Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 07:38 AM EDT

PDB ID	:	6P84
Title	:	E.coli LpxD in complex with compound 2o
Authors	:	Ma, X.; Shia, S.
Deposited on	:	2019-06-06
Resolution	:	1.70 Å(reported)

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

MolProbity	:	FAILED
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)	:	2.35.1

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.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8593 atoms, of which 57 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-3-O-(3-hydroxymyristoyl)glucosamine N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total 2468	C 1541	N 438	O 470	S 19	0	0	0
1	B	339	Total 2509	C 1564	N 448	O 478	S 19	0	2	0
1	C	337	Total 2498	C 1559	N 445	O 474	S 20	0	3	0

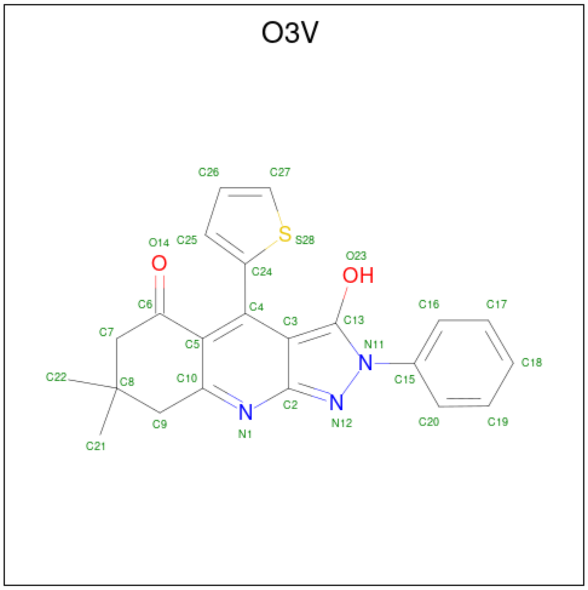
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q0P6M7
A	0	SER	-	expression tag	UNP Q0P6M7
A	1	GLY	-	expression tag	UNP Q0P6M7
A	2	GLY	-	expression tag	UNP Q0P6M7
B	-1	GLY	-	expression tag	UNP Q0P6M7
B	0	SER	-	expression tag	UNP Q0P6M7
B	1	GLY	-	expression tag	UNP Q0P6M7
B	2	GLY	-	expression tag	UNP Q0P6M7
C	-1	GLY	-	expression tag	UNP Q0P6M7
C	0	SER	-	expression tag	UNP Q0P6M7
C	1	GLY	-	expression tag	UNP Q0P6M7
C	2	GLY	-	expression tag	UNP Q0P6M7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0

- Molecule 3 is 3-hydroxy-7,7-dimethyl-2-phenyl-4-(thiophen-2-yl)-2,6,7,8-tetrahydro-5H-pyrazolo[3,4-b]quinolin-5-one (three-letter code: O3V) (formula: $C_{22}H_{19}N_3O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 47	C 22	H 19	N 3	O 2	S 1	19	0
3	B	1	Total 47	C 22	H 19	N 3	O 2	S 1	19	0
3	C	1	Total 47	C 22	H 19	N 3	O 2	S 1	19	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total 304	O 304	0	0
4	B	333	Total 333	O 333	0	0
4	C	338	Total 338	O 338	0	0

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

3 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.58Å 96.58Å 216.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.42 – 1.70	Depositor
% Data completeness (in resolution range)	87.9 (45.42-1.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.169 , 0.196	Depositor
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.526	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
Total number of atoms	8593	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
3	O3V	B	501	-	31,32,32	1.27	3 (9%)	28,49,49	0.98	2 (7%)
3	O3V	A	403	-	31,32,32	1.16	3 (9%)	28,49,49	0.95	0
3	O3V	C	501	-	31,32,32	1.18	4 (12%)	28,49,49	1.07	3 (10%)

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
3	O3V	B	501	-	-	1/8/34/34	0/5/5/5
3	O3V	A	403	-	-	0/8/34/34	0/5/5/5
3	O3V	C	501	-	-	1/8/34/34	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	O3V	C13-C3	-4.56	1.39	1.45
3	A	403	O3V	C9-C10	3.43	1.53	1.50
3	A	403	O3V	C13-C3	-3.38	1.41	1.45
3	C	501	O3V	C4-C24	-3.11	1.45	1.48
3	C	501	O3V	C13-C3	-2.62	1.41	1.45
3	B	501	O3V	C4-C24	-2.37	1.45	1.48
3	C	501	O3V	C9-C10	2.21	1.52	1.50
3	A	403	O3V	C5-C10	2.12	1.45	1.41
3	B	501	O3V	C5-C10	2.09	1.45	1.41
3	C	501	O3V	C5-C10	2.05	1.45	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	O3V	C8-C7-C6	-2.91	109.50	113.73
3	C	501	O3V	C24-C4-C3	-2.61	114.98	121.06
3	B	501	O3V	C24-C4-C3	-2.39	115.51	121.06
3	C	501	O3V	C8-C9-C10	-2.06	112.49	114.12
3	B	501	O3V	C5-C10-N1	2.06	125.65	122.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

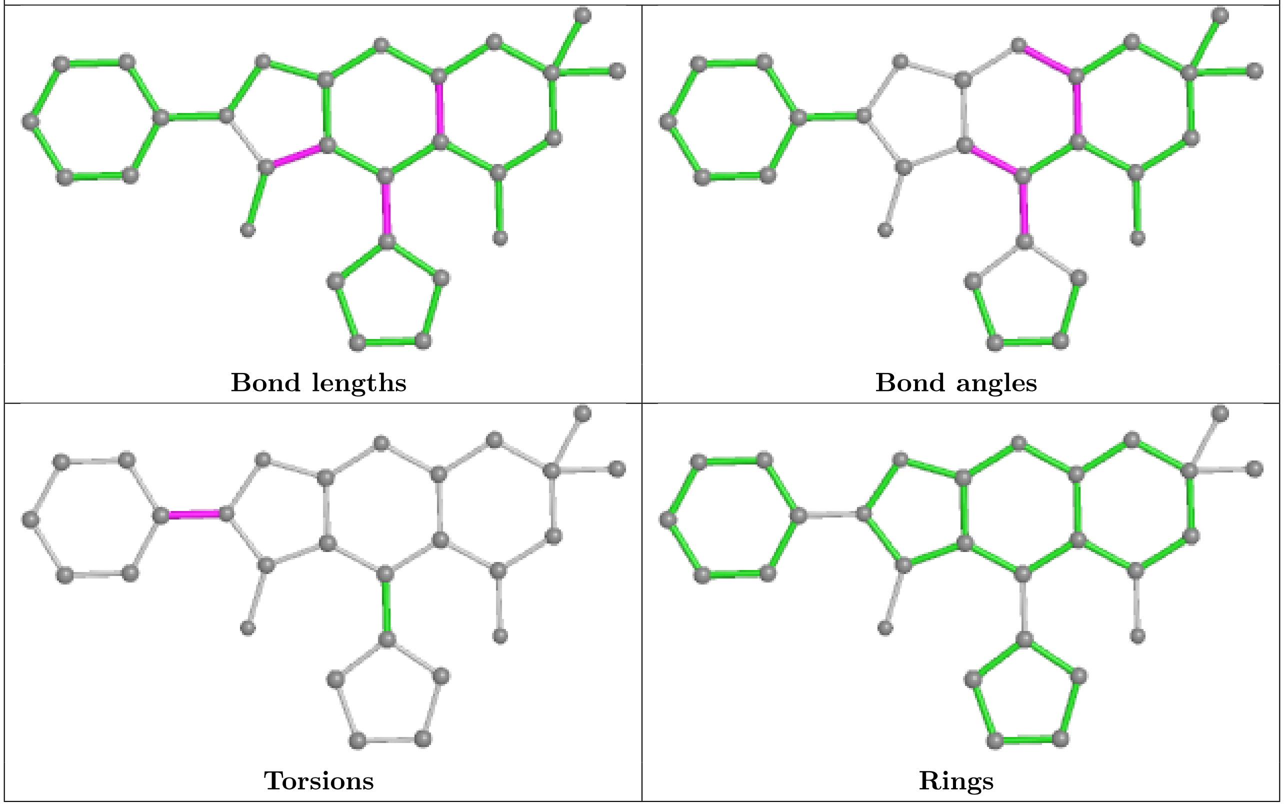
Mol	Chain	Res	Type	Atoms
3	B	501	O3V	C16-C15-N11-C13
3	C	501	O3V	C16-C15-N11-C13

There are no ring outliers.

No monomer is involved in short contacts.

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 O3V B 501



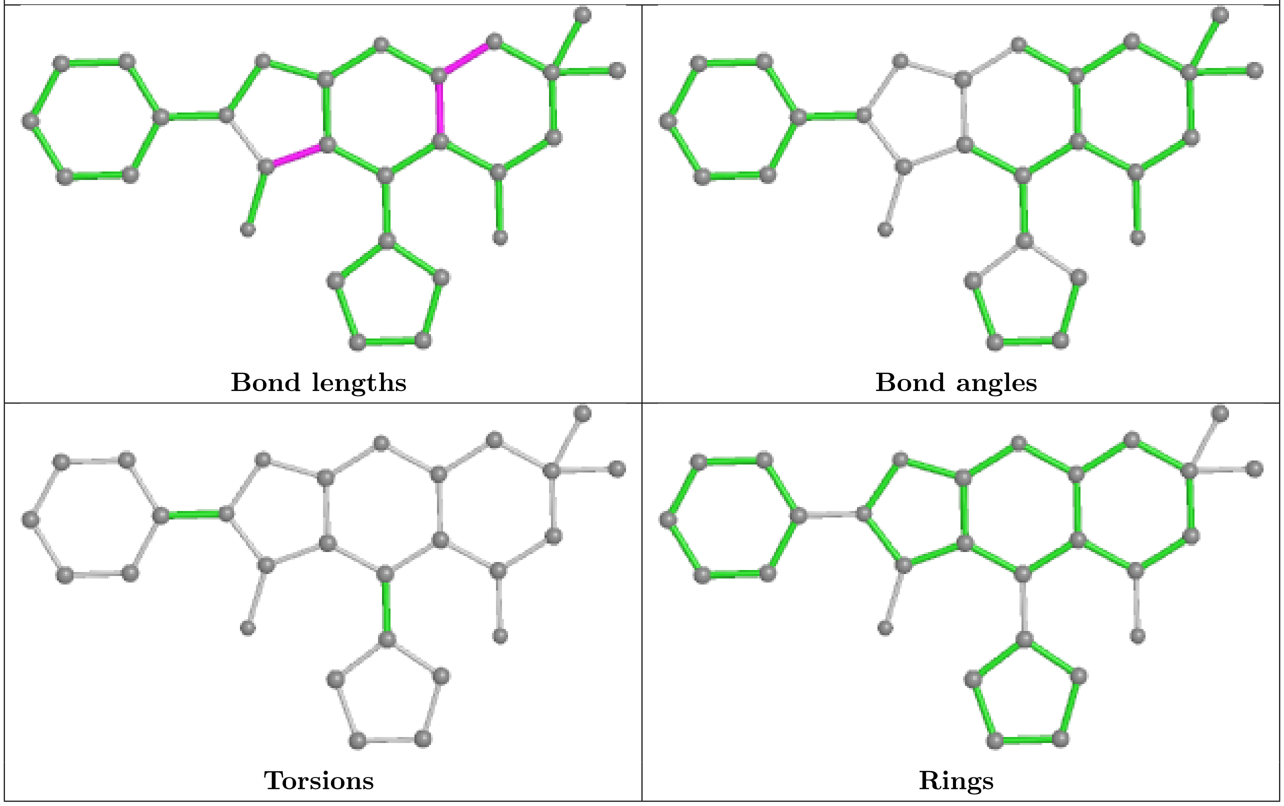
Bond lengths

Bond angles

Torsions

Rings

Ligand O3V A 403



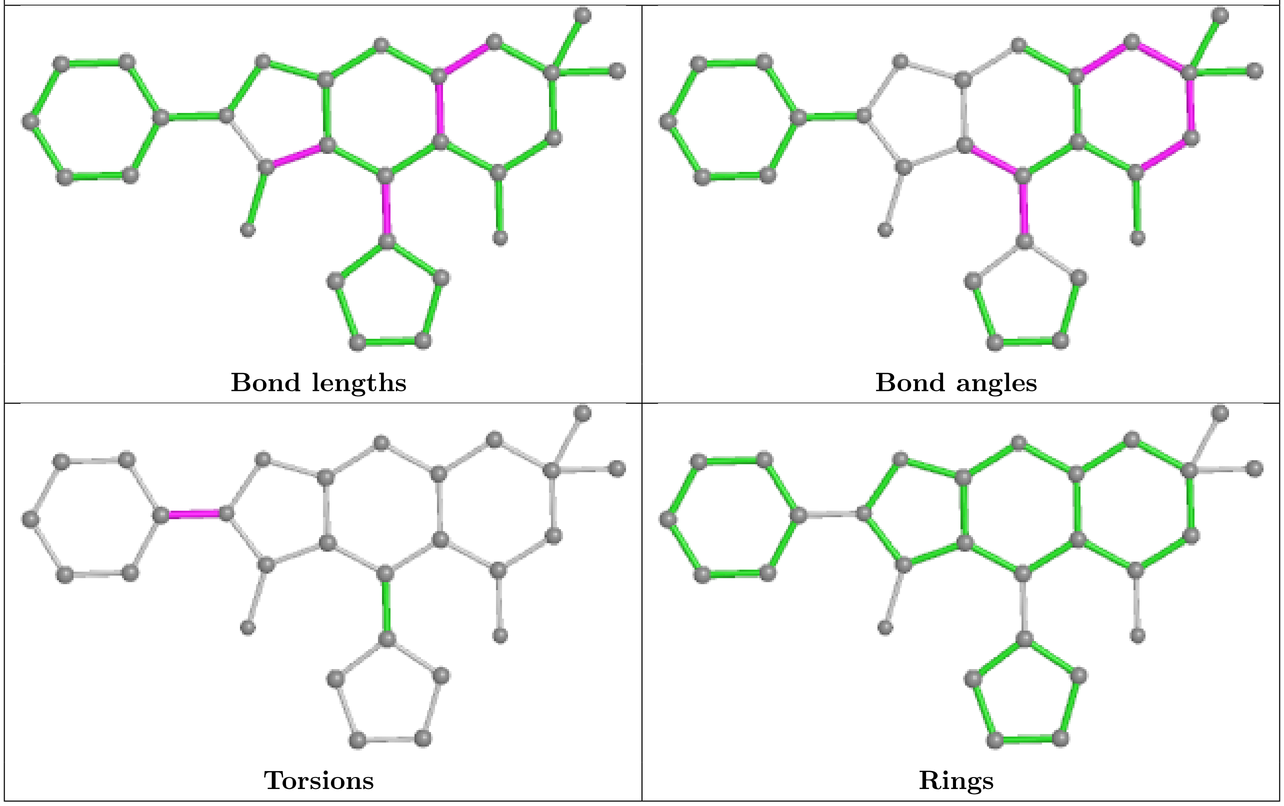
Bond lengths

Bond angles

Torsions

Rings

Ligand O3V C 501



Bond lengths

Bond angles

Torsions

Rings

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

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

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

5.3 Carbohydrates ⓘ

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

5.4 Ligands ⓘ

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

5.5 Other polymers ⓘ

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