



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:00 am BST

PDB ID : 6BK0
Title : Crystal structure of Os79 Q202A from *O. sativa* in complex with UDP.
Authors : Wetterhorn, K.; Gabardi, K.; Rayment, I.
Deposited on : 2017-11-07
Resolution : 1.47 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

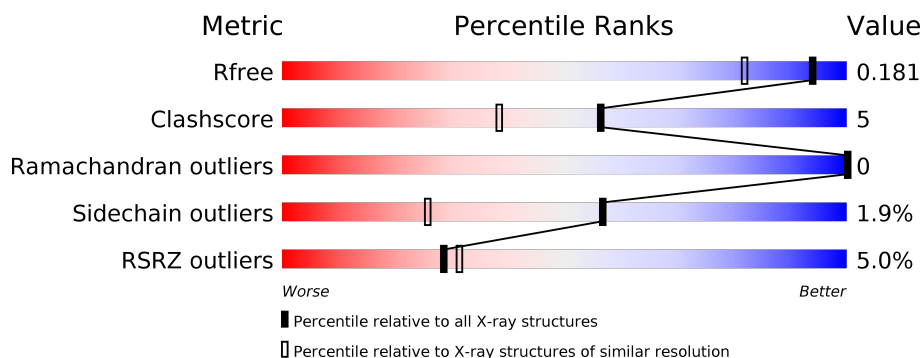
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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 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	467	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4067 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.

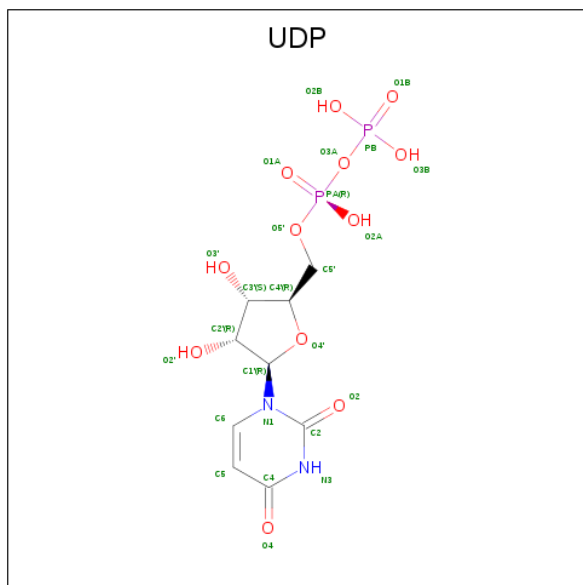
- Molecule 1 is a protein called UDP-glycosyltransferase 79.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3459	2198	607	635	19	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q7XT97
A	202	ALA	GLN	engineered mutation	UNP Q7XT97

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

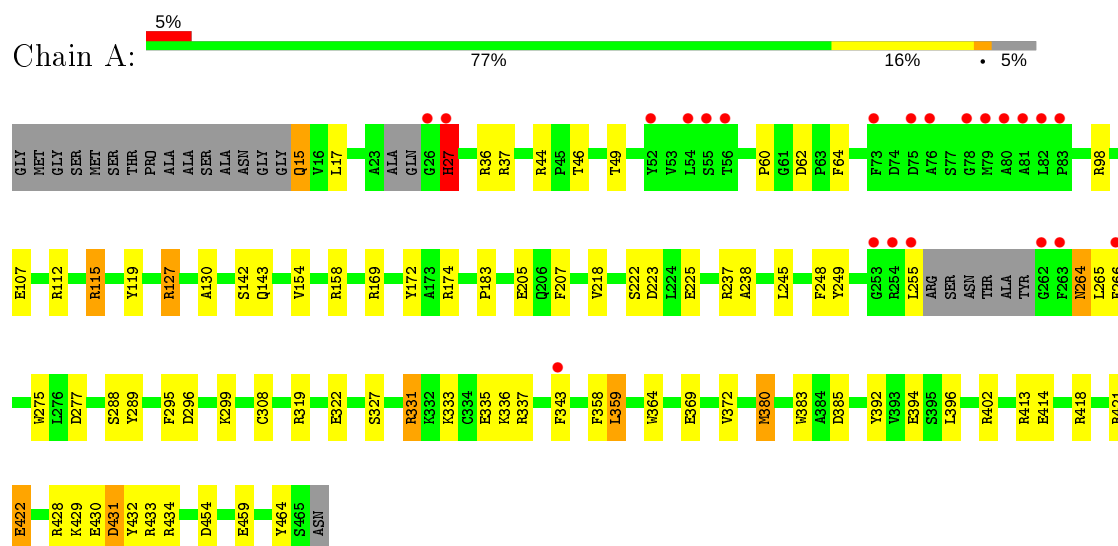


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	583	Total 583	O 583	0	0

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 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: UDP-glycosyltransferase 79



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.41Å 83.23Å 99.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.46 – 1.47 43.46 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.46-1.47) 99.9 (43.46-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.71 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.153 , 0.181 0.153 , 0.181	Depositor DCC
R_{free} test set	4150 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	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	4067	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: 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	1.58	30/3558 (0.8%)	1.62	62/4834 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLN	CD-NE2	-11.71	1.03	1.32
1	A	394	GLU	CD-OE2	11.22	1.38	1.25
1	A	385	ASP	CB-CG	-9.85	1.31	1.51
1	A	394	GLU	CG-CD	9.29	1.65	1.51
1	A	249	TYR	CE1-CZ	-8.85	1.27	1.38
1	A	127	ARG	CZ-NH2	-7.50	1.23	1.33
1	A	414	GLU	CD-OE2	7.08	1.33	1.25
1	A	434	ARG	CD-NE	-7.06	1.34	1.46
1	A	422	GLU	CG-CD	-6.22	1.42	1.51
1	A	394	GLU	CD-OE1	-6.18	1.18	1.25
1	A	225	GLU	CB-CG	-6.18	1.40	1.52
1	A	222	SER	CB-OG	-6.16	1.34	1.42
1	A	422	GLU	C-O	6.01	1.34	1.23
1	A	275	TRP	CZ3-CH2	-5.98	1.30	1.40
1	A	364	TRP	CG-CD1	5.95	1.45	1.36
1	A	429	LYS	CE-NZ	5.87	1.63	1.49
1	A	308	CYS	CB-SG	5.79	1.92	1.82
1	A	369	GLU	CG-CD	-5.68	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	GLU	CG-CD	5.47	1.60	1.51
1	A	392	TYR	CE1-CZ	-5.40	1.31	1.38
1	A	288	SER	CB-OG	5.40	1.49	1.42
1	A	459	GLU	CA-CB	-5.35	1.42	1.53
1	A	130	ALA	CA-CB	5.32	1.63	1.52
1	A	380	MET	SD-CE	-5.25	1.48	1.77
1	A	429	LYS	CB-CG	-5.25	1.38	1.52
1	A	335	GLU	CD-OE1	-5.25	1.19	1.25
1	A	430	GLU	CG-CD	5.21	1.59	1.51
1	A	432	TYR	CB-CG	-5.15	1.44	1.51
1	A	183	PRO	N-CA	-5.15	1.38	1.47
1	A	327	SER	CB-OG	-5.06	1.35	1.42

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ARG	NE-CZ-NH2	21.30	130.95	120.30
1	A	454	ASP	CB-CG-OD1	-15.27	104.56	118.30
1	A	319	ARG	NE-CZ-NH2	14.59	127.60	120.30
1	A	127	ARG	NE-CZ-NH2	13.65	127.13	120.30
1	A	158	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	364	TRP	CD1-NE1-CE2	10.78	118.70	109.00
1	A	459	GLU	OE1-CD-OE2	10.66	136.09	123.30
1	A	169	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	A	237	ARG	NE-CZ-NH2	10.15	125.37	120.30
1	A	385	ASP	CB-CG-OD1	9.51	126.86	118.30
1	A	331	ARG	NE-CZ-NH1	-9.50	115.55	120.30
1	A	402	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	A	364	TRP	NE1-CE2-CZ2	9.09	140.40	130.40
1	A	433	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	223	ASP	CB-CG-OD2	8.43	125.89	118.30
1	A	413	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	322	GLU	OE1-CD-OE2	-8.01	113.69	123.30
1	A	421	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	418	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	359	LEU	CB-CG-CD2	7.58	123.89	111.00
1	A	107	GLU	OE1-CD-OE2	7.52	132.33	123.30
1	A	295	PHE	CB-CG-CD2	-7.42	115.61	120.80
1	A	364	TRP	NE1-CE2-CD2	-7.42	99.88	107.30
1	A	434	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	A	429	LYS	CD-CE-NZ	7.26	128.41	111.70
1	A	249	TYR	CB-CG-CD2	7.25	125.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	454	ASP	OD1-CG-OD2	6.99	136.57	123.30
1	A	459	GLU	CG-CD-OE1	-6.95	104.41	118.30
1	A	277	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	115	ARG	NE-CZ-NH2	6.63	123.62	120.30
1	A	421	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	434	ARG	NH1-CZ-NH2	-6.44	112.32	119.40
1	A	158	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
1	A	37	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	207	PHE	CZ-CE2-CD2	-6.22	112.63	120.10
1	A	174[A]	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	174[B]	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	432	TYR	CB-CG-CD1	6.12	124.67	121.00
1	A	265	LEU	CB-CG-CD2	6.06	121.30	111.00
1	A	289	TYR	CB-CG-CD1	6.04	124.62	121.00
1	A	127	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	112	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	A	431	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	237	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	464	TYR	CB-CG-CD2	5.64	124.39	121.00
1	A	98	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	422	GLU	O-C-N	-5.54	113.83	122.70
1	A	394	GLU	CG-CD-OE1	-5.53	107.25	118.30
1	A	295	PHE	CB-CG-CD1	5.50	124.65	120.80
1	A	337	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	331	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	36	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	434	ARG	CD-NE-CZ	5.41	131.17	123.60
1	A	414	GLU	CG-CD-OE1	5.35	129.00	118.30
1	A	265	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	A	418	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	385	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	15	GLN	N-CA-CB	-5.22	101.21	110.60
1	A	358	PHE	CB-CG-CD1	5.12	124.39	120.80
1	A	154	VAL	O-C-N	-5.11	114.52	122.70
1	A	172	TYR	CD1-CE1-CZ	-5.10	115.21	119.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	A	422	GLU	Mainchain
1	A	64	PHE	Peptide

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	3459	0	3467	35	0
2	A	25	0	11	2	0
3	A	583	0	0	16	3
All	All	4067	0	3478	35	3

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 5.

All (35) 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:333:LYS:HE2	3:A:643:HOH:O	1.27	1.27
1:A:119:TYR:OH	1:A:127:ARG:NH1	1.89	1.05
1:A:359:LEU:HD21	1:A:380:MET:HE2	1.54	0.87
1:A:343:PHE:CD1	3:A:1012:HOH:O	2.30	0.84
1:A:359:LEU:CD2	1:A:380:MET:HE2	2.09	0.83
1:A:27:HIS:HE1	2:A:501:UDP:O3B	1.62	0.81
1:A:27:HIS:CD2	1:A:27:HIS:N	2.54	0.76
1:A:343:PHE:HD1	3:A:1012:HOH:O	1.70	0.72
1:A:359:LEU:HD21	1:A:380:MET:CE	2.21	0.70
1:A:336:LYS:HG2	3:A:1025:HOH:O	1.96	0.65
1:A:359:LEU:CD2	1:A:380:MET:CE	2.75	0.65
1:A:343:PHE:CE1	3:A:1012:HOH:O	2.48	0.62
1:A:333:LYS:CE	3:A:643:HOH:O	2.09	0.60
1:A:27:HIS:N	1:A:27:HIS:HD2	1.97	0.58
1:A:336:LYS:CG	3:A:1025:HOH:O	2.50	0.57
1:A:428:ARG:NH2	3:A:603:HOH:O	2.36	0.57
1:A:264:ASN:ND2	1:A:266:PHE:H	2.04	0.56
1:A:245:LEU:HD12	1:A:372[A]:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:NH1	1:A:431:ASP:OD2	2.39	0.54
1:A:142:SER:HB2	3:A:741:HOH:O	2.08	0.54
1:A:49:THR:HG22	3:A:995:HOH:O	2.09	0.51
1:A:27:HIS:CE1	2:A:501:UDP:O3B	2.52	0.51
1:A:336:LYS:CD	3:A:1025:HOH:O	2.59	0.50
1:A:331:ARG:CD	3:A:626:HOH:O	2.60	0.49
1:A:264:ASN:HD22	1:A:266:PHE:H	1.59	0.48
1:A:44:ARG:HD2	3:A:1063:HOH:O	2.16	0.46
1:A:27:HIS:CD2	1:A:27:HIS:H	2.32	0.45
1:A:396:LEU:HD23	3:A:618:HOH:O	2.17	0.45
1:A:205:GLU:HG3	3:A:960:HOH:O	2.17	0.45
1:A:15:GLN:NE2	3:A:613:HOH:O	2.51	0.44
1:A:15:GLN:CG	1:A:46:THR:OG1	2.67	0.42
1:A:296:ASP:H	1:A:299:LYS:NZ	2.17	0.42
1:A:248:PHE:CE2	1:A:264:ASN:ND2	2.88	0.41
1:A:17:LEU:HD23	1:A:46:THR:HB	2.03	0.41
1:A:218[B]:VAL:HG23	1:A:238:ALA:HB1	2.03	0.40

All (3) 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)
3:A:692:HOH:O	3:A:877:HOH:O[4_545]	2.01	0.19
3:A:604:HOH:O	3:A:725:HOH:O[4_445]	2.10	0.10
3:A:796:HOH:O	3:A:1052:HOH:O[4_455]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/467 (95%)	434 (98%)	9 (2%)	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	372/381 (98%)	365 (98%)	7 (2%)	57 26

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	60	PRO
1	A	62	ASP
1	A	115	ARG
1	A	255	LEU
1	A	264	ASN
1	A	383	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	27	HIS
1	A	29	ASN
1	A	206	GLN
1	A	264	ASN
1	A	456	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	UDP	A	501	-	20,26,26	1.71	3 (15%)	25,40,40	1.79	4 (16%)

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	A	501	-	-	2/14/32/32	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UDP	O4'-C1'	5.62	1.48	1.41
2	A	501	UDP	C2'-C1'	-2.48	1.50	1.53
2	A	501	UDP	O5'-C5'	2.00	1.52	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	UDP	O4'-C1'-C2'	-5.67	98.64	106.93
2	A	501	UDP	C3'-C2'-C1'	4.50	107.75	100.98
2	A	501	UDP	O2B-PB-O1B	2.40	120.08	110.68
2	A	501	UDP	C5-C6-N1	2.14	125.46	120.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

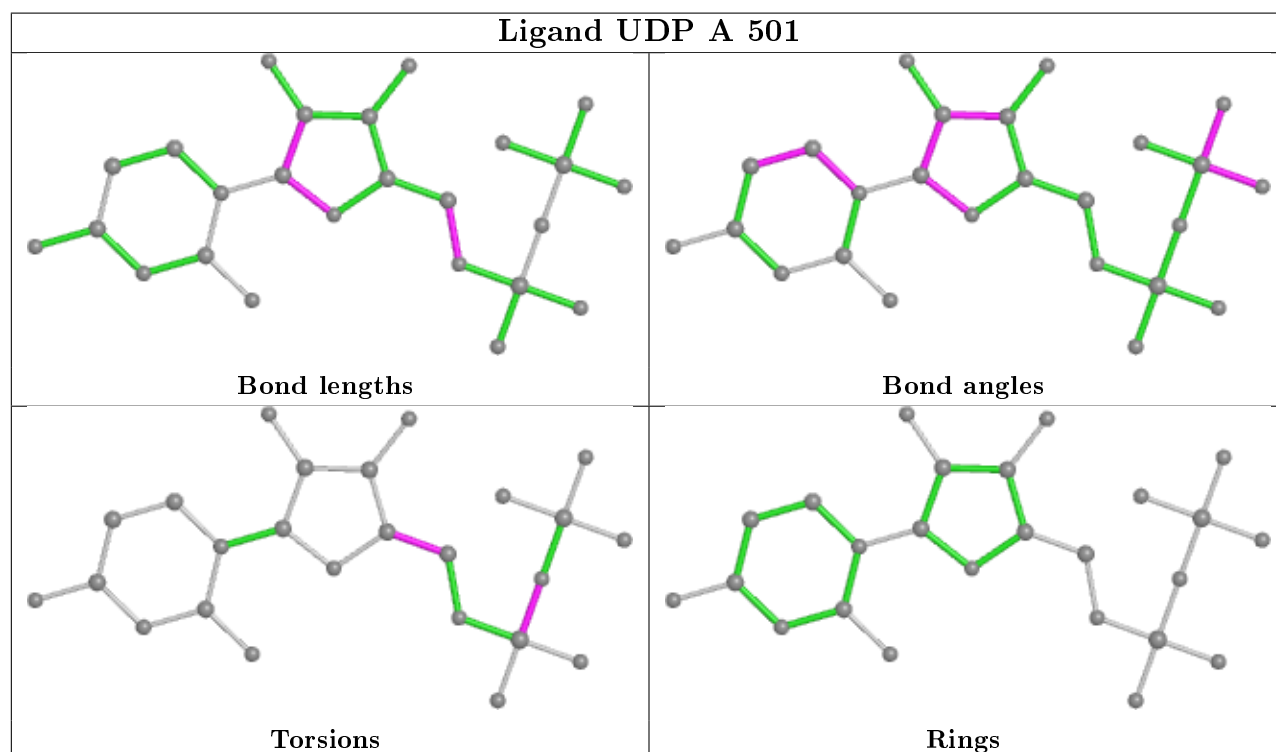
Mol	Chain	Res	Type	Atoms
2	A	501	UDP	PB-O3A-PA-O5'
2	A	501	UDP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	UDP	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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	443/467 (94%)	0.17	22 (4%)	28 31	8, 15, 40, 63	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	LEU	9.7
1	A	253	GLY	7.8
1	A	82	LEU	4.3
1	A	54	LEU	4.3
1	A	266	PHE	4.1
1	A	79	MET	3.9
1	A	26	GLY	3.8
1	A	83	PRO	3.7
1	A	55	SER	3.6
1	A	27	HIS	3.4
1	A	78	GLY	3.4
1	A	80	ALA	3.4
1	A	73	PHE	3.3
1	A	81	ALA	3.2
1	A	56	THR	3.1
1	A	76	ALA	3.1
1	A	262	GLY	3.0
1	A	75	ASP	2.7
1	A	263	PHE	2.7
1	A	52	TYR	2.6
1	A	343	PHE	2.2
1	A	254	ARG	2.1

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](#)

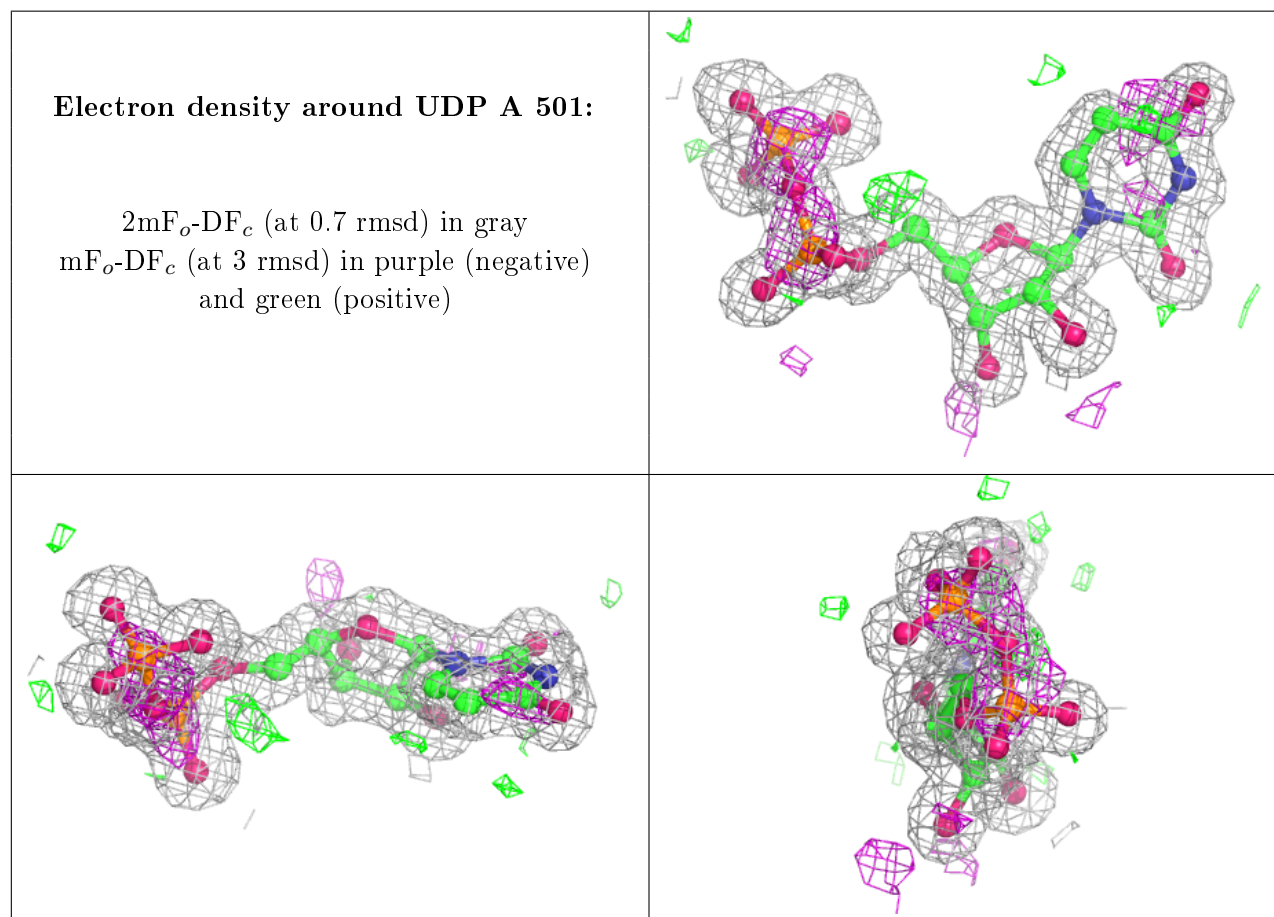
There are no carbohydrates in this entry.

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. 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(\AA^2)	Q<0.9
2	UDP	A	501	25/25	0.97	0.08	13,15,18,20	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.