



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:06 PM UTC

PDB ID : 3EC3 / pdb\_00003ec3  
Title : Crystal structure of the bb fragment of ERp72  
Authors : Kozlov, G.; Gehring, K.  
Deposited on : 2008-08-28  
Resolution : 1.92 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](mailto: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>.

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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)  
Xtrriage (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

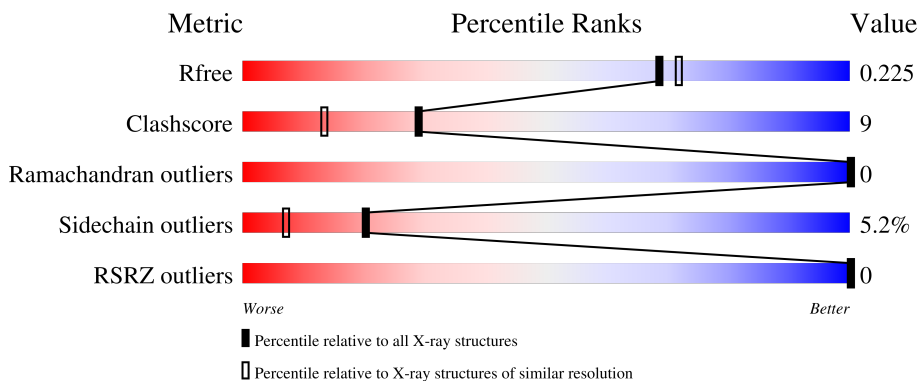
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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  $\geq 3$ , 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	250	 74% 15% • 8%
1	B	250	 79% 12% • 8%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4077 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 Protein disulfide-isomerase A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	231	1852	1191	302	354	5	0	0	0
1	B	229	1837	1180	300	352	5	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	GLY	-	insertion	UNP P38659
A	279	PRO	-	insertion	UNP P38659
A	280	LEU	-	insertion	UNP P38659
A	281	GLY	-	insertion	UNP P38659
A	282	SER	-	insertion	UNP P38659
A	470	GLY	GLU	engineered mutation	UNP P38659
A	497	ARG	GLN	SEE REMARK 999	UNP P38659
A	524	ALA	-	insertion	UNP P38659
A	525	ALA	-	insertion	UNP P38659
A	526	ALA	-	insertion	UNP P38659
A	527	SER	-	insertion	UNP P38659
B	278	GLY	-	insertion	UNP P38659
B	279	PRO	-	insertion	UNP P38659
B	280	LEU	-	insertion	UNP P38659
B	281	GLY	-	insertion	UNP P38659
B	282	SER	-	insertion	UNP P38659
B	470	GLY	GLU	engineered mutation	UNP P38659
B	497	ARG	GLN	SEE REMARK 999	UNP P38659
B	524	ALA	-	insertion	UNP P38659
B	525	ALA	-	insertion	UNP P38659
B	526	ALA	-	insertion	UNP P38659
B	527	SER	-	insertion	UNP P38659

- Molecule 2 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	A	195	Total 195	O 195	0	0
2	B	193	Total 193	O 193	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.17Å 62.17Å 135.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.48 – 1.92 19.48 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.48-1.92) 99.8 (19.48-1.92)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.188 , 0.236 (Not available) , 0.225	Depositor DCC
$R_{free}$ test set	2238 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.489 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.96	1/1889 (0.1%)	0.99	2/2540 (0.1%)
1	B	0.94	1/1874 (0.1%)	0.95	0/2519
All	All	0.95	2/3763 (0.1%)	0.97	2/5059 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	MSE	SE-CE	-8.00	1.71	1.95
1	A	372	MSE	SE-CE	-7.58	1.72	1.95

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ARG	NE-CZ-NH2	-8.33	111.70	119.20
1	A	433	ARG	NE-CZ-NH1	5.54	127.04	121.50

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	1852	0	1829	45	0
1	B	1837	0	1809	19	0
2	A	195	0	0	18	1
2	B	193	0	0	8	1
All	All	4077	0	3638	64	1

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 9.

All (64) 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:299:LYS:HB3	2:B:739:HOH:O	1.45	1.16
1:A:303:ASP:OD1	1:A:406:ARG:NH1	1.83	1.11
1:B:434:ASN:HB3	2:B:638:HOH:O	1.56	1.04
1:A:369:MSE:SE	2:A:707:HOH:O	2.32	0.97
1:A:303:ASP:CG	1:A:406:ARG:HH12	1.79	0.90
1:A:282:SER:HB3	1:A:283:PRO:HD2	1.56	0.86
1:A:504:LYS:HE3	2:B:676:HOH:O	1.81	0.80
1:B:494:ASP:O	1:B:498:GLU:HG3	1.82	0.80
1:A:282:SER:HB3	1:A:283:PRO:CD	2.13	0.79
1:A:284:PRO:HG2	1:A:322:GLN:OE1	1.84	0.78
1:A:353:LEU:HD12	1:A:372:MSE:HE2	1.66	0.76
1:A:434:ASN:HB3	2:A:624:HOH:O	1.87	0.74
1:B:299:LYS:HG3	2:B:692:HOH:O	1.90	0.72
1:A:295:GLN:O	1:A:299:LYS:HD3	1.89	0.71
1:B:353:LEU:HD23	1:B:372:MSE:HE2	1.72	0.70
1:A:468:SER:OG	2:A:713:HOH:O	2.13	0.66
1:A:434:ASN:ND2	2:A:659:HOH:O	2.28	0.65
1:B:434:ASN:CB	2:B:638:HOH:O	2.29	0.64
1:B:291:LEU:HD21	1:B:345:PHE:CD1	2.33	0.63
1:B:284:PRO:HG2	1:B:322:GLN:OE1	1.98	0.63
1:A:435:LYS:NZ	2:A:660:HOH:O	2.32	0.62
1:A:494:ASP:O	1:A:498:GLU:HG3	1.99	0.62
1:A:372:MSE:HE1	1:A:383:ILE:HA	1.84	0.59
1:B:372:MSE:HE1	1:B:383:ILE:HA	1.84	0.59
1:A:340:THR:O	1:A:344:LYS:HG3	2.02	0.58
1:A:477:LEU:HD22	1:A:483:LYS:HG2	1.86	0.57
1:A:291:LEU:HD21	1:A:345:PHE:CD1	2.40	0.56
1:B:457:ALA:O	1:B:461:LYS:HG3	2.06	0.56
1:B:352:LYS:NZ	1:B:373:ASP:OD1	2.33	0.56
1:A:299:LYS:NZ	2:A:654:HOH:O	2.40	0.55
1:A:282:SER:CB	1:A:283:PRO:CD	2.84	0.54
1:A:291:LEU:HD21	1:A:345:PHE:CG	2.43	0.54
1:A:497:ARG:HH21	1:A:501:MSE:HE2	1.72	0.54
1:A:366:GLU:CD	1:A:394:LEU:HB2	2.33	0.53
1:B:330:GLU:O	1:B:405:LYS:HE3	2.09	0.53
1:A:408:SER:HB2	2:A:585:HOH:O	2.07	0.53
1:B:299:LYS:CG	2:B:692:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLN:HG3	2:B:760:HOH:O	2.10	0.52
1:A:394:LEU:HD22	1:A:440:ALA:HB1	1.92	0.51
1:A:353:LEU:HD12	1:A:372:MSE:CE	2.37	0.50
1:A:433:ARG:NH2	2:A:533:HOH:O	2.46	0.48
1:B:291:LEU:HD21	1:B:345:PHE:CG	2.49	0.48
1:A:299:LYS:HD3	1:A:299:LYS:N	2.30	0.47
1:B:431:PHE:CE1	1:B:435:LYS:HE2	2.50	0.47
1:A:299:LYS:HD2	2:A:662:HOH:O	2.15	0.46
1:A:364:LYS:HG3	2:A:540:HOH:O	2.14	0.46
1:A:432:TRP:CE3	1:A:435:LYS:HD2	2.50	0.46
1:A:379:GLU:HG2	2:A:611:HOH:O	2.16	0.45
1:A:434:ASN:CB	2:A:624:HOH:O	2.55	0.45
1:A:369:MSE:CG	2:A:707:HOH:O	2.66	0.43
1:B:282:SER:HB2	1:B:283:PRO:HD2	1.99	0.43
1:A:497:ARG:HH21	1:A:501:MSE:CE	2.32	0.43
1:B:434:ASN:CG	2:B:638:HOH:O	2.59	0.43
1:A:297:PHE:CE1	2:A:628:HOH:O	2.57	0.42
1:A:327:THR:HG21	1:A:384:LYS:NZ	2.34	0.42
1:A:497:ARG:HG3	2:A:598:HOH:O	2.18	0.42
1:B:468:SER:CB	1:B:488:PRO:HG2	2.49	0.42
1:A:430:GLN:OE1	1:A:433:ARG:HD3	2.20	0.41
1:A:512:ILE:HG22	1:A:512:ILE:O	2.20	0.41
1:A:297:PHE:CD1	2:A:628:HOH:O	2.72	0.41
1:A:476:ILE:HG13	1:A:499:PHE:CE1	2.55	0.41
1:A:497:ARG:NH1	2:A:598:HOH:O	2.51	0.41
1:A:301:GLY:HA3	2:A:626:HOH:O	2.21	0.40
1:A:509:LYS:HD3	1:A:509:LYS:HA	1.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:594:HOH:O	2:B:794:HOH:O[1_565]	2.15	0.05

## 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	229/250 (92%)	225 (98%)	4 (2%)	0	100	100
1	B	227/250 (91%)	222 (98%)	5 (2%)	0	100	100
All	All	456/500 (91%)	447 (98%)	9 (2%)	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	201/209 (96%)	189 (94%)	12 (6%)	17	5
1	B	199/209 (95%)	190 (96%)	9 (4%)	24	9
All	All	400/418 (96%)	379 (95%)	21 (5%)	20	7

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	SER
1	A	291	LEU
1	A	353	LEU
1	A	384	LYS
1	A	394	LEU
1	A	408	SER
1	A	458	THR
1	A	461	LYS
1	A	467	GLU
1	A	477	LEU
1	A	479	GLU
1	A	504	LYS
1	B	291	LEU
1	B	347	LYS

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Mol	Chain	Res	Type
1	B	375	GLN
1	B	467	GLU
1	B	477	LEU
1	B	487	GLU
1	B	490	GLU
1	B	496	LEU
1	B	497	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	434	ASN
1	A	473	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	226/250 (90%)	-1.34	0 <a href="#">100</a> <a href="#">100</a>	14, 23, 44, 54	0
1	B	224/250 (89%)	-1.40	0 <a href="#">100</a> <a href="#">100</a>	13, 23, 43, 53	0
All	All	450/500 (90%)	-1.37	0 <a href="#">100</a> <a href="#">100</a>	13, 23, 44, 54	0

There are no RSRZ outliers to report.

### 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.