

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 04:56 AM EDT

PDB ID : 6ML5

Title: ZBTB24 Zinc Fingers 4-8 with 19+1mer DNA Oligonucleotide (Sequence 4)

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Deposited on : 2018-09-26

Resolution : 1.65 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 1.65 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 6 unique types of molecules in this entry. The entry contains 2249 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 Zinc finger and BTB domain-containing protein 24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	142	Total 1132	C 705	N 217	O 196	S 14	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	GLY	-	expression tag	UNP Q80X44
A	371	PRO	-	expression tag	UNP Q80X44
A	372	LEU	-	expression tag	UNP Q80X44
A	373	GLY	-	expression tag	UNP Q80X44
A	374	SER	-	expression tag	UNP Q80X44
A	520	TYR	-	expression tag	UNP Q80X44

• Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*GP*CP*AP*GP*GP*TP*CP*CP*TP*GP*GP*AP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	$\mathbf{AltConf}$	Trace
2	Е	20	Total 409	C 195	N 78	O 117	P 19	0	0	0

• Molecule 3 is a DNA chain called DNA (5'-D(*TP*AP*AP*TP*TP*CP*GP*TP*CP*CP* AP*GP*AP*CP*CP*TP*GP*CP*G)-3').

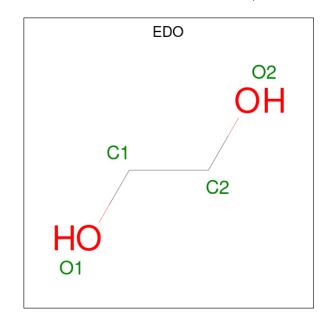
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	20	Total 405	C 194	N 73	O 119	P 19	0	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Zn 5 5	0	0



 \bullet Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0
6	E	70	Total O 70 70	0	0
6	F	67	Total O 67 67	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	46.01Å 68.24 Å 48.58 Å	Depositor	
a, b, c, α , β , γ	90.00° 92.54° 90.00°	Depositor	
Resolution (Å)	27.91 - 1.65	Depositor	
% Data completeness	97.9 (27.91-1.65)	Depositor	
(in resolution range)	,	Depositor	
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.51 (at 1.65Å)	Xtriage	
Refinement program	PHENIX (1.13_2998: ???)	Depositor	
R, R_{free}	0.226 , 0.244	Depositor	
Wilson B-factor $(Å^2)$	16.4	Xtriage	
Anisotropy	0.196	Xtriage	
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.34$	Xtriage	
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage	
Total number of atoms	2249	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	25.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 12.96% 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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	Tuno	Chain	Res	Link	\mathbf{B}	ond leng	gths	Bond angles		
MIOI	Type		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	Е	401	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	A	606	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	A	608	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	A	607	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	Е	402	-	3,3,3	0.45	0	2,2,2	0.37	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
5	EDO	Е	401	-	-	0/1/1/1	-
5	EDO	A	606	-	-	0/1/1/1	-
5	EDO	A	608	-	-	0/1/1/1	_
5	EDO	A	607	-	-	0/1/1/1	-
5	EDO	Е	402	-	-	0/1/1/1	-

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.

