Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 11:03 PM EDT

PDB ID	:	6PQ9
Title	:	Crystal Structure of TLA-1 S70G extended spectrum Beta-lactamase
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Deposited on	:	2019-07-08
Resolution	:	2.19 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 2.19 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.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	308	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2425 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.

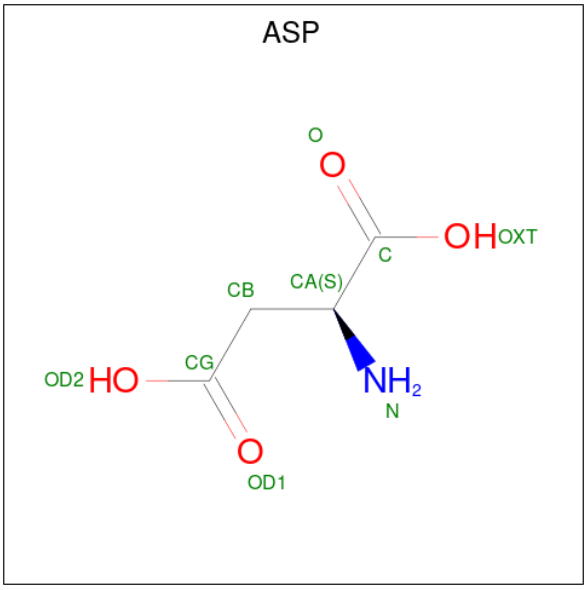
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2187	1395	367	420	5	0	3	0

There is a discrepancy between the modelled and reference sequences:

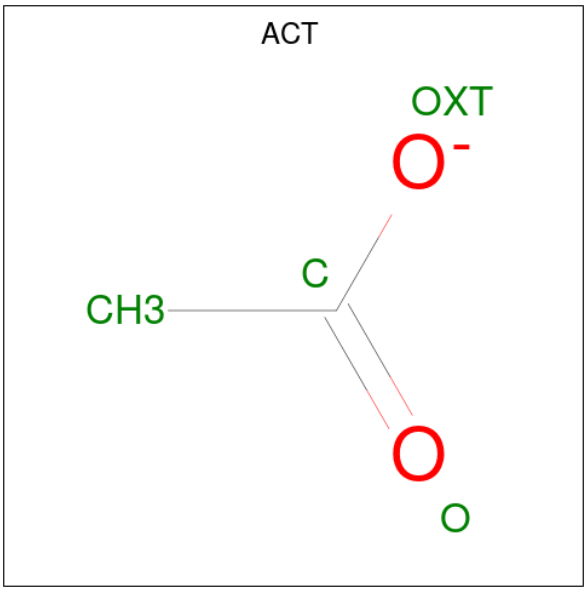
Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	SER	engineered mutation	UNP Q9X6W1

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



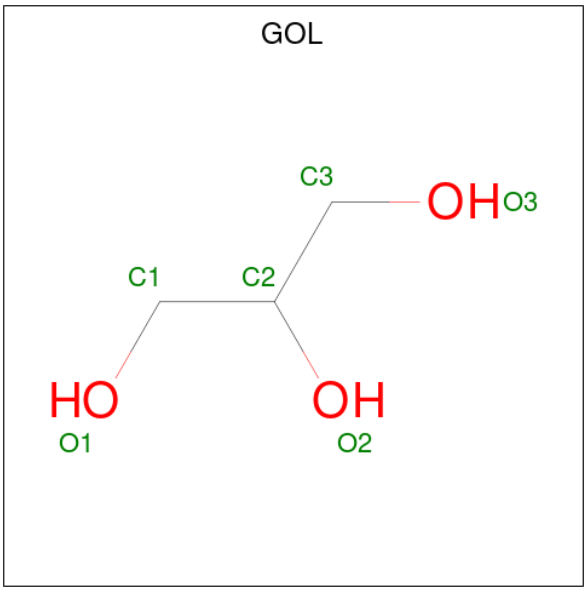
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



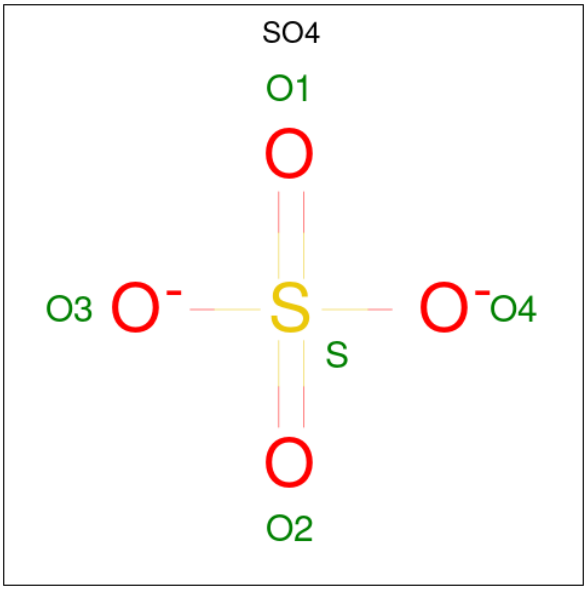
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	185	185	185	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 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.41Å 99.41Å 99.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.19	Depositor
% Data completeness (in resolution range)	99.5 (19.89-2.19)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.191 , 0.238	Depositor
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.018	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k 0.007 for -l,-k,-h	Xtriage
Total number of atoms	2425	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
3	ACT	A	302	-	3,3,3	1.62	1 (33%)	3,3,3	1.63	0
2	ASP	A	301	-	6,7,8	0.97	0	5,8,10	0.90	0
3	ACT	A	303	-	3,3,3	1.55	1 (33%)	3,3,3	1.41	0
3	ACT	A	309	-	3,3,3	1.31	0	3,3,3	1.83	2 (66%)
5	SO4	A	311	-	4,4,4	0.17	0	6,6,6	0.26	0
3	ACT	A	304	-	3,3,3	1.57	1 (33%)	3,3,3	1.46	0
3	ACT	A	305	-	3,3,3	1.62	1 (33%)	3,3,3	1.50	0
3	ACT	A	306	-	3,3,3	1.56	1 (33%)	3,3,3	1.39	0
4	GOL	A	310	-	5,5,5	1.66	1 (20%)	5,5,5	0.92	0
3	ACT	A	307	-	3,3,3	0.93	0	3,3,3	1.57	0
4	GOL	A	308	-	5,5,5	1.64	1 (20%)	5,5,5	1.70	2 (40%)

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	GOL	A	308	-	-	3/4/4/4	-
4	GOL	A	310	-	-	3/4/4/4	-
2	ASP	A	301	-	-	2/5/6/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	310	GOL	C3-C2	3.42	1.65	1.51
4	A	308	GOL	C1-C2	3.21	1.64	1.51
3	A	305	ACT	CH3-C	2.54	1.59	1.49
3	A	302	ACT	CH3-C	2.39	1.59	1.49
3	A	303	ACT	CH3-C	2.30	1.58	1.49
3	A	306	ACT	CH3-C	2.28	1.58	1.49
3	A	304	ACT	CH3-C	2.24	1.58	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	308	GOL	O2-C2-C1	2.91	121.96	109.12
3	A	309	ACT	OXT-C-O	2.30	130.52	122.05
4	A	308	GOL	O2-C2-C3	2.25	119.05	109.12
3	A	309	ACT	O-C-CH3	-2.18	113.85	122.33

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	308	GOL	O2-C2-C3-O3
4	A	308	GOL	O1-C1-C2-C3
4	A	308	GOL	C1-C2-C3-O3
4	A	310	GOL	C1-C2-C3-O3
2	A	301	ASP	CA-CB-CG-OD1
2	A	301	ASP	CA-CB-CG-OD2
4	A	310	GOL	O2-C2-C3-O3
4	A	310	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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.