



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:16 AM UTC

PDB ID : 5IN3 / pdb_00005in3
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)

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

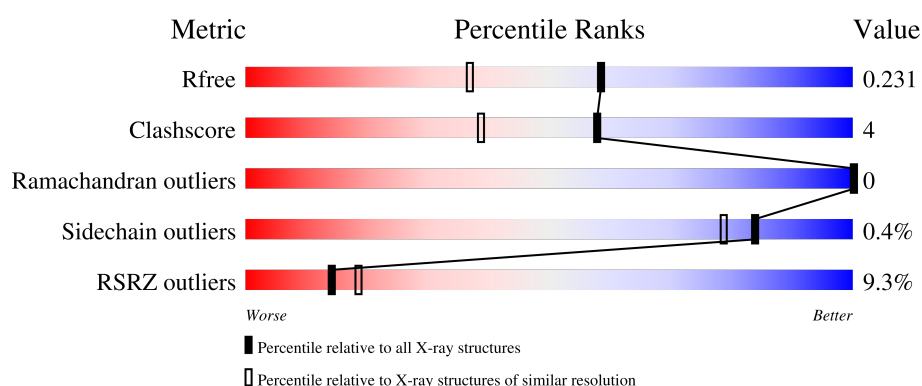
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	7% 74% 6% 19%
1	B	401	8% 75% 7% 18%

2 Entry composition

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
1	B	330	Total	C	H	N	O	S	0	5	0
			5281	1720	2588	477	482	14			
1	A	324	Total	C	H	N	O	S	0	6	0
			5213	1699	2556	467	476	15			

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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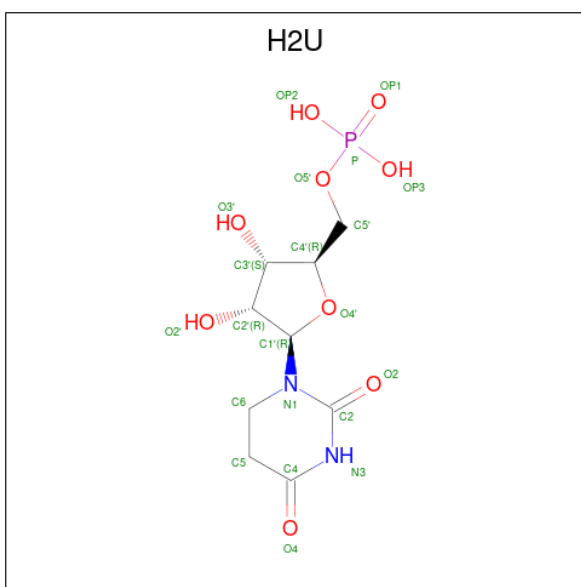
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	HIS	-	expression tag	UNP P07902
A	-17	HIS	-	expression tag	UNP P07902
A	-16	HIS	-	expression tag	UNP P07902
A	-15	HIS	-	expression tag	UNP P07902
A	-14	SER	-	expression tag	UNP P07902
A	-13	SER	-	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 (CCD ID: ZN) (formula: Zn).

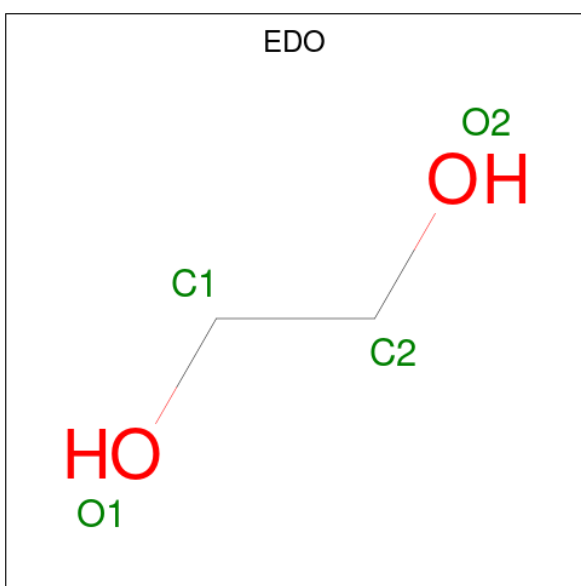
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5,6-DIHYDROURIDINE-5'-MONOPHOSPHATE (CCD ID: H2U) (formula: C₉H₁₅N₂O₉P).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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		

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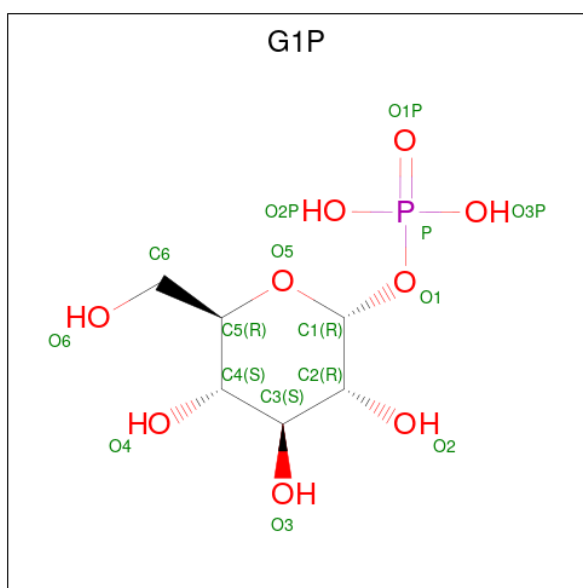
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1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

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

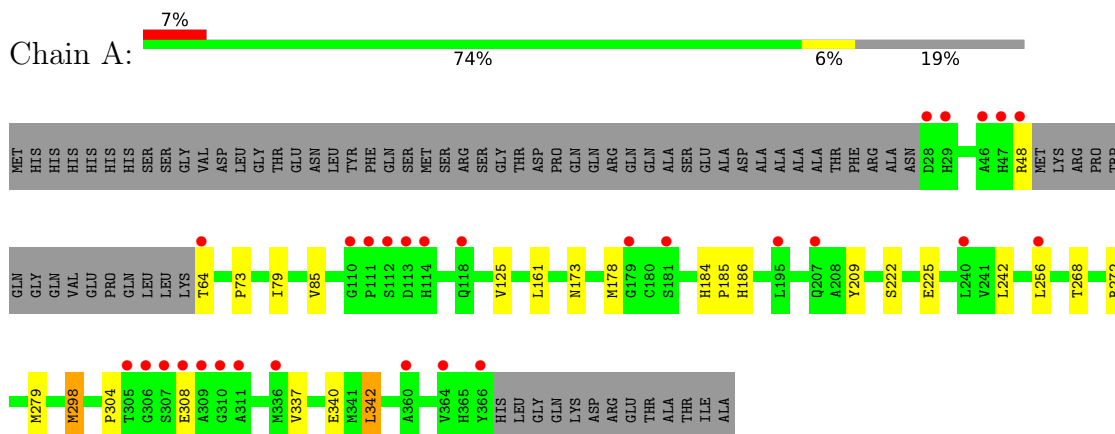
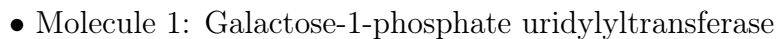


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	O	P	0	0
			27	6	11	9	1		
5	A	1	Total	C	H	O	P	0	0
			27	6	11	9	1		

- 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		

- 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) 99.9 (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)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.228 0.201 , 0.231	Depositor DCC
R_{free} test set	4231 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	0.46	1/2766 (0.0%)	0.60	0/3779
1	B	0.38	0/2805	0.56	0/3832
All	All	0.42	1/5571 (0.0%)	0.58	0/7611

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	MET	SD-CE	-6.03	1.64	1.79

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	2657	2556	2546	25	1
1	B	2693	2588	2567	27	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	3	2
6	B	188	0	0	5	3
All	All	5960	5356	5328	49	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 (49) 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: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:A:298:MET:O	1:A:298:MET:HE3	2.03	0.58
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:279[A]:MET:HE3	6:A:521:HOH:O	2.05	0.57
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:B:172:GLU:H	1:B:298:MET:HE3	1.75	0.52
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:A:298:MET:HE3	1:A:298:MET:C	2.42	0.45
1:B:67:ARG:HH11	4:B:417:EDO:H11	1.81	0.44
1:B:298:MET:HE3	1:B:298:MET:O	2.17	0.44
1:B:241:VAL:HG22	1:B:255:LEU:HD13	1.99	0.44
1:B:172:GLU:N	1:B:298:MET:HE3	2.33	0.44
1:A:64:THR:HG23	1:A:64:THR:O	2.18	0.44
1:A:256:LEU:HD12	1:A:256:LEU:C	2.43	0.44
1:B:281:LYS:NZ	6:B:510:HOH:O	2.51	0.43
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:B:336:MET:SD	1:B:340[B]:GLU:CD	3.02	0.42
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
1:A:242:LEU:HD12	1:A:242:LEU:C	2.45	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	287 (100%)	1 (0%)	86	82
1	B	291/346 (84%)	290 (100%)	1 (0%)	86	82
All	All	579/692 (84%)	577 (100%)	2 (0%)	84	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	342	LEU
1	A	342	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	GLN
1	B	207	GLN
1	B	213	HIS
1	A	206	GLN
1	A	212	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	414	-	3,3,3	0.43	0	2,2,2	0.48	0
4	EDO	B	416	-	3,3,3	0.54	0	2,2,2	1.05	0
3	H2U	A	402	-	18,21,22	4.07	10 (55%)	19,30,33	1.59	3 (15%)
4	EDO	A	406	-	3,3,3	0.36	0	2,2,2	0.51	0
4	EDO	B	404	-	3,3,3	0.45	0	2,2,2	0.44	0
4	EDO	B	409	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	B	414	-	3,3,3	0.46	0	2,2,2	0.42	0
4	EDO	A	411	-	3,3,3	0.65	0	2,2,2	0.08	0
4	EDO	A	410	-	3,3,3	0.59	0	2,2,2	0.12	0
4	EDO	B	405	-	3,3,3	0.59	0	2,2,2	0.22	0
4	EDO	A	405	-	3,3,3	0.48	0	2,2,2	0.25	0
4	EDO	B	406	-	3,3,3	0.39	0	2,2,2	0.49	0
5	G1P	B	418	-	15,16,16	1.82	2 (13%)	24,24,24	1.03	2 (8%)
4	EDO	B	413	-	3,3,3	0.57	0	2,2,2	0.17	0
4	EDO	A	408	-	3,3,3	0.55	0	2,2,2	0.10	0
4	EDO	B	411	-	3,3,3	0.42	0	2,2,2	0.46	0
4	EDO	A	407	-	3,3,3	0.53	0	2,2,2	0.27	0
4	EDO	B	410	-	3,3,3	0.49	0	2,2,2	0.34	0
4	EDO	A	412	-	3,3,3	0.52	0	2,2,2	0.18	0
4	EDO	A	415	-	3,3,3	0.42	0	2,2,2	0.45	0
4	EDO	A	413	-	3,3,3	0.66	0	2,2,2	0.06	0
5	G1P	A	416	-	15,16,16	1.67	2 (13%)	24,24,24	1.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	403	-	3,3,3	0.44	0	2,2,2	0.46	0
4	EDO	B	417	-	3,3,3	0.10	0	2,2,2	0.82	0
4	EDO	B	412	-	3,3,3	0.50	0	2,2,2	0.21	0
3	H2U	B	402	-	18,21,22	4.27	10 (55%)	19,30,33	1.97	5 (26%)
4	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.38	0
4	EDO	A	404	-	3,3,3	0.51	0	2,2,2	0.20	0
4	EDO	B	415	-	3,3,3	0.35	0	2,2,2	0.52	0
4	EDO	A	409	-	3,3,3	0.43	0	2,2,2	0.48	0
4	EDO	B	408	-	3,3,3	0.53	0	2,2,2	0.17	0
4	EDO	B	407	-	3,3,3	0.44	0	2,2,2	0.46	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	414	-	-	0/1/1/1	-
4	EDO	B	416	-	-	1/1/1/1	-
3	H2U	A	402	-	-	2/7/38/39	0/2/2/2
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	B	409	-	-	1/1/1/1	-
4	EDO	B	414	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
4	EDO	A	410	-	-	0/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
5	G1P	B	418	-	-	2/7/27/27	0/1/1/1
4	EDO	B	413	-	-	0/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
4	EDO	B	411	-	-	0/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	B	410	-	-	1/1/1/1	-
4	EDO	A	412	-	-	0/1/1/1	-
4	EDO	A	415	-	-	1/1/1/1	-
4	EDO	A	413	-	-	1/1/1/1	-
5	G1P	A	416	-	-	1/7/27/27	0/1/1/1
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	B	417	-	-	1/1/1/1	-
4	EDO	B	412	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H2U	B	402	-	-	2/7/38/39	0/2/2/2
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	415	-	-	0/1/1/1	-
4	EDO	A	409	-	-	0/1/1/1	-
4	EDO	B	408	-	-	0/1/1/1	-
4	EDO	B	407	-	-	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	10.43	1.50	1.35
3	B	402	H2U	C2-N1	10.08	1.49	1.35
3	B	402	H2U	C3'-C4'	-7.10	1.35	1.53
3	B	402	H2U	C4-N3	6.43	1.48	1.37
3	B	402	H2U	C2-N3	6.28	1.48	1.38
3	A	402	H2U	C4-N3	6.17	1.47	1.37
3	A	402	H2U	C3'-C4'	-6.13	1.37	1.53
3	A	402	H2U	C2-N3	6.00	1.48	1.38
3	B	402	H2U	O4'-C4'	5.64	1.57	1.45
3	B	402	H2U	O4'-C1'	-5.24	1.29	1.42
3	A	402	H2U	O4'-C4'	5.17	1.56	1.45
5	B	418	G1P	P-O1	4.75	1.67	1.59
3	A	402	H2U	O4'-C1'	-4.58	1.31	1.42
5	A	416	G1P	P-O1	4.35	1.67	1.59
5	B	418	G1P	O5-C1	4.19	1.52	1.41
5	A	416	G1P	O5-C1	4.08	1.52	1.41
3	B	402	H2U	O4-C4	-3.37	1.16	1.23
3	B	402	H2U	O2-C2	-2.88	1.18	1.23
3	B	402	H2U	O2'-C2'	-2.59	1.36	1.43
3	A	402	H2U	C6-C5	-2.58	1.45	1.52
3	A	402	H2U	O4-C4	-2.57	1.18	1.23
3	A	402	H2U	O2-C2	-2.47	1.18	1.23
3	A	402	H2U	O3'-C3'	2.41	1.48	1.43
3	B	402	H2U	O3'-C3'	2.10	1.48	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	H2U	O2-C2-N1	-4.38	117.83	123.10
3	B	402	H2U	C5-C4-N3	4.26	121.22	116.69
3	A	402	H2U	N3-C2-N1	3.30	119.97	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	H2U	N3-C2-N1	3.20	119.87	116.65
3	A	402	H2U	C5-C6-N1	3.03	120.70	111.52
3	A	402	H2U	C2'-C3'-C4'	2.83	108.08	102.61
3	B	402	H2U	C4'-O4'-C1'	-2.56	103.81	109.47
5	A	416	G1P	O5-C5-C4	2.54	114.28	109.70
3	B	402	H2U	C5-C6-N1	2.43	118.87	111.52
5	B	418	G1P	C6-C5-C4	-2.38	107.17	113.02
5	B	418	G1P	O5-C5-C4	2.36	113.95	109.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

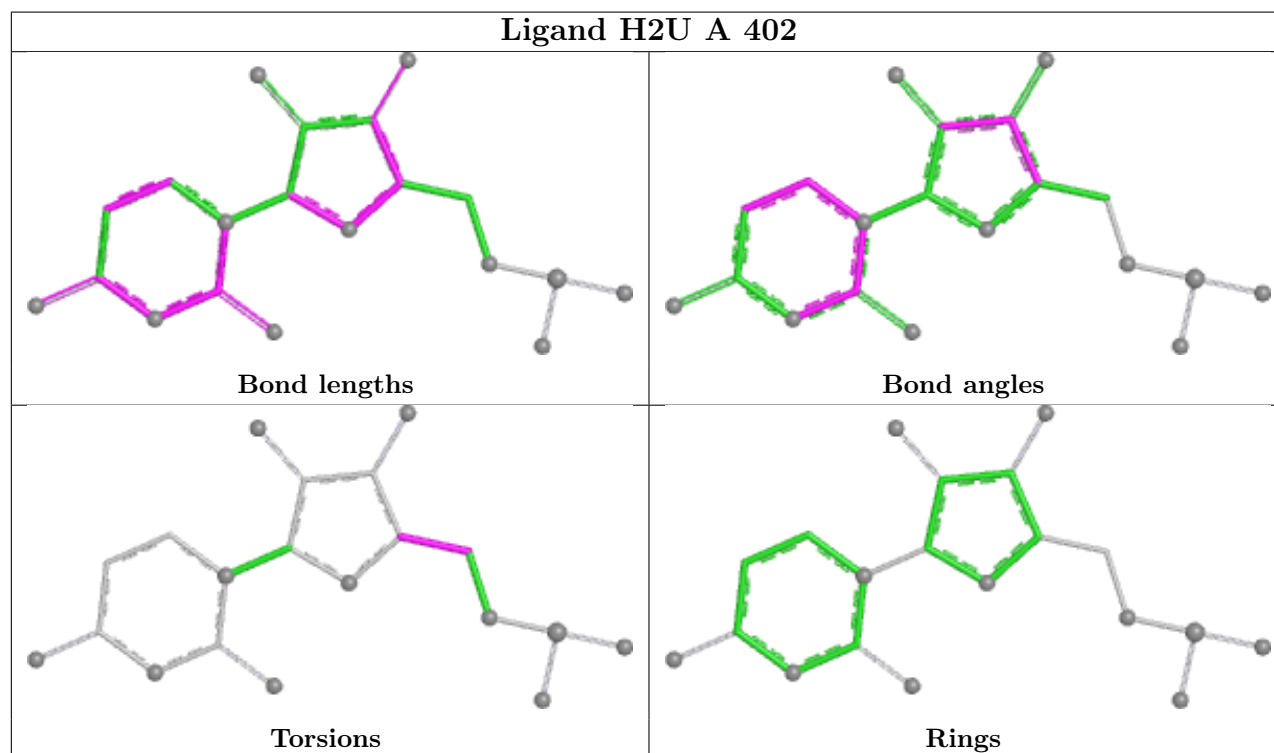
Mol	Chain	Res	Type	Atoms
5	B	418	G1P	C1-O1-P-O1P
4	B	417	EDO	O1-C1-C2-O2
4	A	415	EDO	O1-C1-C2-O2
3	A	402	H2U	O4'-C4'-C5'-O5'
3	A	402	H2U	C3'-C4'-C5'-O5'
4	B	410	EDO	O1-C1-C2-O2
4	A	413	EDO	O1-C1-C2-O2
3	B	402	H2U	O4'-C4'-C5'-O5'
3	B	402	H2U	C3'-C4'-C5'-O5'
4	B	405	EDO	O1-C1-C2-O2
4	B	416	EDO	O1-C1-C2-O2
5	B	418	G1P	C1-O1-P-O2P
4	A	411	EDO	O1-C1-C2-O2
4	B	414	EDO	O1-C1-C2-O2
5	A	416	G1P	C1-O1-P-O1P
4	B	409	EDO	O1-C1-C2-O2

There are no ring outliers.

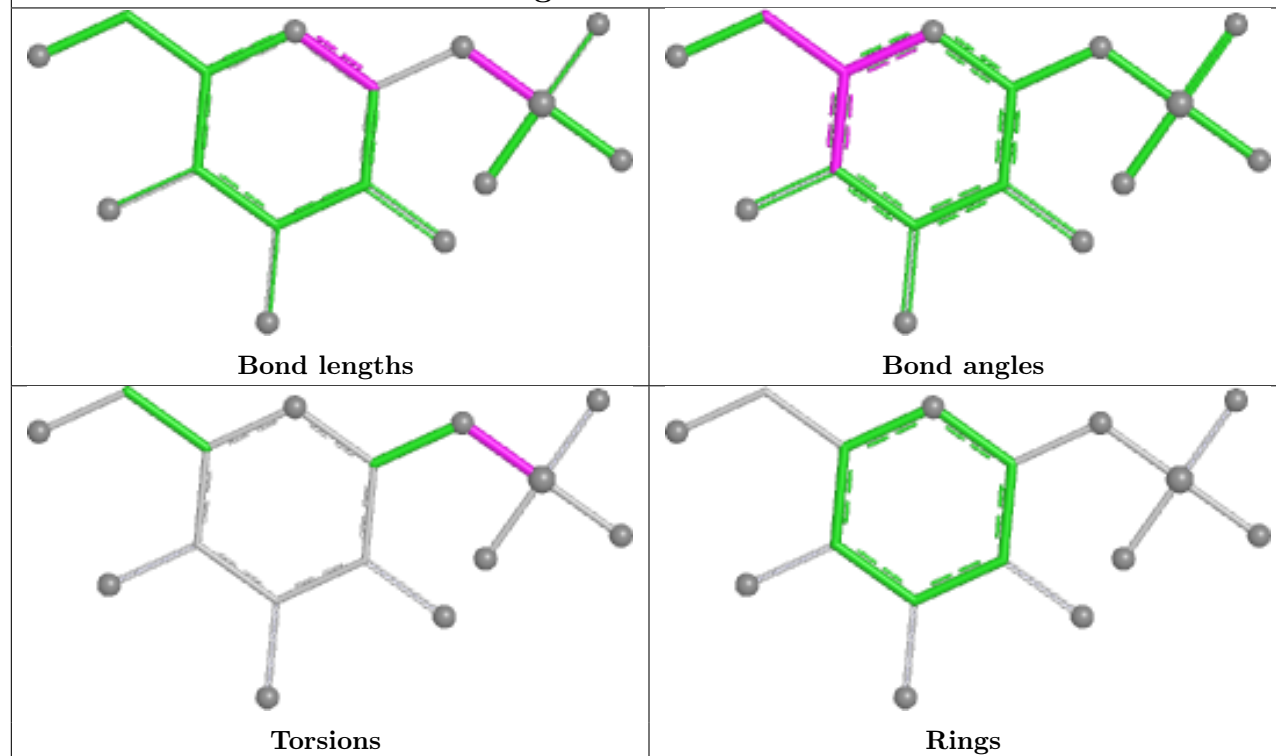
6 monomers are involved in 13 short contacts:

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

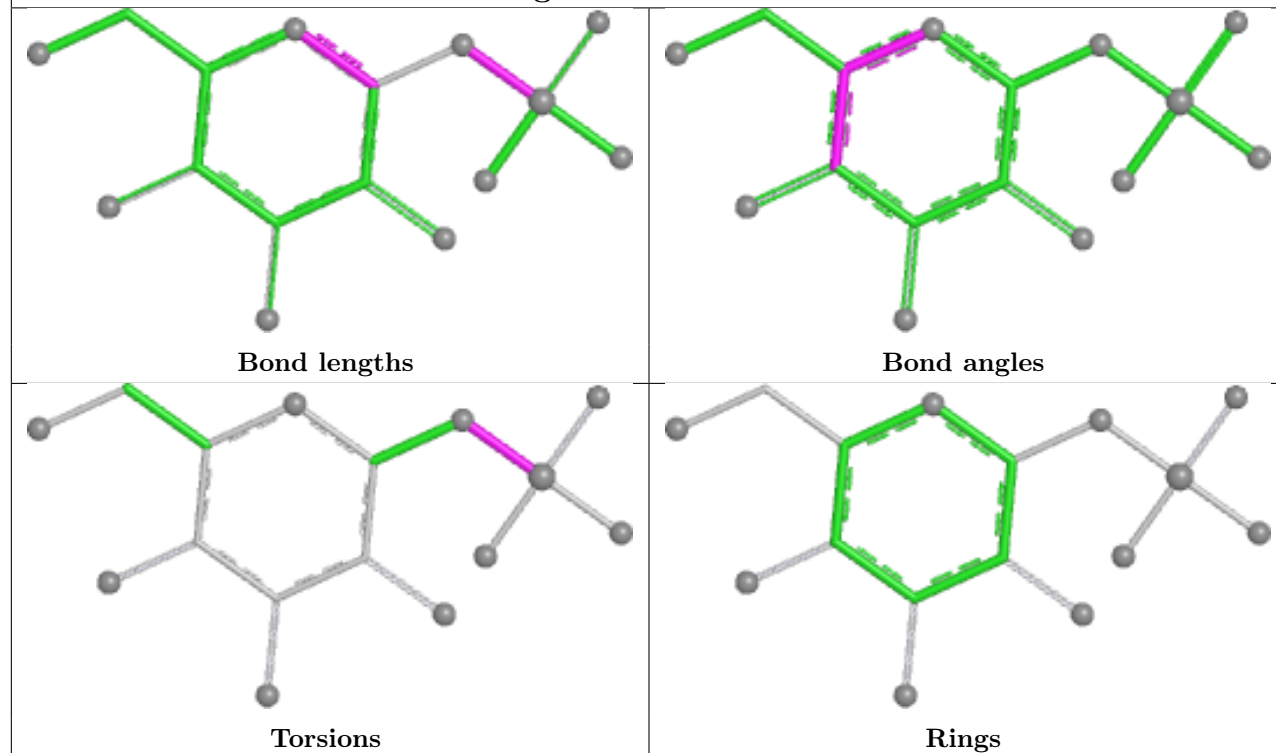
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

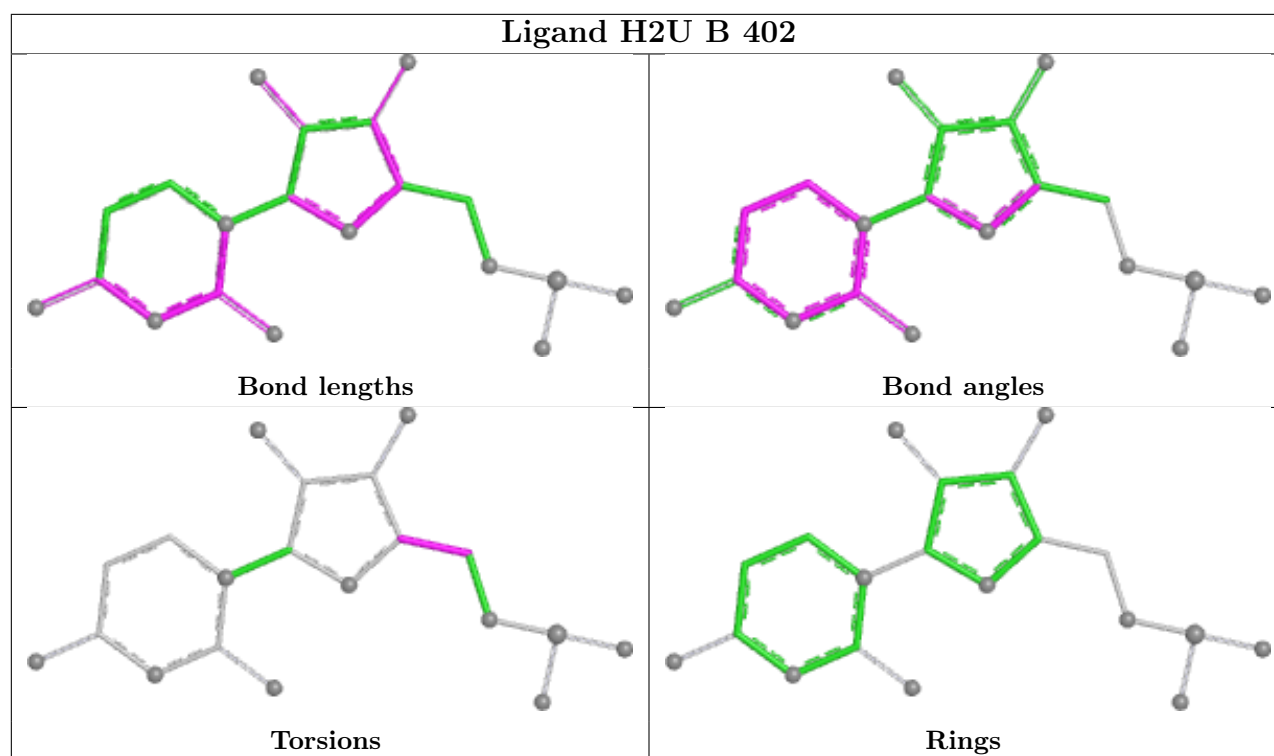


Ligand G1P B 418



Ligand G1P A 416





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, 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%)	0.46	29 (8%) 15 20	14, 32, 61, 87	5 (1%)
1	B	330/401 (82%)	0.65	32 (9%) 13 17	15, 36, 69, 111	3 (0%)
All	All	654/802 (81%)	0.56	61 (9%) 14 18	14, 34, 66, 111	8 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	HIS	6.3
1	A	64	THR	5.2
1	B	256	LEU	4.5
1	A	310	GLY	4.2
1	A	46	ALA	4.1
1	A	48	ARG	4.1
1	B	47	HIS	4.0
1	B	64	THR	3.9
1	B	240	LEU	3.7
1	B	27	ASN	3.5
1	B	112	SER	3.5
1	B	26	ALA	3.5
1	B	22	ALA	3.4
1	B	181	SER	3.4
1	A	306	GLY	3.3
1	B	81	ALA	3.3
1	A	110	GLY	3.2
1	B	46	ALA	3.2
1	A	113	ASP	3.2
1	B	23	THR	3.2
1	A	111	PRO	3.1
1	B	113	ASP	3.1
1	B	305	THR	3.1
1	A	308	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	29	HIS	3.0
1	B	311	ALA	3.0
1	A	112	SER	3.0
1	A	179	GLY	3.0
1	A	256	LEU	2.9
1	B	307	SER	2.9
1	B	366	TYR	2.9
1	B	308	GLU	2.9
1	B	111	PRO	2.8
1	A	28	ASP	2.8
1	A	311	ALA	2.8
1	A	181	SER	2.7
1	B	179	GLY	2.7
1	B	24	PHE	2.7
1	A	195	LEU	2.7
1	B	336	MET	2.7
1	A	307	SER	2.6
1	B	309	ALA	2.6
1	A	336	MET	2.6
1	B	85	VAL	2.6
1	B	79	ILE	2.5
1	B	348	ASP	2.4
1	A	240	LEU	2.4
1	B	48	ARG	2.4
1	A	366	TYR	2.3
1	B	211	SER	2.3
1	A	309	ALA	2.3
1	A	364	VAL	2.3
1	B	110	GLY	2.3
1	B	88	GLN	2.2
1	B	310	GLY	2.2
1	A	207	GLN	2.1
1	A	118	GLN	2.1
1	A	360	ALA	2.1
1	A	114	HIS	2.0
1	A	305	THR	2.0
1	B	360	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	B	414	4/4	0.61	0.21	46,67,80,80	0
4	EDO	A	411	4/4	0.61	0.28	40,58,73,73	0
4	EDO	A	409	4/4	0.62	0.23	51,65,82,82	0
4	EDO	A	413	4/4	0.64	0.28	37,61,81,81	0
4	EDO	B	408	4/4	0.65	0.30	39,73,87,87	0
4	EDO	B	416	4/4	0.69	0.20	45,73,87,88	0
4	EDO	B	413	4/4	0.69	0.26	37,64,84,84	0
4	EDO	A	415	4/4	0.70	0.25	41,80,96,96	0
4	EDO	B	404	4/4	0.73	0.25	46,101,140,143	0
4	EDO	A	414	4/4	0.77	0.19	45,61,73,73	0
4	EDO	B	411	4/4	0.77	0.25	45,75,90,90	0
4	EDO	A	406	4/4	0.78	0.26	40,68,90,90	0
4	EDO	B	406	4/4	0.79	0.15	46,71,86,86	0
4	EDO	A	410	4/4	0.79	0.22	37,68,85,85	0
4	EDO	A	404	4/4	0.80	0.21	36,67,91,91	0
4	EDO	B	407	4/4	0.80	0.19	45,79,95,95	0
4	EDO	B	410	4/4	0.82	0.23	46,85,102,102	0
4	EDO	B	417	4/4	0.83	0.15	40,60,65,72	0
4	EDO	B	409	4/4	0.83	0.20	44,76,101,101	0
4	EDO	B	405	4/4	0.83	0.18	35,52,66,66	0
4	EDO	A	405	4/4	0.84	0.16	44,68,82,82	0
4	EDO	B	415	4/4	0.86	0.28	31,42,51,51	0
4	EDO	B	412	4/4	0.86	0.14	46,60,72,72	0
4	EDO	A	407	4/4	0.86	0.18	32,65,82,82	0
5	G1P	A	416	16/16	0.86	0.15	21,50,66,68	27
5	G1P	B	418	16/16	0.87	0.17	16,44,60,65	27
4	EDO	A	412	4/4	0.88	0.15	40,48,53,53	0
4	EDO	A	408	4/4	0.88	0.17	32,49,77,80	0
4	EDO	B	403	4/4	0.91	0.12	36,58,70,70	0
3	H2U	A	402	20/21	0.93	0.09	22,27,35,39	0
4	EDO	A	403	4/4	0.93	0.13	22,38,45,45	0
3	H2U	B	402	20/21	0.97	0.07	25,31,38,40	0

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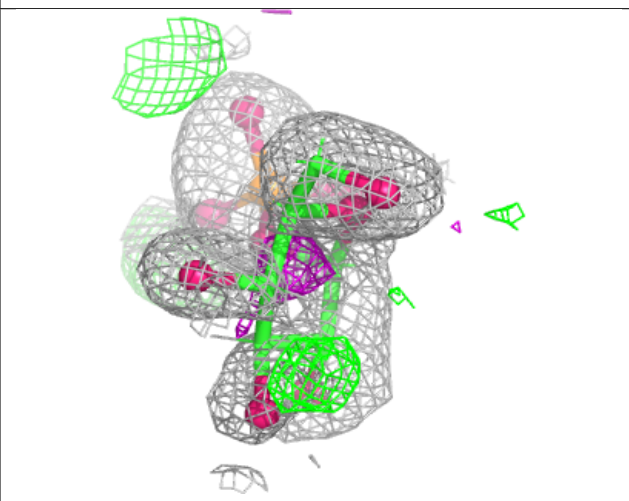
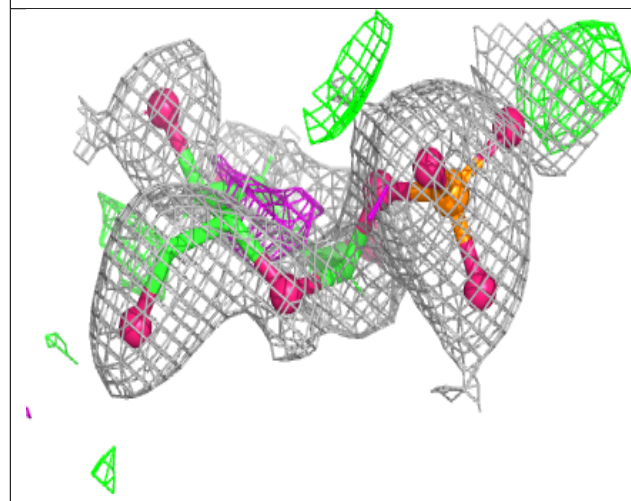
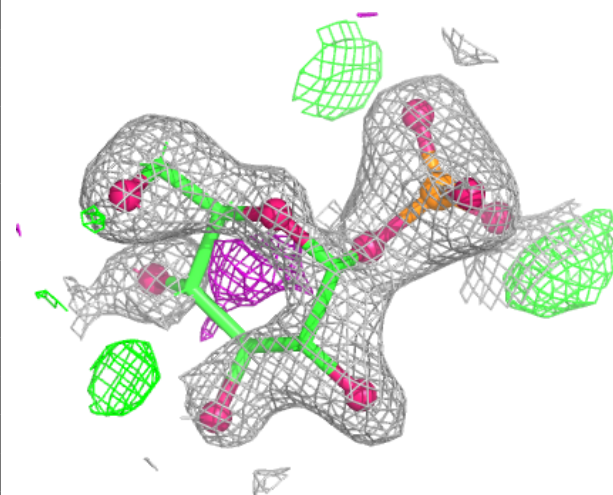
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	401	1/1	0.98	0.04	22,22,22,22	1
2	ZN	A	401	1/1	0.98	0.05	26,26,26,26	1

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.

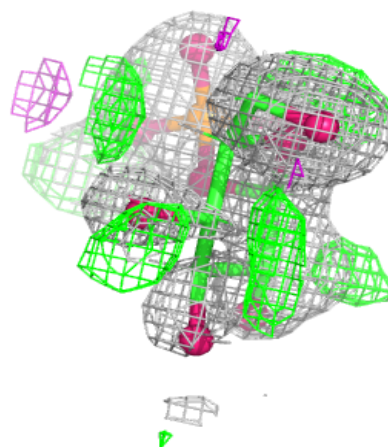
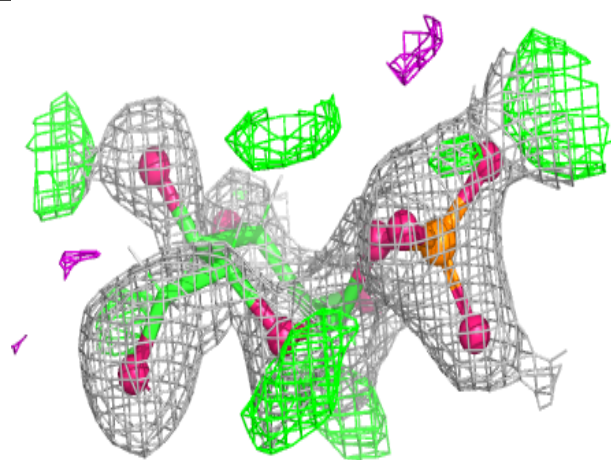
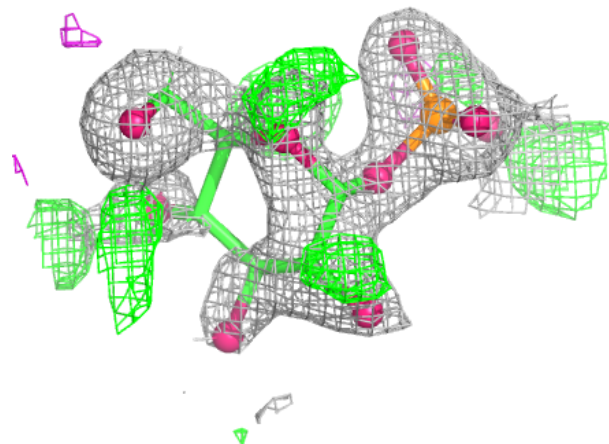
Electron density around G1P A 416:

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



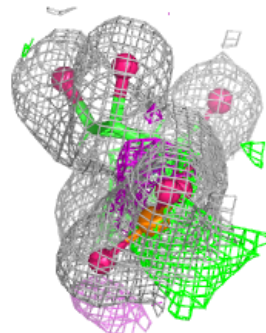
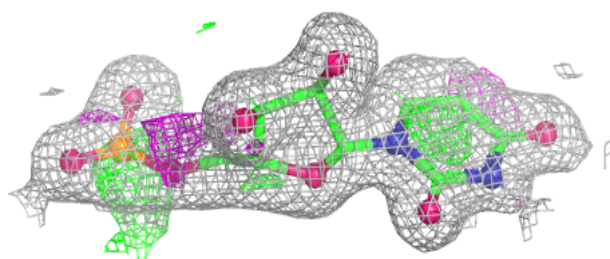
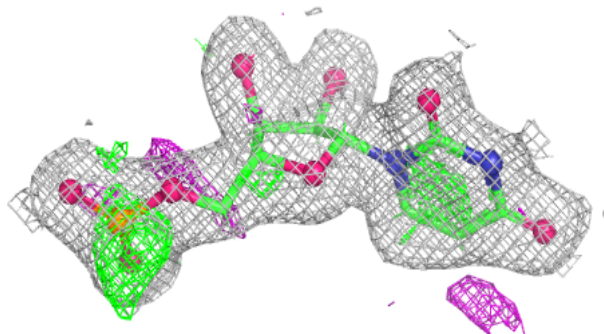
Electron density around G1P B 418:

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

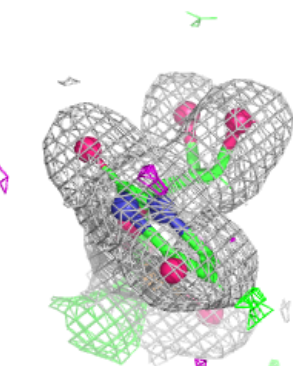
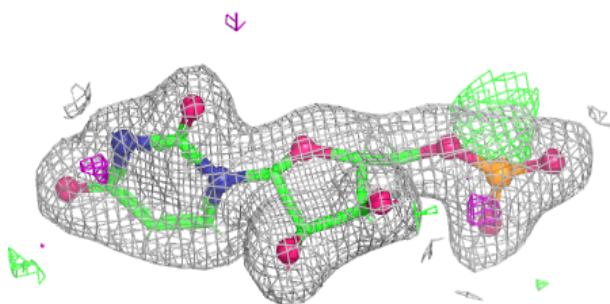
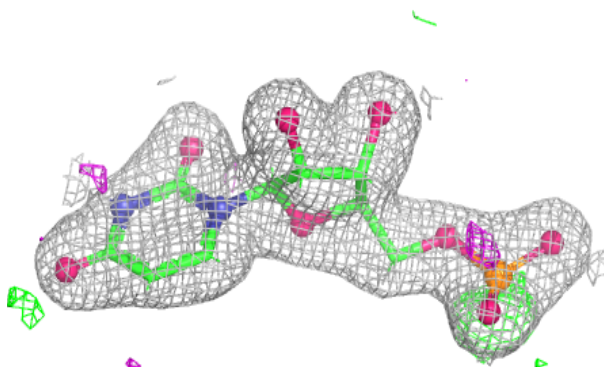


Electron density around H2U A 402:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.