



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 08:12 PM UTC

PDB ID : 5GT8 / pdb_00005gt8
Title : Crystal Structure of apo-CASTOR1
Authors : Guo, L.; Deng, D.
Deposited on : 2016-08-18
Resolution : 2.80 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>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

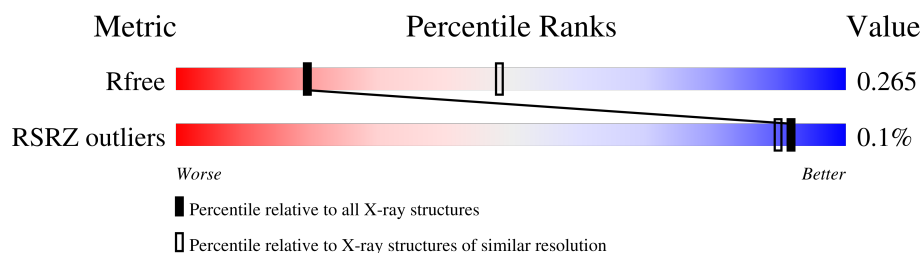
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16411 atoms, of which 8129 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 GATS-like protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	277	Total	C	H	N	O	S	0	1	0
			4253	1386	2126	348	386	7			
1	B	270	Total	C	H	N	O	S	0	0	0
			4109	1345	2046	331	381	6			
1	C	268	Total	C	H	N	O	S	0	0	0
			4022	1323	1987	332	373	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP Q8WTX7
A	-4	GLY	-	expression tag	UNP Q8WTX7
A	-3	SER	-	expression tag	UNP Q8WTX7
A	-2	GLY	-	expression tag	UNP Q8WTX7
A	-1	HIS	-	expression tag	UNP Q8WTX7
A	0	MET	-	expression tag	UNP Q8WTX7
B	-5	ALA	-	expression tag	UNP Q8WTX7
B	-4	GLY	-	expression tag	UNP Q8WTX7
B	-3	SER	-	expression tag	UNP Q8WTX7
B	-2	GLY	-	expression tag	UNP Q8WTX7
B	-1	HIS	-	expression tag	UNP Q8WTX7
B	0	MET	-	expression tag	UNP Q8WTX7
C	-5	ALA	-	expression tag	UNP Q8WTX7
C	-4	GLY	-	expression tag	UNP Q8WTX7
C	-3	SER	-	expression tag	UNP Q8WTX7
C	-2	GLY	-	expression tag	UNP Q8WTX7
C	-1	HIS	-	expression tag	UNP Q8WTX7
C	0	MET	-	expression tag	UNP Q8WTX7

- Molecule 2 is a protein called GATS-like protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	265	Total	C	H	N	O	S	0	0	0
			3983	1311	1970	327	368	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	ALA	-	expression tag	UNP Q8WTX7
D	-4	GLY	-	expression tag	UNP Q8WTX7
D	-3	SER	-	expression tag	UNP Q8WTX7
D	-2	GLY	-	expression tag	UNP Q8WTX7
D	-1	HIS	-	expression tag	UNP Q8WTX7
D	0	MET	-	expression tag	UNP Q8WTX7
D	285	ILE	ALA	engineered mutation	UNP Q8WTX7

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	12	Total	O	0	0
			12	12		
3	C	8	Total	O	0	0
			8	8		
3	D	8	Total	O	0	0
			8	8		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.41 Å 142.60 Å 95.40 Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	47.41 – 2.80 47.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.41-2.80) 94.2 (47.41-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.69 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155: ???	Depositor
R, R_{free}	0.243 , 0.265 0.244 , 0.265	Depositor DCC
R_{free} test set	2002 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.156 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16411	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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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 oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

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 [i](#)

5.1 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	277/335 (82%)	-0.74	0	100 100	32, 62, 94, 109	1 (0%)
1	B	270/335 (80%)	-0.68	0	100 100	37, 68, 92, 108	0
1	C	268/335 (80%)	-0.25	1 (0%)	88 84	50, 87, 127, 151	0
2	D	265/335 (79%)	-0.54	0	100 100	39, 76, 108, 204	0
All	All	1080/1340 (80%)	-0.56	1 (0%)	92 90	32, 72, 111, 204	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	SER	2.5

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.