



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2016 – 05:48 PM EDT

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)

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

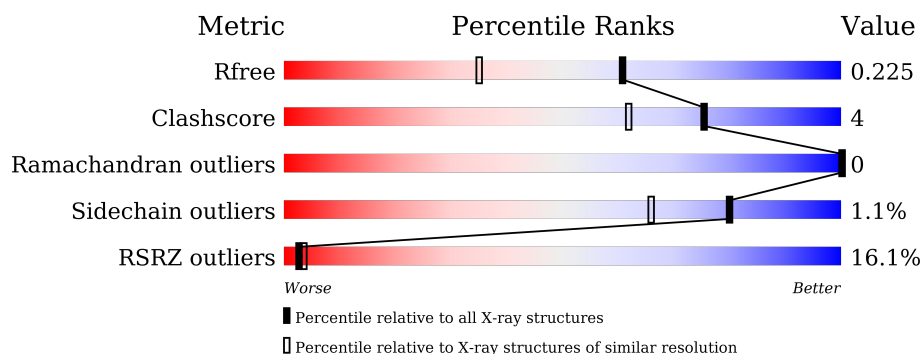
1 Overall quality at a glance ⓘ

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}	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>6%</div> <div>19%</div> </div> </div>
1	B	401	<div> <div>16%</div> <div> <div></div> <div>75%</div> <div>7%</div> <div>18%</div> </div> </div>

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	A	405	-	-	-	X
4	EDO	A	406	-	-	-	X
4	EDO	A	407	-	-	-	X
4	EDO	A	410	-	-	-	X
4	EDO	A	411	-	-	-	X
4	EDO	A	412	-	-	-	X
4	EDO	A	413	-	-	-	X
4	EDO	B	405	-	-	-	X
4	EDO	B	411	-	-	-	X
4	EDO	B	412	-	-	-	X
4	EDO	B	414	-	-	-	X
4	EDO	B	415	-	-	-	X
4	EDO	B	416	-	-	-	X
5	G1P	B	418	-	-	-	X

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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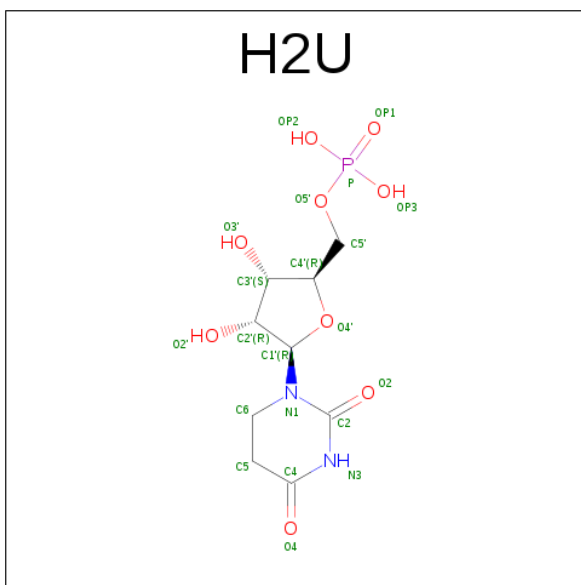
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	HIS	-	expression tag	UNP P07902
A	-17	HIS	-	expression tag	UNP P07902
A	-16	HIS	-	expression tag	UNP P07902
A	-15	HIS	-	expression tag	UNP P07902
A	-14	SER	-	expression tag	UNP P07902
A	-13	SER	-	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 (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
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 (three-letter code: EDO) (formula: C₂H₆O₂).



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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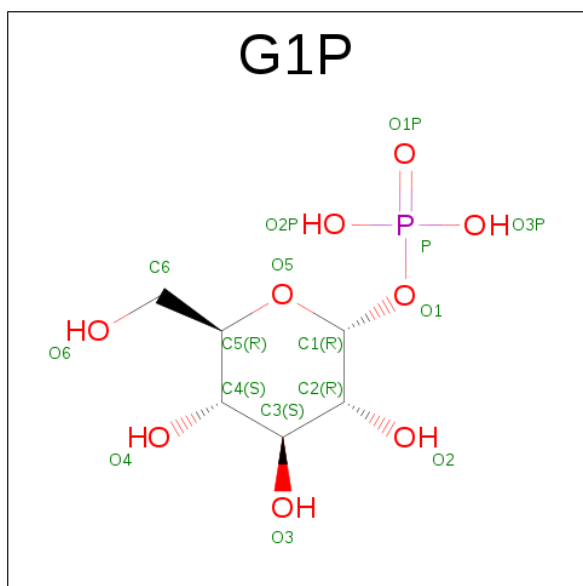
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	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 ALPHA-D-GLUCOSE-1-PHOSPHATE (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		

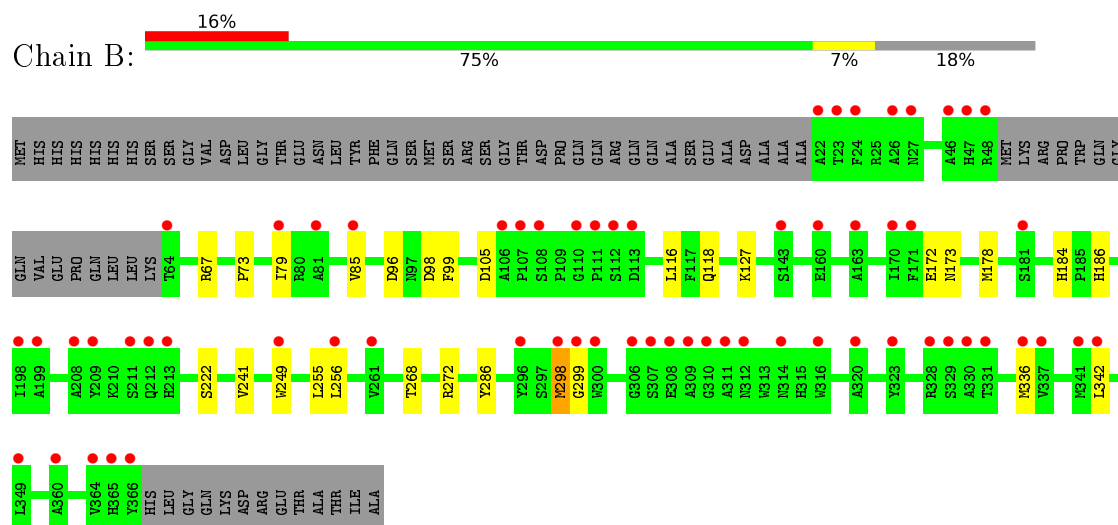
- Molecule 6 is water.

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

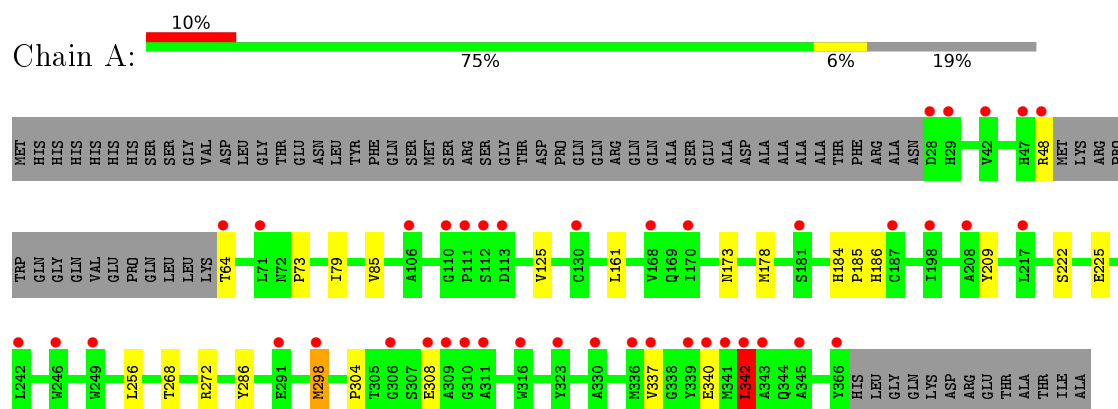
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.228 0.196 , 0.225	Depositor DCC
R_{free} test set	4223 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, ZN, EDO, 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	0.49	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:HE3	1:A:298:MET:O	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:OE1	1:A:225:GLU:HA	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 ⓘ

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 ⓘ

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%)	82	69
1	B	291/346 (84%)	288 (99%)	3 (1%)	82	69
All	All	579/692 (84%)	573 (99%)	6 (1%)	80	69

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

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

5.3.3 RNA ⓘ

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 carbohydrates 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
3	H2U	A	402	-	17,21,22	4.02	10 (58%)	23,30,33	2.64	4 (17%)
4	EDO	A	403	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	A	404	-	3,3,3	0.52	0	2,2,2	0.20	0
4	EDO	A	405	-	3,3,3	0.50	0	2,2,2	0.26	0
4	EDO	A	406	-	3,3,3	0.38	0	2,2,2	0.55	0
4	EDO	A	407	-	3,3,3	0.54	0	2,2,2	0.27	0
4	EDO	A	408	-	3,3,3	0.56	0	2,2,2	0.10	0
4	EDO	A	409	-	3,3,3	0.45	0	2,2,2	0.51	0
4	EDO	A	410	-	3,3,3	0.60	0	2,2,2	0.11	0
4	EDO	A	411	-	3,3,3	0.66	0	2,2,2	0.07	0
4	EDO	A	412	-	3,3,3	0.53	0	2,2,2	0.18	0
4	EDO	A	413	-	3,3,3	0.67	0	2,2,2	0.06	0
4	EDO	A	414	-	3,3,3	0.45	0	2,2,2	0.51	0
4	EDO	A	415	-	3,3,3	0.43	0	2,2,2	0.48	0
5	G1P	A	416	-	15,16,16	1.27	1 (6%)	23,24,24	1.12	1 (4%)
3	H2U	B	402	-	17,21,22	4.19	11 (64%)	23,30,33	2.92	6 (26%)
4	EDO	B	403	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	B	404	-	3,3,3	0.46	0	2,2,2	0.47	0
4	EDO	B	405	-	3,3,3	0.60	0	2,2,2	0.23	0
4	EDO	B	406	-	3,3,3	0.41	0	2,2,2	0.53	0
4	EDO	B	407	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	B	408	-	3,3,3	0.55	0	2,2,2	0.16	0
4	EDO	B	409	-	3,3,3	0.47	0	2,2,2	0.38	0
4	EDO	B	410	-	3,3,3	0.50	0	2,2,2	0.36	0
4	EDO	B	411	-	3,3,3	0.44	0	2,2,2	0.49	0
4	EDO	B	412	-	3,3,3	0.51	0	2,2,2	0.22	0
4	EDO	B	413	-	3,3,3	0.58	0	2,2,2	0.17	0
4	EDO	B	414	-	3,3,3	0.48	0	2,2,2	0.44	0
4	EDO	B	415	-	3,3,3	0.38	0	2,2,2	0.57	0
4	EDO	B	416	-	3,3,3	0.55	0	2,2,2	1.15	0
4	EDO	B	417	-	3,3,3	0.11	0	2,2,2	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	G1P	B	418	-	15,16,16	1.38	1 (6%)	23,24,24	1.00	2 (8%)

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	H2U	C3'-C4'	-6.73	1.35	1.53
3	A	402	H2U	C3'-C4'	-5.81	1.37	1.53
3	B	402	H2U	O4'-C1'	-4.89	1.29	1.42
3	A	402	H2U	O4'-C1'	-4.28	1.31	1.42
3	A	402	H2U	C6-C5	-3.87	1.45	1.52
3	B	402	H2U	O4-C4	-3.18	1.16	1.23
3	B	402	H2U	O2'-C2'	-2.73	1.36	1.43
3	B	402	H2U	O2-C2	-2.62	1.18	1.23
3	B	402	H2U	C6-C5	-2.45	1.48	1.52
3	A	402	H2U	O4-C4	-2.42	1.18	1.23
3	A	402	H2U	O2-C2	-2.25	1.18	1.23
3	B	402	H2U	O3'-C3'	2.21	1.48	1.43
3	A	402	H2U	O3'-C3'	2.53	1.48	1.43
5	A	416	G1P	O5-C1	4.10	1.52	1.41
5	B	418	G1P	O5-C1	4.21	1.52	1.41
3	A	402	H2U	O4'-C4'	5.00	1.56	1.45
3	B	402	H2U	O4'-C4'	5.46	1.57	1.45
3	A	402	H2U	C2-N3	5.60	1.48	1.38
3	B	402	H2U	C2-N3	5.86	1.48	1.38
3	A	402	H2U	C4-N3	6.69	1.47	1.37
3	B	402	H2U	C4-N3	6.97	1.48	1.37
3	B	402	H2U	C2-N1	8.94	1.49	1.35
3	A	402	H2U	C2-N1	9.25	1.50	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	H2U	C4-N3-C2	-8.28	118.26	125.77
3	A	402	H2U	C4-N3-C2	-5.76	120.55	125.77
3	B	402	H2U	O2-C2-N1	-4.07	117.83	123.17
3	B	402	H2U	C4'-O4'-C1'	-2.59	103.81	109.52
5	B	418	G1P	C6-C5-C4	-2.32	107.17	112.99
5	B	418	G1P	O5-C5-C4	2.25	113.95	109.67
5	A	416	G1P	O5-C5-C4	2.42	114.28	109.67
3	A	402	H2U	C2'-C3'-C4'	2.66	108.08	102.64
3	B	402	H2U	N3-C2-N1	3.48	119.87	116.64
3	A	402	H2U	N3-C2-N1	3.59	119.97	116.64
3	B	402	H2U	C5-C4-N3	4.36	121.22	116.62
3	B	402	H2U	C5-C6-N1	7.40	118.87	110.76
3	A	402	H2U	C5-C6-N1	9.07	120.70	110.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

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

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%)	1.14	42 (12%) 5 6	17, 29, 54, 80	0
1	B	330/401 (82%)	1.34	63 (19%) 2 2	21, 32, 61, 99	0
All	All	654/802 (81%)	1.24	105 (16%) 3 3	17, 31, 60, 99	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	THR	10.4
1	A	111	PRO	8.6
1	B	307	SER	7.9
1	A	47	HIS	7.7
1	A	310	GLY	7.7
1	B	22	ALA	7.1
1	A	110	GLY	7.0
1	B	311	ALA	6.9
1	B	310	GLY	6.5
1	B	110	GLY	6.4
1	B	24	PHE	5.8
1	A	48	ARG	5.3
1	B	79	ILE	5.3
1	B	112	SER	5.2
1	A	309	ALA	5.1
1	B	308	GLU	4.9
1	B	309	ALA	4.9
1	B	23	THR	4.7
1	B	27	ASN	4.6
1	B	64	THR	4.5
1	B	256	LEU	4.5
1	B	212	GLN	4.5
1	B	26	ALA	4.5
1	A	342	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	336	MET	4.3
1	B	330	ALA	4.3
1	A	112	SER	4.2
1	A	366	TYR	4.2
1	A	311	ALA	4.2
1	B	111	PRO	4.2
1	A	343	ALA	4.0
1	B	366	TYR	4.0
1	A	28	ASP	4.0
1	B	211	SER	3.6
1	B	331	THR	3.5
1	B	47	HIS	3.5
1	B	323	TYR	3.4
1	B	106	ALA	3.4
1	B	181	SER	3.4
1	A	323	TYR	3.3
1	A	113	ASP	3.3
1	B	81	ALA	3.3
1	B	46	ALA	3.3
1	A	339	TYR	3.2
1	B	48	ARG	3.1
1	B	320	ALA	3.1
1	B	299	GLY	3.0
1	B	306	GLY	3.0
1	B	108	SER	3.0
1	A	340[A]	GLU	2.9
1	B	329	SER	2.9
1	B	300	TRP	2.9
1	A	306	GLY	2.9
1	B	170	ILE	2.9
1	A	29	HIS	2.9
1	B	198	ILE	2.8
1	A	246	TRP	2.8
1	A	341	MET	2.8
1	B	314	ASN	2.8
1	B	208	ALA	2.7
1	A	308	GLU	2.7
1	B	337	VAL	2.7
1	B	364	VAL	2.7
1	B	349	LEU	2.6
1	B	171	PHE	2.6
1	B	199	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	181	SER	2.5
1	B	342	LEU	2.5
1	A	208	ALA	2.5
1	A	249	TRP	2.5
1	A	337	VAL	2.5
1	B	312	ASN	2.5
1	B	316	TRP	2.5
1	A	42	VAL	2.5
1	A	198	ILE	2.5
1	B	160	GLU	2.4
1	B	298	MET	2.4
1	B	336	MET	2.4
1	B	249	TRP	2.4
1	B	365	HIS	2.4
1	A	106	ALA	2.3
1	B	85	VAL	2.3
1	B	360	ALA	2.3
1	A	168	VAL	2.3
1	A	291	GLU	2.2
1	B	328	ARG	2.2
1	A	316	TRP	2.2
1	B	213	HIS	2.2
1	A	71	LEU	2.2
1	B	163	ALA	2.2
1	B	261	VAL	2.1
1	A	345	ALA	2.1
1	A	130	CYS	2.1
1	A	187	CYS	2.1
1	B	143	SER	2.1
1	A	170	ILE	2.1
1	A	217	LEU	2.1
1	A	330	ALA	2.1
1	B	209	TYR	2.1
1	B	113	ASP	2.1
1	B	341[A]	MET	2.0
1	A	298	MET	2.0
1	B	107	PRO	2.0
1	B	296	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	B	411	4/4	0.55	0.61	15.74	45,75,90,90	0
4	EDO	B	414	4/4	0.51	0.33	14.46	46,67,80,80	0
4	EDO	A	406	4/4	0.73	0.25	12.66	40,68,90,90	0
4	EDO	A	413	4/4	0.36	0.38	10.85	37,61,81,81	0
4	EDO	B	412	4/4	0.75	0.51	8.77	46,60,72,72	0
4	EDO	A	410	4/4	0.50	0.25	8.19	37,68,85,85	0
4	EDO	A	411	4/4	0.40	0.27	7.77	40,58,73,73	0
4	EDO	A	405	4/4	0.71	0.29	7.22	44,68,82,82	0
4	EDO	A	407	4/4	0.79	0.22	7.01	32,65,82,82	0
4	EDO	A	412	4/4	0.78	0.17	4.41	40,48,53,53	0
4	EDO	B	416	4/4	0.67	0.27	4.41	45,73,87,88	0
4	EDO	B	415	4/4	0.90	0.25	3.75	31,42,51,51	0
4	EDO	B	405	4/4	0.70	0.33	3.05	35,52,66,66	0
5	G1P	B	418	16/16	0.75	0.27	2.08	16,44,60,65	27
4	EDO	A	404	4/4	0.78	0.30	1.73	36,67,91,91	0
5	G1P	A	416	16/16	0.77	0.28	0.70	21,50,66,68	27
4	EDO	A	408	4/4	0.89	0.23	0.56	32,49,77,80	0
4	EDO	B	406	4/4	0.81	0.26	0.06	46,71,86,86	0
3	H2U	A	402	20/21	0.91	0.14	-0.22	22,27,35,39	0
4	EDO	A	403	4/4	0.93	0.10	-0.54	22,38,45,45	0
3	H2U	B	402	20/21	0.92	0.13	-0.56	25,31,38,40	0
4	EDO	B	410	4/4	0.75	0.17	-0.87	46,85,102,102	0
4	EDO	B	403	4/4	0.91	0.12	-0.90	36,58,70,70	0
2	ZN	B	401	1/1	0.99	0.08	-3.03	22,22,22,22	1
2	ZN	A	401	1/1	0.99	0.10	-6.45	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	B	407	4/4	0.74	0.24	-	45,79,95,95	0
4	EDO	A	415	4/4	0.88	0.23	-	41,80,96,96	0
4	EDO	B	408	4/4	0.46	0.52	-	39,73,87,87	0
4	EDO	A	409	4/4	0.38	0.30	-	51,65,82,82	0
4	EDO	A	414	4/4	0.72	0.34	-	45,61,73,73	0
4	EDO	B	409	4/4	0.82	0.54	-	44,76,101,101	0
4	EDO	B	417	4/4	0.89	0.26	-	40,60,65,72	0
4	EDO	B	413	4/4	0.70	0.34	-	37,64,84,84	0
4	EDO	B	404	4/4	0.73	0.44	-	46,101,140,143	0

6.5 Other polymers [i](#)

There are no such residues in this entry.