



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:33 AM UTC

PDB ID : 5T4I / pdb_00005t4i
Title : A Novel domain in human EXOG converts apoptotic endonuclease to DNA-repair enzyme
Authors : Szymanski, M.R.; Yin, W.Y.
Deposited on : 2016-08-29
Resolution : 2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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>

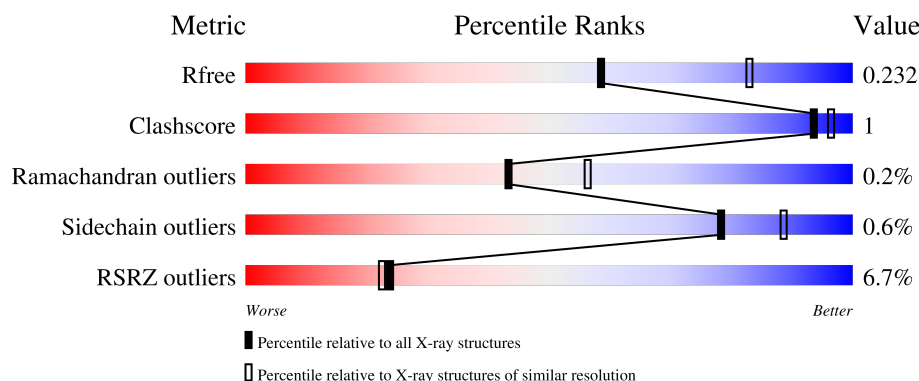
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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Mol	Chain	Length	Quality of chain
3	F	9	11% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10661 atoms, of which 5101 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 Nuclease EXOG, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A										

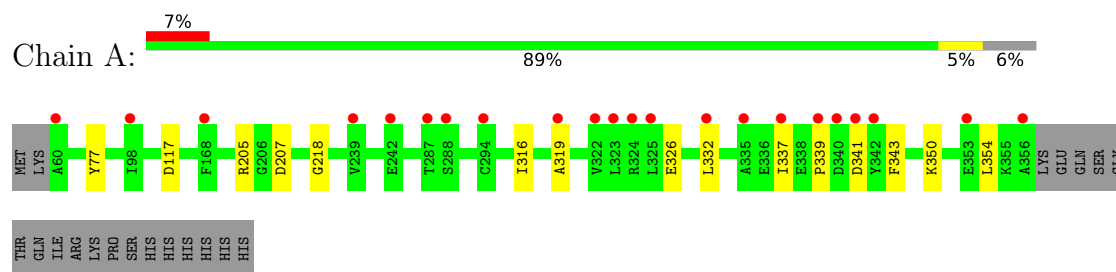
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*AP*CP*GP*TP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	9	Total	C	H	N	O	P	0	0	0
			284	87	102	36	51	8			
3	F	9	Total	C	H	N	O	P	0	0	0
			284	87	102	36	51	8			

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nuclease EXOG, mitochondrial





- Molecule 3: DNA (5'-D(*GP*CP*AP*CP*GP*TP*CP*AP*G)-3')

Chain F:  11%  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.51Å 79.72Å 138.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.03 – 2.39 40.03 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.03-2.39) 97.7 (40.03-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.39	

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/2437	0.32	0/3

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2381	2340	2340	8	0
1	B	2390	2353	2353	4	0
2	C	185	102	102	0	0
2	E	185	102	102	0	0
3	D	182	102	102	0	0
3	F	182	102	102	0	0
4	A	1	0	0	0	0
4	B					

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	296/317 (93%)	291 (98%)	5 (2%)	0	100	100
All	All	591/634 (93%)	580 (98%)	10 (2%)	1 (0%)	43	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ILE

5.3.2 Protein sidechains ⓘ

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/317 (93%)	0.50	22 (7%) 20 19	34, 55, 127, 176	0
1	B	2				

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MN	A	401	1/1	0.90	0.23	59,59,59,59	0
4	MN	B	401	1/1	0.98	0.11	54,54,54,54	0

6.5 Other polymers [i](#)

There are