Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:53 PM EDT

PDB ID : 6PIB

Title : Structure of the Klebsiella pneumoniae LpxH-AZ1 complex

Authors : Cho, J.; Zhou, P.

Deposited on : 2019-06-26

Resolution : 2.26 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

---

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.

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 ⓘ

There are 5 unique types of molecules in this entry. The entry contains 2049 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-2,3-diacylglucosamine hydrolase.

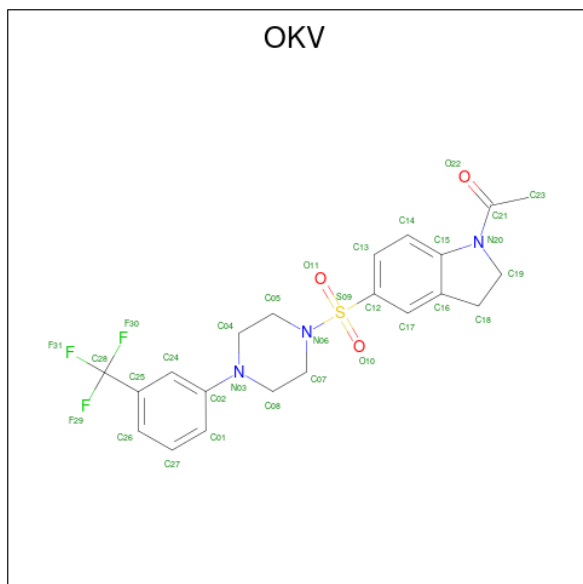| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total 1931	C 1237	N 348	O 338	S 8	0	4	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	insertion	UNP A0A1S0WIC1
A	241	LEU	-	expression tag	UNP A0A1S0WIC1
A	242	GLU	-	expression tag	UNP A0A1S0WIC1
A	243	GLU	-	expression tag	UNP A0A1S0WIC1
A	244	ASN	-	expression tag	UNP A0A1S0WIC1
A	245	LEU	-	expression tag	UNP A0A1S0WIC1
A	246	TYR	-	expression tag	UNP A0A1S0WIC1
A	247	PHE	-	expression tag	UNP A0A1S0WIC1
A	248	GLN	-	expression tag	UNP A0A1S0WIC1
A	249	SER	-	expression tag	UNP A0A1S0WIC1
A	250	HIS	-	expression tag	UNP A0A1S0WIC1
A	251	HIS	-	expression tag	UNP A0A1S0WIC1
A	252	HIS	-	expression tag	UNP A0A1S0WIC1
A	253	HIS	-	expression tag	UNP A0A1S0WIC1
A	254	HIS	-	expression tag	UNP A0A1S0WIC1
A	255	HIS	-	expression tag	UNP A0A1S0WIC1
A	256	HIS	-	expression tag	UNP A0A1S0WIC1
A	257	HIS	-	expression tag	UNP A0A1S0WIC1
A	258	HIS	-	expression tag	UNP A0A1S0WIC1
A	259	HIS	-	expression tag	UNP A0A1S0WIC1

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).
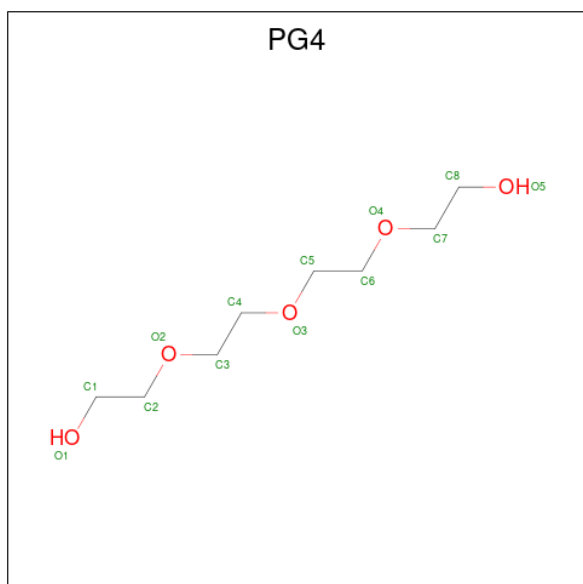
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0

- Molecule 3 is 1-[5-({4-[3-(trifluoromethyl)phenyl]piperazin-1-yl}sulfonyl)-2,3-dihydro-1H-indol-1-yl]ethan-1-one (three-letter code: OKV) (formula: $C_{21}H_{22}F_3N_3O_3S$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	31	21	3	3	3	1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 8	O 5	0	0
4	A	1	Total 13	C 8	O 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	0

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

3 Data and refinement statistics (i)

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	106.75Å 106.75Å 52.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.96 – 2.26	Depositor
% Data completeness (in resolution range)	99.9 (45.96-2.26)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.196 , 0.239	Depositor
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.668	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
Total number of atoms	2049	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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.

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	PG4	A	305	-	12,12,12	0.52	0	11,11,11	0.24	0
3	OKV	A	303	-	34,34,34	2.15	8 (23%)	51,52,52	1.72	10 (19%)
4	PG4	A	306	-	12,12,12	0.52	0	11,11,11	0.30	0
4	PG4	A	304	-	12,12,12	0.53	0	11,11,11	0.22	0

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	PG4	A	305	-	-	4/10/10/10	-
3	OKV	A	303	-	-	1/26/45/45	0/4/4/4
4	PG4	A	306	-	-	6/10/10/10	-
4	PG4	A	304	-	-	8/10/10/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	OKV	C21-N20	6.70	1.45	1.36
3	A	303	OKV	C15-N20	5.35	1.50	1.39
3	A	303	OKV	S09-N06	5.28	1.70	1.63
3	A	303	OKV	C12-S09	3.64	1.81	1.76
3	A	303	OKV	O11-S09	3.06	1.46	1.43
3	A	303	OKV	O10-S09	2.70	1.46	1.43
3	A	303	OKV	C05-N06	-2.16	1.45	1.47
3	A	303	OKV	C07-N06	-2.13	1.45	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	OKV	O11-S09-O10	-5.95	109.88	119.52
3	A	303	OKV	C07-N06-S09	-4.29	109.25	117.05
3	A	303	OKV	C05-N06-S09	-3.71	110.31	117.05
3	A	303	OKV	O11-S09-N06	3.46	109.84	106.69
3	A	303	OKV	C04-C05-N06	3.31	111.44	108.91
3	A	303	OKV	C08-C07-N06	3.26	111.40	108.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	OKV	C12-S09-N06	2.56	110.35	107.30
3	A	303	OKV	C19-C18-C16	2.16	105.71	103.65
3	A	303	OKV	C18-C19-N20	2.07	106.75	104.94
3	A	303	OKV	C16-C15-N20	-2.06	108.53	109.66

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	PG4	O2-C3-C4-O3
4	A	305	PG4	O4-C7-C8-O5
4	A	304	PG4	O3-C5-C6-O4
4	A	304	PG4	O1-C1-C2-O2
4	A	306	PG4	O2-C3-C4-O3
4	A	306	PG4	O3-C5-C6-O4
3	A	303	OKV	C05-N06-S09-O11
4	A	305	PG4	C3-C4-O3-C5
4	A	304	PG4	C5-C6-O4-C7
4	A	304	PG4	C1-C2-O2-C3
4	A	305	PG4	C1-C2-O2-C3
4	A	306	PG4	C1-C2-O2-C3
4	A	304	PG4	C6-C5-O3-C4
4	A	306	PG4	C8-C7-O4-C6
4	A	305	PG4	O3-C5-C6-O4
4	A	306	PG4	C4-C3-O2-C2
4	A	306	PG4	C3-C4-O3-C5
4	A	304	PG4	C3-C4-O3-C5
4	A	304	PG4	C4-C3-O2-C2

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 OKV A 303

Bond lengths   Bond angles

Torsions   Rings
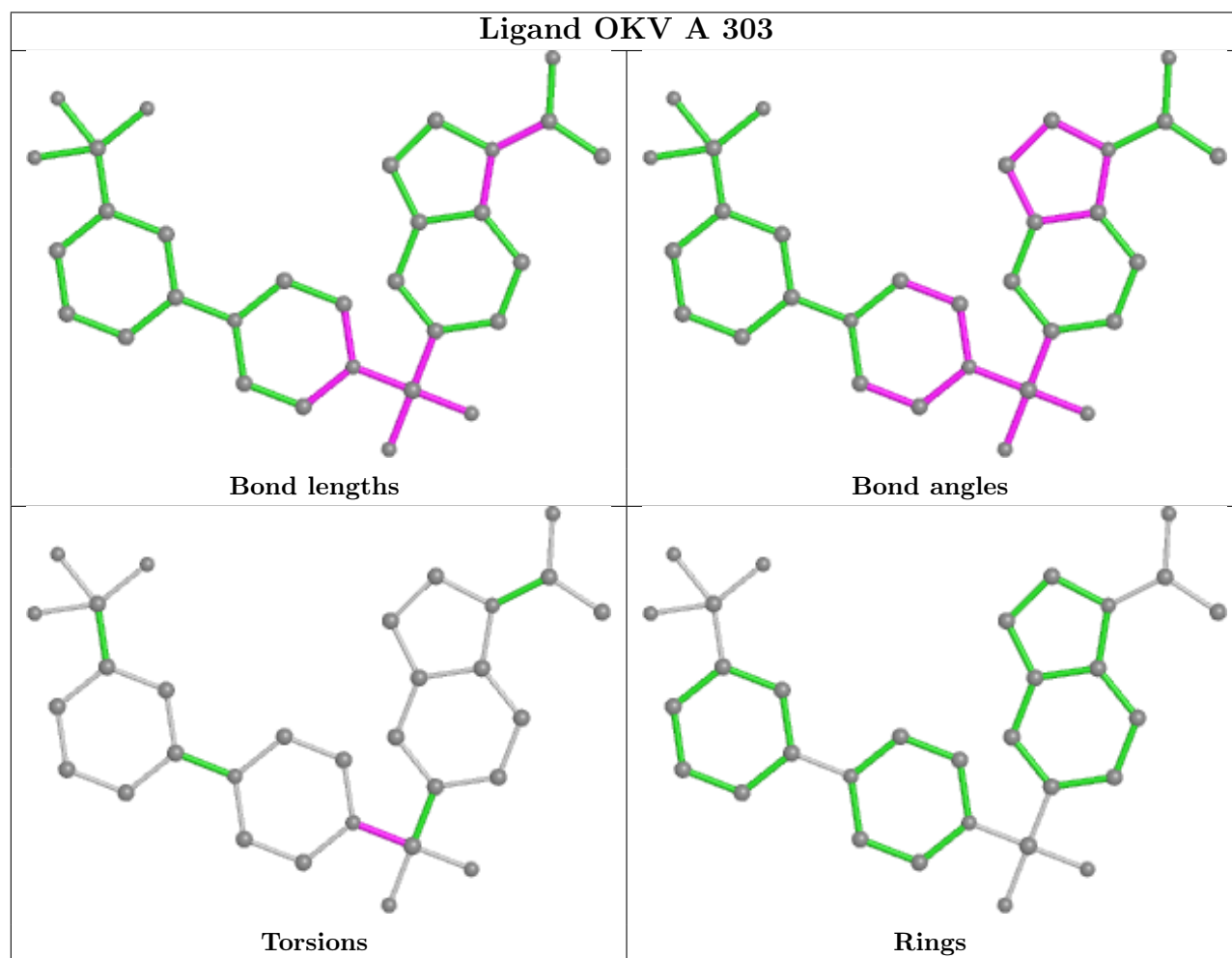
4.7 Other polymers ⓘ

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.