



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 07:57 pm GMT

PDB ID : 2CX3  
Title : Crystal structure of a bacterioferritin comigratory protein peroxiredoxin from the *Aeropyrum pernix* K1 (form-1 crystal)  
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Deposited on : 2005-06-27  
Resolution : 2.64 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

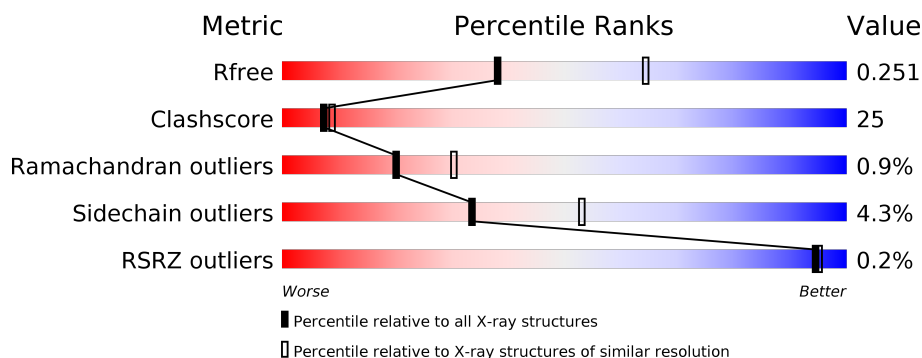
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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))
$R_{free}$	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	164	
1	B	164	
1	C	164	
1	D	164	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5360 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 bacterioferritin comigratory protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	Se	0	0	0
			1289	835	212	237	3	2			
1	B	161	Total	C	N	O	S	Se	0	0	0
			1293	837	213	238	3	2			
1	C	160	Total	C	N	O	S	Se	0	0	0
			1289	835	212	237	3	2			
1	D	160	Total	C	N	O	S	Se	0	0	0
			1289	835	212	237	3	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 14601861
A	60	MSE	MET	MODIFIED RESIDUE	GB 14601861
A	118	MSE	MET	MODIFIED RESIDUE	GB 14601861
B	1	MSE	MET	MODIFIED RESIDUE	GB 14601861
B	60	MSE	MET	MODIFIED RESIDUE	GB 14601861
B	118	MSE	MET	MODIFIED RESIDUE	GB 14601861
C	1	MSE	MET	MODIFIED RESIDUE	GB 14601861
C	60	MSE	MET	MODIFIED RESIDUE	GB 14601861
C	118	MSE	MET	MODIFIED RESIDUE	GB 14601861
D	1	MSE	MET	MODIFIED RESIDUE	GB 14601861
D	60	MSE	MET	MODIFIED RESIDUE	GB 14601861
D	118	MSE	MET	MODIFIED RESIDUE	GB 14601861

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	53	Total	O	0	0
			53	53		
2	B	56	Total	O	0	0
			56	56		

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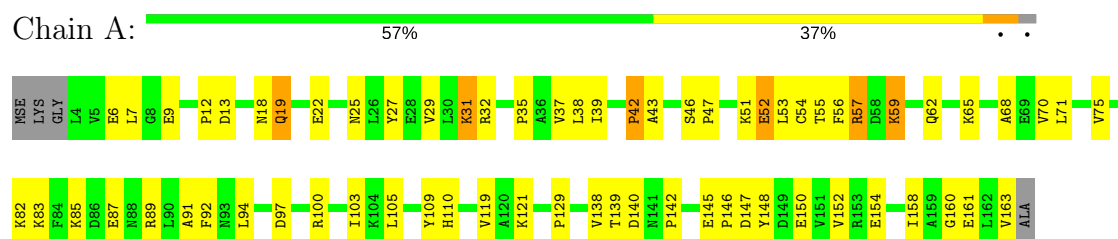
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	42	Total 42	O 42	0	0
2	D	49	Total 49	O 49	0	0

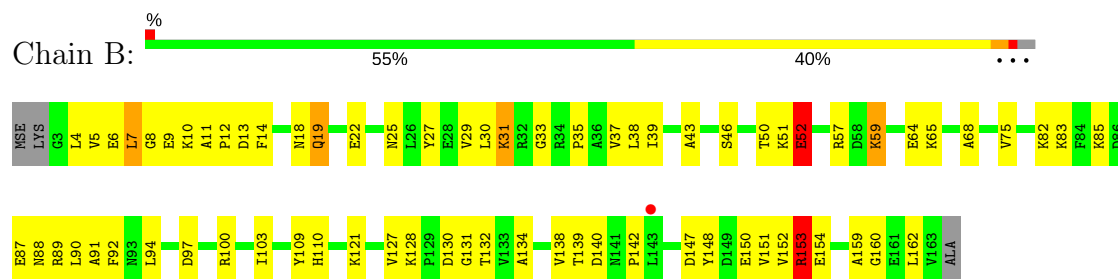
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

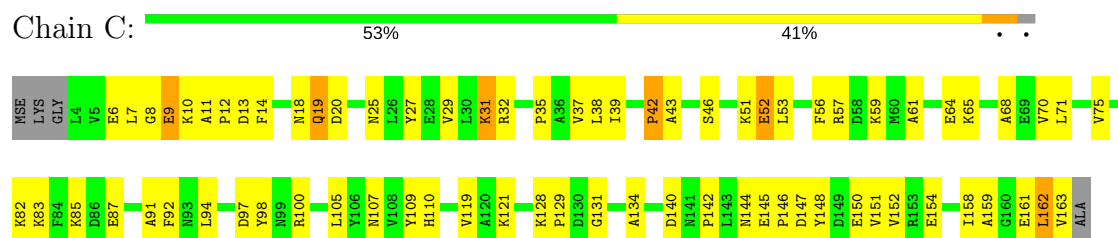
#### • Molecule 1: bacterioferritin comigratory protein



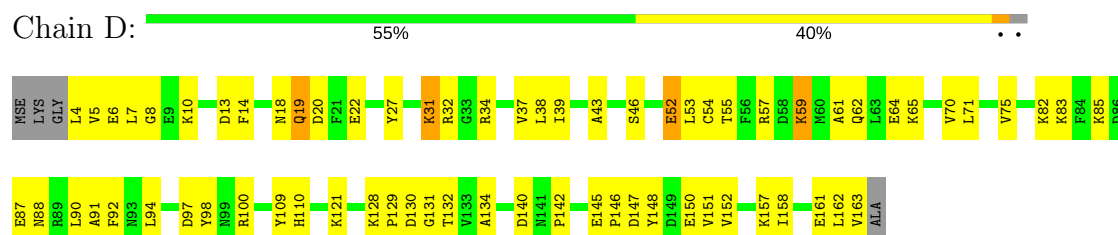
#### • Molecule 1: bacterioferritin comigratory protein



#### • Molecule 1: bacterioferritin comigratory protein



#### • Molecule 1: bacterioferritin comigratory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.99Å 126.99Å 104.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.33 – 2.64 47.33 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.33-2.64) 99.1 (47.33-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.247 0.211 , 0.251	Depositor DCC
$R_{free}$ test set	1223 reflections (4.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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	0.44	0/1316	0.61	0/1782
1	B	0.48	0/1320	0.78	3/1787 (0.2%)
1	C	0.43	0/1316	0.61	0/1782
1	D	0.44	0/1316	0.62	0/1782
All	All	0.45	0/5268	0.66	3/7133 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ARG	NE-CZ-NH1	-14.71	112.95	120.30
1	B	153	ARG	CA-CB-CG	8.78	132.72	113.40
1	B	153	ARG	NE-CZ-NH2	7.77	124.19	120.30

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	1289	0	1298	72	0
1	B	1293	0	1301	66	0
1	C	1289	0	1298	73	0
1	D	1289	0	1298	68	0
2	A	53	0	0	1	0
2	B	56	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	42	0	0	5	0
2	D	49	0	0	2	0
All	All	5360	0	5195	257	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 25.

The worst 5 of 257 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:83:LYS:HE3	1:B:87:GLU:OE1	1.75	0.86
1:D:31:LYS:HE2	2:D:180:HOH:O	1.80	0.82
1:A:83:LYS:HE3	1:A:87:GLU:OE1	1.80	0.81
1:C:19:GLN:HG2	1:C:85:LYS:HD2	1.63	0.81
1:B:37:VAL:HG12	1:B:39:ILE:HD11	1.62	0.80

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	158/164 (96%)	140 (89%)	16 (10%)	2 (1%)	14	20
1	B	159/164 (97%)	137 (86%)	21 (13%)	1 (1%)	28	43
1	C	158/164 (96%)	138 (87%)	18 (11%)	2 (1%)	14	20
1	D	158/164 (96%)	139 (88%)	18 (11%)	1 (1%)	28	43
All	All	633/656 (96%)	554 (88%)	73 (12%)	6 (1%)	20	30

5 of 6 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	B	52	GLU
1	C	9	GLU
1	C	42	PRO
1	D	8	GLY
1	A	42	PRO

### 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	141/140 (101%)	136 (96%)	5 (4%)	41	61
1	B	141/140 (101%)	134 (95%)	7 (5%)	28	45
1	C	141/140 (101%)	134 (95%)	7 (5%)	28	45
1	D	141/140 (101%)	136 (96%)	5 (4%)	41	61
All	All	564/560 (101%)	540 (96%)	24 (4%)	33	53

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	LYS
1	C	31	LYS
1	D	57	ARG
1	B	153	ARG
1	C	19	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	144	ASN
1	C	19	GLN
1	D	62	GLN
1	B	88	ASN
1	D	19	GLN

### 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 carbohydrates 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	158/164 (96%)	0.03	0 <b>100</b> <b>100</b>	41, 65, 81, 90	0
1	B	159/164 (96%)	0.00	1 (0%) <b>89</b> <b>88</b>	34, 64, 87, 96	0
1	C	158/164 (96%)	0.07	0 <b>100</b> <b>100</b>	43, 67, 86, 92	0
1	D	158/164 (96%)	-0.03	0 <b>100</b> <b>100</b>	30, 65, 85, 94	0
All	All	633/656 (96%)	0.02	1 (0%) <b>94</b> <b>95</b>	30, 65, 85, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	LEU	2.9

### 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 carbohydrates 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.