Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 09:55 PM EDT

PDB ID	:	4L0U
Title	:	Crystal structure of Plasmodium vivax Prx1a
Authors	:	Gretes, M.C.; Karplus, P.A.
Deposited on	:	2013-06-01
Resolution	:	2.50 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:

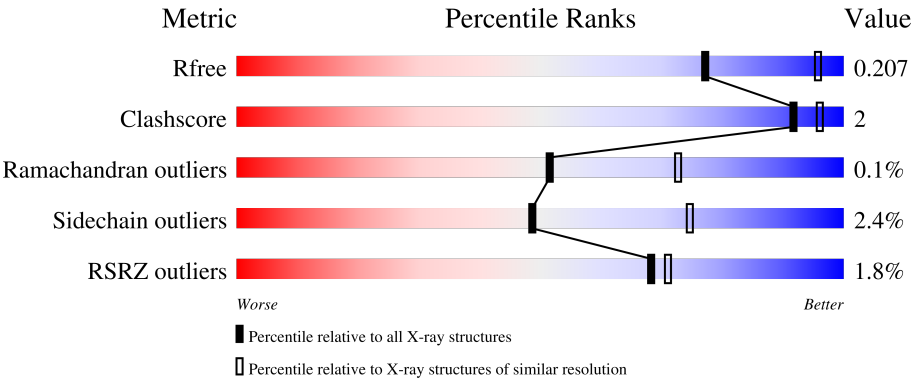
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	213	77% 21%
1	B	213	77% 20%
1	C	213	77% 19%
1	D	213	78% 20%
1	E	213	75% 24%

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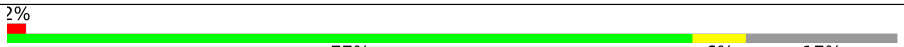
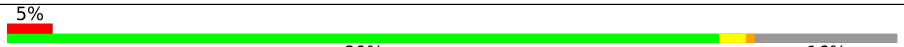
Mol	Chain	Length	Quality of chain
1	F	213	
1	G	213	
1	H	213	
1	I	213	
1	J	213	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	C	201	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13753 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 2-Cys peroxiredoxin, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1330	865	217	245	3			
1	B	171	Total	C	N	O	S	0	0	0
			1350	878	220	248	4			
1	C	172	Total	C	N	O	S	0	1	0
			1356	881	221	249	5			
1	D	171	Total	C	N	O	S	0	1	0
			1353	880	220	248	5			
1	E	162	Total	C	N	O	S	0	0	0
			1283	836	210	234	3			
1	F	169	Total	C	N	O	S	0	0	0
			1332	868	218	242	4			
1	G	171	Total	C	N	O	S	0	0	0
			1346	875	219	248	4			
1	H	167	Total	C	N	O	S	0	0	0
			1322	861	216	242	3			
1	I	177	Total	C	N	O	S	0	0	0
			1395	906	229	256	4			
1	J	179	Total	C	N	O	S	0	1	0
			1418	922	233	258	5			

There are 190 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP A5K421
A	-16	GLY	-	expression tag	UNP A5K421
A	-15	SER	-	expression tag	UNP A5K421
A	-14	SER	-	expression tag	UNP A5K421
A	-13	HIS	-	expression tag	UNP A5K421
A	-12	HIS	-	expression tag	UNP A5K421
A	-11	HIS	-	expression tag	UNP A5K421
A	-10	HIS	-	expression tag	UNP A5K421
A	-9	HIS	-	expression tag	UNP A5K421

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP A5K421
A	-7	SER	-	expression tag	UNP A5K421
A	-6	SER	-	expression tag	UNP A5K421
A	-5	GLY	-	expression tag	UNP A5K421
A	-4	LEU	-	expression tag	UNP A5K421
A	-3	VAL	-	expression tag	UNP A5K421
A	-2	PRO	-	expression tag	UNP A5K421
A	-1	ARG	-	expression tag	UNP A5K421
A	0	GLY	-	expression tag	UNP A5K421
A	1	SER	-	expression tag	UNP A5K421
B	-17	MET	-	expression tag	UNP A5K421
B	-16	GLY	-	expression tag	UNP A5K421
B	-15	SER	-	expression tag	UNP A5K421
B	-14	SER	-	expression tag	UNP A5K421
B	-13	HIS	-	expression tag	UNP A5K421
B	-12	HIS	-	expression tag	UNP A5K421
B	-11	HIS	-	expression tag	UNP A5K421
B	-10	HIS	-	expression tag	UNP A5K421
B	-9	HIS	-	expression tag	UNP A5K421
B	-8	HIS	-	expression tag	UNP A5K421
B	-7	SER	-	expression tag	UNP A5K421
B	-6	SER	-	expression tag	UNP A5K421
B	-5	GLY	-	expression tag	UNP A5K421
B	-4	LEU	-	expression tag	UNP A5K421
B	-3	VAL	-	expression tag	UNP A5K421
B	-2	PRO	-	expression tag	UNP A5K421
B	-1	ARG	-	expression tag	UNP A5K421
B	0	GLY	-	expression tag	UNP A5K421
B	1	SER	-	expression tag	UNP A5K421
C	-17	MET	-	expression tag	UNP A5K421
C	-16	GLY	-	expression tag	UNP A5K421
C	-15	SER	-	expression tag	UNP A5K421
C	-14	SER	-	expression tag	UNP A5K421
C	-13	HIS	-	expression tag	UNP A5K421
C	-12	HIS	-	expression tag	UNP A5K421
C	-11	HIS	-	expression tag	UNP A5K421
C	-10	HIS	-	expression tag	UNP A5K421
C	-9	HIS	-	expression tag	UNP A5K421
C	-8	HIS	-	expression tag	UNP A5K421
C	-7	SER	-	expression tag	UNP A5K421
C	-6	SER	-	expression tag	UNP A5K421
C	-5	GLY	-	expression tag	UNP A5K421

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP A5K421
C	-3	VAL	-	expression tag	UNP A5K421
C	-2	PRO	-	expression tag	UNP A5K421
C	-1	ARG	-	expression tag	UNP A5K421
C	0	GLY	-	expression tag	UNP A5K421
C	1	SER	-	expression tag	UNP A5K421
D	-17	MET	-	expression tag	UNP A5K421
D	-16	GLY	-	expression tag	UNP A5K421
D	-15	SER	-	expression tag	UNP A5K421
D	-14	SER	-	expression tag	UNP A5K421
D	-13	HIS	-	expression tag	UNP A5K421
D	-12	HIS	-	expression tag	UNP A5K421
D	-11	HIS	-	expression tag	UNP A5K421
D	-10	HIS	-	expression tag	UNP A5K421
D	-9	HIS	-	expression tag	UNP A5K421
D	-8	HIS	-	expression tag	UNP A5K421
D	-7	SER	-	expression tag	UNP A5K421
D	-6	SER	-	expression tag	UNP A5K421
D	-5	GLY	-	expression tag	UNP A5K421
D	-4	LEU	-	expression tag	UNP A5K421
D	-3	VAL	-	expression tag	UNP A5K421
D	-2	PRO	-	expression tag	UNP A5K421
D	-1	ARG	-	expression tag	UNP A5K421
D	0	GLY	-	expression tag	UNP A5K421
D	1	SER	-	expression tag	UNP A5K421
E	-17	MET	-	expression tag	UNP A5K421
E	-16	GLY	-	expression tag	UNP A5K421
E	-15	SER	-	expression tag	UNP A5K421
E	-14	SER	-	expression tag	UNP A5K421
E	-13	HIS	-	expression tag	UNP A5K421
E	-12	HIS	-	expression tag	UNP A5K421
E	-11	HIS	-	expression tag	UNP A5K421
E	-10	HIS	-	expression tag	UNP A5K421
E	-9	HIS	-	expression tag	UNP A5K421
E	-8	HIS	-	expression tag	UNP A5K421
E	-7	SER	-	expression tag	UNP A5K421
E	-6	SER	-	expression tag	UNP A5K421
E	-5	GLY	-	expression tag	UNP A5K421
E	-4	LEU	-	expression tag	UNP A5K421
E	-3	VAL	-	expression tag	UNP A5K421
E	-2	PRO	-	expression tag	UNP A5K421
E	-1	ARG	-	expression tag	UNP A5K421

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP A5K421
E	1	SER	-	expression tag	UNP A5K421
F	-17	MET	-	expression tag	UNP A5K421
F	-16	GLY	-	expression tag	UNP A5K421
F	-15	SER	-	expression tag	UNP A5K421
F	-14	SER	-	expression tag	UNP A5K421
F	-13	HIS	-	expression tag	UNP A5K421
F	-12	HIS	-	expression tag	UNP A5K421
F	-11	HIS	-	expression tag	UNP A5K421
F	-10	HIS	-	expression tag	UNP A5K421
F	-9	HIS	-	expression tag	UNP A5K421
F	-8	HIS	-	expression tag	UNP A5K421
F	-7	SER	-	expression tag	UNP A5K421
F	-6	SER	-	expression tag	UNP A5K421
F	-5	GLY	-	expression tag	UNP A5K421
F	-4	LEU	-	expression tag	UNP A5K421
F	-3	VAL	-	expression tag	UNP A5K421
F	-2	PRO	-	expression tag	UNP A5K421
F	-1	ARG	-	expression tag	UNP A5K421
F	0	GLY	-	expression tag	UNP A5K421
F	1	SER	-	expression tag	UNP A5K421
G	-17	MET	-	expression tag	UNP A5K421
G	-16	GLY	-	expression tag	UNP A5K421
G	-15	SER	-	expression tag	UNP A5K421
G	-14	SER	-	expression tag	UNP A5K421
G	-13	HIS	-	expression tag	UNP A5K421
G	-12	HIS	-	expression tag	UNP A5K421
G	-11	HIS	-	expression tag	UNP A5K421
G	-10	HIS	-	expression tag	UNP A5K421
G	-9	HIS	-	expression tag	UNP A5K421
G	-8	HIS	-	expression tag	UNP A5K421
G	-7	SER	-	expression tag	UNP A5K421
G	-6	SER	-	expression tag	UNP A5K421
G	-5	GLY	-	expression tag	UNP A5K421
G	-4	LEU	-	expression tag	UNP A5K421
G	-3	VAL	-	expression tag	UNP A5K421
G	-2	PRO	-	expression tag	UNP A5K421
G	-1	ARG	-	expression tag	UNP A5K421
G	0	GLY	-	expression tag	UNP A5K421
G	1	SER	-	expression tag	UNP A5K421
H	-17	MET	-	expression tag	UNP A5K421
H	-16	GLY	-	expression tag	UNP A5K421

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-15	SER	-	expression tag	UNP A5K421
H	-14	SER	-	expression tag	UNP A5K421
H	-13	HIS	-	expression tag	UNP A5K421
H	-12	HIS	-	expression tag	UNP A5K421
H	-11	HIS	-	expression tag	UNP A5K421
H	-10	HIS	-	expression tag	UNP A5K421
H	-9	HIS	-	expression tag	UNP A5K421
H	-8	HIS	-	expression tag	UNP A5K421
H	-7	SER	-	expression tag	UNP A5K421
H	-6	SER	-	expression tag	UNP A5K421
H	-5	GLY	-	expression tag	UNP A5K421
H	-4	LEU	-	expression tag	UNP A5K421
H	-3	VAL	-	expression tag	UNP A5K421
H	-2	PRO	-	expression tag	UNP A5K421
H	-1	ARG	-	expression tag	UNP A5K421
H	0	GLY	-	expression tag	UNP A5K421
H	1	SER	-	expression tag	UNP A5K421
I	-17	MET	-	expression tag	UNP A5K421
I	-16	GLY	-	expression tag	UNP A5K421
I	-15	SER	-	expression tag	UNP A5K421
I	-14	SER	-	expression tag	UNP A5K421
I	-13	HIS	-	expression tag	UNP A5K421
I	-12	HIS	-	expression tag	UNP A5K421
I	-11	HIS	-	expression tag	UNP A5K421
I	-10	HIS	-	expression tag	UNP A5K421
I	-9	HIS	-	expression tag	UNP A5K421
I	-8	HIS	-	expression tag	UNP A5K421
I	-7	SER	-	expression tag	UNP A5K421
I	-6	SER	-	expression tag	UNP A5K421
I	-5	GLY	-	expression tag	UNP A5K421
I	-4	LEU	-	expression tag	UNP A5K421
I	-3	VAL	-	expression tag	UNP A5K421
I	-2	PRO	-	expression tag	UNP A5K421
I	-1	ARG	-	expression tag	UNP A5K421
I	0	GLY	-	expression tag	UNP A5K421
I	1	SER	-	expression tag	UNP A5K421
J	-17	MET	-	expression tag	UNP A5K421
J	-16	GLY	-	expression tag	UNP A5K421
J	-15	SER	-	expression tag	UNP A5K421
J	-14	SER	-	expression tag	UNP A5K421
J	-13	HIS	-	expression tag	UNP A5K421
J	-12	HIS	-	expression tag	UNP A5K421

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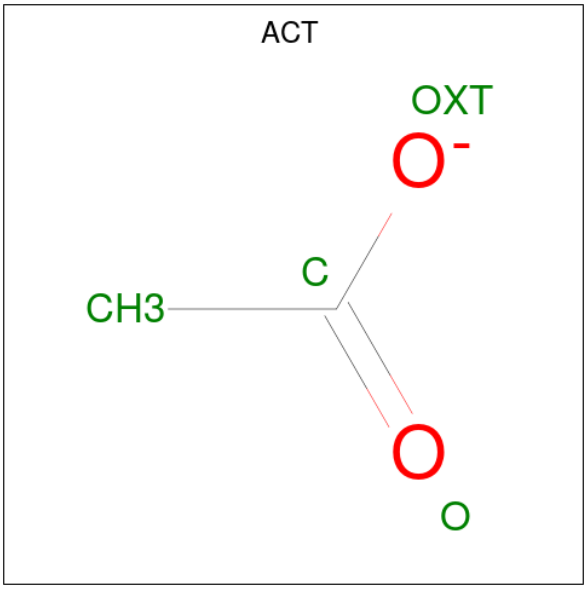
Chain	Residue	Modelled	Actual	Comment	Reference
J	-11	HIS	-	expression tag	UNP A5K421
J	-10	HIS	-	expression tag	UNP A5K421
J	-9	HIS	-	expression tag	UNP A5K421
J	-8	HIS	-	expression tag	UNP A5K421
J	-7	SER	-	expression tag	UNP A5K421
J	-6	SER	-	expression tag	UNP A5K421
J	-5	GLY	-	expression tag	UNP A5K421
J	-4	LEU	-	expression tag	UNP A5K421
J	-3	VAL	-	expression tag	UNP A5K421
J	-2	PRO	-	expression tag	UNP A5K421
J	-1	ARG	-	expression tag	UNP A5K421
J	0	GLY	-	expression tag	UNP A5K421
J	1	SER	-	expression tag	UNP A5K421

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0

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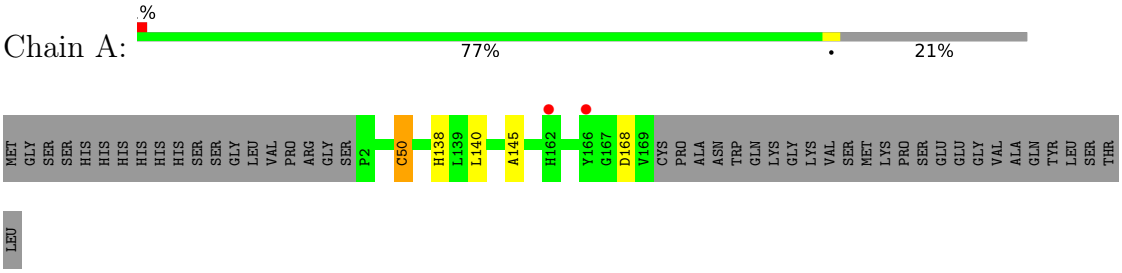
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	18	Total O 18 18	0	0
3	C	33	Total O 33 33	0	0
3	D	25	Total O 25 25	0	0
3	E	22	Total O 22 22	0	0
3	F	22	Total O 22 22	0	0
3	G	21	Total O 21 21	0	0
3	H	31	Total O 31 31	0	0
3	I	35	Total O 35 35	0	0
3	J	35	Total O 35 35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

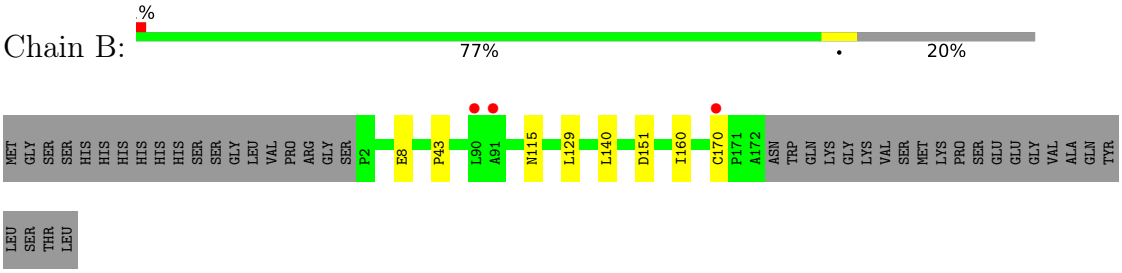
• Molecule 1: 2-Cys peroxiredoxin, putative

Chain A:



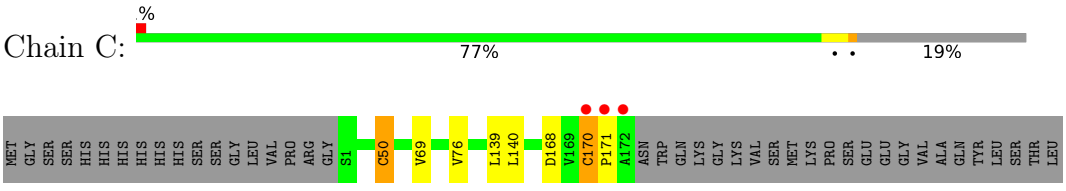
• Molecule 1: 2-Cys peroxiredoxin, putative

Chain B:



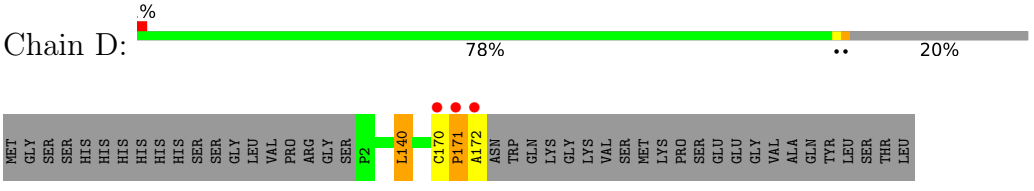
• Molecule 1: 2-Cys peroxiredoxin, putative

Chain C:



• Molecule 1: 2-Cys peroxiredoxin, putative

Chain D:

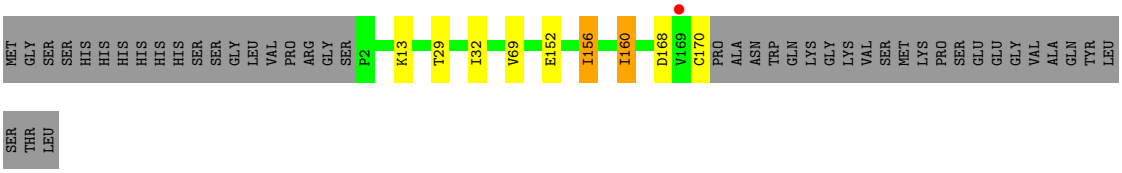


• Molecule 1: 2-Cys peroxiredoxin, putative

Chain E:

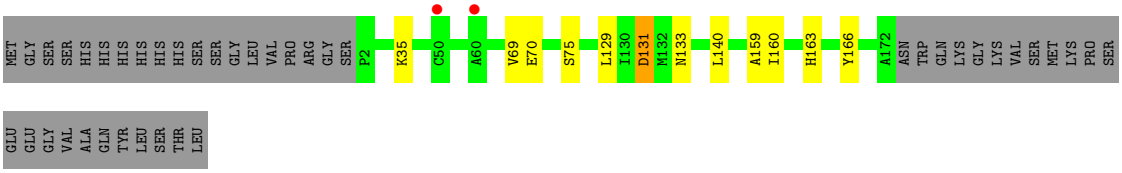
• Molecule 1: 2-Cys peroxiredoxin, putative

Chain F:



• Molecule 1: 2-Cys peroxiredoxin, putative

Chain G:

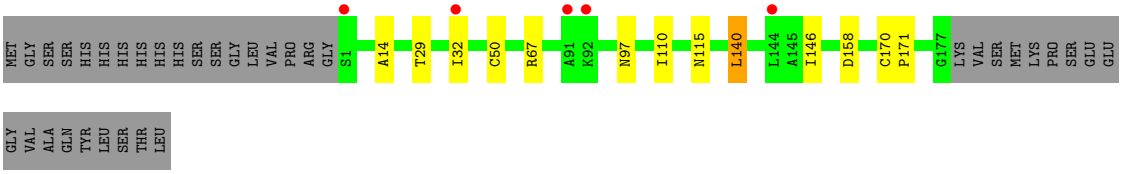


• Molecule 1: 2-Cys peroxiredoxin, putative

Chain H:

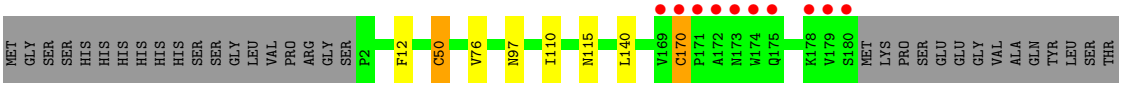
• Molecule 1: 2-Cys peroxiredoxin, putative

Chain I:



• Molecule 1: 2-Cys peroxiredoxin, putative

Chain J:



LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.55Å 149.59Å 131.91Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	40.25 – 2.50 40.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.25-2.50) 94.7 (40.25-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.176 , 0.212 0.176 , 0.207	Depositor DCC
R_{free} test set	4302 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13753	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.47	0/1360	0.66	1/1841 (0.1%)
1	B	0.47	0/1381	0.62	0/1871
1	C	0.54	1/1390 (0.1%)	0.81	5/1885 (0.3%)
1	D	0.46	0/1387	0.63	0/1880
1	E	0.50	0/1312	0.68	0/1777
1	F	0.48	0/1362	0.66	0/1844
1	G	0.51	0/1377	0.66	0/1867
1	H	0.49	0/1352	0.66	0/1830
1	I	0.50	0/1428	0.68	1/1937 (0.1%)
1	J	0.55	0/1454	0.75	2/1970 (0.1%)
All	All	0.50	1/13803 (0.0%)	0.68	9/18702 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	PRO	N-CD	5.12	1.55	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	50[A]	CYS	CA-C-O	8.12	137.16	120.10
1	C	50[B]	CYS	CA-C-O	8.12	137.16	120.10
1	J	50[A]	CYS	CA-C-O	5.97	132.65	120.10
1	J	50[B]	CYS	CA-C-O	5.97	132.65	120.10
1	C	170	CYS	C-N-CD	5.66	140.28	128.40
1	I	146	ILE	N-CA-C	-5.44	96.32	111.00
1	C	50[A]	CYS	CA-C-N	-5.34	102.14	117.10
1	C	50[B]	CYS	CA-C-N	-5.34	102.14	117.10
1	A	50	CYS	N-CA-C	5.24	125.14	111.00

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	1330	0	1329	4	0
1	B	1350	0	1353	5	0
1	C	1356	0	1356	5	0
1	D	1353	0	1359	13	0
1	E	1283	0	1293	1	0
1	F	1332	0	1338	3	0
1	G	1346	0	1342	6	0
1	H	1322	0	1325	3	0
1	I	1395	0	1387	11	0
1	J	1418	0	1423	7	0
2	A	4	0	3	0	0
2	C	4	0	3	0	0
3	A	18	0	0	0	0
3	B	18	0	0	0	0
3	C	33	0	0	0	0
3	D	25	0	0	0	0
3	E	22	0	0	0	0
3	F	22	0	0	0	0
3	G	21	0	0	0	0
3	H	31	0	0	0	0
3	I	35	0	0	2	0
3	J	35	0	0	0	0
All	All	13753	0	13511	41	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.

All (41) 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:D:171:PRO:HB2	1:D:172:ALA:CA	1.61	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:PRO:CB	1:D:172:ALA:HA	1.64	1.25
1:C:50[A]:CYS:SG	1:D:170:CYS:HB3	2.02	0.99
1:I:50:CYS:HG	1:J:170:CYS:HG	1.00	0.95
1:C:50[A]:CYS:SG	1:D:170:CYS:CB	2.62	0.87
1:D:170:CYS:HB2	1:D:171:PRO:HA	1.57	0.83
1:D:170:CYS:HA	1:D:171:PRO:O	1.82	0.78
1:I:170:CYS:HG	1:J:50[A]:CYS:HG	0.76	0.75
1:C:50[A]:CYS:HG	1:D:170:CYS:CB	2.04	0.70
1:D:171:PRO:HB2	1:D:172:ALA:HA	0.76	0.67
1:I:67:ARG:NH1	1:I:158:ASP:OD1	2.27	0.67
1:I:140:LEU:HD12	1:J:140:LEU:HD12	1.82	0.60
1:A:145:ALA:O	1:B:170:CYS:HB3	2.05	0.57
1:D:170:CYS:HB2	1:D:171:PRO:CA	2.34	0.56
1:I:67:ARG:NE	3:I:209:HOH:O	2.40	0.55
1:H:144:LEU:HB2	1:H:146:ILE:HD13	1.90	0.54
1:D:171:PRO:CG	1:D:172:ALA:HA	2.36	0.54
1:G:163:HIS:O	1:G:166:TYR:O	2.28	0.52
1:I:170:CYS:HG	1:J:50[B]:CYS:HG	1.57	0.52
1:G:129:LEU:HD23	1:G:160:ILE:HD13	1.91	0.52
1:J:12:PHE:HB2	1:J:110:ILE:HD12	1.91	0.51
1:E:152:GLU:HG3	1:F:152:GLU:HG3	1.95	0.49
1:A:140:LEU:HD12	1:B:140:LEU:HD13	1.94	0.49
1:C:140:LEU:HD12	1:D:140:LEU:HD12	1.95	0.49
1:G:159:ALA:HB1	1:H:146:ILE:HG13	1.96	0.48
1:I:67:ARG:CZ	3:I:209:HOH:O	2.61	0.48
1:D:171:PRO:HB2	1:D:172:ALA:C	2.33	0.46
1:I:140:LEU:CD1	1:J:140:LEU:HD12	2.45	0.44
1:A:138:HIS:HE1	1:B:140:LEU:HD11	1.83	0.43
1:G:35:LYS:HE2	1:G:70:GLU:HB2	2.00	0.43
1:I:29:THR:O	1:I:32:ILE:HG22	2.17	0.43
1:H:129:LEU:HD23	1:H:160:ILE:HD13	2.00	0.43
1:I:14:ALA:HB2	1:I:110:ILE:HD11	2.01	0.42
1:A:140:LEU:HD12	1:B:140:LEU:CD1	2.50	0.42
1:G:35:LYS:HE3	1:G:35:LYS:HB3	1.82	0.41
1:F:29:THR:HA	1:F:32:ILE:HG12	2.02	0.41
1:C:50[A]:CYS:SG	1:D:170:CYS:SG	3.10	0.41
1:B:129:LEU:HD23	1:B:160:ILE:HD13	2.02	0.41
1:I:170:CYS:SG	1:J:50[B]:CYS:SG	3.08	0.41
1:G:131:ASP:HB3	1:G:133:ASN:H	1.85	0.41
1:F:156:ILE:O	1:F:160:ILE:HG23	2.22	0.40

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	166/213 (78%)	160 (96%)	6 (4%)	0	100 100
1	B	169/213 (79%)	162 (96%)	6 (4%)	1 (1%)	25 43
1	C	171/213 (80%)	166 (97%)	5 (3%)	0	100 100
1	D	170/213 (80%)	164 (96%)	5 (3%)	1 (1%)	25 43
1	E	160/213 (75%)	154 (96%)	6 (4%)	0	100 100
1	F	167/213 (78%)	163 (98%)	4 (2%)	0	100 100
1	G	169/213 (79%)	163 (96%)	6 (4%)	0	100 100
1	H	165/213 (78%)	158 (96%)	7 (4%)	0	100 100
1	I	175/213 (82%)	171 (98%)	4 (2%)	0	100 100
1	J	178/213 (84%)	173 (97%)	5 (3%)	0	100 100
All	All	1690/2130 (79%)	1634 (97%)	54 (3%)	2 (0%)	51 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	171	PRO
1	B	43	PRO

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	145/184 (79%)	143 (99%)	2 (1%)	67 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	148/184 (80%)	145 (98%)	3 (2%)	55 79
1	C	148/184 (80%)	143 (97%)	5 (3%)	37 63
1	D	149/184 (81%)	148 (99%)	1 (1%)	84 94
1	E	141/184 (77%)	139 (99%)	2 (1%)	67 86
1	F	145/184 (79%)	139 (96%)	6 (4%)	30 55
1	G	147/184 (80%)	143 (97%)	4 (3%)	44 71
1	H	144/184 (78%)	140 (97%)	4 (3%)	43 70
1	I	151/184 (82%)	147 (97%)	4 (3%)	46 72
1	J	155/184 (84%)	151 (97%)	4 (3%)	46 72
All	All	1473/1840 (80%)	1438 (98%)	35 (2%)	49 74

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	168	ASP
1	B	8	GLU
1	B	115	ASN
1	B	151	ASP
1	C	69	VAL
1	C	76	VAL
1	C	139	LEU
1	C	168	ASP
1	C	170	CYS
1	D	140	LEU
1	E	150	VAL
1	E	151	ASP
1	F	13	LYS
1	F	69	VAL
1	F	156	ILE
1	F	160	ILE
1	F	168	ASP
1	F	170	CYS
1	G	69	VAL
1	G	75	SER
1	G	131	ASP
1	G	140	LEU
1	H	26	VAL
1	H	35	LYS

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Mol	Chain	Res	Type
1	H	146	ILE
1	H	165	LYS
1	I	97	ASN
1	I	115	ASN
1	I	140	LEU
1	I	171	PRO
1	J	76	VAL
1	J	97	ASN
1	J	115	ASN
1	J	170	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	C	201	-	3,3,3	1.29	1 (33%)	3,3,3	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ACT	A	201	-	3,3,3	0.87	0	3,3,3	1.11	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	ACT	CH3-C	2.03	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	168/213 (78%)	-0.23	2 (1%) 79 80	38, 55, 83, 112	0
1	B	171/213 (80%)	-0.19	3 (1%) 68 71	41, 54, 82, 106	0
1	C	172/213 (80%)	-0.24	3 (1%) 70 72	34, 47, 74, 131	0
1	D	171/213 (80%)	-0.21	3 (1%) 68 71	38, 54, 80, 125	0
1	E	162/213 (76%)	-0.39	0 100 100	38, 51, 75, 118	0
1	F	169/213 (79%)	-0.20	1 (0%) 89 90	37, 52, 78, 108	0
1	G	171/213 (80%)	-0.26	2 (1%) 79 80	36, 53, 76, 89	0
1	H	167/213 (78%)	-0.40	1 (0%) 89 90	33, 48, 75, 96	0
1	I	177/213 (83%)	-0.20	5 (2%) 53 56	34, 50, 72, 81	0
1	J	179/213 (84%)	-0.16	10 (5%) 24 25	33, 44, 95, 111	0
All	All	1707/2130 (80%)	-0.25	30 (1%) 68 71	33, 51, 80, 131	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	172	ALA	8.4
1	J	179	VAL	6.4
1	D	171	PRO	4.8
1	B	91	ALA	4.6
1	J	180	SER	4.5
1	A	166	TYR	4.0
1	H	166	TYR	3.5
1	J	173	ASN	3.4
1	J	175	GLN	3.3
1	J	172	ALA	3.2
1	C	172	ALA	3.2
1	J	170	CYS	3.2
1	I	92	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	174	TRP	2.9
1	D	170	CYS	2.8
1	C	171	PRO	2.7
1	J	178	LYS	2.6
1	I	91	ALA	2.6
1	J	171	PRO	2.6
1	B	90	LEU	2.5
1	A	162	HIS	2.3
1	I	32	ILE	2.3
1	F	169	VAL	2.3
1	G	60	ALA	2.3
1	C	170	CYS	2.2
1	G	50	CYS	2.1
1	I	144	LEU	2.1
1	I	1	SER	2.1
1	J	169	VAL	2.1
1	B	170	CYS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	C	201	4/4	0.65	0.45	70,72,73,78	0
2	ACT	A	201	4/4	0.90	0.18	53,57,60,61	0

6.5 Other polymers (i)

There are no such residues in this entry.