



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 03:59 AM BST

PDB ID : 6LLW
Title : Crystal Structure of Fagopyrum esculentum M UGT708C1 complexed with UDP
Authors : Wang, X.; Liu, M.
Deposited on : 2019-12-23
Resolution : 2.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

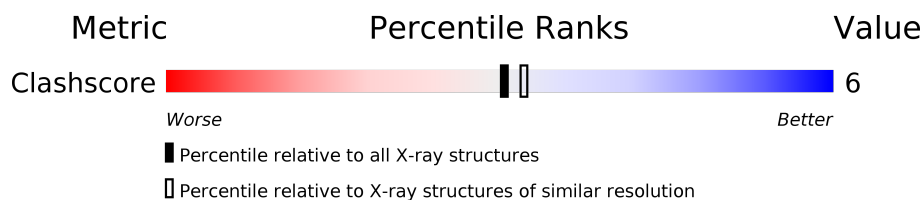
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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))
Clashscore	141614	1487 (2.26-2.26)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	457	 82% 12% • 5%
1	B	457	 84% 9% 7%

2 Entry composition [i](#)

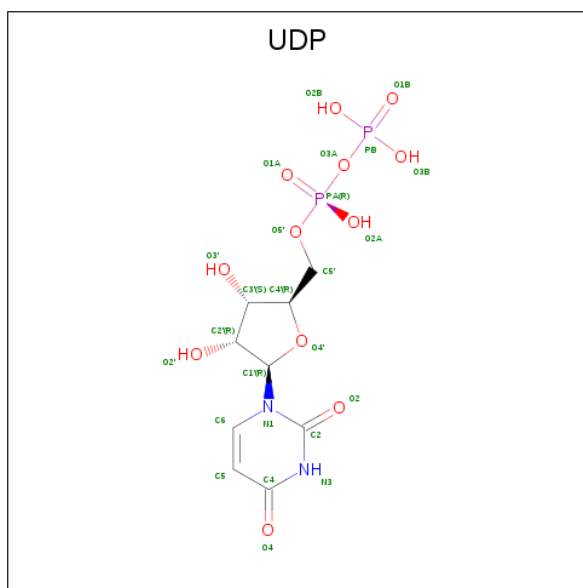
There are 3 unique types of molecules in this entry. The entry contains 7040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 708C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3359	2156	565	624	14			
1	B	424	Total	C	N	O	S	0	0	0
			3283	2110	552	607	14			

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total 162	O 162	0	0
3	B	186	Total 186	O 186	0	0

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.31Å 144.10Å 69.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.19 – 2.26	Depositor
% Data completeness (in resolution range)	98.2 (40.19-2.26)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.46 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.171 , 0.215	Depositor
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.079	Xtriage
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
Total number of atoms	7040	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.62	3/3450 (0.1%)	0.76	7/4696 (0.1%)
1	B	0.59	5/3372 (0.1%)	0.64	1/4589 (0.0%)
All	All	0.60	8/6822 (0.1%)	0.70	8/9285 (0.1%)

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	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLY	C-O	-6.12	1.13	1.23
1	A	247	GLY	C-O	-5.69	1.14	1.23
1	A	48	TYR	CE1-CZ	-5.50	1.31	1.38
1	B	122	PRO	N-CD	5.24	1.55	1.47
1	B	59	PRO	N-CD	5.20	1.55	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	PRO	O-C-N	-18.65	92.86	122.70
1	A	248	PRO	CA-N-CD	-11.39	95.56	111.50
1	A	58	ILE	C-N-CD	-6.79	105.66	120.60
1	A	248	PRO	N-CA-C	6.40	128.74	112.10
1	A	121	PRO	C-N-CD	5.21	139.34	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	GLY	Peptide
1	A	59	PRO	Mainchain

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	3359	0	3305	41	0
1	B	3283	0	3233	34	0
2	A	25	0	11	3	0
2	B	25	0	11	3	0
3	A	162	0	0	4	0
3	B	186	0	0	6	0
All	All	7040	0	6560	75	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 6.

The worst 5 of 75 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:280:ARG:O	3:A:1001:HOH:O	1.64	1.15
1:B:358:HIS:HD2	3:B:1039:HOH:O	1.52	0.90
1:A:279:ASN:ND2	2:A:900:UDP:O2B	2.05	0.88
1:B:358:HIS:CD2	3:B:1039:HOH:O	2.27	0.82
1:B:130:PHE:HZ	1:B:202:THR:HA	1.43	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	900	-	20,26,26	2.26	10 (50%)	25,40,40	1.15	2 (8%)
2	UDP	A	900	-	20,26,26	2.63	11 (55%)	25,40,40	1.05	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	B	900	-	-	2/14/32/32	0/2/2/2
2	UDP	A	900	-	-	2/14/32/32	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	UDP	C6-N1	-4.58	1.30	1.35
2	B	900	UDP	PA-O2A	-4.20	1.35	1.55
2	A	900	UDP	C2-N3	-4.20	1.29	1.38
2	B	900	UDP	C6-N1	-3.76	1.31	1.35
2	A	900	UDP	PA-O1A	-3.69	1.37	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	UDP	O3B-PB-O2B	3.36	120.47	107.64
2	A	900	UDP	O3B-PB-O3A	2.99	114.67	104.64
2	B	900	UDP	O3B-PB-O1B	-2.46	101.04	110.68
2	A	900	UDP	O2A-PA-O5'	2.04	117.24	107.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	UDP	O4'-C4'-C5'-O5'
2	A	900	UDP	O4'-C4'-C5'-O5'
2	B	900	UDP	C3'-C4'-C5'-O5'
2	A	900	UDP	C3'-C4'-C5'-O5'

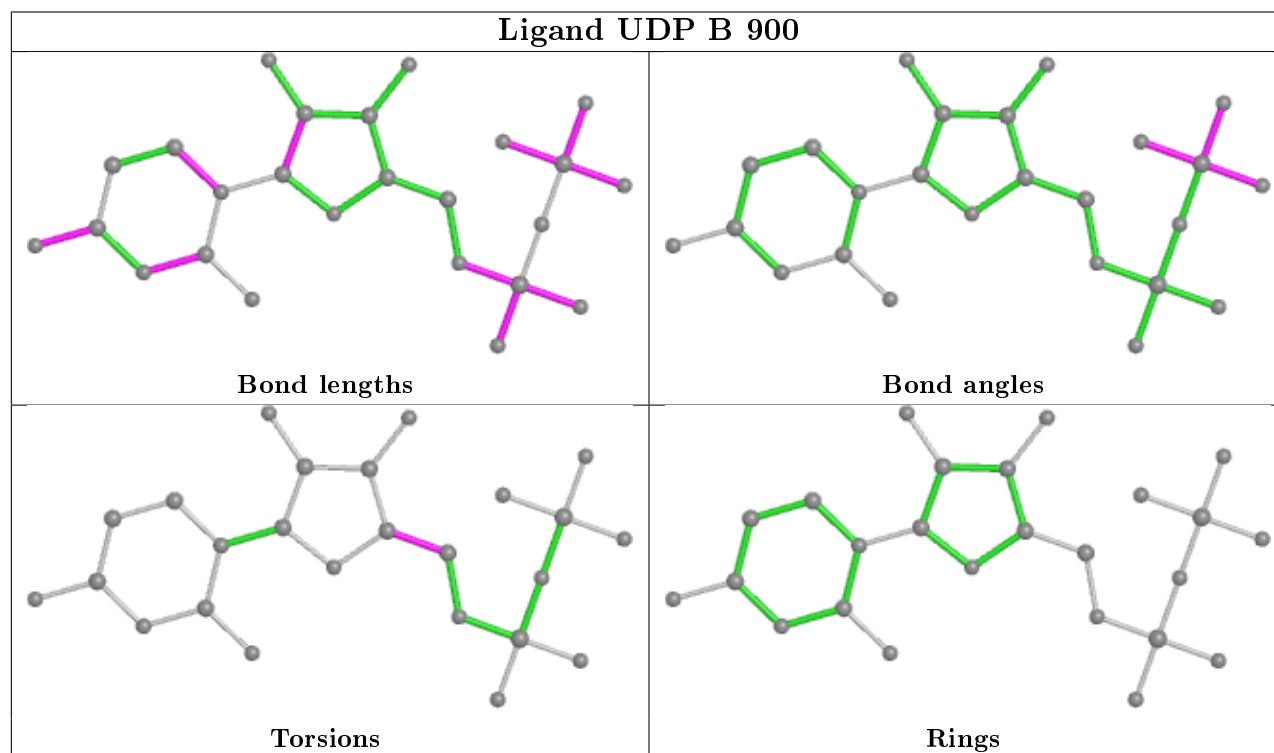
There are no ring outliers.

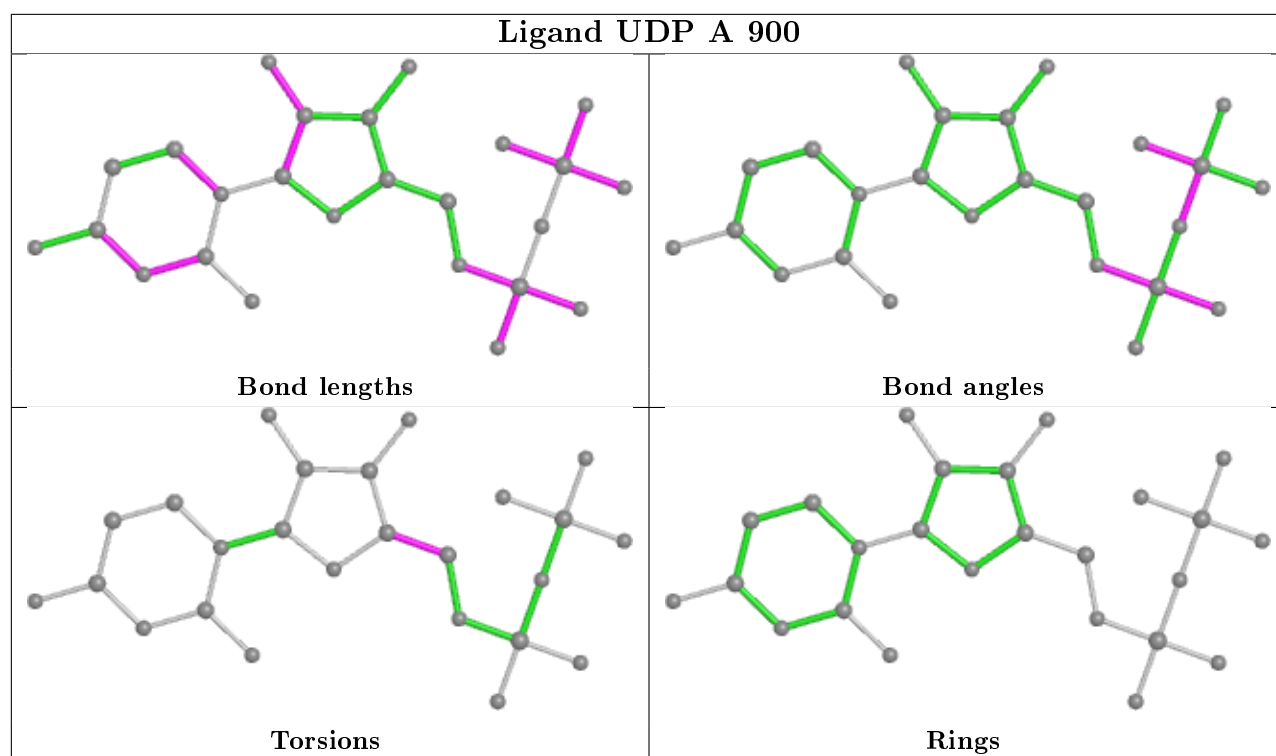
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	UDP	3	0
2	A	900	UDP	3	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 ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.