Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:07 AM JST

PDB ID	:	6INI
Title	:	a glycosyltransferase complex with UDP and the product
Authors	:	Zhu, X.; Yang, T.; Naismith, J.H.
Deposited on	:	2018-10-25
Resolution	:	1.70 Å(reported)

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

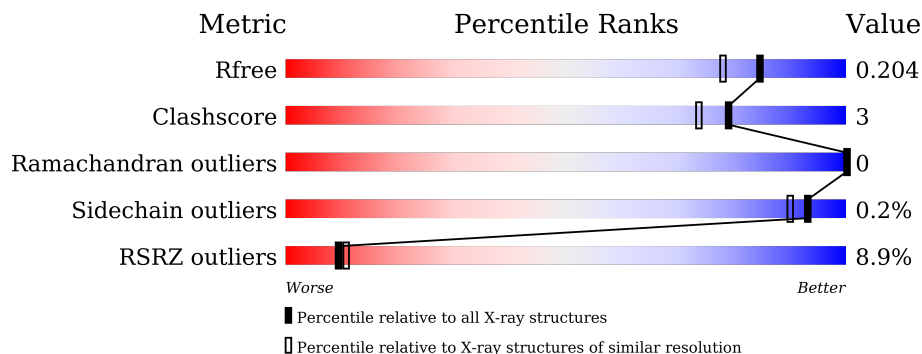|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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	Percentile Ranks	Value
Rfree		0.204
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.2%
RSRZ outliers		8.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

◻Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	466	9% 91% 6% ·

2 Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4049 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 76G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3655	2347	617	679	12	0	8	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	LEU	-	expression tag	UNP Q6VAB4
A	460	GLU	-	expression tag	UNP Q6VAB4
A	461	HIS	-	expression tag	UNP Q6VAB4
A	462	HIS	-	expression tag	UNP Q6VAB4
A	463	HIS	-	expression tag	UNP Q6VAB4
A	464	HIS	-	expression tag	UNP Q6VAB4
A	465	HIS	-	expression tag	UNP Q6VAB4
A	466	HIS	-	expression tag	UNP Q6VAB4

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).
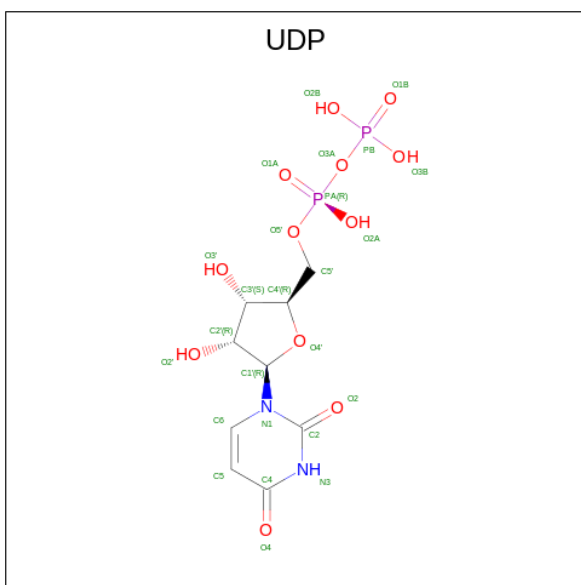
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 4 is (8alpha,9beta,10alpha,13alpha)-13-{[beta-D-glucopyranosyl-(1->2)-[beta-D-glucopyranosyl-(1->3)]-beta-D-glucopyranosyl]oxy}kaur-16-en-18-oic acid (three-letter code: AUO) (formula: $C_{38}H_{60}O_{18}$).
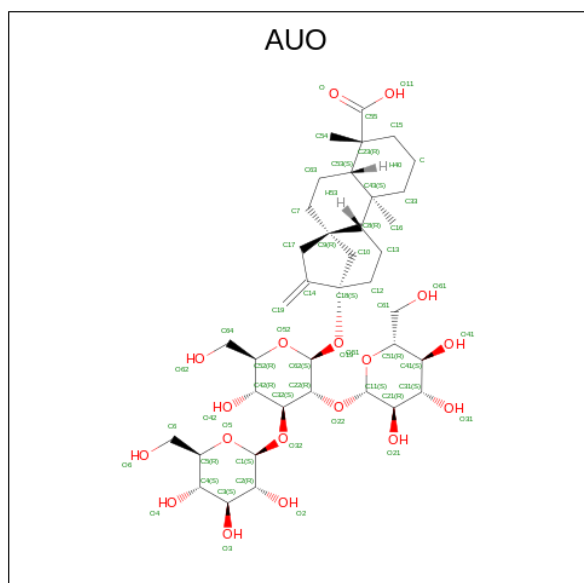
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 56	C 38	O 18	0	0

- Molecule 5 is 1-O-[(8alpha,9beta,10alpha,13alpha)-13-(beta-D-glucopyranosyloxy)-18-oxoka ur-16-en-18-yl]-beta-D-glucopyranose (three-letter code: AQ9) (formula: $C_{32}H_{50}O_{13}$).
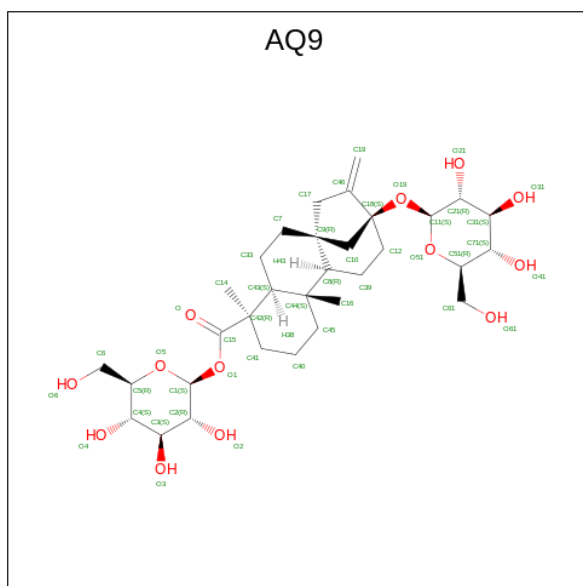
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 34	C 26	O 8	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	273	Total 273	O 273	0	0

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: UDP-glycosyltransferase 76G1
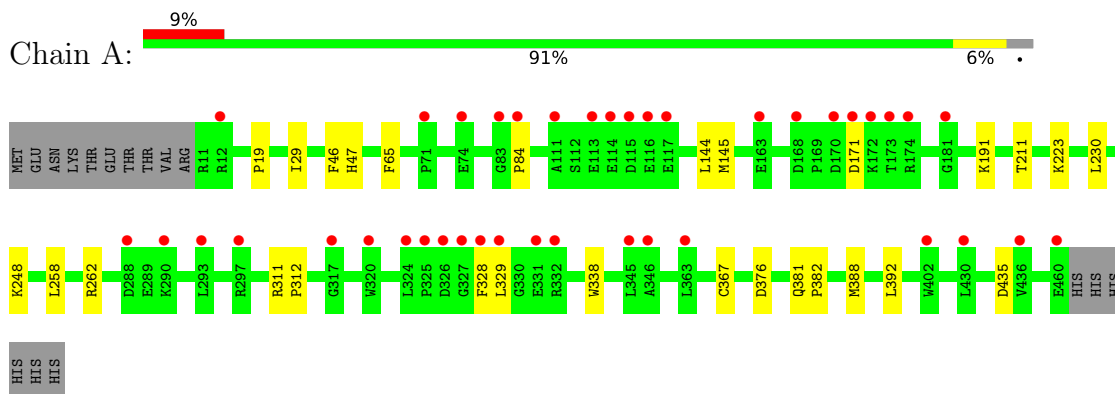
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.66Å 97.66Å 89.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.88 – 1.70 42.88 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.88-1.70) 99.1 (42.88-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.161 , 0.190 0.175 , 0.204	Depositor DCC
R_{free} test set	2725 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.7	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4049	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, AUO, AQ9, 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	0.67	0/3762	0.74	0/5102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3655	0	3643	20	0
2	A	25	0	11	0	0
3	A	6	0	8	1	0
4	A	56	0	0	1	0
5	A	34	0	0	0	0
6	A	273	0	0	2	0
All	All	4049	0	3662	21	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 3.

All (21) 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:19:PRO:HB3	1:A:29[A]:ILE:HG21	1.63	0.81
1:A:223:LYS:HG3	1:A:230:LEU:HD11	1.68	0.74
1:A:388:MET:SD	1:A:392:LEU:HD12	2.34	0.67
3:A:502:GOL:H32	6:A:626:HOH:O	1.97	0.64
1:A:248:LYS:HE2	1:A:435:ASP:OD1	2.03	0.58
1:A:258:LEU:HD13	1:A:311[A]:ARG:CZ	2.38	0.54
1:A:171:ASP:O	1:A:191:LYS:HE3	2.09	0.51
1:A:311[A]:ARG:CZ	1:A:312:PRO:HD2	2.44	0.47
1:A:248:LYS:CE	1:A:435:ASP:OD1	2.63	0.47
1:A:29[B]:ILE:HG12	1:A:144:LEU:HD23	1.97	0.46
1:A:19:PRO:HD2	1:A:46:PHE:O	2.16	0.45
1:A:328:PHE:O	1:A:329:LEU:HB2	2.18	0.43
1:A:248:LYS:HD2	1:A:367:CYS:HB3	2.01	0.43
1:A:248:LYS:NZ	1:A:435:ASP:OD1	2.50	0.43
1:A:328:PHE:O	1:A:329:LEU:CB	2.66	0.43
1:A:47:HIS:O	1:A:65:PHE:HA	2.18	0.43
1:A:262:ARG:N	6:A:601:HOH:O	2.34	0.43
1:A:145[B]:MET:CE	1:A:211:THR:HG21	2.50	0.41
1:A:311[A]:ARG:HD3	1:A:338:TRP:CE3	2.55	0.41
1:A:84:PRO:O	4:A:503:AUO:O11	2.39	0.40
1:A:381:GLN:N	1:A:382:PRO:HD2	2.37	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	456/466 (98%)	445 (98%)	11 (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	409/417 (98%)	408 (100%)	1 (0%)	93	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	#$|Z| > 2$
4	AUO	A	503	-	60,62,62	0.77	1 (1%)	91,99,99	1.57	16 (17%)
3	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.30	0
5	AQ9	A	504	-	38,38,50	1.21	2 (5%)	61,63,81	1.42	10 (16%)
2	UDP	A	501	-	24,26,26	1.21	3 (12%)	37,40,40	1.38	5 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AUO	A	503	-	-	4/25/146/146	0/8/7/7
3	GOL	A	502	-	-	2/4/4/4	-
5	AQ9	A	504	-	-	0/12/93/120	0/6/5/6
2	UDP	A	501	-	-	2/16/32/32	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	AQ9	O1-C15	6.04	1.45	1.34
2	A	501	UDP	C4-N3	-2.93	1.33	1.38
2	A	501	UDP	C2-N3	-2.56	1.33	1.38
2	A	501	UDP	C5-C4	-2.15	1.38	1.43
5	A	504	AQ9	C39-C8	2.15	1.57	1.53
4	A	503	AUO	C43-C53	-2.01	1.53	1.56

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	AUO	C10-C9-C17	4.86	104.45	100.01
4	A	503	AUO	O32-C1-O5	-4.32	98.60	110.67
4	A	503	AUO	C54-C23-C15	-3.78	103.46	109.43
4	A	503	AUO	C17-C14-C18	3.58	110.72	107.32
5	A	504	AQ9	C12-C39-C8	3.53	117.92	111.07
2	A	501	UDP	O4-C4-C5	-3.48	119.04	125.16
4	A	503	AUO	O5-C5-C4	-3.47	103.39	109.69
5	A	504	AQ9	C10-C9-C17	3.35	103.08	100.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	AUO	O32-C1-C2	3.34	116.74	108.10
2	A	501	UDP	O3B-PB-O2B	3.26	120.11	107.64
2	A	501	UDP	C5-C4-N3	3.11	119.50	114.84
4	A	503	AUO	C9-C8-C43	-2.97	114.06	116.63
4	A	503	AUO	C7-C9-C17	-2.90	107.74	112.91
4	A	503	AUO	C1-O32-C32	2.79	124.87	117.96
4	A	503	AUO	C15-C23-C53	2.76	111.50	108.34
4	A	503	AUO	O4-C4-C5	2.72	116.06	109.30
4	A	503	AUO	C10-C9-C8	2.71	112.95	108.46
2	A	501	UDP	N3-C2-N1	2.60	118.34	114.89
2	A	501	UDP	C4-N3-C2	-2.59	123.16	126.58
5	A	504	AQ9	C17-C9-C8	-2.58	106.03	111.09
4	A	503	AUO	O5-C5-C6	-2.57	100.03	106.44
5	A	504	AQ9	C8-C44-C43	2.54	110.24	106.77
4	A	503	AUO	C6-C5-C4	2.51	118.88	113.00
5	A	504	AQ9	C17-C46-C18	2.44	109.60	107.58
5	A	504	AQ9	C41-C42-C43	2.41	111.09	108.34
5	A	504	AQ9	C10-C18-C46	-2.39	100.80	102.09
5	A	504	AQ9	C40-C45-C44	2.31	116.05	113.17
4	A	503	AUO	O52-C52-C64	2.20	111.91	106.44
5	A	504	AQ9	O1-C15-C42	2.12	113.89	111.70
5	A	504	AQ9	O19-C18-C12	2.10	112.19	107.83
4	A	503	AUO	C17-C9-C8	-2.01	107.14	111.09

There are no chirality outliers.
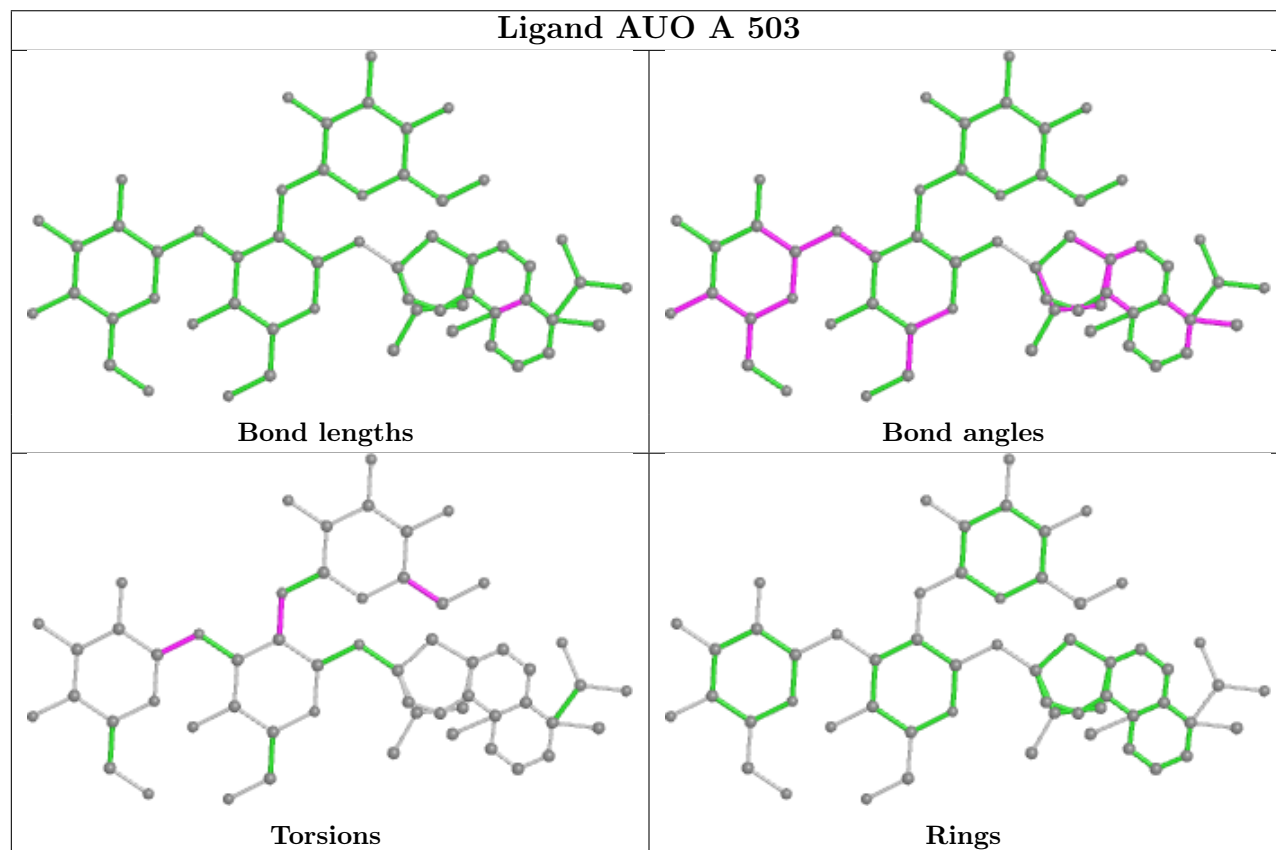
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
4	A	503	AUO	C2-C1-O32-C32
4	A	503	AUO	O5-C1-O32-C32
4	A	503	AUO	O51-C51-C61-O61
4	A	503	AUO	C32-C22-O22-C11
2	A	501	UDP	PB-O3A-PA-O5'
2	A	501	UDP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	AUO	1	0
3	A	502	GOL	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AUO A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand AQ9 A 504

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP A 501

Bond lengths

Bond angles

Torsions

Rings
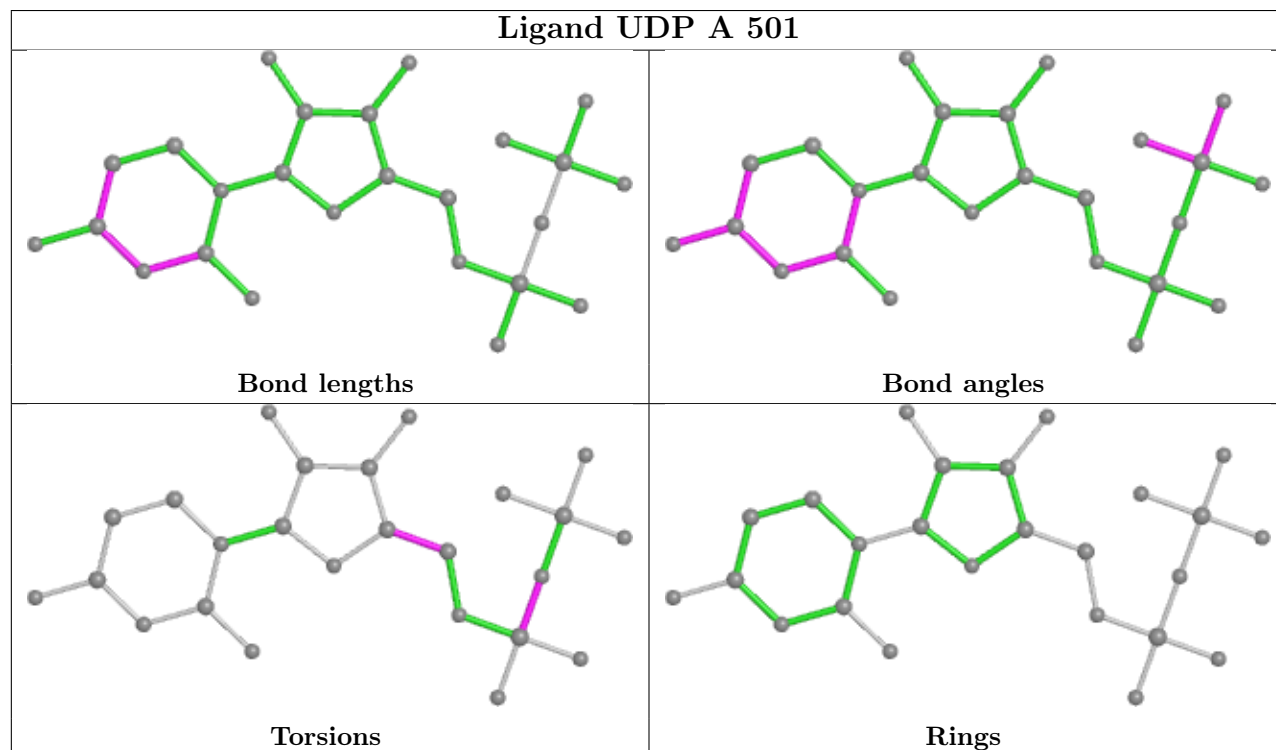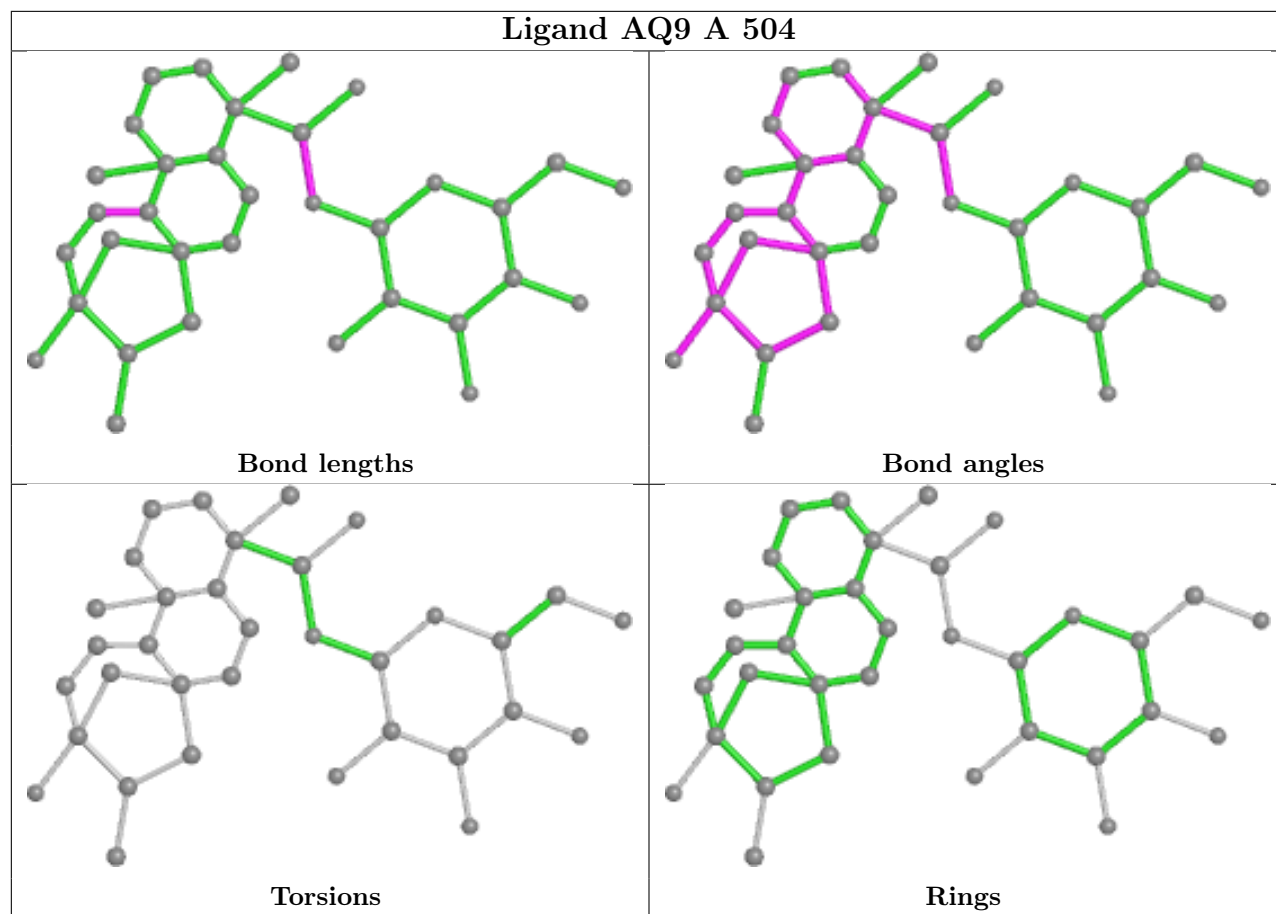
5.7 Other polymers ⓘ

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 ⓘ

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	450/466 (96%)	0.32	40 (8%)	9	11	16, 29, 67, 86	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	LEU	8.0
1	A	328	PHE	6.0
1	A	326	ASP	5.0
1	A	12	ARG	5.0
1	A	114	GLU	4.8
1	A	168	ASP	4.6
1	A	331	GLU	4.5
1	A	324	LEU	4.4
1	A	327	GLY	4.3
1	A	115	ASP	4.0
1	A	460	GLU	3.9
1	A	173	THR	3.5
1	A	71	PRO	3.4
1	A	293	LEU	3.4
1	A	181	GLY	3.3
1	A	83	GLY	3.2
1	A	170	ASP	3.1
1	A	436	VAL	3.1
1	A	84	PRO	3.0
1	A	290	LYS	3.0
1	A	325	PRO	2.9
1	A	74	GLU	2.9
1	A	113	GLU	2.8
1	A	297	ARG	2.8
1	A	116	GLU	2.7
1	A	288	ASP	2.6
1	A	171	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	320	TRP	2.6
1	A	163	GLU	2.5
1	A	111	ALA	2.5
1	A	117	GLU	2.4
1	A	402	TRP	2.3
1	A	430	LEU	2.3
1	A	172	LYS	2.2
1	A	345	LEU	2.2
1	A	174	ARG	2.2
1	A	346	ALA	2.1
1	A	317	GLY	2.1
1	A	332	ARG	2.1
1	A	363	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	AQ9	A	504	34/45	0.75	0.26	37,43,54,58	0
3	GOL	A	502	6/6	0.80	0.16	38,40,48,50	0
4	AUO	A	503	56/56	0.92	0.10	23,28,41,49	0
2	UDP	A	501	25/25	0.98	0.09	20,22,26,31	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.
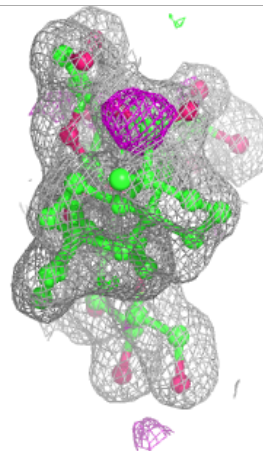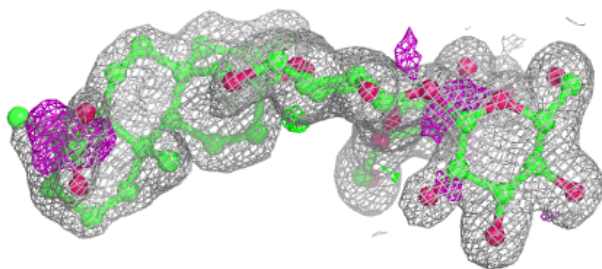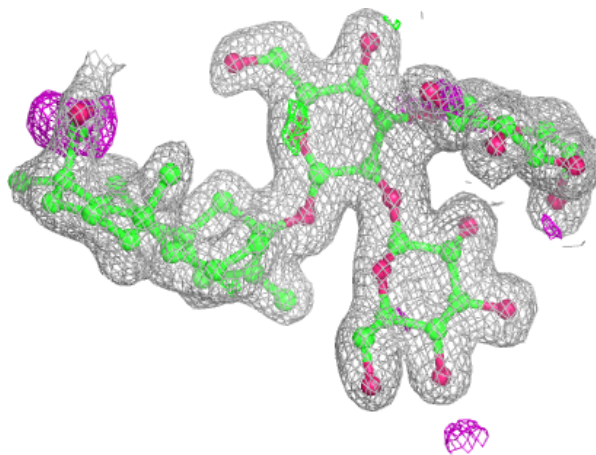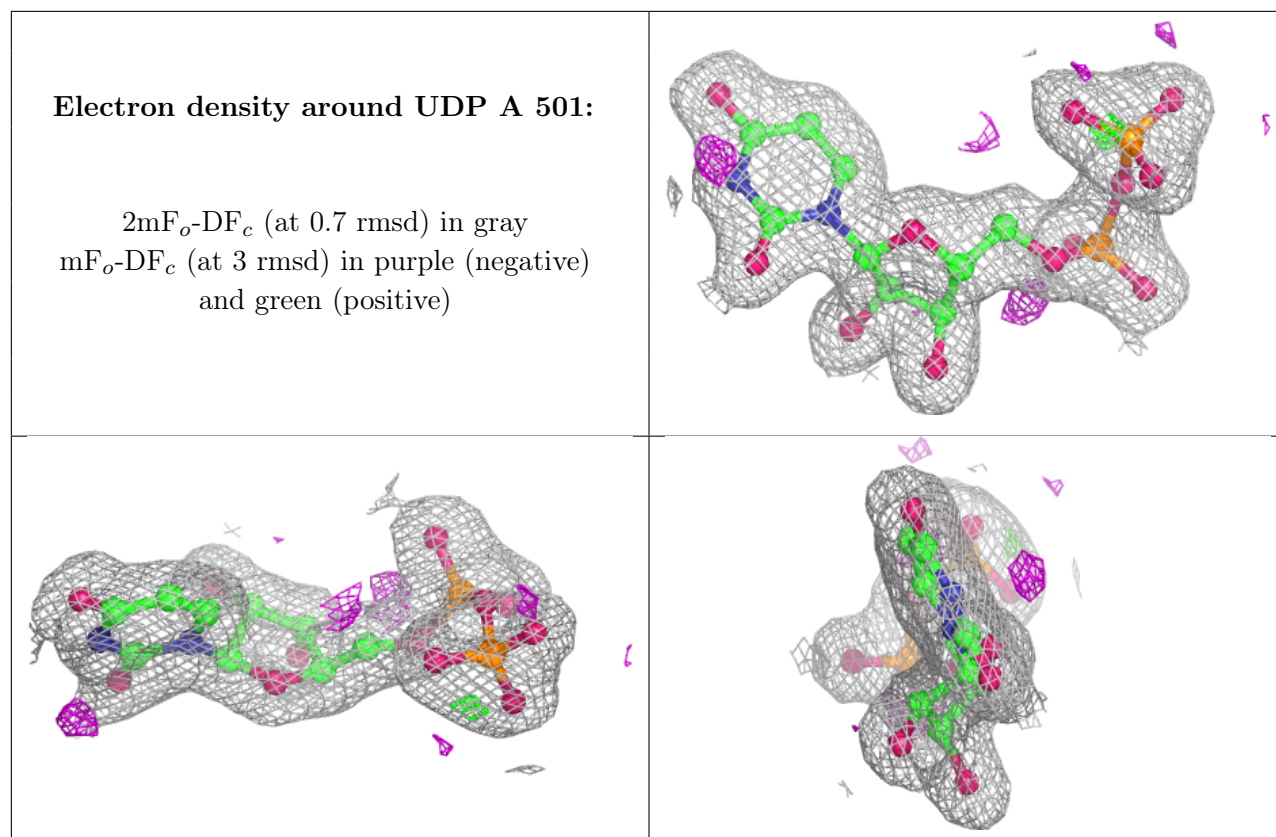
Electron density around AQ9 A 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
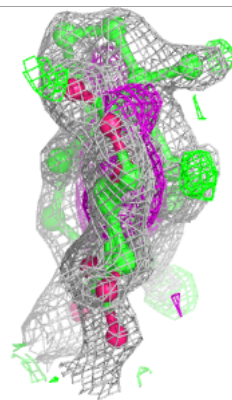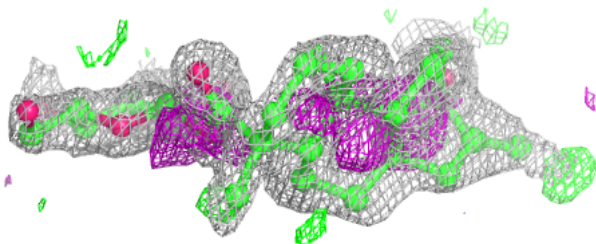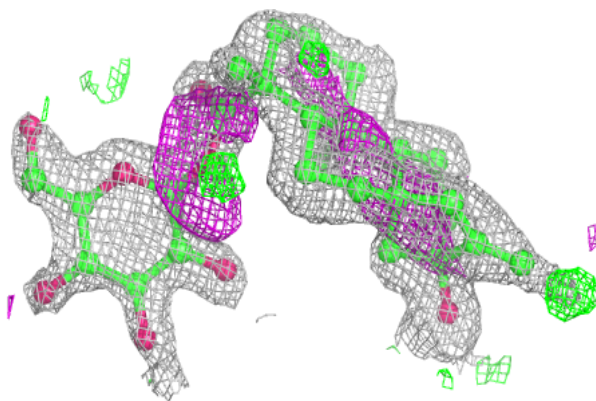
Electron density around AUO A 503:

$2mF_o$-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 ⓘ

There are no such residues in this entry.