



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 01:00 PM EDT

PDB ID : 5EF5 / pdb_00005ef5
Title : Crystal structure of Chaetomium thermophilum Raptor
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Maier, T.
Deposited on : 2015-10-23
Resolution : 4.30 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 ⓘ 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	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 4.30 Å.

There are no overall percentile quality scores available for this entry.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10164 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 Raptor from Chaetomium thermophilum.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	E	1004	Total	C	N	O	0	0	0
			5019	3012	1004	1003			
1	A	1029	Total	C	N	O	0	0	0
			5145	3087	1029	1029			

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	183.83Å 183.83Å 272.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 4.30	Depositor
% Data completeness (in resolution range)	99.7 (48.98-4.30)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 4.29Å)	Xtriage
Refinement program	PHENIX dev_1992	Depositor
R, R_{free}	0.371 , 0.391	Depositor
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10164	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	11
1	E	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3030:UNK	C	4513:UNK	N	41.13
1	E	3040:UNK	C	4522:UNK	N	40.48
1	A	1557:UNK	C	3009:UNK	N	26.55
1	E	1565:UNK	C	3018:UNK	N	24.12
1	A	176:UNK	C	177:UNK	N	18.75
1	A	633:UNK	C	1505:UNK	N	17.54
1	E	49:UNK	C	50:UNK	N	16.92
1	E	612:UNK	C	1514:UNK	N	15.77
1	A	49:UNK	C	50:UNK	N	14.80
1	A	4630:UNK	C	4631:UNK	N	14.15
1	E	127:UNK	C	128:UNK	N	13.83
1	A	144:UNK	C	145:UNK	N	13.26
1	E	159:UNK	C	160:UNK	N	13.23
1	E	4638:UNK	C	4639:UNK	N	11.32
1	E	315:UNK	C	316:UNK	N	9.40
1	A	332:UNK	C	333:UNK	N	8.55
1	A	109:UNK	C	110:UNK	N	8.40
1	A	4799:UNK	C	4800:UNK	N	8.16
1	A	24:UNK	C	25:UNK	N	7.43
1	E	97:UNK	C	98:UNK	N	7.18
1	E	120:UNK	C	121:UNK	N	7.04
1	E	24:UNK	C	25:UNK	N	5.75

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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5.3 Carbohydrates ⓘ

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5.4 Ligands ⓘ

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5.5 Other polymers ⓘ

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