



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:31 AM UTC

PDB ID : 4FH8 / pdb_00004fh8
Title : Crystal Structure of Peroxiredoxin-1 from the human hookworm *Ancylostoma ceylanicum*
Authors : Nguyen, J.B.; Modis, Y.
Deposited on : 2012-06-05
Resolution : 2.11 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
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

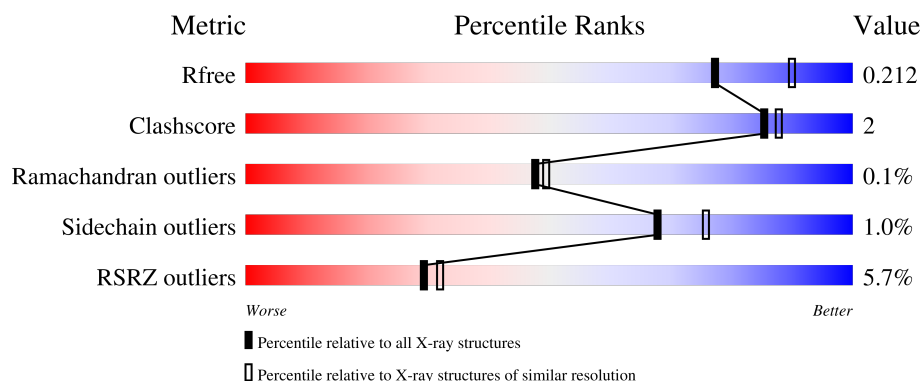
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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.



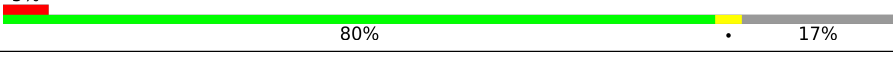
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	204	4% 79% 16%
1	B	204	3% 78% 5% 16%
1	C	204	3% 79% 18%
1	D	204	8% 79% 16%
1	E	204	3% 76% 5% 18%

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Mol	Chain	Length	Quality of chain
1	F	204	 4% 81% 17%
1	G	204	 3% 76% 5% 18%
1	H	204	 6% 79% 17%
1	I	204	 6% 77% 6% 17%
1	J	204	 5% 80% 17%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14009 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 AcePrx-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1348	877	220	246	5			
1	B	171	Total	C	N	O	S	0	0	0
			1353	880	222	246	5			
1	C	168	Total	C	N	O	S	0	0	0
			1330	866	217	243	4			
1	D	171	Total	C	N	O	S	0	0	0
			1353	880	222	246	5			
1	E	167	Total	C	N	O	S	0	0	0
			1321	861	216	240	4			
1	F	170	Total	C	N	O	S	0	0	0
			1347	877	221	245	4			
1	G	167	Total	C	N	O	S	0	0	0
			1321	861	216	240	4			
1	H	170	Total	C	N	O	S	0	0	0
			1347	877	221	245	4			
1	I	169	Total	C	N	O	S	0	0	0
			1337	871	218	244	4			
1	J	170	Total	C	N	O	S	0	0	0
			1347	877	221	245	4			

- Molecule 2 is water.

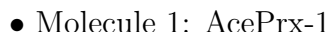
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	67	Total	O	0	0
			67	67		
2	C	47	Total	O	0	0
			47	47		
2	D	46	Total	O	0	0
			46	46		

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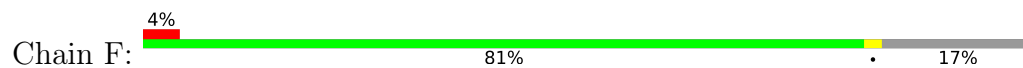
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	45	Total 45	O 45	0	0
2	F	51	Total 51	O 51	0	0
2	G	50	Total 50	O 50	0	0
2	H	69	Total 69	O 69	0	0
2	I	69	Total 69	O 69	0	0
2	J	70	Total 70	O 70	0	0

- Molecule 1: AcePrx-1



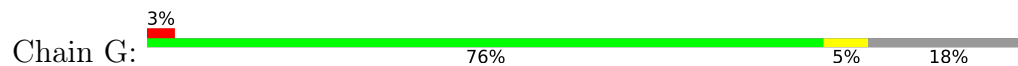
TYR
PHE
ASN
LYS
ALA
ASN

• Molecule 1: AcePrx-1



MET HIS HIS HIS HIS HIS HIS HO M1 F47 V48 C49 P50 T51 N106 H107 D131 P132 G167 E168 V169 CYS PRO ALA GLY TRP THR PRO GLY LYS ASP THR ILE LYS PRO ALA VAL LYS GLU SER LYS GLU TYR PHE ASN LYS ALA ASN

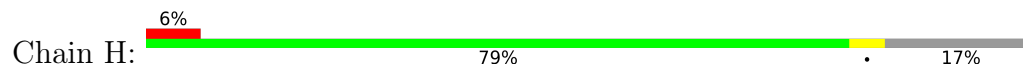
• Molecule 1: AcePrx-1



MET HIS HIS HIS HIS HIS HIS HO M1 V48 C49 E52 I53 V68 V78 D96 N106 H107 Q108 D131 P132 V157 K166 H166 G167 VAL CYS PRO ALA GLY TRP THR PRO GLY LYS ASP THR ILE LYS PRO ALA VAL LYS GLU SER LYS GLU TYR PHE ASN

LYS
ALA
ASN

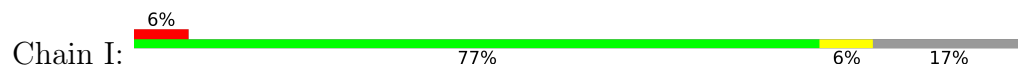
• Molecule 1: AcePrx-1



MET HIS HIS HIS HIS HIS HIS HO M1 D12 G21 K32 P42 F47 V48 C49 S80 D118 D119 D131 P132 L144 T163 G167 E168 V169 CYS PRO ALA GLY TRP THR PRO GLY LYS ASP THR ILE LYS PRO ALA VAL LYS GLU SER LYS GLU TYR PHE

ASN
LYS
ALA
ASN

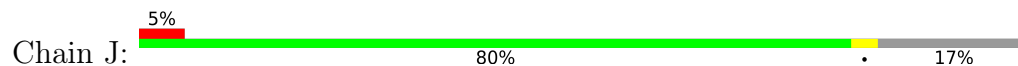
• Molecule 1: AcePrx-1



MET HIS HIS HIS HIS HIS HIS HO M1 K16 A17 V18 F23 K32 Y35 V48 C49 P50 V63 V78 K90 H106 H107 Q108 D118 D119 D131 P132 V157 G167 E168 V169 CYS PRO ALA GLY TRP THR PRO GLY LYS ASP THR ILE LYS PRO ALA VAL LYS GLU SER LYS GLU TYR PHE

VAL
LYS
GLU
SER
LYS
GLU
TYR
PHE
ASN
LYS
ALA
ASN

• Molecule 1: AcePrx-1



MET HIS HIS HIS HIS HIS HO M1 K32 Y35 T46 C49 N106 H107 Q108 D118 D131 P132 V157 G167 E168 V169 CYS PRO ALA GLY TRP THR PRO GLY LYS ASP THR ILE LYS PRO ALA VAL LYS GLU SER LYS GLU TYR PHE ASN LYS ALA ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.69Å 146.28Å 136.03Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	46.55 – 2.11 46.55 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.55-2.11) 99.7 (46.55-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.214 0.193 , 0.212	Depositor DCC
R_{free} test set	7231 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.8	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	0.97	EDS
Total number of atoms	14009	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% 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	0.55	0/1382	0.73	0/1874
1	B	0.57	0/1388	0.72	0/1882
1	C	0.53	0/1364	0.71	0/1849
1	D	0.55	0/1388	0.73	0/1882
1	E	0.53	0/1355	0.73	0/1837
1	F	0.56	0/1382	0.72	0/1874
1	G	0.54	0/1355	0.73	0/1837
1	H	0.57	0/1382	0.70	0/1874
1	I	0.53	0/1371	0.74	0/1859
1	J	0.56	0/1382	0.72	0/1874
All	All	0.55	0/13749	0.72	0/18642

There are no bond length outliers.

There are no bond angle outliers.

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	1348	0	1339	5	0
1	B	1353	0	1344	8	0
1	C	1330	0	1323	4	0
1	D	1353	0	1344	5	0
1	E	1321	0	1318	6	0
1	F	1347	0	1340	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1321	0	1318	6	0
1	H	1347	0	1340	4	0
1	I	1337	0	1333	13	0
1	J	1347	0	1340	7	0
2	A	91	0	0	0	0
2	B	67	0	0	0	0
2	C	47	0	0	0	0
2	D	46	0	0	1	0
2	E	45	0	0	0	0
2	F	51	0	0	1	0
2	G	50	0	0	0	0
2	H	69	0	0	0	0
2	I	69	0	0	0	0
2	J	70	0	0	2	0
All	All	14009	0	13339	60	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 2.

The worst 5 of 60 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:I:23:PHE:CE1	1:I:78:VAL:HG12	2.33	0.64
1:A:68:VAL:HG21	1:A:157:VAL:HG11	1.82	0.59
1:B:106:ASN:HB3	1:B:108:GLN:H	1.68	0.58
1:A:49:CYS:HB2	1:B:170:CYS:SG	2.43	0.58
1:I:23:PHE:CD1	1:I:78:VAL:HG12	2.41	0.55

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	169/204 (83%)	166 (98%)	3 (2%)	0	100	100
1	B	169/204 (83%)	166 (98%)	3 (2%)	0	100	100
1	C	166/204 (81%)	163 (98%)	3 (2%)	0	100	100
1	D	169/204 (83%)	167 (99%)	2 (1%)	0	100	100
1	E	165/204 (81%)	163 (99%)	1 (1%)	1 (1%)	21	18
1	F	168/204 (82%)	165 (98%)	3 (2%)	0	100	100
1	G	165/204 (81%)	163 (99%)	2 (1%)	0	100	100
1	H	168/204 (82%)	165 (98%)	3 (2%)	0	100	100
1	I	167/204 (82%)	163 (98%)	4 (2%)	0	100	100
1	J	168/204 (82%)	166 (99%)	2 (1%)	0	100	100
All	All	1674/2040 (82%)	1647 (98%)	26 (2%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	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	146/175 (83%)	145 (99%)	1 (1%)	76	83
1	B	147/175 (84%)	147 (100%)	0	100	100
1	C	144/175 (82%)	143 (99%)	1 (1%)	76	83
1	D	147/175 (84%)	144 (98%)	3 (2%)	48	55
1	E	143/175 (82%)	141 (99%)	2 (1%)	59	67
1	F	146/175 (83%)	145 (99%)	1 (1%)	76	83
1	G	143/175 (82%)	140 (98%)	3 (2%)	47	54
1	H	146/175 (83%)	143 (98%)	3 (2%)	47	54
1	I	145/175 (83%)	145 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	146/175 (83%)	146 (100%)	0	100	100
All	All	1453/1750 (83%)	1439 (99%)	14 (1%)	68	76

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	0	HIS
1	G	1	MET
1	H	118	ASP
1	H	0	HIS
1	H	80	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	106	ASN
1	J	158	GLN
1	D	166	HIS
1	F	158	GLN
1	G	91	HIS

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	171/204 (83%)	0.10	9 (5%) 32 35	28, 37, 59, 90	0
1	B	171/204 (83%)	0.35	7 (4%) 41 44	33, 45, 71, 107	0
1	C	168/204 (82%)	0.30	6 (3%) 46 49	35, 50, 70, 89	0
1	D	171/204 (83%)	0.60	17 (9%) 13 14	36, 51, 87, 115	0
1	E	167/204 (81%)	0.37	7 (4%) 40 43	37, 51, 72, 84	0
1	F	170/204 (83%)	0.43	9 (5%) 32 35	35, 47, 76, 99	0
1	G	167/204 (81%)	0.35	7 (4%) 40 43	34, 48, 68, 82	0
1	H	170/204 (83%)	0.32	12 (7%) 22 24	33, 44, 64, 98	0
1	I	169/204 (82%)	0.34	13 (7%) 19 21	29, 42, 67, 101	0
1	J	170/204 (83%)	0.40	10 (5%) 28 30	32, 46, 68, 109	0
All	All	1694/2040 (83%)	0.35	97 (5%) 29 32	28, 46, 71, 115	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	169	VAL	10.1
1	H	169	VAL	9.9
1	J	169	VAL	9.9
1	F	169	VAL	9.3
1	D	169	VAL	7.3

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

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.