Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 09:36 PM EDT

PDB ID	:	6VYE
Title	:	6-phosphogluconolactonase from Trypanosoma cruzi
Authors	:	Merritt, E.A.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on	:	2020-02-26
Resolution	:	1.95 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
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 1.95 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 4317 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.

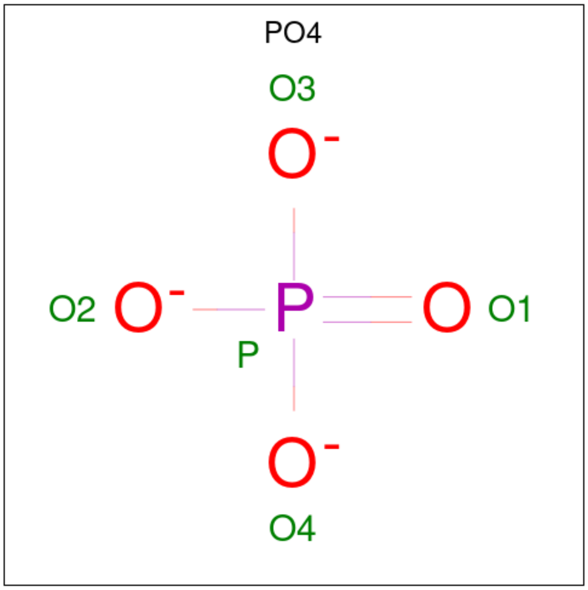
- Molecule 1 is a protein called 6-phosphogluconolactonase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total 2021	C 1286	N 351	O 372	S 12	0	0	0
1	B	266	Total 2047	C 1301	N 354	O 379	S 13	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

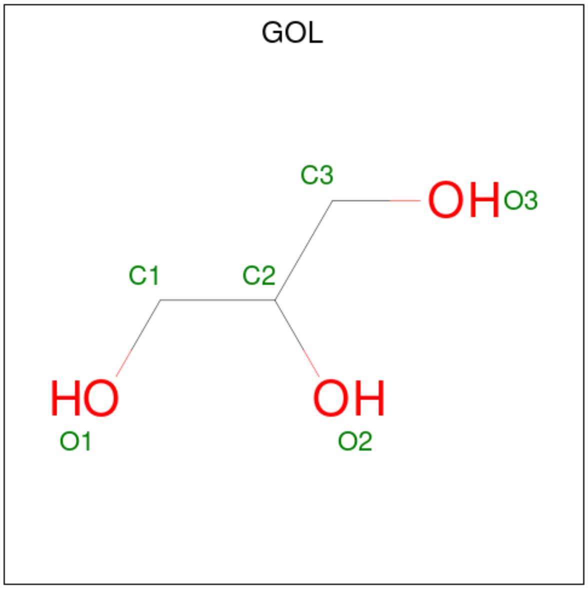
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q4CQA8
A	-6	ALA	-	expression tag	UNP Q4CQA8
A	-5	HIS	-	expression tag	UNP Q4CQA8
A	-4	HIS	-	expression tag	UNP Q4CQA8
A	-3	HIS	-	expression tag	UNP Q4CQA8
A	-2	HIS	-	expression tag	UNP Q4CQA8
A	-1	HIS	-	expression tag	UNP Q4CQA8
A	0	HIS	-	expression tag	UNP Q4CQA8
A	97	ARG	HIS	conflict	UNP Q4CQA8
A	259	GLU	GLY	conflict	UNP Q4CQA8
B	-7	MET	-	initiating methionine	UNP Q4CQA8
B	-6	ALA	-	expression tag	UNP Q4CQA8
B	-5	HIS	-	expression tag	UNP Q4CQA8
B	-4	HIS	-	expression tag	UNP Q4CQA8
B	-3	HIS	-	expression tag	UNP Q4CQA8
B	-2	HIS	-	expression tag	UNP Q4CQA8
B	-1	HIS	-	expression tag	UNP Q4CQA8
B	0	HIS	-	expression tag	UNP Q4CQA8
B	97	ARG	HIS	conflict	UNP Q4CQA8
B	259	GLU	GLY	conflict	UNP Q4CQA8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	113	Total O 113 113	0	0
4	B	103	Total O 103 103	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 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.77Å 63.39Å 79.32Å 90.00° 94.91° 90.00°	Depositor
Resolution (Å)	49.50 – 1.95	Depositor
% Data completeness (in resolution range)	95.3 (49.50-1.95)	Depositor
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.231 , 0.270	Depositor
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.110	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4317	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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 ⓘ

6 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	PO4	B	301	-	4,4,4	0.65	0	6,6,6	0.73	0
3	GOL	A	304	-	5,5,5	0.09	0	5,5,5	0.29	0
2	PO4	A	301	-	4,4,4	1.67	1 (25%)	6,6,6	1.06	0
3	GOL	B	302	-	5,5,5	0.16	0	5,5,5	0.35	0
3	GOL	A	303	-	5,5,5	0.21	0	5,5,5	0.45	0
2	PO4	A	302	-	4,4,4	1.48	1 (25%)	6,6,6	0.65	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
3	GOL	A	304	-	-	2/4/4/4	-
3	GOL	B	302	-	-	4/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	PO4	P-O1	2.24	1.56	1.50
2	A	301	PO4	P-O4	-2.18	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	GOL	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-C3
3	A	304	GOL	C1-C2-C3-O3
3	B	302	GOL	C1-C2-C3-O3
3	B	302	GOL	O2-C2-C3-O3
3	A	304	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-O2
3	B	302	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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.