



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:41 am BST

PDB ID : 5XBQ
Title : Peroxiredoxin from *Pyrococcus horikoshii* (6m mutant)
Authors : Nakamura, T.; Uegaki, K.
Deposited on : 2017-03-21
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

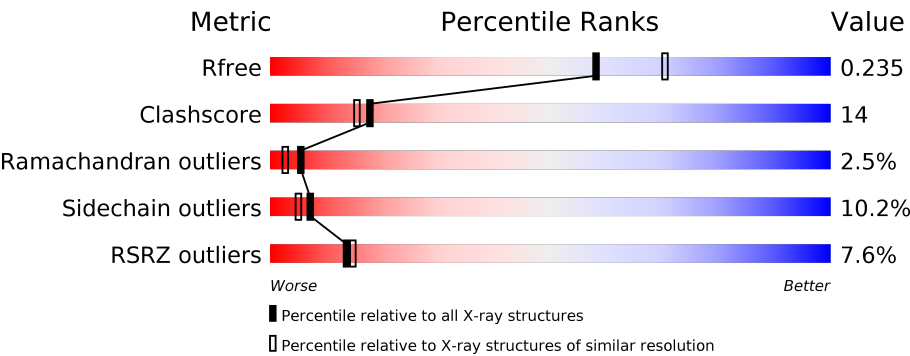
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 ≥ 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	216	<div><div>6%</div><div>69%26%...</div></div>
1	B	216	<div><div>9%</div><div>61%31%7%..</div></div>
1	C	216	<div><div>6%</div><div>58%30%11%. </div></div>
1	D	216	<div><div>10%</div><div>66%26%7%. </div></div>
1	E	216	<div><div>8%</div><div>67%26%6%. </div></div>
1	F	216	<div><div>9%</div><div>65%31%.. </div></div>

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Mol	Chain	Length	Quality of chain
1	G	216	
1	H	216	
1	I	216	
1	J	216	
1	K	216	
1	L	216	

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
1	OCS	F	46	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20842 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	B	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	C	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	D	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	E	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	F	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	G	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	H	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	I	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	J	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	K	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			
1	L	214	Total	C	N	O	S	0	0	0
			1725	1117	283	320	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	VAL	engineered mutation	UNP O58966
A	76	GLU	PHE	engineered mutation	UNP O58966
A	77	ASP	SER	engineered mutation	UNP O58966
A	79	SER	ILE	engineered mutation	UNP O58966
A	80	ALA	LYS	engineered mutation	UNP O58966

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Chain	Residue	Modelled	Actual	Comment	Reference
A	208	SER	TRP	engineered mutation	UNP O58966
B	19	ARG	VAL	engineered mutation	UNP O58966
B	76	GLU	PHE	engineered mutation	UNP O58966
B	77	ASP	SER	engineered mutation	UNP O58966
B	79	SER	ILE	engineered mutation	UNP O58966
B	80	ALA	LYS	engineered mutation	UNP O58966
B	208	SER	TRP	engineered mutation	UNP O58966
C	19	ARG	VAL	engineered mutation	UNP O58966
C	76	GLU	PHE	engineered mutation	UNP O58966
C	77	ASP	SER	engineered mutation	UNP O58966
C	79	SER	ILE	engineered mutation	UNP O58966
C	80	ALA	LYS	engineered mutation	UNP O58966
C	208	SER	TRP	engineered mutation	UNP O58966
D	19	ARG	VAL	engineered mutation	UNP O58966
D	76	GLU	PHE	engineered mutation	UNP O58966
D	77	ASP	SER	engineered mutation	UNP O58966
D	79	SER	ILE	engineered mutation	UNP O58966
D	80	ALA	LYS	engineered mutation	UNP O58966
D	208	SER	TRP	engineered mutation	UNP O58966
E	19	ARG	VAL	engineered mutation	UNP O58966
E	76	GLU	PHE	engineered mutation	UNP O58966
E	77	ASP	SER	engineered mutation	UNP O58966
E	79	SER	ILE	engineered mutation	UNP O58966
E	80	ALA	LYS	engineered mutation	UNP O58966
E	208	SER	TRP	engineered mutation	UNP O58966
F	19	ARG	VAL	engineered mutation	UNP O58966
F	76	GLU	PHE	engineered mutation	UNP O58966
F	77	ASP	SER	engineered mutation	UNP O58966
F	79	SER	ILE	engineered mutation	UNP O58966
F	80	ALA	LYS	engineered mutation	UNP O58966
F	208	SER	TRP	engineered mutation	UNP O58966
G	19	ARG	VAL	engineered mutation	UNP O58966
G	76	GLU	PHE	engineered mutation	UNP O58966
G	77	ASP	SER	engineered mutation	UNP O58966
G	79	SER	ILE	engineered mutation	UNP O58966
G	80	ALA	LYS	engineered mutation	UNP O58966
G	208	SER	TRP	engineered mutation	UNP O58966
H	19	ARG	VAL	engineered mutation	UNP O58966
H	76	GLU	PHE	engineered mutation	UNP O58966
H	77	ASP	SER	engineered mutation	UNP O58966
H	79	SER	ILE	engineered mutation	UNP O58966
H	80	ALA	LYS	engineered mutation	UNP O58966

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Chain	Residue	Modelled	Actual	Comment	Reference
H	208	SER	TRP	engineered mutation	UNP O58966
I	19	ARG	VAL	engineered mutation	UNP O58966
I	76	GLU	PHE	engineered mutation	UNP O58966
I	77	ASP	SER	engineered mutation	UNP O58966
I	79	SER	ILE	engineered mutation	UNP O58966
I	80	ALA	LYS	engineered mutation	UNP O58966
I	208	SER	TRP	engineered mutation	UNP O58966
J	19	ARG	VAL	engineered mutation	UNP O58966
J	76	GLU	PHE	engineered mutation	UNP O58966
J	77	ASP	SER	engineered mutation	UNP O58966
J	79	SER	ILE	engineered mutation	UNP O58966
J	80	ALA	LYS	engineered mutation	UNP O58966
J	208	SER	TRP	engineered mutation	UNP O58966
K	19	ARG	VAL	engineered mutation	UNP O58966
K	76	GLU	PHE	engineered mutation	UNP O58966
K	77	ASP	SER	engineered mutation	UNP O58966
K	79	SER	ILE	engineered mutation	UNP O58966
K	80	ALA	LYS	engineered mutation	UNP O58966
K	208	SER	TRP	engineered mutation	UNP O58966
L	19	ARG	VAL	engineered mutation	UNP O58966
L	76	GLU	PHE	engineered mutation	UNP O58966
L	77	ASP	SER	engineered mutation	UNP O58966
L	79	SER	ILE	engineered mutation	UNP O58966
L	80	ALA	LYS	engineered mutation	UNP O58966
L	208	SER	TRP	engineered mutation	UNP O58966

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	16	Total O 16 16	0	0
2	C	17	Total O 17 17	0	0
2	D	6	Total O 6 6	0	0
2	E	15	Total O 15 15	0	0
2	F	10	Total O 10 10	0	0
2	G	11	Total O 11 11	0	0

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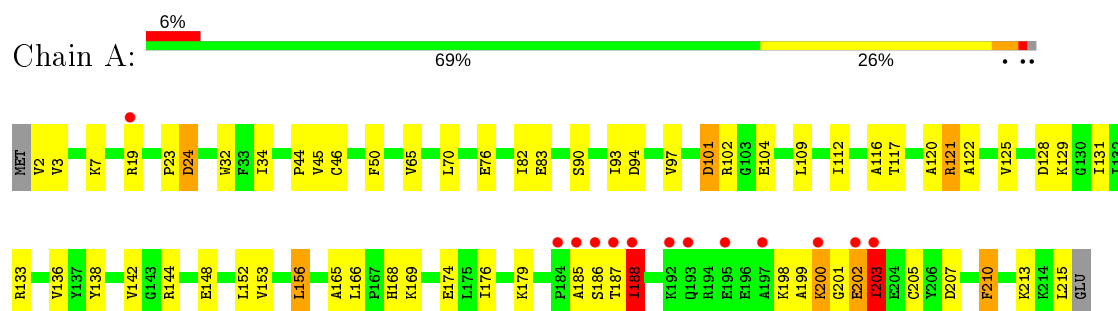
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	11	Total 11	O 11	0	0
2	I	18	Total 18	O 18	0	0
2	J	11	Total 11	O 11	0	0
2	K	9	Total 9	O 9	0	0
2	L	9	Total 9	O 9	0	0

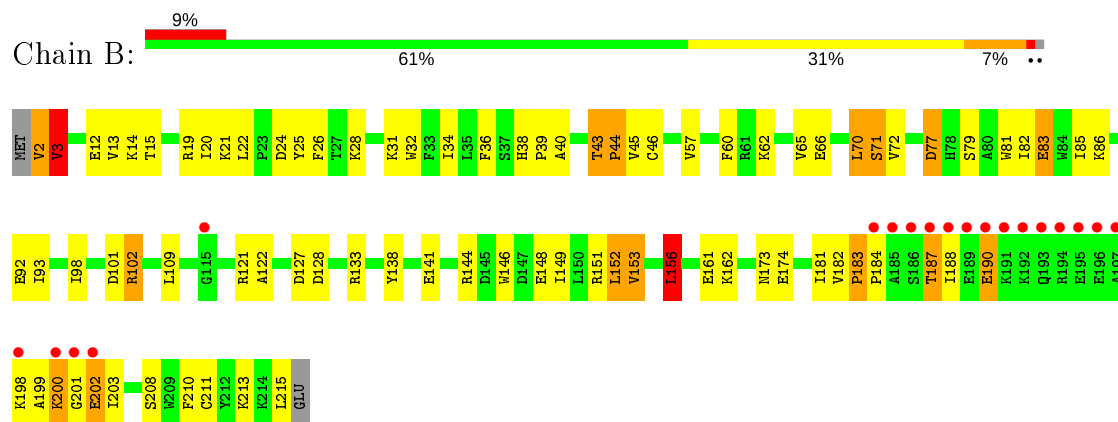
3 Residue-property plots [i](#)

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.

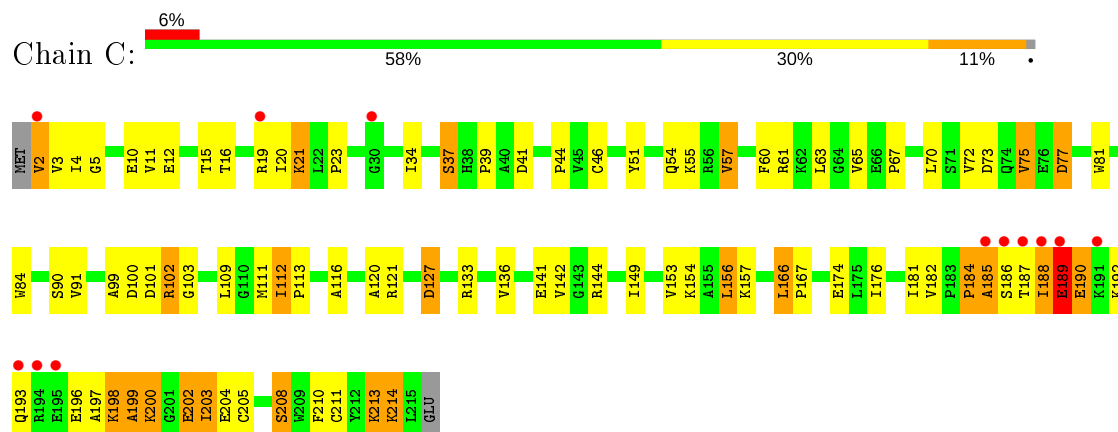
• Molecule 1: Peroxiredoxin



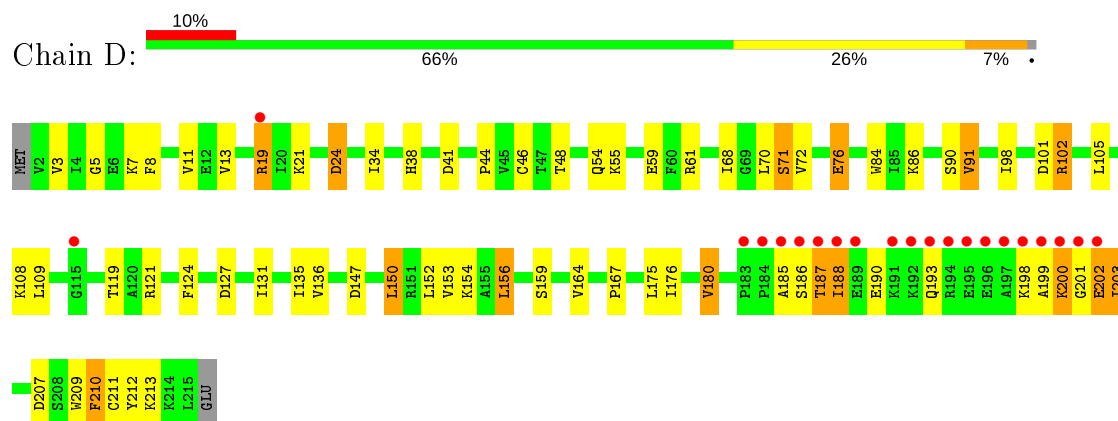
• Molecule 1: Peroxiredoxin



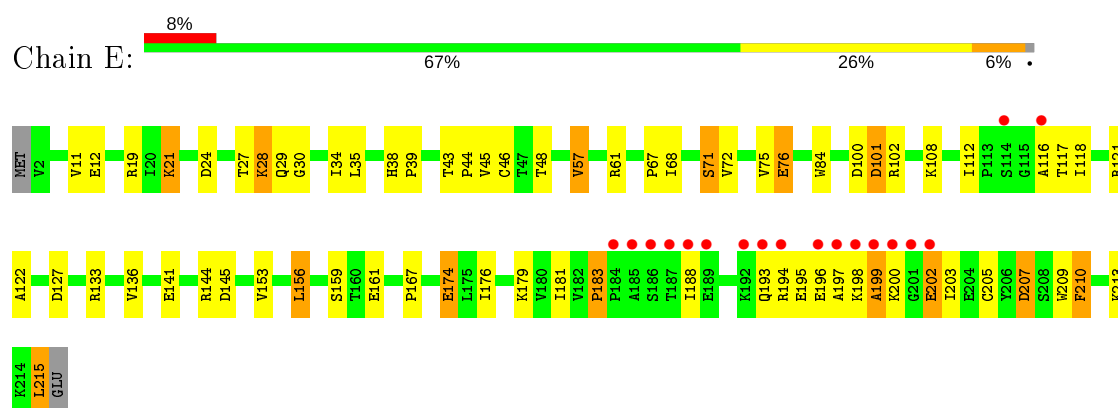
• Molecule 1: Peroxiredoxin



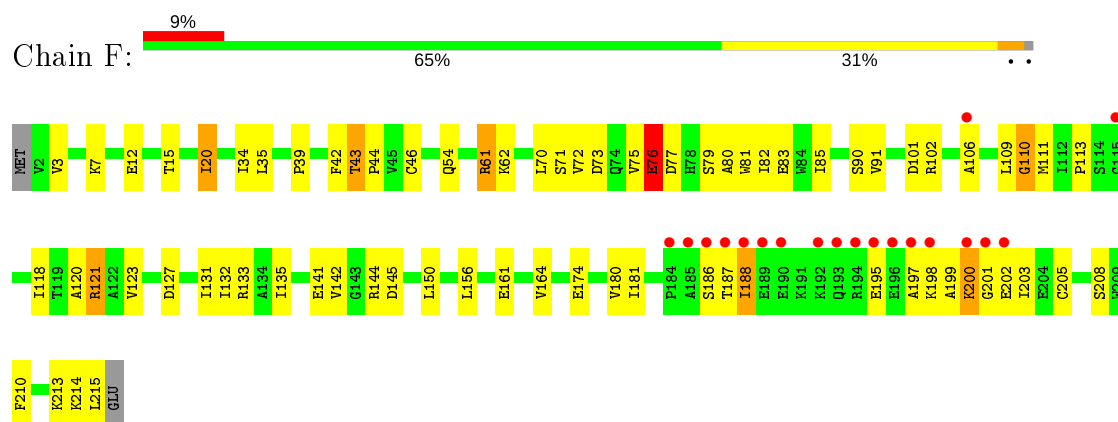
● Molecule 1: Peroxiredoxin



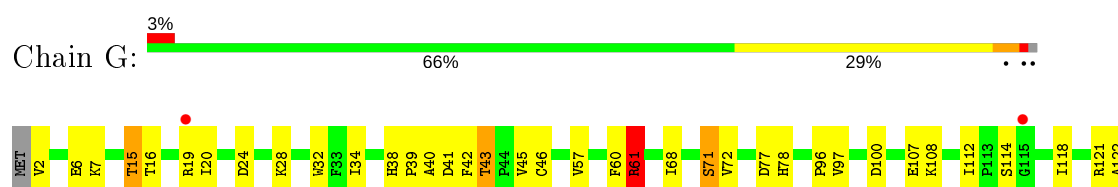
● Molecule 1: Peroxiredoxin



● Molecule 1: Peroxiredoxin

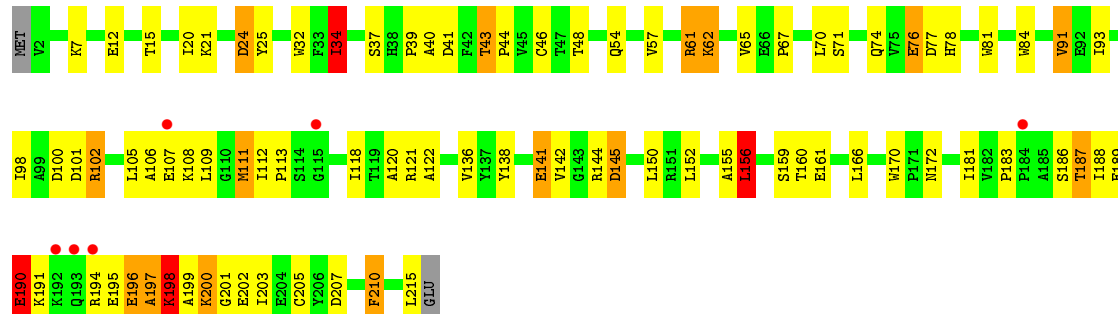


● Molecule 1: Peroxiredoxin

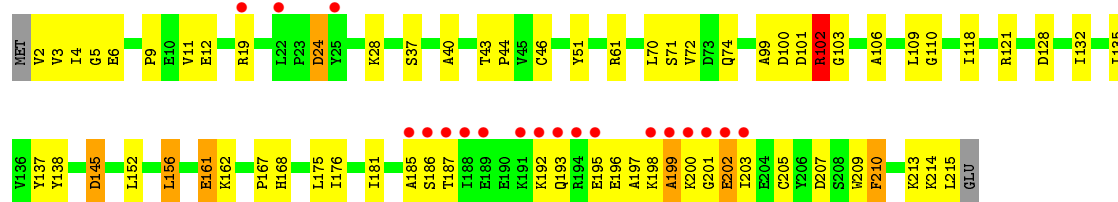




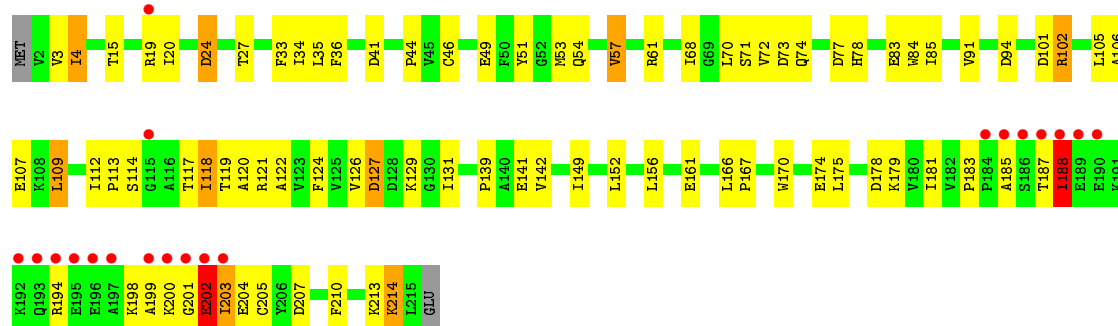
- Molecule 1: Peroxiredoxin



- Molecule 1: Peroxiredoxin

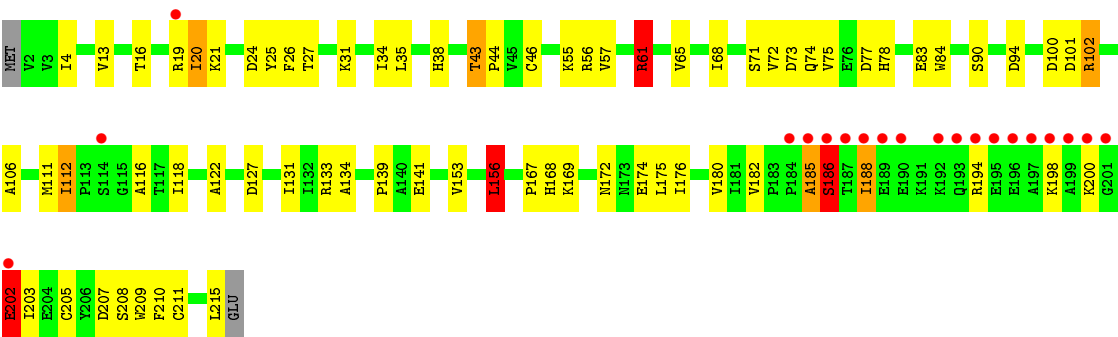


- Molecule 1: Peroxiredoxin

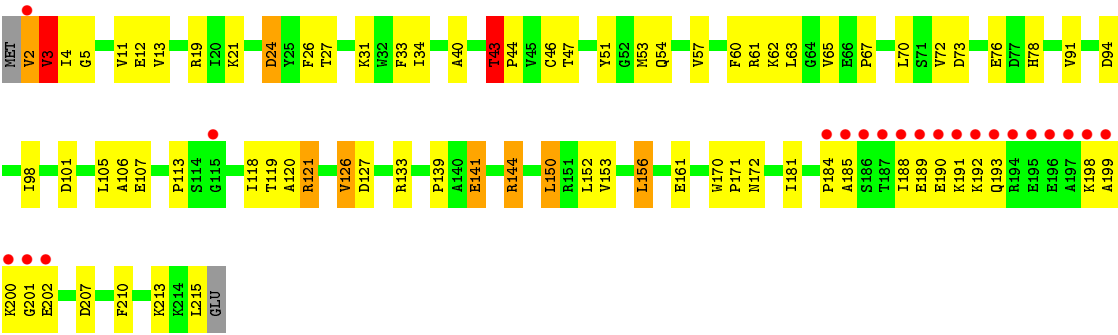


- Molecule 1: Peroxiredoxin





● Molecule 1: Peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.58 Å 98.60 Å 137.57 Å 90.00° 119.95° 90.00°	Depositor
Resolution (Å)	39.73 – 2.25 39.73 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.73-2.25) 99.7 (39.73-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	678.50 (at 2.24 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.232 0.198 , 0.235	Depositor DCC
R_{free} test set	7632 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.046 for l,k,-h-l 0.046 for -h-l,k,h 0.000 for -h-l,-k,l 0.000 for h,-k,-h-l 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20842	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0440e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.00	1/1758 (0.1%)	1.06	4/2380 (0.2%)
1	B	1.01	3/1758 (0.2%)	1.13	9/2380 (0.4%)
1	C	1.02	2/1758 (0.1%)	1.13	8/2380 (0.3%)
1	D	0.94	1/1758 (0.1%)	1.05	7/2380 (0.3%)
1	E	1.05	3/1758 (0.2%)	1.13	9/2380 (0.4%)
1	F	0.97	1/1758 (0.1%)	1.09	9/2380 (0.4%)
1	G	1.05	3/1758 (0.2%)	1.07	5/2380 (0.2%)
1	H	0.98	2/1758 (0.1%)	1.16	10/2380 (0.4%)
1	I	0.97	0/1758	1.07	4/2380 (0.2%)
1	J	0.99	0/1758	1.11	5/2380 (0.2%)
1	K	0.98	1/1758 (0.1%)	1.06	5/2380 (0.2%)
1	L	0.98	3/1758 (0.2%)	1.01	4/2380 (0.2%)
All	All	1.00	20/21096 (0.1%)	1.09	79/28560 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	K	0	1
1	L	0	1
All	All	0	8

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	SER	CB-OG	-10.62	1.28	1.42
1	E	174	GLU	CD-OE2	-8.69	1.16	1.25
1	G	141	GLU	CD-OE2	-7.30	1.17	1.25
1	H	141	GLU	CD-OE2	-6.83	1.18	1.25
1	E	183	PRO	C-O	-6.53	1.10	1.23

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	61	ARG	NE-CZ-NH1	-13.71	113.44	120.30
1	E	61	ARG	NE-CZ-NH2	13.05	126.82	120.30
1	E	61	ARG	NE-CZ-NH1	-12.55	114.02	120.30
1	J	61	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	K	61	ARG	NE-CZ-NH2	9.84	125.22	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	183	PRO	Peptide
1	B	2	VAL	Peptide
1	C	196	GLU	Peptide
1	E	202	GLU	Peptide
1	G	200	LYS	Peptide

5.2 Too-close contacts ⓘ

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	1725	0	1727	48	0
1	B	1725	0	1728	50	0
1	C	1725	0	1727	70	0
1	D	1725	0	1728	50	0
1	E	1725	0	1728	43	0
1	F	1725	0	1727	51	0
1	G	1725	0	1727	44	0
1	H	1725	0	1728	69	0
1	I	1725	0	1727	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1725	0	1728	60	0
1	K	1725	0	1728	52	0
1	L	1725	0	1727	47	0
2	A	9	0	0	0	0
2	B	16	0	0	1	0
2	C	17	0	0	0	0
2	D	6	0	0	1	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
2	G	11	0	0	0	0
2	H	11	0	0	0	0
2	I	18	0	0	0	0
2	J	11	0	0	0	0
2	K	9	0	0	0	0
2	L	9	0	0	2	0
All	All	20842	0	20730	565	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 14.

The worst 5 of 565 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:J:179:LYS:HE2	1:J:204:GLU:OE2	1.37	1.20
1:C:185:ALA:HB3	1:C:186:SER:HA	1.41	1.02
1:J:179:LYS:CE	1:J:204:GLU:OE2	2.14	0.95
1:F:43:THR:HG21	1:F:46:OCS:OD3	1.66	0.94
1:F:109:LEU:HD12	1:F:111:MET:HE3	1.51	0.91

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	211/216 (98%)	191 (90%)	14 (7%)	6 (3%)	5	2
1	B	211/216 (98%)	179 (85%)	23 (11%)	9 (4%)	2	0
1	C	211/216 (98%)	181 (86%)	21 (10%)	9 (4%)	2	0
1	D	211/216 (98%)	185 (88%)	23 (11%)	3 (1%)	11	7
1	E	211/216 (98%)	189 (90%)	17 (8%)	5 (2%)	6	3
1	F	211/216 (98%)	192 (91%)	16 (8%)	3 (1%)	11	7
1	G	211/216 (98%)	194 (92%)	16 (8%)	1 (0%)	29	29
1	H	211/216 (98%)	191 (90%)	12 (6%)	8 (4%)	3	1
1	I	211/216 (98%)	193 (92%)	16 (8%)	2 (1%)	17	14
1	J	211/216 (98%)	183 (87%)	25 (12%)	3 (1%)	11	7
1	K	211/216 (98%)	183 (87%)	22 (10%)	6 (3%)	5	2
1	L	211/216 (98%)	188 (89%)	15 (7%)	8 (4%)	3	1
All	All	2532/2592 (98%)	2249 (89%)	220 (9%)	63 (2%)	5	3

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	LYS
1	A	203	ILE
1	B	184	PRO
1	B	190	GLU
1	C	185	ALA

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	185/187 (99%)	172 (93%)	13 (7%)	15	13
1	B	185/187 (99%)	166 (90%)	19 (10%)	7	5
1	C	185/187 (99%)	159 (86%)	26 (14%)	3	2
1	D	185/187 (99%)	166 (90%)	19 (10%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	185/187 (99%)	168 (91%)	17 (9%)	9	7
1	F	185/187 (99%)	165 (89%)	20 (11%)	6	4
1	G	185/187 (99%)	172 (93%)	13 (7%)	15	13
1	H	185/187 (99%)	162 (88%)	23 (12%)	4	3
1	I	185/187 (99%)	171 (92%)	14 (8%)	13	12
1	J	185/187 (99%)	158 (85%)	27 (15%)	3	1
1	K	185/187 (99%)	171 (92%)	14 (8%)	13	12
1	L	185/187 (99%)	164 (89%)	21 (11%)	5	3
All	All	2220/2244 (99%)	1994 (90%)	226 (10%)	7	5

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	101	ASP
1	G	213	LYS
1	L	21	LYS
1	F	150	LEU
1	G	7	LYS

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	H	74	GLN
1	I	74	GLN
1	K	193	GLN
1	F	74	GLN
1	K	74	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OCS	G	46	1	7,8,9	2.23	2 (28%)	6,11,13	2.66	2 (33%)
1	OCS	K	46	1	7,8,9	1.83	2 (28%)	6,11,13	2.18	3 (50%)
1	OCS	A	46	1	7,8,9	3.08	3 (42%)	6,11,13	4.06	5 (83%)
1	OCS	E	46	1	7,8,9	2.37	3 (42%)	6,11,13	3.94	2 (33%)
1	OCS	C	46	1	7,8,9	3.47	4 (57%)	6,11,13	3.03	3 (50%)
1	OCS	J	46	1	7,8,9	1.87	1 (14%)	6,11,13	4.91	5 (83%)
1	OCS	H	46	1	7,8,9	1.88	2 (28%)	6,11,13	2.44	1 (16%)
1	OCS	L	46	1	7,8,9	3.14	2 (28%)	6,11,13	4.57	4 (66%)
1	OCS	B	46	1	7,8,9	2.15	3 (42%)	6,11,13	9.93	5 (83%)
1	OCS	F	46	1	7,8,9	2.68	2 (28%)	6,11,13	3.75	4 (66%)
1	OCS	D	46	1	7,8,9	2.09	2 (28%)	6,11,13	4.65	6 (100%)
1	OCS	I	46	1	7,8,9	3.02	2 (28%)	6,11,13	2.08	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	G	46	1	-	0/4/7/9	-
1	OCS	K	46	1	-	0/4/7/9	-
1	OCS	A	46	1	-	0/4/7/9	-
1	OCS	E	46	1	-	0/4/7/9	-
1	OCS	C	46	1	-	0/4/7/9	-
1	OCS	J	46	1	-	0/4/7/9	-
1	OCS	H	46	1	-	0/4/7/9	-
1	OCS	L	46	1	-	0/4/7/9	-
1	OCS	B	46	1	-	1/4/7/9	-
1	OCS	F	46	1	-	0/4/7/9	-
1	OCS	D	46	1	-	0/4/7/9	-
1	OCS	I	46	1	-	0/4/7/9	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	OCS	OD3-SG	7.69	1.67	1.45
1	L	46	OCS	OD1-SG	7.62	1.67	1.45
1	I	46	OCS	OD1-SG	7.03	1.65	1.45
1	A	46	OCS	OD3-SG	6.77	1.65	1.45
1	F	46	OCS	OD3-SG	6.08	1.63	1.45

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	OCS	OD1-SG-CB	18.21	128.58	106.94
1	B	46	OCS	OD2-SG-OD3	-9.63	87.74	111.27
1	E	46	OCS	OD3-SG-CB	8.68	117.26	106.94
1	D	46	OCS	OD2-SG-CB	8.32	119.00	105.74
1	J	46	OCS	OD3-SG-CB	8.27	116.77	106.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	46	OCS	CA-CB-SG-OD1

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	46	OCS	2	0
1	K	46	OCS	2	0
1	A	46	OCS	1	0
1	E	46	OCS	2	0
1	C	46	OCS	2	0
1	J	46	OCS	1	0
1	H	46	OCS	2	0
1	L	46	OCS	1	0
1	B	46	OCS	3	0
1	F	46	OCS	4	0
1	D	46	OCS	1	0
1	I	46	OCS	1	0

5.5 Carbohydrates

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, 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	213/216 (98%)	0.03	13 (6%) 21 23	11, 23, 84, 100	0
1	B	213/216 (98%)	0.24	19 (8%) 9 10	13, 25, 111, 125	0
1	C	213/216 (98%)	0.19	12 (5%) 24 26	15, 26, 80, 112	0
1	D	213/216 (98%)	0.35	21 (9%) 7 7	15, 27, 109, 146	0
1	E	213/216 (98%)	0.33	18 (8%) 10 12	15, 25, 105, 141	0
1	F	213/216 (98%)	0.53	19 (8%) 9 10	14, 25, 119, 165	0
1	G	213/216 (98%)	0.00	7 (3%) 46 48	14, 24, 71, 93	0
1	H	213/216 (98%)	0.10	6 (2%) 53 55	14, 25, 84, 108	0
1	I	213/216 (98%)	0.35	19 (8%) 9 10	13, 25, 97, 149	0
1	J	213/216 (98%)	0.41	20 (9%) 8 9	13, 24, 109, 142	0
1	K	213/216 (98%)	0.41	20 (9%) 8 9	14, 27, 109, 132	0
1	L	213/216 (98%)	0.44	21 (9%) 7 7	14, 28, 108, 129	0
All	All	2556/2592 (98%)	0.28	195 (7%) 13 15	11, 25, 100, 165	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	185	ALA	22.0
1	I	188	ILE	12.2
1	F	188	ILE	11.2
1	E	186	SER	10.6
1	J	185	ALA	10.2

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
1	OCS	C	46	9/10	0.96	0.11	19,21,36,38	0
1	OCS	H	46	9/10	0.96	0.15	19,23,43,45	0
1	OCS	L	46	9/10	0.96	0.12	17,19,35,39	0
1	OCS	A	46	9/10	0.97	0.11	17,21,37,40	0
1	OCS	B	46	9/10	0.97	0.12	20,21,33,34	0
1	OCS	F	46	9/10	0.97	0.11	18,19,39,48	0
1	OCS	D	46	9/10	0.97	0.13	15,16,31,38	0
1	OCS	I	46	9/10	0.97	0.10	20,24,39,39	0
1	OCS	G	46	9/10	0.98	0.14	20,22,40,42	0
1	OCS	E	46	9/10	0.98	0.09	19,19,35,40	0
1	OCS	K	46	9/10	0.98	0.09	20,22,38,42	0
1	OCS	J	46	9/10	0.99	0.13	14,18,41,41	0

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.