	1:A:225:GLU:OE1	2.19	0.41
1:B:336:MET:HB3	6:B:571:HOH:O	2.21	0.41

All (4) 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)
4:A:414:EDO:O2	6:B:687:HOH:O[2_555]	1.85	0.35
1:A:308:GLU:OE1	6:B:633:HOH:O[2_555]	1.97	0.23
4:A:409:EDO:O1	6:A:733:HOH:O[1_655]	1.97	0.23
6:B:684:HOH:O	6:A:505:HOH:O[4_545]	2.04	0.16

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	326/401 (81%)	318 (98%)	8 (2%)	0	100	100
1	B	331/401 (82%)	321 (97%)	10 (3%)	0	100	100
All	All	657/802 (82%)	639 (97%)	18 (3%)	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	288/346 (83%)	285 (99%)	3 (1%)	76	63
1	B	291/346 (84%)	288 (99%)	3 (1%)	76	63
All	All	579/692 (84%)	573 (99%)	6 (1%)	73	63

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	286	TYR
1	B	298	MET
1	B	342	LEU
1	A	286	TYR
1	A	298	MET
1	A	342	LEU

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

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	406	-	3,3,3	0.38	0	2,2,2	0.48	0
4	EDO	A	414	-	3,3,3	0.46	0	2,2,2	0.44	0
4	EDO	B	413	-	3,3,3	0.60	0	2,2,2	0.12	0
4	EDO	A	412	-	3,3,3	0.55	0	2,2,2	0.13	0
4	EDO	B	409	-	3,3,3	0.49	0	2,2,2	0.32	0
4	EDO	B	416	-	3,3,3	0.57	0	2,2,2	1.05	0
4	EDO	A	411	-	3,3,3	0.68	0	2,2,2	0.06	0
4	EDO	B	406	-	3,3,3	0.41	0	2,2,2	0.46	0
4	EDO	A	404	-	3,3,3	0.54	0	2,2,2	0.14	0
4	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.40	0
5	G1P	A	416	-	15,16,16	1.65	2 (13%)	23,24,24	1.08	1 (4%)
4	EDO	A	407	-	3,3,3	0.56	0	2,2,2	0.22	0
4	EDO	A	410	-	3,3,3	0.62	0	2,2,2	0.06	0
4	EDO	A	405	-	3,3,3	0.52	0	2,2,2	0.20	0
5	G1P	B	418	-	15,16,16	1.79	2 (13%)	23,24,24	1.00	2 (8%)
4	EDO	B	403	-	3,3,3	0.47	0	2,2,2	0.42	0
4	EDO	B	412	-	3,3,3	0.52	0	2,2,2	0.17	0
4	EDO	B	405	-	3,3,3	0.63	0	2,2,2	0.19	0
4	EDO	B	414	-	3,3,3	0.49	0	2,2,2	0.38	0
3	H2U	A	402	-	18,21,22	3.99	10 (55%)	21,30,33	2.02	4 (19%)
4	EDO	B	407	-	3,3,3	0.47	0	2,2,2	0.42	0
3	H2U	B	402	-	18,21,22	4.19	10 (55%)	21,30,33	2.70	6 (28%)
4	EDO	B	408	-	3,3,3	0.57	0	2,2,2	0.11	0
4	EDO	B	417	-	3,3,3	0.10	0	2,2,2	0.80	0
4	EDO	A	408	-	3,3,3	0.58	0	2,2,2	0.05	0
4	EDO	A	413	-	3,3,3	0.69	0	2,2,2	0.06	0
4	EDO	A	409	-	3,3,3	0.46	0	2,2,2	0.44	0
4	EDO	A	415	-	3,3,3	0.44	0	2,2,2	0.41	0
4	EDO	B	410	-	3,3,3	0.51	0	2,2,2	0.30	0
4	EDO	B	415	-	3,3,3	0.38	0	2,2,2	0.51	0
4	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	411	-	3,3,3	0.46	0	2,2,2	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	A	414	-	-	0/1/1/1	-
4	EDO	B	413	-	-	0/1/1/1	-
4	EDO	A	412	-	-	0/1/1/1	-
4	EDO	B	409	-	-	0/1/1/1	-
4	EDO	B	416	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
5	G1P	A	416	-	-	1/7/27/27	0/1/1/1
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	A	410	-	-	0/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
5	G1P	B	418	-	-	2/7/27/27	0/1/1/1
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	B	412	-	-	0/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	B	414	-	-	1/1/1/1	-
3	H2U	A	402	-	-	3/7/38/39	0/2/2/2
4	EDO	B	407	-	-	0/1/1/1	-
3	H2U	B	402	-	-	3/7/38/39	0/2/2/2
4	EDO	B	408	-	-	0/1/1/1	-
4	EDO	B	417	-	-	1/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
4	EDO	A	413	-	-	1/1/1/1	-
4	EDO	A	409	-	-	0/1/1/1	-
4	EDO	A	415	-	-	1/1/1/1	-
4	EDO	B	410	-	-	1/1/1/1	-
4	EDO	B	415	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	B	411	-	-	0/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	H2U	C2-N1	10.12	1.50	1.35
3	B	402	H2U	C2-N1	9.78	1.49	1.35
3	B	402	H2U	C3'-C4'	-7.04	1.35	1.53
3	B	402	H2U	C4-N3	6.30	1.48	1.37
3	B	402	H2U	C2-N3	6.14	1.48	1.38
3	A	402	H2U	C3'-C4'	-6.08	1.37	1.53
3	A	402	H2U	C4-N3	6.05	1.47	1.37
3	A	402	H2U	C2-N3	5.86	1.48	1.38
3	B	402	H2U	O4'-C4'	5.61	1.57	1.45
3	A	402	H2U	O4'-C4'	5.14	1.56	1.45
3	B	402	H2U	O4'-C1'	-5.12	1.29	1.42
5	B	418	G1P	P-O1	4.52	1.67	1.59
3	A	402	H2U	O4'-C1'	-4.47	1.31	1.42
5	B	418	G1P	O5-C1	4.23	1.52	1.41
5	A	416	G1P	P-O1	4.15	1.67	1.59
5	A	416	G1P	O5-C1	4.12	1.52	1.41
3	B	402	H2U	O4-C4	-3.30	1.16	1.23
3	B	402	H2U	O2-C2	-2.78	1.18	1.23
3	B	402	H2U	O2'-C2'	-2.73	1.36	1.43
3	A	402	H2U	O3'-C3'	2.53	1.48	1.43
3	A	402	H2U	O4-C4	-2.51	1.18	1.23
3	A	402	H2U	C6-C5	-2.42	1.45	1.52
3	A	402	H2U	O2-C2	-2.39	1.18	1.23
3	B	402	H2U	O3'-C3'	2.20	1.48	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	H2U	C4-N3-C2	-9.08	118.26	125.79
3	A	402	H2U	C4-N3-C2	-6.32	120.55	125.79
3	B	402	H2U	O2-C2-N1	-4.20	117.83	123.11
3	B	402	H2U	C5-C4-N3	4.07	121.22	116.65
3	A	402	H2U	N3-C2-N1	3.13	119.97	116.65
3	B	402	H2U	N3-C2-N1	3.04	119.87	116.65
3	A	402	H2U	C2'-C3'-C4'	2.80	108.08	102.64
3	A	402	H2U	C5-C6-N1	2.76	120.70	111.61
3	B	402	H2U	C4'-O4'-C1'	-2.57	103.81	109.47
5	A	416	G1P	O5-C5-C4	2.53	114.28	109.69
5	B	418	G1P	C6-C5-C4	-2.49	107.17	113.00
5	B	418	G1P	O5-C5-C4	2.34	113.95	109.69
3	B	402	H2U	C5-C6-N1	2.20	118.87	111.61

There are no chirality outliers.

All (17) torsion outliers are listed below:

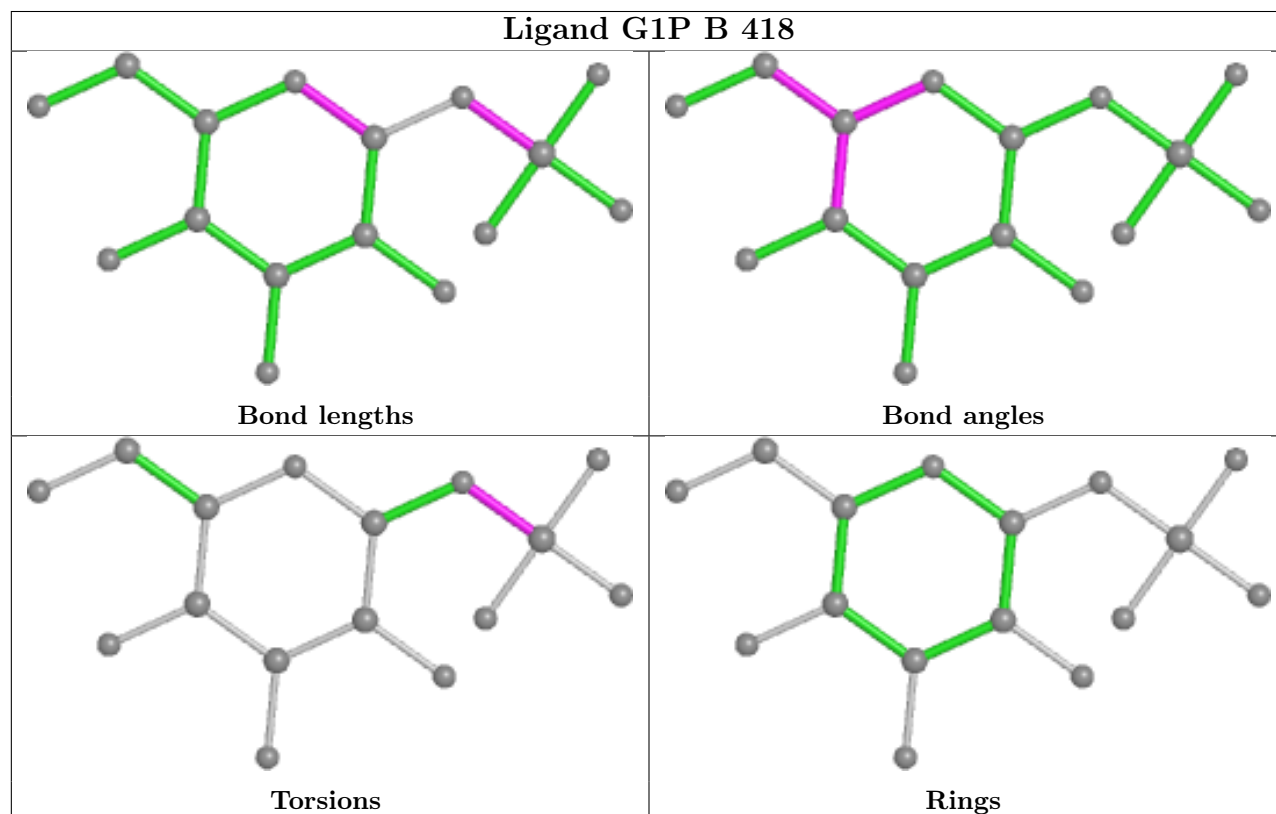
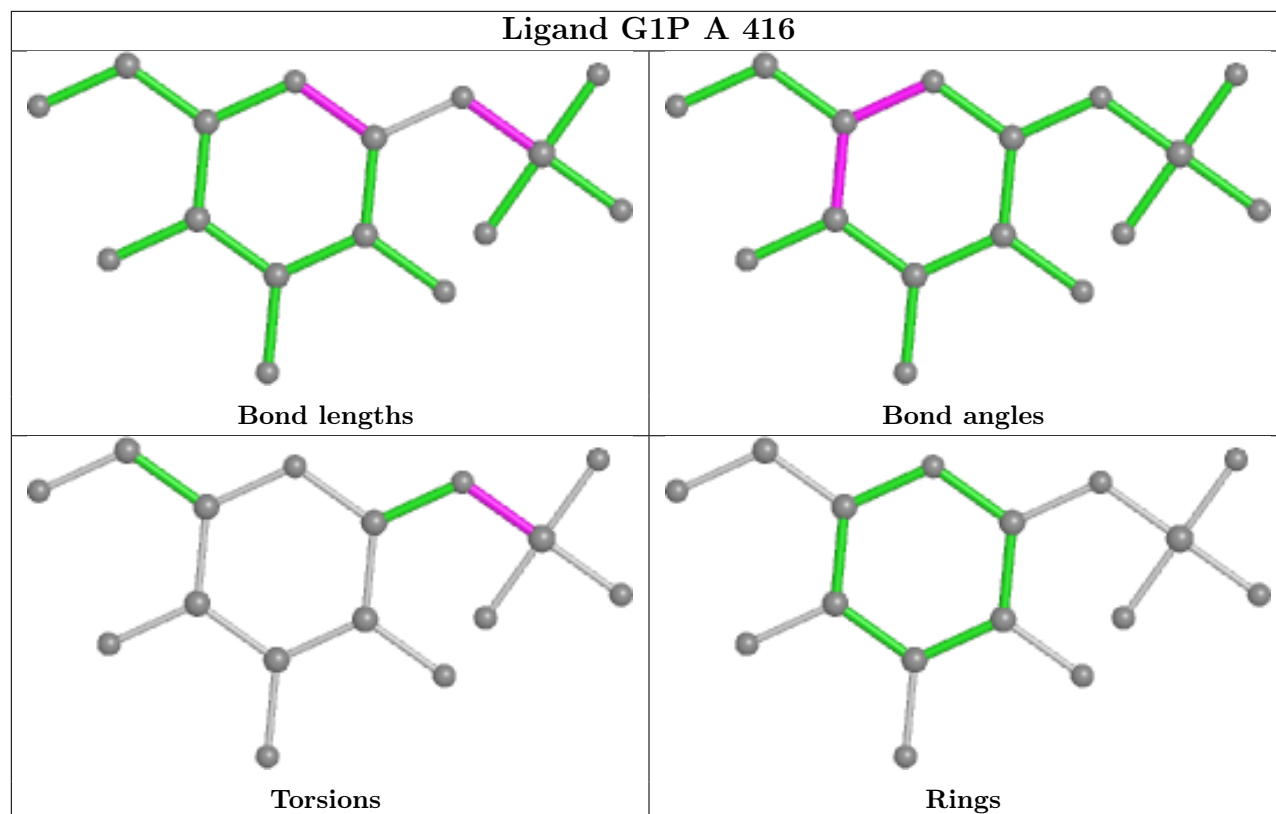
Mol	Chain	Res	Type	Atoms
3	A	402	H2U	O4'-C4'-C5'-O5'
3	B	402	H2U	O4'-C4'-C5'-O5'
3	A	402	H2U	C3'-C4'-C5'-O5'
3	B	402	H2U	C3'-C4'-C5'-O5'
4	B	410	EDO	O1-C1-C2-O2
4	B	417	EDO	O1-C1-C2-O2
4	A	413	EDO	O1-C1-C2-O2
4	A	415	EDO	O1-C1-C2-O2
4	B	405	EDO	O1-C1-C2-O2
5	B	418	G1P	C1-O1-P-O1P
5	A	416	G1P	C1-O1-P-O1P
5	B	418	G1P	C1-O1-P-O2P
4	B	416	EDO	O1-C1-C2-O2
4	A	411	EDO	O1-C1-C2-O2
4	B	414	EDO	O1-C1-C2-O2
3	B	402	H2U	C2'-C1'-N1-C6
3	A	402	H2U	C2'-C1'-N1-C6

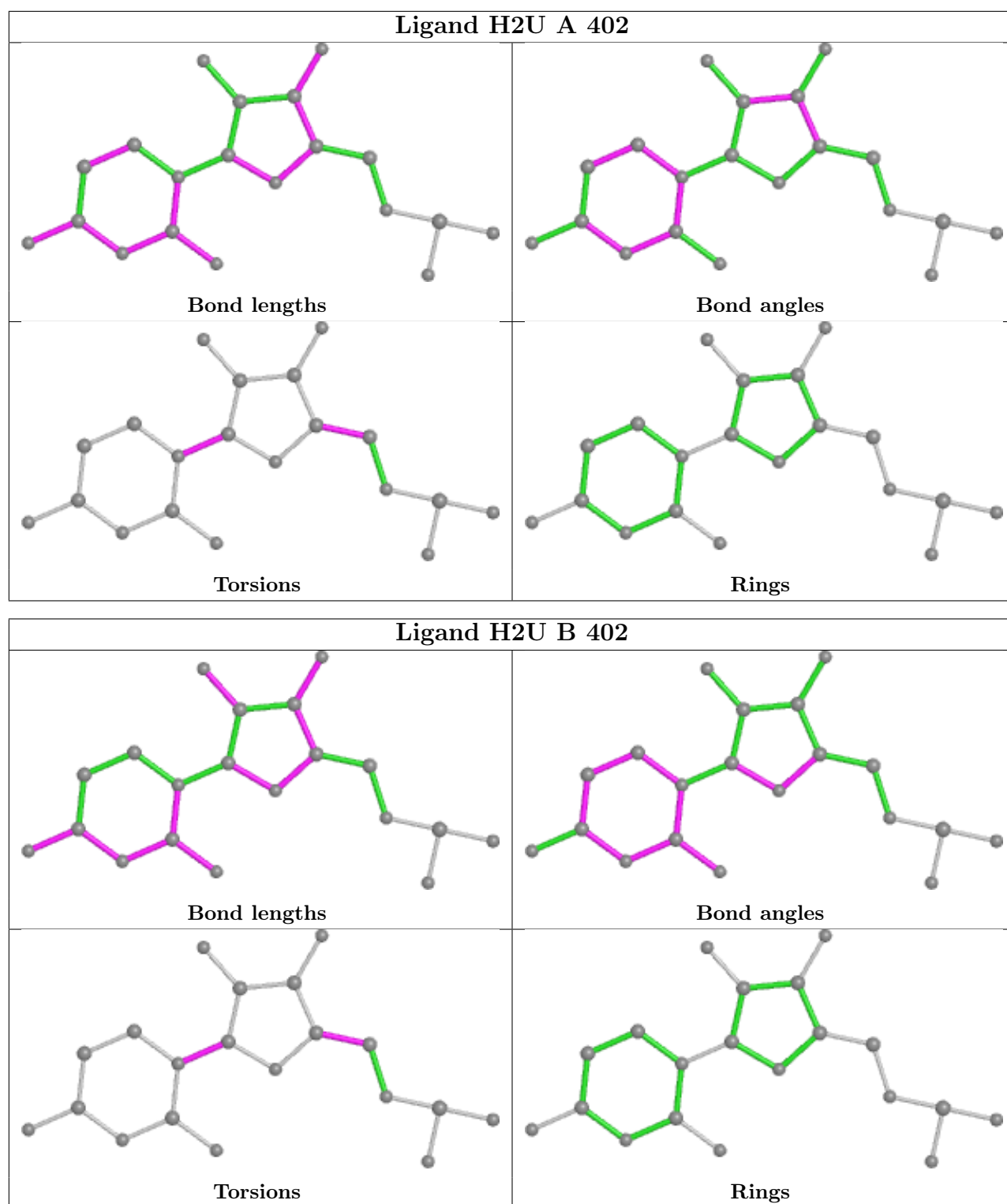
There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	414	EDO	0	1
3	A	402	H2U	3	0
4	B	407	EDO	2	0
3	B	402	H2U	4	0
4	B	417	EDO	2	0
4	A	409	EDO	0	1

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/401 (80%)	1.15	41 (12%) 3 4	17, 29, 54, 80	0
1	B	330/401 (82%)	1.35	64 (19%) 1 1	21, 32, 61, 99	0
All	All	654/802 (81%)	1.25	105 (16%) 1 2	17, 31, 60, 99	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	THR	10.5
1	A	111	PRO	8.4
1	B	307	SER	8.0
1	A	47	HIS	7.8
1	A	310	GLY	7.7
1	B	22	ALA	7.1
1	B	311	ALA	7.0
1	A	110	GLY	6.8
1	B	110	GLY	6.6
1	B	310	GLY	6.5
1	B	24	PHE	5.6
1	B	79	ILE	5.4
1	A	48	ARG	5.3
1	B	112	SER	5.3
1	A	309	ALA	5.3
1	B	308	GLU	5.0
1	B	309	ALA	4.9
1	B	23	THR	4.7
1	B	64	THR	4.6
1	B	256	LEU	4.5
1	B	212	GLN	4.5
1	B	27	ASN	4.5
1	A	112	SER	4.4
1	B	26	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	330	ALA	4.4
1	A	366	TYR	4.3
1	A	336	MET	4.3
1	A	342	LEU	4.3
1	B	111	PRO	4.2
1	A	311	ALA	4.2
1	B	366	TYR	4.1
1	A	28	ASP	4.1
1	A	343	ALA	4.0
1	B	211	SER	3.8
1	B	331	THR	3.5
1	B	106	ALA	3.4
1	B	47	HIS	3.4
1	B	81	ALA	3.4
1	B	323	TYR	3.4
1	A	113	ASP	3.4
1	A	323	TYR	3.3
1	B	181	SER	3.3
1	B	46	ALA	3.3
1	B	306	GLY	3.2
1	A	339	TYR	3.2
1	B	320	ALA	3.1
1	B	48	ARG	3.1
1	A	29	HIS	3.0
1	B	299	GLY	3.0
1	B	108	SER	3.0
1	B	329	SER	3.0
1	A	340[A]	GLU	2.9
1	B	170	ILE	2.9
1	B	300	TRP	2.9
1	B	208	ALA	2.9
1	B	314	ASN	2.9
1	B	198	ILE	2.9
1	A	306	GLY	2.9
1	A	246	TRP	2.8
1	A	341	MET	2.8
1	B	337	VAL	2.7
1	A	308	GLU	2.7
1	B	364	VAL	2.6
1	B	171	PHE	2.6
1	B	199	ALA	2.6
1	B	316	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	208	ALA	2.5
1	A	249	TRP	2.5
1	B	312	ASN	2.5
1	A	42	VAL	2.5
1	A	337	VAL	2.5
1	B	342	LEU	2.5
1	B	349	LEU	2.5
1	A	181	SER	2.5
1	B	160	GLU	2.5
1	A	198	ILE	2.5
1	B	336	MET	2.4
1	B	85	VAL	2.4
1	B	298	MET	2.4
1	A	106	ALA	2.4
1	B	365	HIS	2.4
1	B	249	TRP	2.4
1	A	291	GLU	2.3
1	A	168	VAL	2.3
1	B	360	ALA	2.3
1	B	163	ALA	2.2
1	A	71	LEU	2.2
1	B	328	ARG	2.2
1	A	316	TRP	2.2
1	A	330	ALA	2.2
1	B	261	VAL	2.2
1	A	170	ILE	2.2
1	A	345	ALA	2.2
1	A	130	CYS	2.1
1	A	187	CYS	2.1
1	B	213	HIS	2.1
1	B	113	ASP	2.1
1	B	209	TYR	2.1
1	B	143	SER	2.1
1	A	217	LEU	2.1
1	B	107	PRO	2.1
1	B	341[A]	MET	2.1
1	B	296	TYR	2.0
1	B	187	CYS	2.0
1	A	242	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

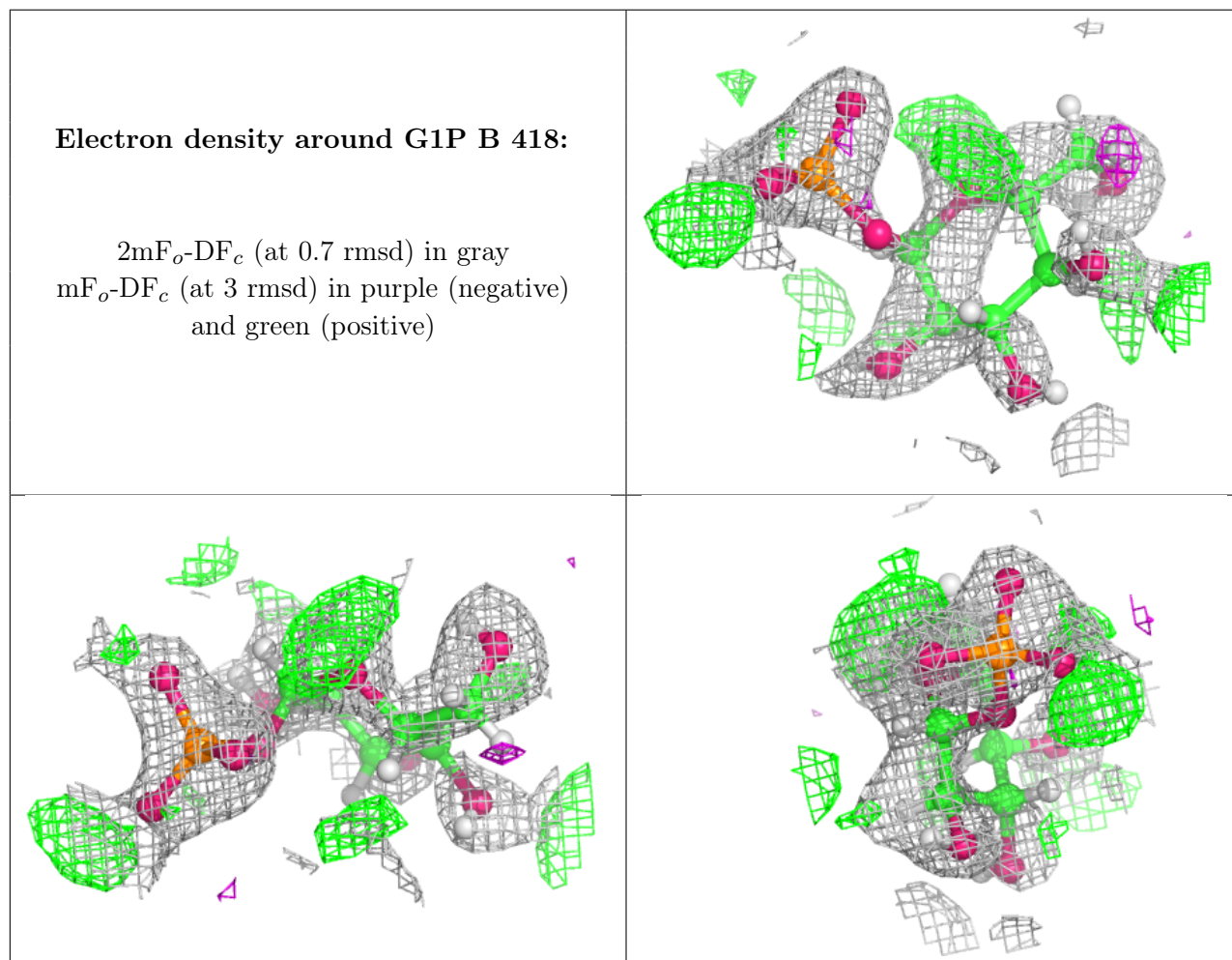
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	413	4/4	0.36	0.38	37,61,81,81	0
4	EDO	A	409	4/4	0.38	0.31	51,65,82,82	0
4	EDO	A	411	4/4	0.40	0.28	40,58,73,73	0
4	EDO	B	408	4/4	0.47	0.51	39,73,87,87	0
4	EDO	B	414	4/4	0.51	0.32	46,67,80,80	0
4	EDO	A	410	4/4	0.51	0.25	37,68,85,85	0
4	EDO	B	411	4/4	0.55	0.60	45,75,90,90	0
4	EDO	B	416	4/4	0.67	0.28	45,73,87,88	0
4	EDO	B	405	4/4	0.69	0.32	35,52,66,66	0
4	EDO	B	413	4/4	0.70	0.35	37,64,84,84	0
4	EDO	A	405	4/4	0.71	0.29	44,68,82,82	0
4	EDO	A	414	4/4	0.72	0.33	45,61,73,73	0
4	EDO	A	406	4/4	0.73	0.25	40,68,90,90	0
4	EDO	B	404	4/4	0.73	0.45	46,101,140,143	0
4	EDO	B	407	4/4	0.74	0.23	45,79,95,95	0
4	EDO	B	410	4/4	0.75	0.17	46,85,102,102	0
4	EDO	B	412	4/4	0.75	0.53	46,60,72,72	0
5	G1P	B	418	16/16	0.75	0.27	16,44,60,65	27
5	G1P	A	416	16/16	0.76	0.28	21,50,66,68	27
4	EDO	A	404	4/4	0.78	0.29	36,67,91,91	0
4	EDO	A	412	4/4	0.78	0.18	40,48,53,53	0
4	EDO	A	407	4/4	0.79	0.22	32,65,82,82	0
4	EDO	B	406	4/4	0.81	0.26	46,71,86,86	0
4	EDO	B	409	4/4	0.83	0.55	44,76,101,101	0
4	EDO	A	415	4/4	0.88	0.23	41,80,96,96	0
4	EDO	A	408	4/4	0.89	0.22	32,49,77,80	0
4	EDO	B	417	4/4	0.89	0.26	40,60,65,72	0

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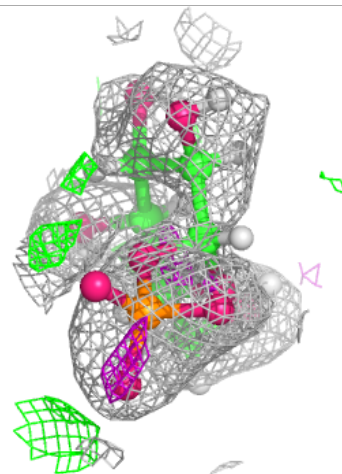
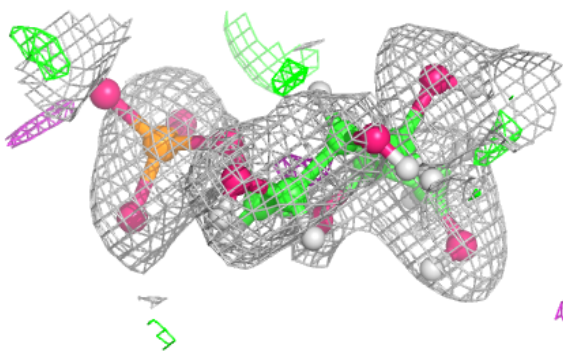
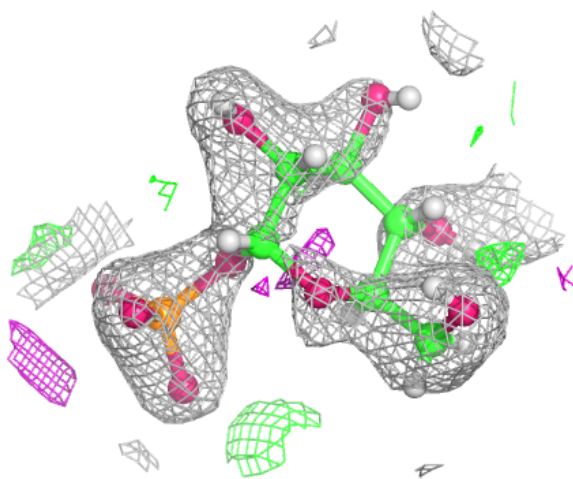
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	415	4/4	0.90	0.24	31,42,51,51	0
4	EDO	B	403	4/4	0.91	0.12	36,58,70,70	0
3	H2U	A	402	20/21	0.92	0.14	22,27,35,39	0
3	H2U	B	402	20/21	0.92	0.13	25,31,38,40	0
4	EDO	A	403	4/4	0.93	0.10	22,38,45,45	0
2	ZN	A	401	1/1	0.98	0.10	26,26,26,26	1
2	ZN	B	401	1/1	0.99	0.08	22,22,22,22	1

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.



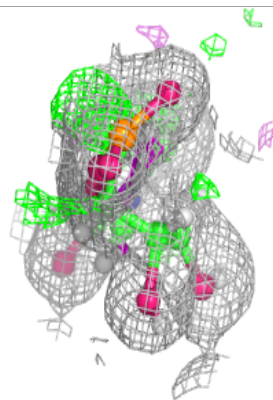
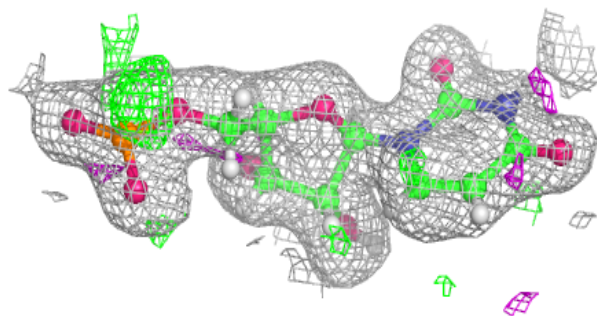
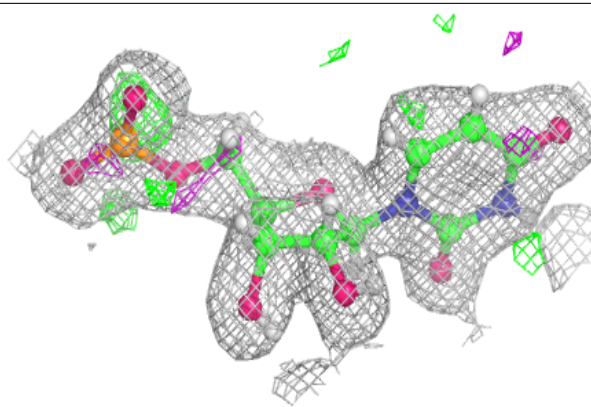
Electron density around G1P A 416:

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

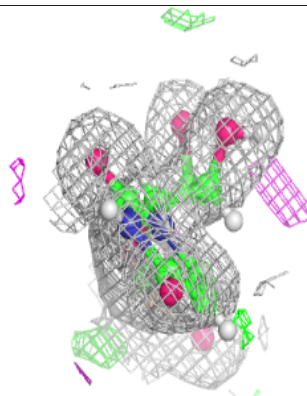
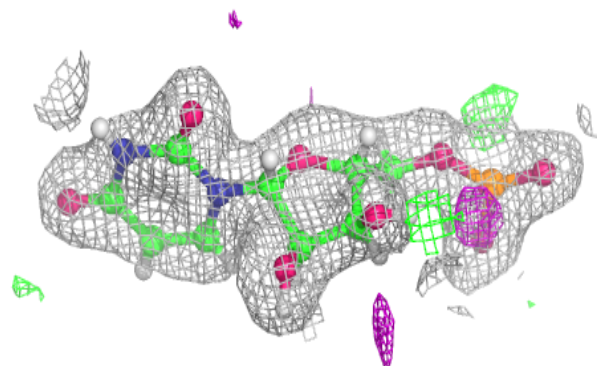
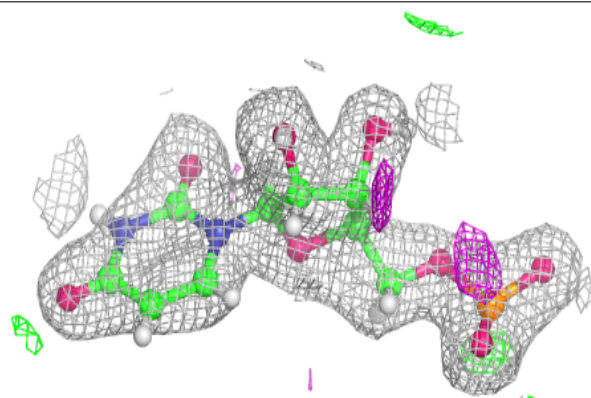


Electron density around H2U A 402:

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

**Electron density around H2U B 402:**

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



6.5 Other polymers

There are no such residues in this entry.