



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3K9E / pdb_00003k9e
Title : Crystal structure of a putative Ribokinase II (Apo Form) from E.coli
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Deposited on : 2009-10-15
Resolution : 2.05 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

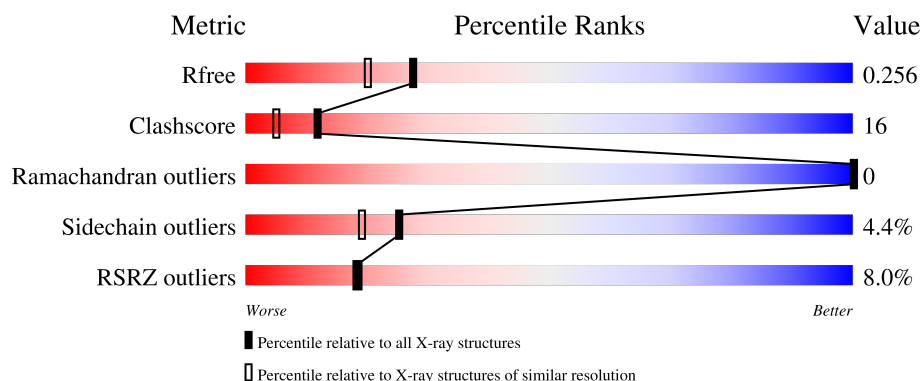
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	330	 4% 68% 24% • 7%
1	B	330	 10% 59% 33% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4900 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 PUTATIVE RIBOKINASE II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	Se	0	0	0
			2350	1491	405	439	7	8			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2376	1506	409	446	7	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MSE	-	expression tag	UNP Q8FD38
A	-3	SER	-	expression tag	UNP Q8FD38
A	-2	LEU	-	expression tag	UNP Q8FD38
A	321	GLU	-	expression tag	UNP Q8FD38
A	322	GLY	-	expression tag	UNP Q8FD38
A	323	HIS	-	expression tag	UNP Q8FD38
A	324	HIS	-	expression tag	UNP Q8FD38
A	325	HIS	-	expression tag	UNP Q8FD38
A	326	HIS	-	expression tag	UNP Q8FD38
A	327	HIS	-	expression tag	UNP Q8FD38
A	328	HIS	-	expression tag	UNP Q8FD38
B	-4	MSE	-	expression tag	UNP Q8FD38
B	-3	SER	-	expression tag	UNP Q8FD38
B	-2	LEU	-	expression tag	UNP Q8FD38
B	321	GLU	-	expression tag	UNP Q8FD38
B	322	GLY	-	expression tag	UNP Q8FD38
B	323	HIS	-	expression tag	UNP Q8FD38
B	324	HIS	-	expression tag	UNP Q8FD38
B	325	HIS	-	expression tag	UNP Q8FD38
B	326	HIS	-	expression tag	UNP Q8FD38
B	327	HIS	-	expression tag	UNP Q8FD38
B	328	HIS	-	expression tag	UNP Q8FD38

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total 103	O 103	0	0
2	B	71	Total 71	O 71	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.73Å 87.67Å 112.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.33 – 2.05 47.33 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.9 (47.33-2.05) 90.0 (47.33-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.257 0.228 , 0.256	Depositor DCC
R_{free} test set	1452 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4900	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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	0.42	0/2394	0.92	8/3229 (0.2%)
1	B	0.40	0/2421	0.90	5/3267 (0.2%)
All	All	0.41	0/4815	0.91	13/6496 (0.2%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	SER	N-CA-C	-7.31	100.68	110.55
1	B	303	GLU	N-CA-C	-6.52	104.26	111.36
1	A	239	GLU	N-CA-C	6.16	116.69	108.38
1	A	84	LEU	CA-C-N	5.96	126.11	119.32
1	A	84	LEU	C-N-CA	5.96	126.11	119.32

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	2350	0	2306	56	0
1	B	2376	0	2330	92	0
2	A	103	0	0	3	0
2	B	71	0	0	22	0
All	All	4900	0	4636	148	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 16.

The worst 5 of 148 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:21:GLN:O	1:B:95:THR:HG21	1.60	0.99
1:A:305:GLU:HB2	2:A:397:HOH:O	1.69	0.92
1:A:44:GLN:HE22	1:A:299:SER:H	1.14	0.90
1:B:15:MSE:HE3	1:B:33:TYR:CD2	2.09	0.87
1:B:233:SER:HB2	2:B:380:HOH:O	1.75	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	303/330 (92%)	297 (98%)	6 (2%)	0	100	100
1	B	309/330 (94%)	294 (95%)	15 (5%)	0	100	100
All	All	612/660 (93%)	591 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	250/259 (96%)	241 (96%)	9 (4%)	31	26
1	B	253/259 (98%)	240 (95%)	13 (5%)	21	14
All	All	503/518 (97%)	481 (96%)	22 (4%)	25	19

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	115	LYS
1	B	168	ILE
1	B	158	ASN
1	B	217	GLU
1	A	242	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	HIS
1	B	229	ASN
1	B	279	GLN
1	B	238	ASN
1	B	240	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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	299/330 (90%)	0.29	14 (4%) 36 36	24, 35, 57, 72	0
1	B	303/330 (91%)	0.79	34 (11%) 10 9	26, 44, 69, 81	0
All	All	602/660 (91%)	0.54	48 (7%) 18 18	24, 39, 65, 81	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	HIS	4.8
1	B	241	PHE	4.3
1	B	311	HIS	4.0
1	B	242	HIS	3.9
1	B	237	ALA	3.8

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.