



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:26 PM UTC

PDB ID : 1VM7 / pdb_00001vm7
Title : Crystal structure of Ribokinase (TM0960) from *Thermotoga maritima* at 2.15 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2004-09-08
Resolution : 2.15 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	:	4-5-2 with Phenix2.0
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

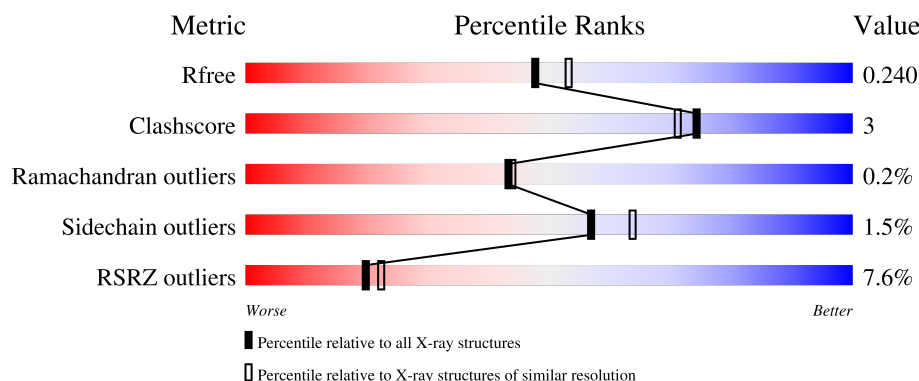
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	311	9% 87% 8% • •
1	B	311	6% 86% 9% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4816 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 ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2262	1457	365	436	4			
1	B	297	Total	C	N	O	S	0	0	0
			2275	1463	370	438	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9X055
A	-10	GLY	-	expression tag	UNP Q9X055
A	-9	SER	-	expression tag	UNP Q9X055
A	-8	ASP	-	expression tag	UNP Q9X055
A	-7	LYS	-	expression tag	UNP Q9X055
A	-6	ILE	-	expression tag	UNP Q9X055
A	-5	HIS	-	expression tag	UNP Q9X055
A	-4	HIS	-	expression tag	UNP Q9X055
A	-3	HIS	-	expression tag	UNP Q9X055
A	-2	HIS	-	expression tag	UNP Q9X055
A	-1	HIS	-	expression tag	UNP Q9X055
A	0	HIS	-	expression tag	UNP Q9X055
B	-11	MET	-	expression tag	UNP Q9X055
B	-10	GLY	-	expression tag	UNP Q9X055
B	-9	SER	-	expression tag	UNP Q9X055
B	-8	ASP	-	expression tag	UNP Q9X055
B	-7	LYS	-	expression tag	UNP Q9X055
B	-6	ILE	-	expression tag	UNP Q9X055
B	-5	HIS	-	expression tag	UNP Q9X055
B	-4	HIS	-	expression tag	UNP Q9X055
B	-3	HIS	-	expression tag	UNP Q9X055
B	-2	HIS	-	expression tag	UNP Q9X055
B	-1	HIS	-	expression tag	UNP Q9X055
B	0	HIS	-	expression tag	UNP Q9X055

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	138	Total 138	O 138	0	0
2	B	141	Total 141	O 141	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.14Å 45.27Å 77.26Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	60.40 – 2.15 60.40 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (60.40-2.15) 98.0 (60.40-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.190 , 0.235 0.198 , 0.240	Depositor DCC
R_{free} test set	1676 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4816	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.90	2/2301 (0.1%)	0.94	3/3117 (0.1%)
1	B	0.85	1/2314 (0.0%)	0.91	1/3133 (0.0%)
All	All	0.88	3/4615 (0.1%)	0.92	4/6250 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	ASN	C-N	10.77	1.48	1.33
1	A	298	ASN	C-O	10.49	1.37	1.24
1	B	159	ALA	C-O	-5.40	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ILE	CA-C-N	-5.99	114.10	120.03
1	A	286	ILE	C-N-CA	-5.99	114.10	120.03
1	A	298	ASN	CA-C-O	-5.71	112.34	120.51
1	B	217	ASP	CB-CA-C	-5.58	101.20	110.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2262	0	2241	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2275	0	2285	16	0
2	A	138	0	0	0	0
2	B	141	0	0	4	0
All	All	4816	0	4526	28	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:NZ	2:B:368:HOH:O	2.37	0.58
1:B:89:LEU:HD12	1:B:115:GLU:HG2	1.84	0.58
1:B:22:PHE:HZ	1:B:103:GLN:HG3	1.71	0.56
1:B:22:PHE:CZ	1:B:103:GLN:HG3	2.41	0.55
1:A:148:LYS:HG2	1:A:171:TYR:CE2	2.42	0.55
1:A:12:ASN:ND2	1:A:14:ASP:OD1	2.41	0.54
1:A:70:ASP:O	1:A:74:GLU:HG3	2.07	0.53
1:B:228:LYS:O	1:B:228:LYS:HD3	2.08	0.53
1:B:18:LYS:NZ	2:B:406:HOH:O	2.34	0.51
1:A:141:GLU:HG3	1:A:142:THR:N	2.30	0.47
1:A:2:PHE:CD2	1:A:55:LYS:HE3	2.50	0.47
1:A:3:LEU:HB2	1:A:257:SER:HA	1.98	0.46
1:B:262:PRO:O	1:B:266:VAL:HG23	2.16	0.46
1:B:13:ILE:HG21	1:B:68:TYR:CD2	2.52	0.45
1:B:227:GLU:CB	1:B:229:LYS:CD	2.95	0.45
1:B:214:LYS:NZ	2:B:435:HOH:O	2.50	0.45
1:B:121:ILE:HB	1:B:123:TRP:CE2	2.52	0.45
1:A:89:LEU:HD12	1:A:115:GLU:HG2	1.99	0.44
1:A:218:LYS:O	1:A:230:HIS:NE2	2.48	0.44
1:A:198:LYS:HE3	1:A:198:LYS:HA	2.00	0.44
1:B:124:ASN:O	1:B:127:SER:OG	2.33	0.43
1:A:93:ARG:HG3	1:A:95:PHE:CE1	2.53	0.43
1:A:13:ILE:CG2	1:A:36:VAL:HG13	2.50	0.42
1:B:175:LEU:HG	1:B:177:PRO:HD3	2.02	0.41
1:A:41:LYS:HE3	1:A:159:ALA:HB1	2.02	0.41
1:B:204:LEU:O	2:B:361:HOH:O	2.22	0.41
1:B:6:SER:HA	1:B:58:ARG:O	2.21	0.41
1:B:59:PHE:CE1	1:B:61:THR:HB	2.56	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/311 (96%)	290 (98%)	6 (2%)	1 (0%)	36	34
1	B	295/311 (95%)	288 (98%)	7 (2%)	0	100	100
All	All	592/622 (95%)	578 (98%)	13 (2%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ASN

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/259 (90%)	231 (99%)	3 (1%)	61	68
1	B	242/259 (93%)	238 (98%)	4 (2%)	53	60
All	All	476/518 (92%)	469 (98%)	7 (2%)	57	64

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	198	LYS
1	A	237	LYS
1	B	151	ASN
1	B	228	LYS

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Mol	Chain	Res	Type
1	B	229	LYS
1	B	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	B	124	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	299/311 (96%)	0.91	27 (9%) 15 16	30, 34, 38, 43	0
1	B	297/311 (95%)	0.78	18 (6%) 27 31	30, 34, 38, 42	0
All	All	596/622 (95%)	0.84	45 (7%) 20 22	30, 34, 38, 43	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	LEU	5.1
1	B	298	ASN	4.4
1	A	299	LEU	3.5
1	B	88	SER	3.5
1	A	193	PHE	3.3
1	B	228	LYS	3.2
1	A	161	ALA	3.1
1	A	194	LEU	3.1
1	B	190	PHE	3.1
1	A	239	VAL	3.0
1	A	71	LEU	3.0
1	A	216	GLY	2.9
1	A	1	MET	2.8
1	A	225	LYS	2.8
1	B	294	ALA	2.7
1	A	120	LEU	2.6
1	A	232	PRO	2.6
1	B	239	VAL	2.6
1	A	230	HIS	2.6
1	A	40	GLY	2.6
1	A	280	LEU	2.6
1	A	297	LYS	2.5
1	B	162	GLN	2.5
1	A	89	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	294	ALA	2.5
1	A	191	GLY	2.5
1	B	2	PHE	2.4
1	B	207	GLY	2.4
1	B	184	ALA	2.3
1	A	233	THR	2.3
1	B	281	GLY	2.3
1	B	297	LYS	2.2
1	B	296	LEU	2.2
1	A	241	THR	2.2
1	A	226	ASN	2.2
1	A	190	PHE	2.1
1	A	224	ASN	2.1
1	B	230	HIS	2.1
1	B	198	LYS	2.1
1	B	229	LYS	2.1
1	A	2	PHE	2.1
1	A	123	TRP	2.1
1	A	12	ASN	2.0
1	A	236	VAL	2.0
1	B	71	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.