

Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 02:54 AM EDT

PDB ID : 6OZW

Title: Crystal structure of the 65-kilodalton amino-terminal fragment of DNA topoi-

somerase I from Streptococcus mutans

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Deposited on : 2019-05-16

Resolution : 2.06 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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the ① 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 2.06 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 4700 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 DNA topoisomerase 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	538	Total	С	N	О	S	0	0	0
	A	000	4339	2770	750	810	9	U		

There are 20 discrepancies between the modelled and reference sequences:

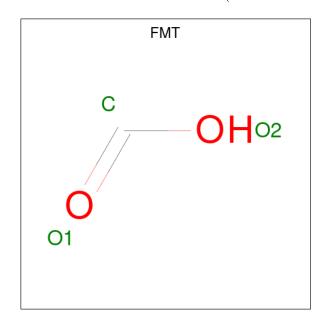
Chain	Residue	Modelled	Actual	Comment	Reference	
A	-19	MET	-	initiating methionine	UNP Q8DUD3	
A	-18	GLY	-	expression tag	UNP Q8DUD3	
A	-17	SER	-	expression tag	UNP Q8DUD3	
A	-16	SER	-	expression tag	UNP Q8DUD3	
A	-15	HIS	-	expression tag	UNP Q8DUD3	
A	-14	HIS	-	expression tag	UNP Q8DUD3	
A	-13	HIS	-	expression tag	UNP Q8DUD3	
A	-12	HIS	-	expression tag	UNP Q8DUD3	
A	-11	HIS	-	expression tag	UNP Q8DUD3	
A	-10	HIS	-	expression tag	UNP Q8DUD3	
A	-9	SER	-	expression tag	UNP Q8DUD3	
A	-8	SER	-	expression tag	UNP Q8DUD3	
A	-7	GLY	-	expression tag	UNP Q8DUD3	
A	-6	LEU	-	expression tag	UNP Q8DUD3	
A	-5	VAL	-	expression tag	UNP Q8DUD3	
A	-4	PRO	ı	expression tag	UNP Q8DUD3	
A	-3	ARG	ı	expression tag	UNP Q8DUD3	
A	-2	GLY	-	expression tag	UNP Q8DUD3	
A	-1	SER	=	expression tag	UNP Q8DUD3	
A	0	HIS	-	expression tag	UNP Q8DUD3	

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Mg 6 6	0	0



 \bullet Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: $\mathrm{CH_2O_2}).$



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

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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	313	Total O 313 313	0	0

 $\operatorname{MolProbity}$ 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 21 21 2	Depositor
Cell constants	88.58Å 98.37Å 72.71Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 - 2.06	Depositor
% Data completeness	82.1 (49.18-2.06)	Depositor
(in resolution range)	02.1 (43.10-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.84 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.200 , 0.268	Depositor
Wilson B-factor (\mathring{A}^2)	24.8	Xtriage
Anisotropy	0.220	Xtriage
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4700	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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).

Mal	Trino	Chain	Res	Link	В	Bond lengths		В	ond ang	gles
Mol	Type	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	FMT	A	618	-	2,2,2	0.63	0	1,1,1	0.17	0
3	FMT	A	614	-	2,2,2	0.66	0	1,1,1	0.23	0
3	FMT	A	612	-	2,2,2	0.59	0	1,1,1	0.12	0
3	FMT	A	619	-	2,2,2	0.66	0	1,1,1	0.12	0
3	FMT	A	620	-	2,2,2	0.67	0	1,1,1	0.22	0
3	FMT	A	611	-	2,2,2	0.67	0	1,1,1	0.18	0
3	FMT	A	617	-	2,2,2	0.66	0	1,1,1	0.17	0
3	FMT	A	615	-	2,2,2	0.66	0	1,1,1	0.22	0
3	FMT	A	610	-	2,2,2	0.67	0	1,1,1	0.23	0
3	FMT	A	608	-	2,2,2	0.62	0	1,1,1	0.11	0
3	FMT	A	616	-	2,2,2	0.62	0	1,1,1	0.10	0
3	FMT	A	609	-	2,2,2	0.69	0	1,1,1	0.30	0
3	FMT	A	607	-	2,2,2	0.61	0	1,1,1	0.02	0
3	FMT	A	613	-	2,2,2	0.68	0	1,1,1	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

