



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:20 PM EDT

PDB ID : 1FGX / pdb_00001fgx
Title : CRYSTAL STRUCTURE OF THE BOVINE BETA 1,4 GALACTOSYLTRANSFERASE (B4GALT1) CATALYTIC DOMAIN COMPLEXED WITH UMP
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Deposited on : 2000-07-29
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

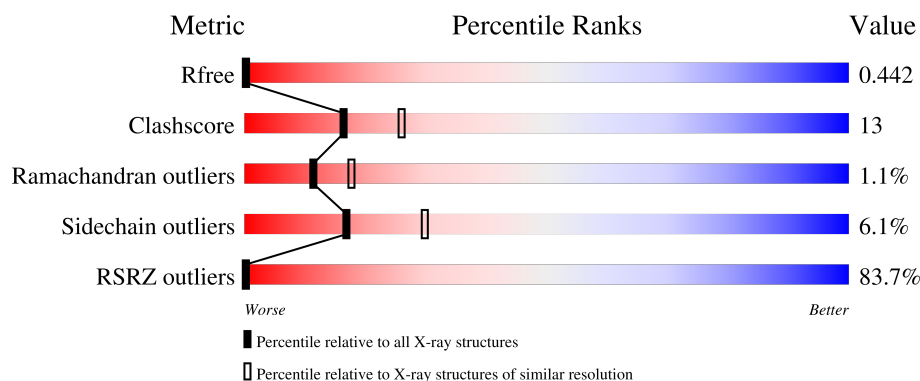
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	288	74% 60% 28% 6% 6%
1	B	288	85% 61% 27% 6% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4609 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

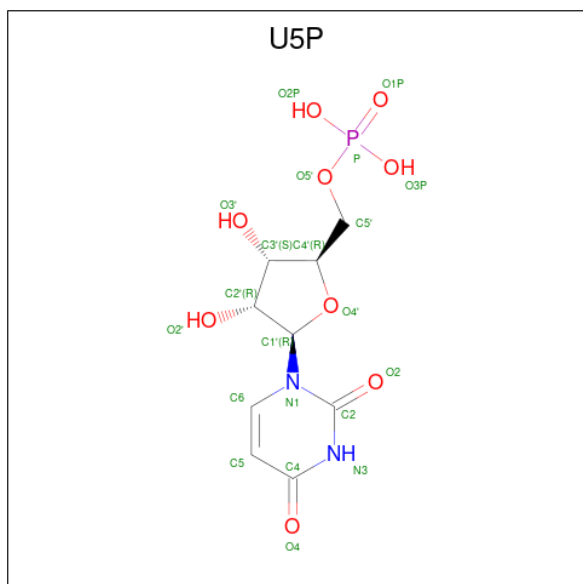
- Molecule 1 is a protein called BETA 1,4 GALACTOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2219	1425	382	398	14			
1	B	273	Total	C	N	O	S	0	0	0
			2224	1428	383	399	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	PRO	LEU	SEE REMARK 999	UNP P08037
B	187	PRO	LEU	SEE REMARK 999	UNP P08037

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: C₉H₁₃N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total 73	O 73	0	0
3	B	72	Total 72	O 72	0	0

- Molecule 1: BETA 1,4 GALACTOSYLTRANSFERASE



P357	Q358	R359	F360	D361	A364	H365	T366	K367	E368	T369	M370	L371	S372	D373	G374	L375	M376	S377	L378	T379	Y380	M381	V382	L383	E384	V385	Q386	R387	Y388	P389	L390	Y391	T392	K393	I394	T395	V396	D397	I398	G399	T400	P401	S402
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.50Å 161.00Å 107.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.28 – 2.40 29.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.28-2.40) 91.8 (29.28-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.225 , 0.268 0.401 , 0.442	Depositor DCC
R_{free} test set	1026 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	4609	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: U5P

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	0.88	1/2279 (0.0%)	1.25	20/3086 (0.6%)
1	B	0.89	0/2284	1.26	24/3093 (0.8%)
All	All	0.89	1/4563 (0.0%)	1.26	44/6179 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	MET	SD-CE	7.02	1.97	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLY	N-CA-C	9.53	135.76	113.18
1	B	182	VAL	N-CA-C	9.04	121.19	107.99
1	A	213	TYR	N-CA-C	8.62	122.26	109.24
1	B	334	ARG	CA-C-N	-8.49	112.11	120.52
1	B	334	ARG	C-N-CA	-8.49	112.11	120.52
1	A	275	VAL	N-CA-C	8.40	119.20	110.72
1	B	223	GLU	N-CA-C	-7.36	102.91	113.21
1	B	213	TYR	N-CA-C	7.32	120.53	109.41
1	A	310	ASN	N-CA-C	6.83	121.77	113.17
1	B	275	VAL	N-CA-C	6.79	118.40	111.00
1	B	310	ASN	N-CA-C	6.77	121.24	112.92
1	A	151	ILE	CA-C-N	-6.68	112.77	119.92
1	A	151	ILE	C-N-CA	-6.68	112.77	119.92
1	A	390	LEU	N-CA-C	6.50	121.37	113.38
1	A	329	GLY	N-CA-C	6.33	123.66	114.10
1	B	368	GLU	N-CA-C	6.28	118.20	111.36
1	A	271	ARG	N-CA-C	6.16	118.98	109.07
1	B	314	TRP	N-CA-C	6.13	120.02	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	SER	N-CA-C	-6.12	101.40	110.46
1	A	182	VAL	N-CA-C	6.08	117.05	108.36
1	B	390	LEU	N-CA-C	6.04	120.78	113.17
1	A	202	LEU	N-CA-C	5.96	119.73	112.23
1	B	369	THR	N-CA-C	5.95	120.70	113.38
1	B	273	ILE	N-CA-C	5.89	116.93	111.45
1	A	335	PRO	N-CA-C	-5.88	102.37	111.13
1	A	212	ASP	N-CA-C	-5.72	97.11	107.75
1	A	251	SER	N-CA-C	5.70	118.76	109.24
1	B	271	ARG	N-CA-C	5.60	118.09	109.07
1	B	254	ASP	N-CA-C	5.57	118.86	112.57
1	A	205	ILE	N-CA-C	5.54	116.18	110.36
1	A	320	ASP	N-CA-C	-5.52	105.34	111.36
1	B	188	PHE	N-CA-C	5.47	117.38	109.07
1	A	369	THR	N-CA-C	5.43	120.06	113.38
1	B	151	ILE	CA-C-N	-5.41	114.13	119.92
1	B	151	ILE	C-N-CA	-5.41	114.13	119.92
1	B	284	LEU	CA-C-N	5.37	125.44	119.32
1	B	284	LEU	C-N-CA	5.37	125.44	119.32
1	B	320	ASP	N-CA-C	-5.32	105.56	111.36
1	A	254	ASP	N-CA-C	5.17	118.42	112.57
1	B	338	VAL	N-CA-C	-5.15	106.12	111.58
1	B	212	ASP	N-CA-C	-5.12	98.97	107.99
1	B	149	PHE	N-CA-C	5.12	116.58	110.44
1	A	137	GLU	N-CA-C	-5.02	102.08	110.17
1	B	344	MET	CB-CG-SD	5.02	127.77	112.70

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	2219	0	2187	56	4
1	B	2224	0	2189	61	4
2	B	21	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	73	0	0	4	1
3	B	72	0	0	6	1
All	All	4609	0	4387	115	5

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 13.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LYS:HZ2	1:B:344:MET:HB2	1.40	0.86
1:B:279:LYS:NZ	1:B:344:MET:HB2	1.99	0.77
1:A:230:LYS:HD3	1:A:398:ILE:HB	1.66	0.77
1:A:222:GLY:O	1:A:223:GLU:HB2	1.86	0.76
1:A:131:LEU:HD13	1:A:177:ILE:HD11	1.73	0.71
1:A:151:ILE:HG13	1:A:151:ILE:O	1.92	0.69
1:B:158:ILE:HD11	1:B:200:TYR:HB2	1.74	0.68
1:A:274:SER:O	1:A:277:MET:HE2	1.95	0.67
1:B:280:PHE:CZ	1:B:357:PRO:HD3	2.31	0.66
1:B:154:ASP:OD2	1:B:156:LYS:HB2	1.97	0.64
1:A:154:ASP:OD2	1:A:156:LYS:HB2	1.98	0.63
1:A:344:MET:HG2	1:A:346:ARG:HG2	1.80	0.63
1:B:259:ASN:OD1	1:B:261:HIS:HB2	2.00	0.61
1:A:158:ILE:HD11	1:A:200:TYR:HB2	1.83	0.60
1:B:150:ASN:O	1:B:152:PRO:HD3	2.01	0.60
1:B:312:TRP:CD2	1:B:401:PRO:HG3	2.38	0.59
1:A:202:LEU:O	1:A:206:LEU:HG	2.03	0.59
1:B:234:VAL:HG11	1:B:396:VAL:HG11	1.84	0.58
1:A:232:LEU:HD22	1:A:250:PHE:HD2	1.69	0.58
1:B:132:THR:O	1:B:133:ALA:HB2	2.02	0.58
1:A:205:ILE:O	1:A:209:GLN:HG3	2.04	0.57
1:A:358:GLN:NE2	1:B:358:GLN:HG3	2.19	0.57
1:A:275:VAL:HG22	1:A:334:ARG:HD3	1.85	0.57
1:A:150:ASN:O	1:A:152:PRO:HD3	2.05	0.56
1:A:279:LYS:HD3	1:A:344:MET:SD	2.45	0.56
1:A:234:VAL:HG11	1:A:396:VAL:HG11	1.88	0.56
1:B:167:LEU:CD1	1:B:387:ARG:HB3	2.36	0.56
1:B:349:ARG:CZ	1:B:351:LYS:HB3	2.35	0.55
1:B:131:LEU:HD22	1:B:176:CYS:HA	1.88	0.55
1:B:132:THR:O	1:B:133:ALA:CB	2.54	0.55
1:B:244:ASP:O	1:B:244:ASP:CG	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLN:HE21	1:B:358:GLN:HG3	1.73	0.54
1:B:138:SER:HB3	1:B:141:LEU:HD13	1.90	0.54
1:A:259:ASN:OD1	1:A:261:HIS:HB2	2.07	0.53
1:A:233:ASN:HB3	1:A:378:LEU:HD22	1.90	0.53
1:B:151:ILE:HD12	1:B:151:ILE:O	2.09	0.52
1:B:225:MET:CE	1:B:225:MET:HA	2.39	0.52
1:B:226:PHE:HB2	2:B:101:U5P:H1'	1.90	0.52
1:A:151:ILE:O	1:A:151:ILE:CG1	2.57	0.52
1:B:312:TRP:CG	1:B:401:PRO:HG3	2.45	0.52
1:A:278:ASP:OD2	1:A:279:LYS:N	2.43	0.52
1:B:141:LEU:HD23	1:B:261:HIS:CE1	2.45	0.52
1:B:267:PHE:CD1	1:B:271:ARG:HD3	2.45	0.52
1:A:187:PRO:HD3	1:A:232:LEU:HD21	1.92	0.51
1:B:272:HIS:HB3	1:B:334:ARG:HG2	1.93	0.51
1:B:221:ALA:O	1:B:222:GLY:O	2.28	0.51
1:A:281:GLY:O	1:A:282:PHE:HB2	2.10	0.51
1:B:167:LEU:HD11	1:B:387:ARG:HB3	1.92	0.51
1:B:197:TYR:CE1	1:B:347:HIS:HE1	2.29	0.51
1:A:188:PHE:C	1:A:188:PHE:CD1	2.88	0.50
1:A:228:ARG:HB2	3:A:509:HOH:O	2.10	0.50
1:B:328:ARG:NH2	3:B:522:HOH:O	2.06	0.50
1:B:278:ASP:OD2	1:B:279:LYS:N	2.45	0.50
1:B:280:PHE:CE1	1:B:357:PRO:HD3	2.47	0.50
1:A:180:HIS:CE1	1:A:265:ARG:HD2	2.47	0.50
1:A:379:THR:N	3:A:549:HOH:O	2.13	0.49
1:A:162:ASN:HD22	1:A:207:GLN:HE22	1.58	0.49
1:B:180:HIS:CE1	1:B:265:ARG:HD2	2.48	0.48
1:B:288:GLN:HB3	1:B:322:TYR:CZ	2.47	0.48
1:B:304:ILE:HB	1:B:324:ARG:HB3	1.95	0.48
1:A:324:ARG:HG2	1:A:370:MET:HG3	1.96	0.48
1:B:279:LYS:CE	1:B:344:MET:HB2	2.44	0.48
1:A:271:ARG:NH2	1:A:335:PRO:HB3	2.29	0.48
1:A:225:MET:SD	1:A:312:TRP:HB3	2.55	0.47
1:B:323:ASN:ND2	3:B:582:HOH:O	2.35	0.47
1:A:138:SER:HB3	1:A:141:LEU:HD13	1.96	0.47
1:A:222:GLY:O	1:A:223:GLU:CB	2.56	0.47
1:A:281:GLY:N	1:A:353:ASN:OD1	2.47	0.47
1:A:275:VAL:CG2	1:A:334:ARG:HD3	2.45	0.47
1:B:164:LYS:NZ	3:B:568:HOH:O	2.48	0.47
1:B:212:ASP:OD2	1:B:243:TYR:OH	2.22	0.47
1:B:167:LEU:HD11	1:B:387:ARG:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ASP:OD2	1:B:397:ASP:C	2.58	0.46
1:B:265:ARG:NH1	3:B:641:HOH:O	2.48	0.46
1:B:288:GLN:HG3	1:B:359:ARG:NH2	2.31	0.46
1:A:175:ASP:OD1	1:A:175:ASP:N	2.48	0.46
1:B:172:THR:HG23	1:B:212:ASP:CG	2.41	0.45
1:A:167:LEU:C	1:A:167:LEU:HD13	2.41	0.45
1:B:279:LYS:NZ	1:B:344:MET:CB	2.77	0.45
1:B:198:TRP:CZ2	1:B:202:LEU:HG	2.52	0.45
1:A:167:LEU:CD1	1:A:387:ARG:HB3	2.47	0.44
1:A:328:ARG:HE	1:A:328:ARG:HB3	1.55	0.44
1:A:218:ILE:HG22	1:A:231:LEU:HD22	2.00	0.44
1:B:288:GLN:OE1	1:B:288:GLN:N	2.52	0.43
1:A:153:VAL:HG23	1:A:196:LYS:HB3	2.00	0.43
1:B:187:PRO:HD3	1:B:232:LEU:HD21	2.00	0.43
1:B:360:PHE:HA	3:B:585:HOH:O	2.19	0.43
1:B:347:HIS:O	1:B:348:SER:C	2.61	0.43
1:A:149:PHE:CE2	1:A:345:ILE:HG12	2.54	0.43
1:A:267:PHE:CD1	1:A:271:ARG:HD3	2.54	0.42
1:B:240:LEU:HD23	1:B:240:LEU:HA	1.86	0.42
1:A:347:HIS:O	1:A:348:SER:C	2.60	0.42
1:B:195:LEU:HD22	1:B:199:LEU:HG	2.01	0.42
1:B:209:GLN:O	1:B:210:GLN:HB2	2.19	0.42
1:A:135:PRO:HG3	1:A:139:PRO:HD3	2.02	0.42
1:A:167:LEU:HD11	1:A:387:ARG:HB3	2.02	0.42
1:B:142:VAL:O	1:B:142:VAL:HG12	2.19	0.42
1:B:287:VAL:HG23	3:B:559:HOH:O	2.19	0.42
1:A:363:ILE:HG23	3:A:551:HOH:O	2.19	0.42
1:A:272:HIS:HB3	1:A:334:ARG:HG2	2.01	0.42
1:A:304:ILE:HB	1:A:324:ARG:HB3	2.02	0.42
1:B:375:LEU:HD12	1:B:375:LEU:HA	1.80	0.42
1:B:279:LYS:HD2	1:B:344:MET:HB2	2.01	0.42
1:A:344:MET:O	1:A:346:ARG:HG3	2.20	0.41
1:A:378:LEU:HA	3:A:549:HOH:O	2.19	0.41
1:B:347:HIS:O	1:B:349:ARG:N	2.52	0.41
1:A:361:ASP:OD1	1:A:363:ILE:HG22	2.20	0.41
1:A:171:TYR:CD2	1:A:171:TYR:C	2.98	0.41
1:B:254:ASP:HA	1:B:345:ILE:HD12	2.02	0.41
1:B:305:ASN:O	1:B:305:ASN:CG	2.64	0.41
1:B:202:LEU:O	1:B:206:LEU:HG	2.21	0.41
1:A:198:TRP:CZ2	1:A:202:LEU:HG	2.56	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ARG:O	1:B:232:LEU:HG	2.21	0.40
1:A:167:LEU:HD11	1:A:387:ARG:CB	2.51	0.40

All (5) 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)
1:A:200:TYR:OH	1:B:160:GLN:OE1[6_554]	1.36	0.84
1:A:161:GLN:OE1	1:B:161:GLN:OE1[6_554]	1.63	0.57
1:A:161:GLN:NE2	1:B:161:GLN:OE1[6_554]	1.66	0.54
1:A:161:GLN:CD	1:B:161:GLN:OE1[6_554]	1.82	0.38
3:A:553:HOH:O	3:B:522:HOH:O[3_555]	2.10	0.10

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	270/288 (94%)	252 (93%)	15 (6%)	3 (1%)	11	18
1	B	271/288 (94%)	250 (92%)	18 (7%)	3 (1%)	11	18
All	All	541/576 (94%)	502 (93%)	33 (6%)	6 (1%)	11	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	LYS
1	B	133	ALA
1	B	222	GLY
1	B	348	SER
1	A	135	PRO
1	A	348	SER

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	245/259 (95%)	229 (94%)	16 (6%)	15	27
1	B	245/259 (95%)	231 (94%)	14 (6%)	18	33
All	All	490/518 (95%)	460 (94%)	30 (6%)	17	30

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	175	ASP
1	A	188	PHE
1	A	189	ARG
1	A	195	LEU
1	A	223	GLU
1	A	224	SER
1	A	263	THR
1	A	270	PRO
1	A	336	ASN
1	A	343	ARG
1	A	344	MET
1	A	346	ARG
1	A	350	ASP
1	A	351	LYS
1	A	400	THR
1	B	141	LEU
1	B	149	PHE
1	B	166	LYS
1	B	175	ASP
1	B	189	ARG
1	B	195	LEU
1	B	223	GLU
1	B	225	MET
1	B	244	ASP
1	B	263	THR
1	B	265	ARG

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Mol	Chain	Res	Type
1	B	270	PRO
1	B	302	LEU
1	B	368	GLU

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

Mol	Chain	Res	Type
1	A	161	GLN
1	A	162	ASN
1	A	210	GLN
1	A	219	ASN
1	A	310	ASN
1	A	358	GLN
1	B	161	GLN
1	B	210	GLN
1	B	219	ASN
1	B	310	ASN
1	B	347	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	U5P	B	101	-	22,22,22	1.92	9 (40%)	32,33,33	1.78	9 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	U5P	B	101	-	-	7/10/26/26	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	U5P	P-O3P	3.96	1.69	1.54
2	B	101	U5P	C1'-N1	3.63	1.57	1.47
2	B	101	U5P	O3'-C3'	2.59	1.49	1.43
2	B	101	U5P	C6-N1	2.45	1.43	1.38
2	B	101	U5P	C5'-C4'	2.35	1.58	1.51
2	B	101	U5P	C2-N1	2.26	1.42	1.38
2	B	101	U5P	C2-N3	2.14	1.41	1.38
2	B	101	U5P	C4-N3	2.04	1.42	1.38
2	B	101	U5P	O4'-C4'	2.01	1.49	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	U5P	O5'-P-O1P	4.34	118.16	106.44
2	B	101	U5P	O4'-C1'-N1	3.89	117.17	108.36
2	B	101	U5P	O5'-C5'-C4'	2.80	118.53	108.99
2	B	101	U5P	O2-C2-N1	-2.52	119.51	122.80
2	B	101	U5P	O3P-P-O5'	-2.47	100.24	106.67
2	B	101	U5P	C2'-C1'-N1	2.37	119.84	113.25
2	B	101	U5P	C2'-C3'-C4'	-2.30	98.17	102.61
2	B	101	U5P	C6-N1-C2	-2.23	118.28	121.00
2	B	101	U5P	O3P-P-O1P	2.03	118.76	110.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

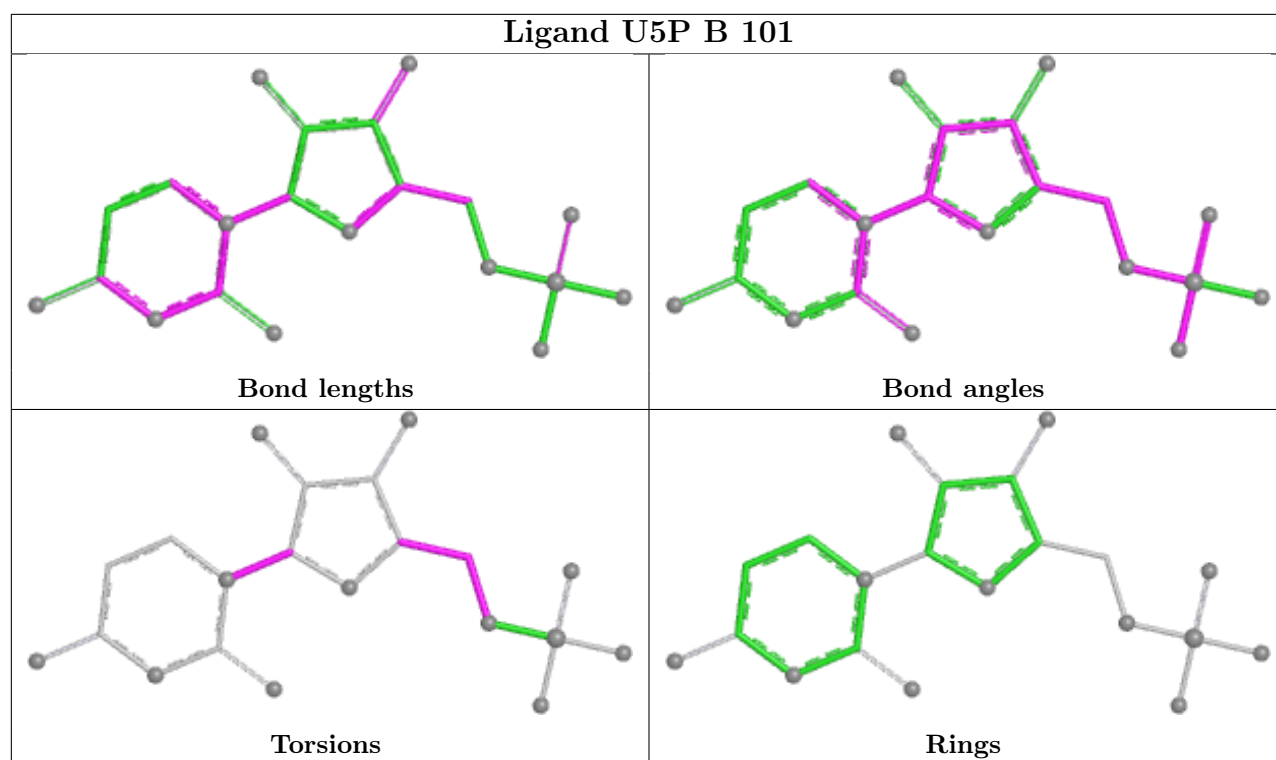
Mol	Chain	Res	Type	Atoms
2	B	101	U5P	O4'-C1'-N1-C2
2	B	101	U5P	O4'-C1'-N1-C6
2	B	101	U5P	C4'-C5'-O5'-P
2	B	101	U5P	C2'-C1'-N1-C6
2	B	101	U5P	C2'-C1'-N1-C2
2	B	101	U5P	C3'-C4'-C5'-O5'
2	B	101	U5P	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	101	U5P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [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	272/288 (94%)	2.99	212 (77%) 0 0	39, 57, 94, 98	0
1	B	273/288 (94%)	3.50	244 (89%) 0 0	34, 54, 90, 98	0
All	All	545/576 (94%)	3.25	456 (83%) 0 0	34, 56, 93, 98	0

All (456) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	LEU	8.2
1	B	391	TYR	7.9
1	A	138	SER	7.6
1	A	176	CYS	7.4
1	B	138	SER	7.4
1	A	267	PHE	7.3
1	B	384	GLU	6.9
1	B	197	TYR	6.8
1	B	166	LYS	6.7
1	B	385	VAL	6.6
1	B	242	ASP	6.5
1	A	353	ASN	6.4
1	A	164	LYS	6.4
1	B	388	TYR	6.3
1	B	186	ILE	6.3
1	A	245	TYR	6.3
1	B	213	TYR	6.3
1	A	131	LEU	6.2
1	B	214	GLY	6.0
1	A	171	TYR	6.0
1	B	236	PHE	5.9
1	B	171	TYR	5.9
1	B	263	THR	5.8
1	A	153	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	179	PRO	5.8
1	B	176	CYS	5.8
1	B	200	TYR	5.8
1	A	332	VAL	5.8
1	B	223	GLU	5.7
1	B	245	TYR	5.7
1	A	273	ILE	5.6
1	B	394	ILE	5.5
1	A	240	LEU	5.5
1	B	157	LEU	5.5
1	B	229	ALA	5.5
1	A	170	ARG	5.5
1	A	266	CYS	5.4
1	B	158	ILE	5.4
1	A	248	PHE	5.4
1	B	395	THR	5.4
1	B	155	LEU	5.4
1	B	165	VAL	5.3
1	B	170	ARG	5.3
1	B	314	TRP	5.3
1	B	153	VAL	5.2
1	A	180	HIS	5.2
1	B	243	TYR	5.2
1	B	237	LYS	5.2
1	B	247	CYS	5.2
1	B	382	VAL	5.1
1	B	185	ILE	5.1
1	A	242	ASP	5.1
1	A	390	LEU	5.1
1	B	295	ALA	5.1
1	B	266	CYS	5.1
1	B	167	LEU	5.1
1	B	377	SER	5.1
1	A	169	GLY	5.1
1	A	360	PHE	5.0
1	A	173	PRO	5.0
1	B	227	ASN	5.0
1	B	387	ARG	4.9
1	A	283	SER	4.9
1	A	211	LEU	4.9
1	A	177	ILE	4.9
1	B	188	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	387	ARG	4.8
1	B	322	TYR	4.8
1	A	174	MET	4.8
1	B	187	PRO	4.8
1	B	180	HIS	4.8
1	A	243	TYR	4.8
1	B	326	ALA	4.7
1	B	281	GLY	4.7
1	B	330	MET	4.6
1	B	198	TRP	4.6
1	B	306	GLY	4.6
1	A	151	ILE	4.6
1	A	158	ILE	4.6
1	B	134	CYS	4.6
1	B	256	ILE	4.6
1	B	398	ILE	4.6
1	B	160	GLN	4.6
1	B	393	LYS	4.6
1	B	146	LEU	4.5
1	B	217	VAL	4.5
1	B	152	PRO	4.5
1	A	162	ASN	4.5
1	A	331	SER	4.5
1	B	337	ALA	4.5
1	B	164	LYS	4.5
1	B	195	LEU	4.5
1	B	380	TYR	4.5
1	A	246	ASN	4.5
1	A	160	GLN	4.5
1	A	386	GLN	4.5
1	B	386	GLN	4.5
1	A	183	ALA	4.5
1	A	157	LEU	4.5
1	B	202	LEU	4.5
1	B	383	LEU	4.5
1	A	236	PHE	4.4
1	B	268	SER	4.4
1	A	339	ILE	4.4
1	B	205	ILE	4.4
1	B	347	HIS	4.4
1	A	295	ALA	4.4
1	A	224	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	137	GLU	4.3
1	A	260	ASP	4.3
1	B	397	ASP	4.3
1	B	257	PRO	4.3
1	A	261	HIS	4.3
1	B	264	TYR	4.3
1	B	332	VAL	4.3
1	A	140	LEU	4.3
1	A	200	TYR	4.3
1	B	144	PRO	4.2
1	A	292	GLY	4.2
1	A	141	LEU	4.2
1	B	201	TYR	4.2
1	B	184	ILE	4.2
1	B	390	LEU	4.2
1	A	291	GLY	4.2
1	B	130	SER	4.2
1	A	134	CYS	4.1
1	B	199	LEU	4.1
1	B	211	LEU	4.1
1	B	221	ALA	4.1
1	A	132	THR	4.1
1	B	378	LEU	4.1
1	B	307	PHE	4.1
1	B	312	TRP	4.1
1	A	143	GLY	4.1
1	B	173	PRO	4.1
1	B	178	SER	4.0
1	B	177	ILE	4.0
1	B	231	LEU	4.0
1	B	376	ASN	4.0
1	B	204	PRO	4.0
1	B	344	MET	4.0
1	A	333	SER	4.0
1	B	331	SER	4.0
1	B	172	THR	4.0
1	B	192	GLN	4.0
1	A	222	GLY	3.9
1	A	142	VAL	3.9
1	B	216	TYR	3.9
1	B	399	GLY	3.9
1	A	175	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	159	GLU	3.9
1	B	139	PRO	3.9
1	B	175	ASP	3.9
1	B	210	GLN	3.9
1	B	135	PRO	3.9
1	A	370	MET	3.8
1	B	276	ALA	3.8
1	A	150	ASN	3.8
1	A	326	ALA	3.8
1	B	131	LEU	3.8
1	A	139	PRO	3.8
1	A	247	CYS	3.8
1	B	219	ASN	3.8
1	A	155	LEU	3.8
1	A	214	GLY	3.7
1	A	302	LEU	3.7
1	B	299	GLN	3.7
1	B	174	MET	3.7
1	B	196	LYS	3.7
1	B	208	ARG	3.7
1	B	226	PHE	3.7
1	B	392	THR	3.6
1	B	222	GLY	3.6
1	B	141	LEU	3.6
1	A	207	GLN	3.6
1	B	163	PRO	3.6
1	B	162	ASN	3.6
1	B	336	ASN	3.6
1	A	165	VAL	3.6
1	B	215	ILE	3.6
1	B	304	ILE	3.6
1	B	145	MET	3.5
1	A	239	ALA	3.5
1	A	233	ASN	3.5
1	A	203	HIS	3.5
1	B	189	ARG	3.5
1	A	199	LEU	3.5
1	A	345	ILE	3.5
1	A	334	ARG	3.5
1	A	391	TYR	3.5
1	A	163	PRO	3.5
1	A	237	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	349	ARG	3.5
1	A	172	THR	3.4
1	B	253	VAL	3.4
1	A	168	GLY	3.4
1	B	270	PRO	3.4
1	A	215	ILE	3.4
1	B	261	HIS	3.4
1	B	259	ASN	3.4
1	B	381	MET	3.4
1	B	396	VAL	3.4
1	A	322	TYR	3.4
1	A	351	LYS	3.4
1	B	235	GLY	3.4
1	A	147	ILE	3.4
1	A	337	ALA	3.4
1	B	339	ILE	3.4
1	A	197	TYR	3.4
1	B	149	PHE	3.4
1	A	262	ASN	3.4
1	A	181	LYS	3.4
1	B	240	LEU	3.4
1	A	133	ALA	3.4
1	B	260	ASP	3.3
1	A	135	PRO	3.3
1	A	217	VAL	3.3
1	B	296	LEU	3.3
1	B	273	ILE	3.3
1	A	137	GLU	3.3
1	B	364	ALA	3.3
1	A	213	TYR	3.3
1	A	388	TYR	3.3
1	A	300	GLN	3.3
1	B	379	THR	3.3
1	A	330	MET	3.3
1	A	286	TYR	3.3
1	B	375	LEU	3.3
1	B	168	GLY	3.3
1	A	204	PRO	3.2
1	B	389	PRO	3.2
1	A	312	TRP	3.2
1	A	178	SER	3.2
1	A	301	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	300	GLN	3.2
1	A	275	VAL	3.2
1	A	338	VAL	3.2
1	A	184	ILE	3.2
1	A	378	LEU	3.2
1	B	206	LEU	3.2
1	A	289	TYR	3.2
1	A	342	CYS	3.2
1	B	161	GLN	3.2
1	B	209	GLN	3.2
1	B	301	PHE	3.2
1	A	202	LEU	3.2
1	A	371	LEU	3.2
1	B	357	PRO	3.2
1	B	218	ILE	3.2
1	A	149	PHE	3.1
1	A	198	TRP	3.1
1	B	203	HIS	3.1
1	B	246	ASN	3.1
1	A	392	THR	3.1
1	B	238	GLU	3.1
1	A	381	MET	3.1
1	B	277	MET	3.1
1	B	325	LEU	3.1
1	A	362	ARG	3.1
1	B	358	GLN	3.1
1	A	166	LYS	3.1
1	A	179	PRO	3.1
1	B	355	PRO	3.1
1	A	251	SER	3.1
1	B	255	LEU	3.1
1	A	366	THR	3.1
1	B	311	TYR	3.1
1	A	161	GLN	3.1
1	B	239	ALA	3.0
1	B	282	PHE	3.0
1	B	371	LEU	3.0
1	B	318	ASP	3.0
1	B	294	SER	3.0
1	A	182	VAL	3.0
1	B	142	VAL	3.0
1	A	395	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	258	MET	3.0
1	A	335	PRO	3.0
1	A	375	LEU	3.0
1	B	372	SER	3.0
1	A	241	LYS	3.0
1	B	292	GLY	3.0
1	A	249	VAL	3.0
1	B	151	ILE	3.0
1	A	263	THR	3.0
1	A	369	THR	3.0
1	A	206	LEU	3.0
1	B	350	ASP	3.0
1	A	336	ASN	3.0
1	B	150	ASN	3.0
1	B	194	HIS	3.0
1	B	319	ASP	3.0
1	B	333	SER	3.0
1	B	334	ARG	2.9
1	A	156	LYS	2.9
1	A	216	TYR	2.9
1	A	268	SER	2.9
1	B	356	ASN	2.9
1	A	296	LEU	2.9
1	A	380	TYR	2.9
1	B	374	GLY	2.9
1	A	201	TYR	2.9
1	B	143	GLY	2.9
1	B	274	SER	2.9
1	B	402	SER	2.9
1	B	345	ILE	2.9
1	B	249	VAL	2.9
1	B	265	ARG	2.9
1	B	352	LYS	2.9
1	A	258	MET	2.9
1	A	205	ILE	2.8
1	A	208	ARG	2.8
1	A	265	ARG	2.8
1	A	257	PRO	2.8
1	A	358	GLN	2.8
1	B	248	PHE	2.8
1	B	297	SER	2.8
1	B	234	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	285	PRO	2.8
1	B	315	GLY	2.8
1	B	303	SER	2.8
1	A	212	ASP	2.8
1	A	350	ASP	2.8
1	B	346	ARG	2.8
1	B	233	ASN	2.8
1	B	182	VAL	2.8
1	B	228	ARG	2.8
1	B	252	ASP	2.8
1	A	282	PHE	2.8
1	A	374	GLY	2.7
1	A	377	SER	2.7
1	B	368	GLU	2.7
1	B	293	VAL	2.7
1	A	195	LEU	2.7
1	B	132	THR	2.7
1	B	367	LYS	2.7
1	A	152	PRO	2.7
1	A	145	MET	2.7
1	A	284	LEU	2.7
1	A	319	ASP	2.7
1	A	305	ASN	2.7
1	A	277	MET	2.7
1	A	348	SER	2.7
1	B	348	SER	2.7
1	B	183	ALA	2.7
1	A	210	GLN	2.7
1	A	154	ASP	2.6
1	A	186	ILE	2.6
1	A	323	ASN	2.6
1	B	207	GLN	2.6
1	B	289	TYR	2.6
1	B	329	GLY	2.6
1	B	343	ARG	2.6
1	B	370	MET	2.6
1	A	293	VAL	2.6
1	B	148	GLU	2.6
1	A	221	ALA	2.6
1	A	288	GLN	2.6
1	B	288	GLN	2.6
1	A	364	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	2.6
1	B	244	ASP	2.6
1	A	136	GLU	2.6
1	B	193	GLU	2.6
1	A	376	ASN	2.6
1	B	308	PRO	2.5
1	B	232	LEU	2.5
1	A	310	ASN	2.5
1	B	230	LYS	2.5
1	B	291	GLY	2.5
1	A	321	ILE	2.5
1	A	244	ASP	2.5
1	B	220	GLN	2.5
1	A	356	ASN	2.5
1	B	190	ASN	2.5
1	A	298	LYS	2.5
1	B	341	LYS	2.5
1	B	156	LYS	2.4
1	B	140	LEU	2.4
1	B	191	ARG	2.4
1	A	253	VAL	2.4
1	A	281	GLY	2.4
1	B	169	GLY	2.4
1	B	340	GLY	2.4
1	A	318	ASP	2.4
1	B	212	ASP	2.4
1	A	220	GLN	2.4
1	A	264	TYR	2.4
1	B	225	MET	2.4
1	A	398	ILE	2.4
1	A	192	GLN	2.4
1	B	271	ARG	2.4
1	B	360	PHE	2.4
1	A	193	GLU	2.4
1	B	298	LYS	2.4
1	B	224	SER	2.4
1	A	299	GLN	2.4
1	B	262	ASN	2.4
1	B	323	ASN	2.4
1	B	133	ALA	2.4
1	A	185	ILE	2.3
1	A	394	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	347	HIS	2.3
1	B	365	HIS	2.3
1	A	344	MET	2.3
1	B	342	CYS	2.3
1	A	250	PHE	2.3
1	B	280	PHE	2.3
1	B	181	LYS	2.3
1	A	227	ASN	2.3
1	A	401	PRO	2.3
1	A	379	THR	2.3
1	A	402	SER	2.3
1	B	361	ASP	2.3
1	A	349	ARG	2.3
1	A	194	HIS	2.3
1	A	307	PHE	2.3
1	A	382	VAL	2.3
1	A	259	ASN	2.3
1	A	209	GLN	2.3
1	B	250	PHE	2.3
1	A	255	LEU	2.2
1	B	251	SER	2.2
1	B	284	LEU	2.2
1	A	361	ASP	2.2
1	B	359	ARG	2.2
1	B	267	PHE	2.2
1	A	352	LYS	2.2
1	A	329	GLY	2.2
1	A	373	ASP	2.2
1	B	373	ASP	2.2
1	A	385	VAL	2.1
1	B	287	VAL	2.1
1	B	154	ASP	2.1
1	A	144	PRO	2.1
1	A	270	PRO	2.1
1	B	327	PHE	2.1
1	B	366	THR	2.1
1	B	335	PRO	2.1
1	A	190	ASN	2.1
1	A	346	ARG	2.1
1	B	324	ARG	2.1
1	A	306	GLY	2.1
1	A	324	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	GLU	2.1
1	A	256	ILE	2.1
1	A	311	TYR	2.1
1	A	287	VAL	2.0
1	A	359	ARG	2.0
1	A	363	ILE	2.0
1	A	317	GLU	2.0
1	B	309	ASN	2.0
1	A	314	TRP	2.0
1	A	308	PRO	2.0
1	A	357	PRO	2.0
1	B	254	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

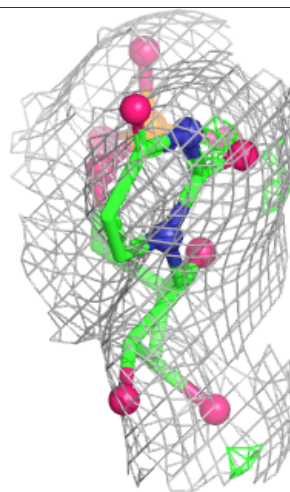
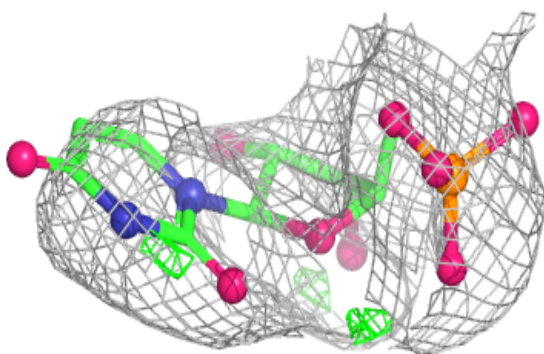
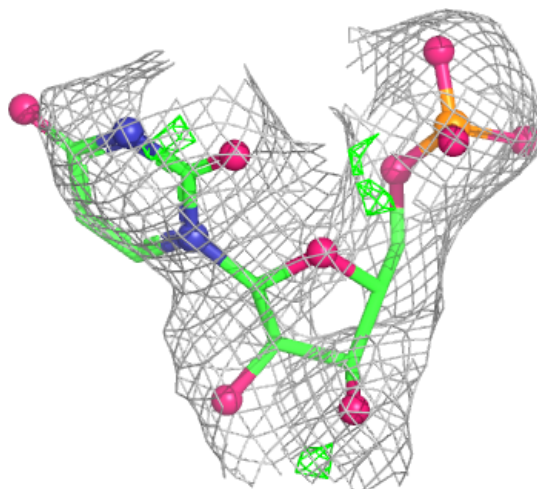
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	U5P	B	101	21/21	0.53	0.21	92,98,98,98	0

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

Electron density around U5P B 101:

$2mF_o-DF_c$ (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.