Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 11:36 PM EDT

PDB ID	:	6TZC
Title	:	Crystal Structure of African Swine Fever Virus A179L with the Autophagy Regulator Beclin
Authors	:	Banjara, S.; Kvansakul, M.; Hinds, M.G.
Deposited on	:	2019-08-12
Resolution	:	2.41 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.

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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 5 unique types of molecules in this entry. The entry contains 8408 atoms, of which 4089 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 Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	367	5569	1824	2740	453	546	6	0	6	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP P0AEX9
A	393	ASN	-	expression tag	UNP P0AEX9
A	394	SER	-	expression tag	UNP P0AEX9
A	395	SER	-	expression tag	UNP P0AEX9
A	396	SER	-	expression tag	UNP P0AEX9

- Molecule 2 is a protein called Apoptosis regulator Bcl-2 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	144	2343	767	1162	187	220	7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	149	HIS	-	expression tag	UNP P42485
B	150	HIS	-	expression tag	UNP P42485
B	151	HIS	-	expression tag	UNP P42485
B	152	HIS	-	expression tag	UNP P42485
B	153	HIS	-	expression tag	UNP P42485
B	154	HIS	-	expression tag	UNP P42485

- Molecule 3 is a protein called Beclin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	20	325	99	165	28	31	2	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
4	D	2	45	12	22	11	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	76	76	76	0	0
5	B	49	49	49	0	0
5	C	1	1	1	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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.56Å 44.35Å 129.02Å 90.00° 94.53° 90.00°	Depositor
Resolution (Å)	51.58 – 2.41	Depositor
% Data completeness (in resolution range)	98.9 (51.58-2.41)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.39Å)	Xtriage
Refinement program	AMBER 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.214 , 0.253	Depositor
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.551	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8408	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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 (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

2 monosaccharides 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	GLC	D	1	4	12,12,12	1.18	3 (25%)	17,17,17	1.68	5 (29%)
4	GLC	D	2	4	11,11,12	0.89	1 (9%)	15,15,17	1.33	2 (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	GLC	D	1	4	-	0/2/22/22	0/1/1/1
4	GLC	D	2	4	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	GLC	O5-C1	-2.23	1.40	1.43
4	D	1	GLC	O4-C4	-2.22	1.37	1.43
4	D	1	GLC	C6-C5	2.20	1.59	1.51
4	D	1	GLC	C4-C5	-2.03	1.48	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	GLC	O5-C1-C2	2.66	115.04	110.28
4	D	1	GLC	C1-O5-C5	-2.41	109.11	113.66
4	D	2	GLC	O5-C5-C6	2.39	110.95	107.20
4	D	1	GLC	C6-C5-C4	2.35	118.52	113.00
4	D	2	GLC	O2-C2-C3	-2.29	105.55	110.14
4	D	1	GLC	O5-C5-C4	2.28	113.83	109.69
4	D	1	GLC	O3-C3-C4	2.19	115.41	110.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	GLC	O5-C5-C6-O6

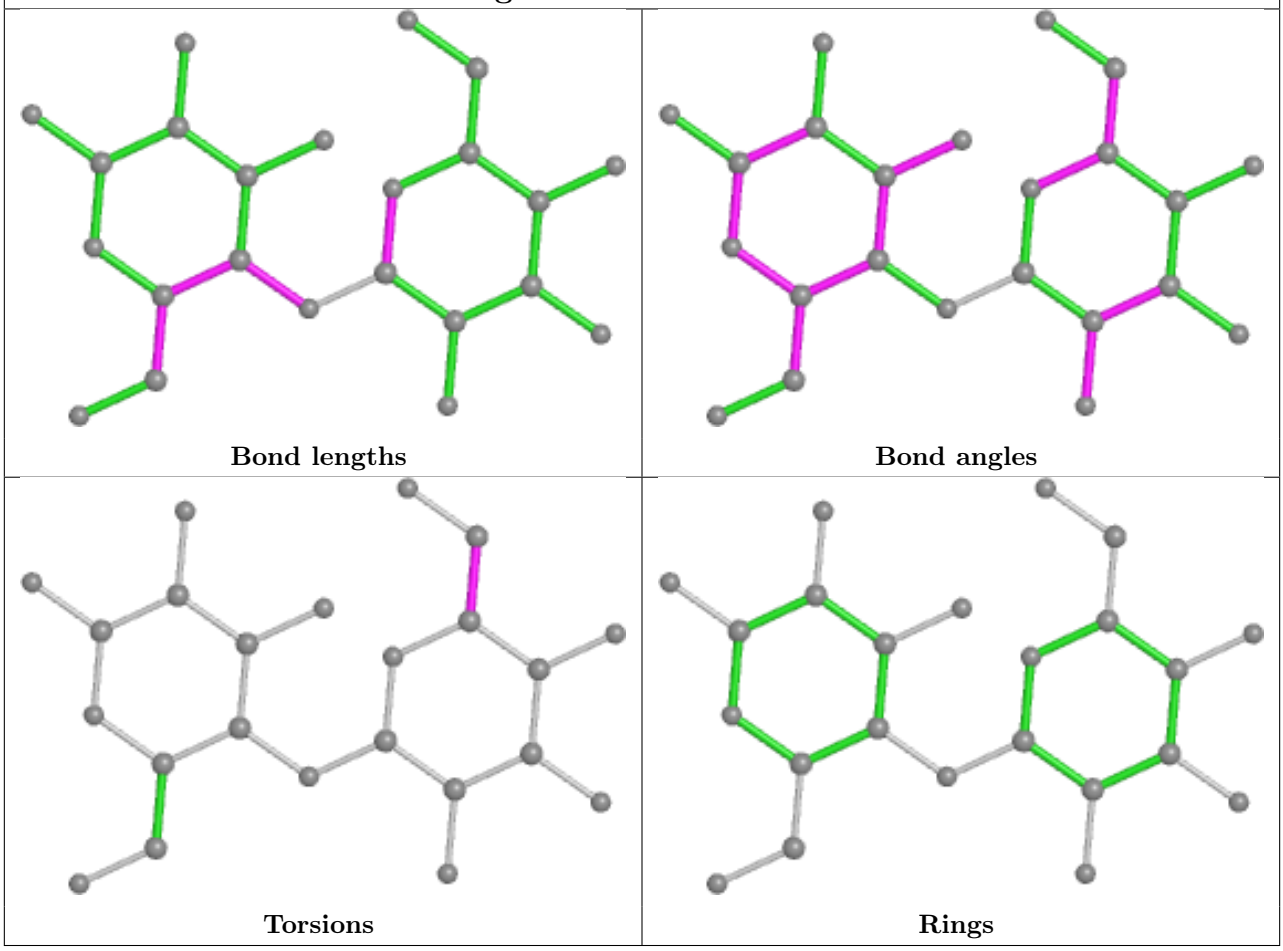
There are no ring outliers.

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 oligosaccharide.

Oligosaccharide Chain D



4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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