



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:40 PM UTC

PDB ID : 8H5D / pdb_00008h5d
Title : Crystal structure of YojK mutant in complex with UDP
Authors : Hou, X.D.; Yang, S.; Yin, D.J.; Rao, Y.J.
Deposited on : 2022-10-12
Resolution : 2.50 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

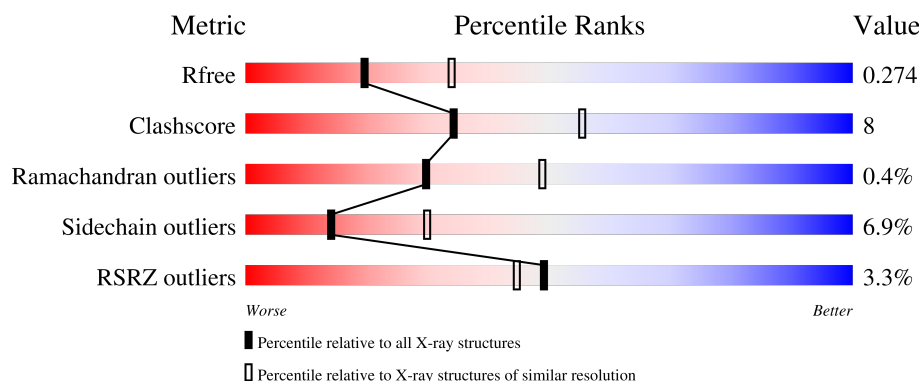
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	414	
1	B	414	

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
3	GOL	A	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6525 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3160	2015	521	607	17			
1	B	384	Total	C	N	O	S	0	0	0
			3063	1953	503	593	14			

There are 28 discrepancies between the modelled and reference sequences:

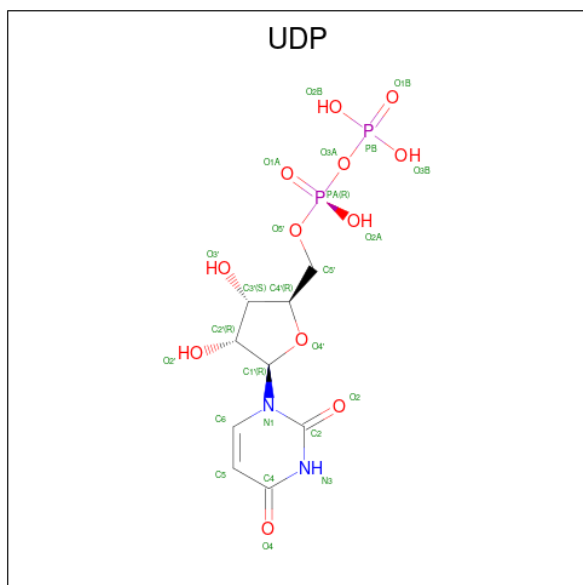
Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLU	SER	engineered mutation	UNP O31853
A	218	HIS	ALA	engineered mutation	UNP O31853
A	241	THR	ILE	engineered mutation	UNP O31853
A	327	ASN	GLY	engineered mutation	UNP O31853
A	369	LYS	ALA	engineered mutation	UNP O31853
A	406	ALA	-	expression tag	UNP O31853
A	407	LEU	-	expression tag	UNP O31853
A	408	GLU	-	expression tag	UNP O31853
A	409	HIS	-	expression tag	UNP O31853
A	410	HIS	-	expression tag	UNP O31853
A	411	HIS	-	expression tag	UNP O31853
A	412	HIS	-	expression tag	UNP O31853
A	413	HIS	-	expression tag	UNP O31853
A	414	HIS	-	expression tag	UNP O31853
B	158	GLU	SER	engineered mutation	UNP O31853
B	218	HIS	ALA	engineered mutation	UNP O31853
B	241	THR	ILE	engineered mutation	UNP O31853
B	327	ASN	GLY	engineered mutation	UNP O31853
B	369	LYS	ALA	engineered mutation	UNP O31853
B	406	ALA	-	expression tag	UNP O31853
B	407	LEU	-	expression tag	UNP O31853
B	408	GLU	-	expression tag	UNP O31853
B	409	HIS	-	expression tag	UNP O31853
B	410	HIS	-	expression tag	UNP O31853
B	411	HIS	-	expression tag	UNP O31853

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Chain	Residue	Modelled	Actual	Comment	Reference
B	412	HIS	-	expression tag	UNP O31853
B	413	HIS	-	expression tag	UNP O31853
B	414	HIS	-	expression tag	UNP O31853

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

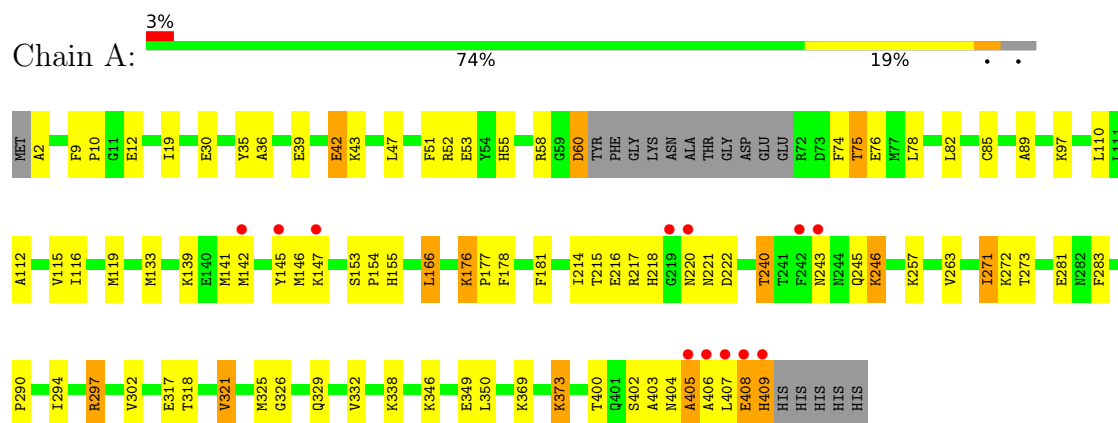
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	113	Total	O	0	0
			113	113		

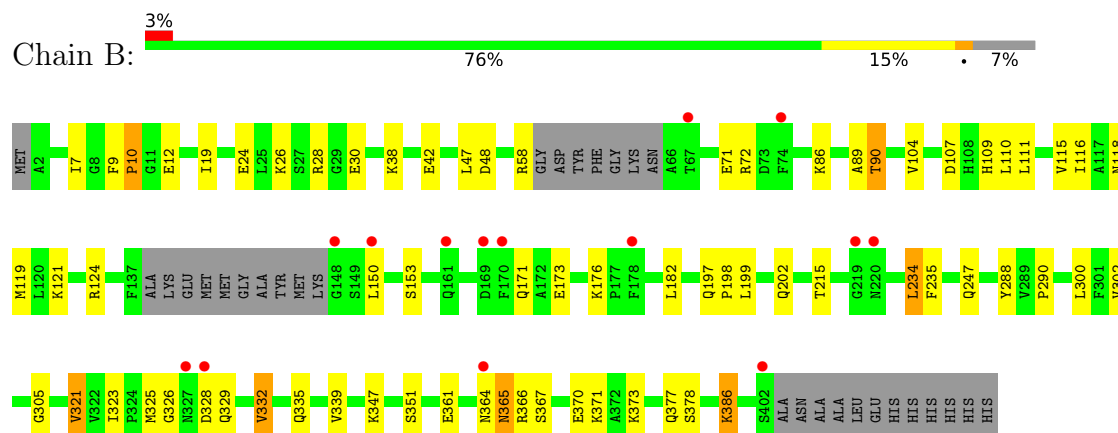
3 Residue-property plots

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: Glycosyltransferase



• Molecule 1: Glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.75Å 79.98Å 99.24Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	62.35 – 2.50 62.35 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (62.35-2.50) 99.7 (62.35-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.179 , 0.273 0.187 , 0.274	Depositor DCC
R_{free} test set	1264 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6525	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: GOL, UDP

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	1.08	0/3223	1.53	6/4339 (0.1%)
1	B	1.07	1/3123 (0.0%)	1.55	11/4206 (0.3%)
All	All	1.08	1/6346 (0.0%)	1.54	17/8545 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	PRO	C-O	-5.82	1.19	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ASP	CA-C-N	6.46	129.58	120.28
1	B	107	ASP	C-N-CA	6.46	129.58	120.28
1	B	365	ASN	CB-CA-C	6.01	119.75	110.14
1	B	365	ASN	CA-C-N	5.89	128.09	120.44
1	B	365	ASN	C-N-CA	5.89	128.09	120.44
1	A	221	ASN	CA-C-N	5.64	132.32	121.54
1	A	221	ASN	C-N-CA	5.64	132.32	121.54
1	B	290	PRO	CA-C-N	5.33	127.42	120.28
1	B	290	PRO	C-N-CA	5.33	127.42	120.28
1	B	378	SER	CA-C-N	5.28	127.30	120.44
1	B	378	SER	C-N-CA	5.28	127.30	120.44
1	A	406	ALA	N-CA-C	-5.25	106.74	112.72
1	B	328	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	405	ALA	CA-C-N	5.11	130.95	122.73
1	A	405	ALA	C-N-CA	5.11	130.95	122.73
1	B	351	SER	CA-C-O	-5.04	115.86	121.51
1	A	218	HIS	CB-CA-C	5.02	118.97	109.37

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	3160	0	3105	61	0
1	B	3063	0	3002	37	0
2	A	25	0	11	1	0
2	B	25	0	11	0	0
3	A	6	0	8	4	0
4	A	133	0	0	4	0
4	B	113	0	0	5	0
All	All	6525	0	6137	94	0

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 8.

All (94) 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:110:LEU:HA	3:A:502:GOL:H32	1.47	0.96
1:B:89:ALA:HA	1:B:116:ILE:HD11	1.54	0.88
1:B:19:ILE:HG23	1:B:47:LEU:HD11	1.57	0.85
1:A:89:ALA:HA	1:A:116:ILE:HD11	1.67	0.75
1:A:402:SER:HA	1:B:90:THR:HG21	1.69	0.75
1:A:75:THR:HG23	1:A:155:HIS:HB2	1.70	0.74
1:B:325:MET:HE1	1:B:347:LYS:HG3	1.70	0.70
1:A:271:ILE:HG22	4:A:639:HOH:O	1.92	0.69
1:A:42:GLU:H	1:A:42:GLU:CD	2.02	0.68
1:B:104:VAL:O	1:B:124:ARG:HA	1.94	0.68
1:A:297:ARG:HH11	1:A:297:ARG:CG	2.09	0.65
1:B:361:GLU:O	1:B:365:ASN:HB3	1.96	0.65
1:B:305:GLY:O	1:B:332:VAL:HG21	1.98	0.64
1:B:364:ASN:HB3	4:B:707:HOH:O	1.99	0.62
1:A:145:TYR:HB3	4:A:703:HOH:O	2.00	0.61
1:A:55:HIS:HE1	1:A:60:ASP:O	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLU:HG2	1:B:386:LYS:HA	1.83	0.60
1:B:325:MET:HE3	1:B:325:MET:HA	1.83	0.60
1:B:326:GLY:O	1:B:329:GLN:HB2	2.01	0.60
1:A:402:SER:HA	1:B:90:THR:CG2	2.33	0.58
1:A:317:GLU:OE1	1:A:373:LYS:HG3	2.04	0.58
1:B:373:LYS:O	1:B:377:GLN:HG3	2.06	0.56
1:A:145:TYR:CB	4:A:703:HOH:O	2.55	0.55
1:A:55:HIS:CE1	1:A:60:ASP:O	2.58	0.55
1:A:133:MET:CE	1:A:141:MET:HE2	2.36	0.55
1:A:133:MET:HE2	1:A:141:MET:HE2	1.90	0.54
1:B:234:LEU:HD13	1:B:300:LEU:HD23	1.90	0.54
1:A:409:HIS:C	1:A:409:HIS:CD2	2.86	0.53
1:A:82:LEU:HD22	1:A:166:LEU:HD13	1.91	0.53
1:B:199:LEU:HB3	1:B:202:GLN:HG3	1.91	0.53
1:A:297:ARG:HH11	1:A:297:ARG:HG3	1.75	0.52
1:A:35:TYR:CZ	1:A:52:ARG:HD2	2.45	0.51
1:A:240:THR:HB	2:A:501:UDP:O2B	2.10	0.51
1:B:9:PHE:CG	1:B:10:PRO:HD2	2.45	0.51
1:A:19:ILE:HG23	1:A:47:LEU:HD11	1.92	0.51
1:A:302:VAL:HG22	1:A:321:VAL:HG13	1.91	0.51
1:B:361:GLU:O	1:B:365:ASN:CB	2.59	0.50
1:B:302:VAL:HG13	1:B:321:VAL:HG22	1.94	0.50
1:A:176:LYS:HD2	1:A:178:PHE:HB2	1.93	0.49
1:A:403:ALA:C	1:A:405:ALA:H	2.19	0.49
1:A:2:ALA:N	1:A:30:GLU:OE2	2.45	0.49
1:B:30:GLU:HA	1:B:30:GLU:OE1	2.13	0.49
1:B:118:ASN:ND2	1:B:171:GLN:HB2	2.28	0.48
1:A:346:LYS:HB2	1:A:349:GLU:HG3	1.96	0.48
1:A:263:VAL:HG11	1:A:283:PHE:CZ	2.49	0.48
1:A:36:ALA:HB3	1:A:51:PHE:HE1	1.79	0.47
1:A:12:GLU:CD	1:A:43:LYS:HE3	2.39	0.47
1:B:364:ASN:CB	4:B:707:HOH:O	2.58	0.47
1:A:263:VAL:CG1	1:A:283:PHE:CE2	2.98	0.46
1:A:408:GLU:HG3	1:B:119:MET:HE3	1.96	0.46
1:A:297:ARG:HB3	4:A:665:HOH:O	2.15	0.46
1:A:263:VAL:HG11	1:A:283:PHE:CE2	2.51	0.45
1:B:197:GLN:HG3	1:B:198:PRO:O	2.15	0.45
1:A:39:GLU:OE2	1:A:58:ARG:NH2	2.50	0.45
1:B:109:HIS:HD2	4:B:650:HOH:O	1.99	0.44
1:A:85:CYS:HA	3:A:502:GOL:H11	1.99	0.44
1:A:110:LEU:HG	3:A:502:GOL:HO1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HD3	1:A:178:PHE:H	1.83	0.44
1:A:220:ASN:HA	1:A:290:PRO:HB3	1.99	0.44
1:A:290:PRO:O	1:A:294:ILE:HG12	2.17	0.44
1:A:78:LEU:HD23	1:A:181:PHE:CZ	2.53	0.44
1:A:112:ALA:O	1:A:116:ILE:HG12	2.18	0.43
1:A:246:LYS:HE2	1:A:271:ILE:HD11	2.00	0.43
1:B:7:ILE:HG22	1:B:110:LEU:CD2	2.48	0.43
1:A:85:CYS:CA	3:A:502:GOL:H11	2.48	0.43
1:B:305:GLY:O	1:B:332:VAL:CG2	2.67	0.43
1:A:400:THR:O	1:A:404:ASN:N	2.36	0.43
1:B:364:ASN:HA	4:B:707:HOH:O	2.19	0.43
1:A:217:ARG:O	1:A:220:ASN:ND2	2.50	0.43
1:B:182:LEU:HB2	4:B:630:HOH:O	2.18	0.43
1:A:153:SER:HA	1:A:154:PRO:HD3	1.92	0.43
1:B:150:LEU:O	1:B:153:SER:HB3	2.19	0.42
1:A:145:TYR:HD1	1:A:146:MET:H	1.66	0.42
1:B:26:LYS:NZ	1:B:48:ASP:HB3	2.35	0.42
1:A:214:ILE:O	1:A:215:THR:HG23	2.20	0.42
1:B:339:VAL:O	1:B:371:LYS:HE3	2.20	0.42
1:A:176:LYS:CD	1:A:178:PHE:H	2.32	0.42
1:B:234:LEU:HD12	1:B:235:PHE:N	2.35	0.42
1:A:115:VAL:CG1	1:A:119:MET:HE3	2.50	0.42
1:A:216:GLU:HG2	1:A:220:ASN:HD21	1.85	0.42
1:A:325:MET:HE3	1:A:325:MET:HB2	1.86	0.42
1:A:133:MET:HE2	1:A:141:MET:CE	2.49	0.41
1:A:402:SER:CA	1:B:90:THR:HG21	2.46	0.41
1:A:9:PHE:CG	1:A:10:PRO:HD2	2.55	0.41
1:B:12:GLU:OE1	1:B:288:TYR:OH	2.25	0.41
1:B:42:GLU:H	1:B:42:GLU:CD	2.29	0.41
1:A:36:ALA:O	1:A:53:GLU:HA	2.21	0.41
1:A:176:LYS:HD3	1:A:177:PRO:N	2.36	0.41
1:B:366:ARG:O	1:B:370:GLU:HG3	2.21	0.41
1:A:240:THR:O	1:A:240:THR:CG2	2.69	0.41
1:A:75:THR:HG23	1:A:155:HIS:CB	2.44	0.40
1:A:74:PHE:HD2	1:A:146:MET:HE2	1.85	0.40
1:A:326:GLY:O	1:A:329:GLN:HB2	2.21	0.40
1:B:111:LEU:O	1:B:115:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

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	393/414 (95%)	370 (94%)	21 (5%)	2 (0%)	24	43
1	B	378/414 (91%)	355 (94%)	22 (6%)	1 (0%)	36	55
All	All	771/828 (93%)	725 (94%)	43 (6%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	222	ASP
1	B	173	GLU

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	343/357 (96%)	314 (92%)	29 (8%)	10	22
1	B	335/357 (94%)	317 (95%)	18 (5%)	20	41
All	All	678/714 (95%)	631 (93%)	47 (7%)	14	30

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	60	ASP
1	A	75	THR

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Mol	Chain	Res	Type
1	A	76	GLU
1	A	97	LYS
1	A	142	MET
1	A	147	LYS
1	A	166	LEU
1	A	176	LYS
1	A	240	THR
1	A	243	ASN
1	A	245	GLN
1	A	246	LYS
1	A	257	LYS
1	A	271	ILE
1	A	272	LYS
1	A	273	THR
1	A	281	GLU
1	A	297	ARG
1	A	318	THR
1	A	321	VAL
1	A	332	VAL
1	A	338	LYS
1	A	350	LEU
1	A	369	LYS
1	A	373	LYS
1	A	407	LEU
1	A	408	GLU
1	A	409	HIS
1	B	28	ARG
1	B	38	LYS
1	B	58	ARG
1	B	71	GLU
1	B	72	ARG
1	B	86	LYS
1	B	90	THR
1	B	121	LYS
1	B	176	LYS
1	B	215	THR
1	B	234	LEU
1	B	247	GLN
1	B	321	VAL
1	B	323	ILE
1	B	332	VAL
1	B	335	GLN

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Mol	Chain	Res	Type
1	B	367	SER
1	B	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	91	HIS
1	A	171	GLN
1	A	220	ASN
1	A	243	ASN
1	A	244	ASN
1	A	251	GLN
1	A	327	ASN
1	A	401	GLN
1	A	409	HIS
1	B	98	HIS
1	B	109	HIS
1	B	161	GLN
1	B	327	ASN
1	B	401	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UDP	B	501	-	25,26,26	1.58	4 (16%)	38,40,40	1.58	7 (18%)
3	GOL	A	502	-	5,5,5	0.18	0	5,5,5	0.77	0
2	UDP	A	501	-	25,26,26	1.30	4 (16%)	38,40,40	1.69	6 (15%)

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	UDP	B	501	-	-	3/16/32/32	0/2/2/2
3	GOL	A	502	-	-	2/4/4/4	-
2	UDP	A	501	-	-	3/16/32/32	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UDP	O2-C2	4.13	1.30	1.23
2	B	501	UDP	PA-O3A	3.61	1.63	1.59
2	A	501	UDP	C2-N3	-2.90	1.32	1.38
2	B	501	UDP	C5-C4	-2.67	1.37	1.43
2	A	501	UDP	C5-C4	-2.48	1.38	1.43
2	B	501	UDP	C2-N1	2.11	1.41	1.38
2	A	501	UDP	C6-N1	-2.10	1.33	1.38
2	A	501	UDP	C6-C5	2.04	1.39	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UDP	N3-C2-N1	4.70	121.01	114.89
2	B	501	UDP	O4-C4-C5	-4.24	117.85	125.16
2	A	501	UDP	C4-N3-C2	-4.17	121.44	126.61
2	A	501	UDP	O2A-PA-O3A	4.11	118.39	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UDP	O4'-C1'-N1	3.37	116.00	108.36
2	A	501	UDP	O2-C2-N3	-3.10	115.78	121.49
2	B	501	UDP	C5-C4-N3	2.94	118.92	114.80
2	B	501	UDP	O2-C2-N1	-2.87	119.06	122.80
2	B	501	UDP	C4-N3-C2	-2.74	123.21	126.61
2	B	501	UDP	O4-C4-N3	2.73	123.23	119.27
2	A	501	UDP	C5-C4-N3	2.59	118.42	114.80
2	A	501	UDP	O3A-PB-O1B	-2.26	99.14	111.04
2	B	501	UDP	O3'-C3'-C4'	2.18	117.34	111.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

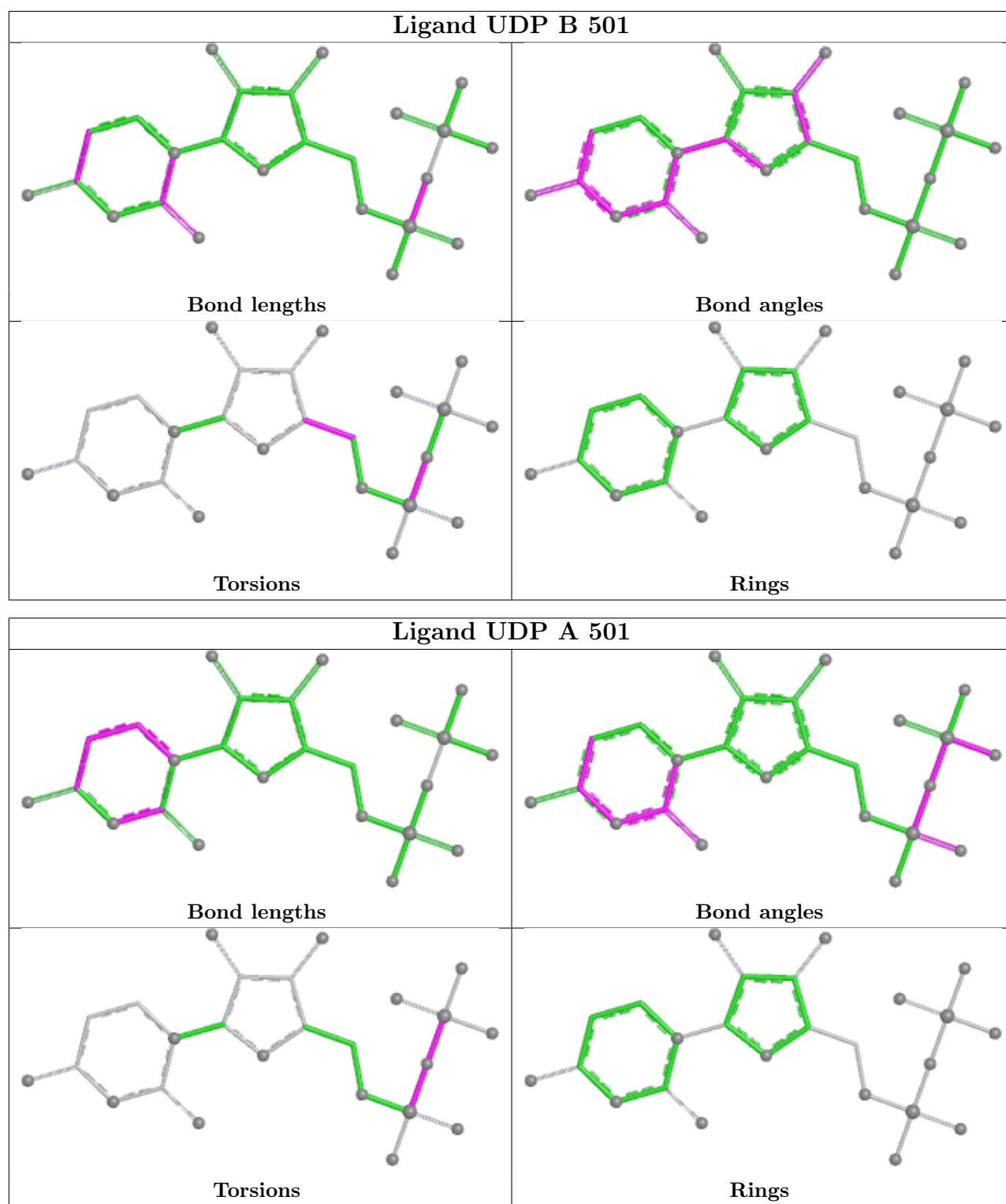
Mol	Chain	Res	Type	Atoms
2	A	501	UDP	PB-O3A-PA-O5'
3	A	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
2	B	501	UDP	C3'-C4'-C5'-O5'
2	B	501	UDP	O4'-C4'-C5'-O5'
2	A	501	UDP	PA-O3A-PB-O1B
2	B	501	UDP	PB-O3A-PA-O5'
2	A	501	UDP	PA-O3A-PB-O3B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	4	0
2	A	501	UDP	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 ⓘ

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	397/414 (95%)	-0.13	12 (3%)	52 48	14, 28, 54, 93	0
1	B	384/414 (92%)	-0.04	14 (3%)	46 41	14, 29, 69, 101	0
All	All	781/828 (94%)	-0.09	26 (3%)	49 45	14, 28, 62, 101	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	MET	4.4
1	A	409	HIS	3.9
1	A	406	ALA	3.6
1	B	178	PHE	3.1
1	A	408	GLU	3.0
1	B	219	GLY	3.0
1	B	169	ASP	3.0
1	A	405	ALA	3.0
1	B	148	GLY	3.0
1	A	145	TYR	2.7
1	B	220	ASN	2.7
1	A	220	ASN	2.6
1	A	242	PHE	2.6
1	A	219	GLY	2.6
1	A	407	LEU	2.4
1	B	74	PHE	2.4
1	A	243	ASN	2.3
1	B	67	THR	2.3
1	B	161	GLN	2.3
1	B	170	PHE	2.3
1	B	402	SER	2.2
1	B	328	ASP	2.2
1	B	150	LEU	2.2
1	B	364	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	147	LYS	2.0
1	B	327	ASN	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](#)

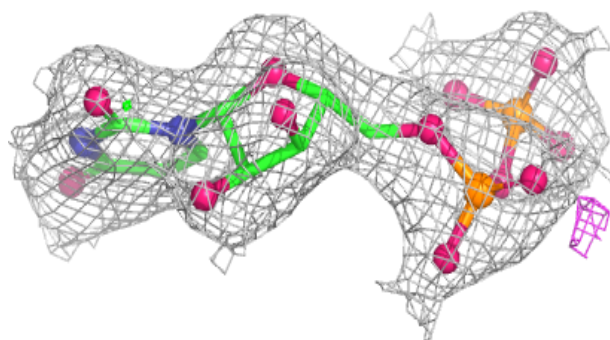
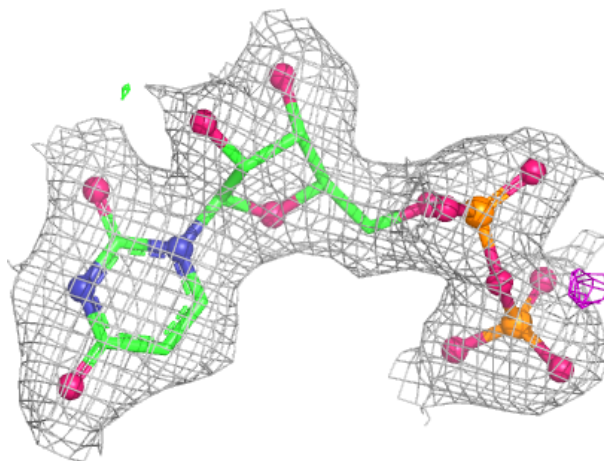
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	GOL	A	502	6/6	0.88	0.22	30,39,44,46	0
2	UDP	B	501	25/25	0.97	0.06	14,18,22,25	0
2	UDP	A	501	25/25	0.98	0.05	15,16,20,22	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.

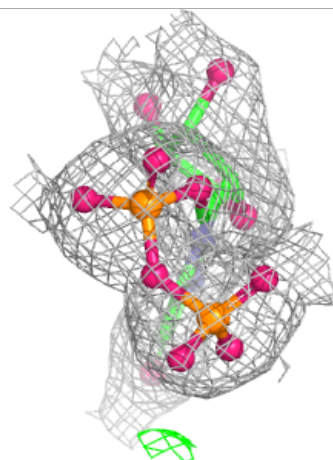
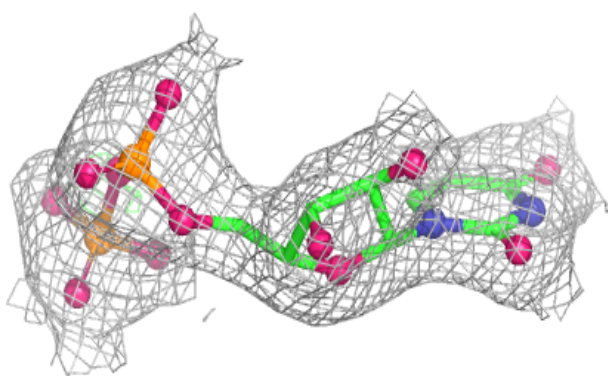
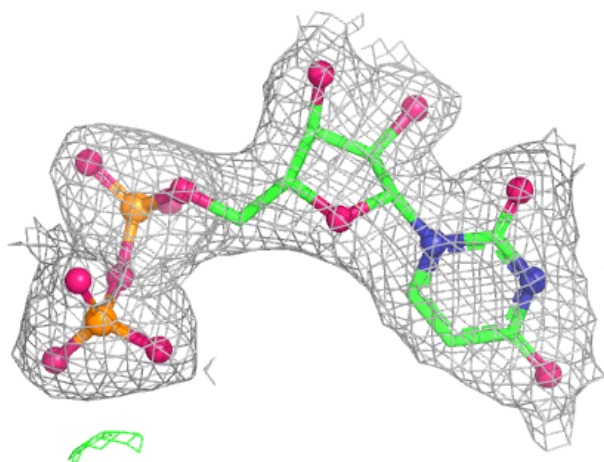
Electron density around UDP B 501:

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



Electron density around UDP A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.