WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 12:13 pm BST

PDB ID	:	3VWU
Title	:	Crystal structure of peroxiredoxin 4 from M. musculus
Authors	:	Inaba, K.; Suzuki, M.
Deposited on	:	2012-09-03
Resolution	:	3.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
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 3.30 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.
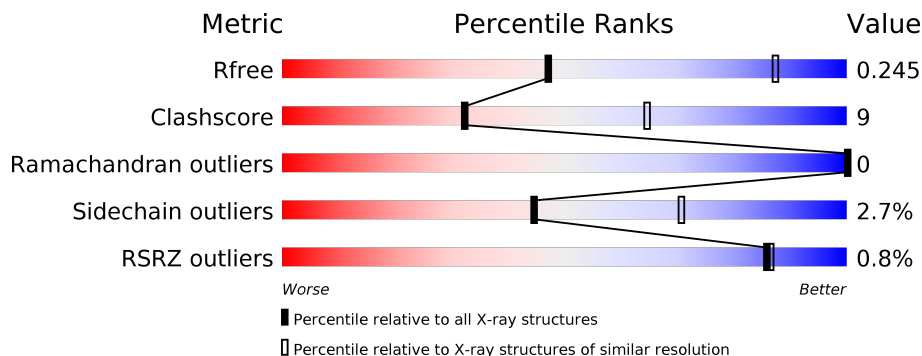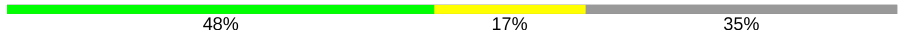

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	255	54% 13% • 33%
1	B	255	54% 11% 35%
1	C	255	56% 11% • 32%
1	D	255	% 52% 14% • 33%
1	E	255	2% 46% 20% • 33%
1	F	255	46% 20% • 33%

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Mol	Chain	Length	Quality of chain
1	G	255	51% 14% 35%
1	H	255	53% 15% 33%
1	I	255	48% 17% 35%
1	J	255	49% 16% 35%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13617 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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1376	894	229	250	3			
1	B	167	Total	C	N	O	S	0	0	0
			1344	870	225	247	2			
1	C	173	Total	C	N	O	S	0	0	0
			1385	899	230	253	3			
1	D	170	Total	C	N	O	S	0	0	0
			1366	883	228	252	3			
1	E	171	Total	C	N	O	S	0	0	0
			1376	889	231	253	3			
1	F	170	Total	C	N	O	S	0	0	0
			1366	883	228	252	3			
1	G	167	Total	C	N	O	S	0	0	0
			1344	870	225	247	2			
1	H	172	Total	C	N	O	S	0	0	0
			1376	894	229	250	3			
1	I	167	Total	C	N	O	S	0	0	0
			1344	870	225	247	2			
1	J	166	Total	C	N	O	S	0	0	0
			1340	868	224	246	2			

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	EXPRESSION TAG	UNP O08807
A	21	GLY	-	EXPRESSION TAG	UNP O08807
A	22	SER	-	EXPRESSION TAG	UNP O08807
A	23	SER	-	EXPRESSION TAG	UNP O08807
A	24	HIS	-	EXPRESSION TAG	UNP O08807
A	25	HIS	-	EXPRESSION TAG	UNP O08807
A	26	HIS	-	EXPRESSION TAG	UNP O08807
A	27	HIS	-	EXPRESSION TAG	UNP O08807
A	28	HIS	-	EXPRESSION TAG	UNP O08807

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP O08807
A	30	SER	-	EXPRESSION TAG	UNP O08807
A	31	SER	-	EXPRESSION TAG	UNP O08807
A	32	GLY	-	EXPRESSION TAG	UNP O08807
A	33	LEU	-	EXPRESSION TAG	UNP O08807
A	34	VAL	-	EXPRESSION TAG	UNP O08807
A	35	PRO	-	EXPRESSION TAG	UNP O08807
A	36	ARG	-	EXPRESSION TAG	UNP O08807
A	37	GLY	-	EXPRESSION TAG	UNP O08807
A	38	SER	-	EXPRESSION TAG	UNP O08807
A	39	HIS	-	EXPRESSION TAG	UNP O08807
A	40	MET	-	EXPRESSION TAG	UNP O08807
A	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
B	20	MET	-	EXPRESSION TAG	UNP O08807
B	21	GLY	-	EXPRESSION TAG	UNP O08807
B	22	SER	-	EXPRESSION TAG	UNP O08807
B	23	SER	-	EXPRESSION TAG	UNP O08807
B	24	HIS	-	EXPRESSION TAG	UNP O08807
B	25	HIS	-	EXPRESSION TAG	UNP O08807
B	26	HIS	-	EXPRESSION TAG	UNP O08807
B	27	HIS	-	EXPRESSION TAG	UNP O08807
B	28	HIS	-	EXPRESSION TAG	UNP O08807
B	29	HIS	-	EXPRESSION TAG	UNP O08807
B	30	SER	-	EXPRESSION TAG	UNP O08807
B	31	SER	-	EXPRESSION TAG	UNP O08807
B	32	GLY	-	EXPRESSION TAG	UNP O08807
B	33	LEU	-	EXPRESSION TAG	UNP O08807
B	34	VAL	-	EXPRESSION TAG	UNP O08807
B	35	PRO	-	EXPRESSION TAG	UNP O08807
B	36	ARG	-	EXPRESSION TAG	UNP O08807
B	37	GLY	-	EXPRESSION TAG	UNP O08807
B	38	SER	-	EXPRESSION TAG	UNP O08807
B	39	HIS	-	EXPRESSION TAG	UNP O08807
B	40	MET	-	EXPRESSION TAG	UNP O08807
B	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
C	20	MET	-	EXPRESSION TAG	UNP O08807
C	21	GLY	-	EXPRESSION TAG	UNP O08807
C	22	SER	-	EXPRESSION TAG	UNP O08807
C	23	SER	-	EXPRESSION TAG	UNP O08807
C	24	HIS	-	EXPRESSION TAG	UNP O08807
C	25	HIS	-	EXPRESSION TAG	UNP O08807
C	26	HIS	-	EXPRESSION TAG	UNP O08807

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Chain	Residue	Modelled	Actual	Comment	Reference
C	27	HIS	-	EXPRESSION TAG	UNP O08807
C	28	HIS	-	EXPRESSION TAG	UNP O08807
C	29	HIS	-	EXPRESSION TAG	UNP O08807
C	30	SER	-	EXPRESSION TAG	UNP O08807
C	31	SER	-	EXPRESSION TAG	UNP O08807
C	32	GLY	-	EXPRESSION TAG	UNP O08807
C	33	LEU	-	EXPRESSION TAG	UNP O08807
C	34	VAL	-	EXPRESSION TAG	UNP O08807
C	35	PRO	-	EXPRESSION TAG	UNP O08807
C	36	ARG	-	EXPRESSION TAG	UNP O08807
C	37	GLY	-	EXPRESSION TAG	UNP O08807
C	38	SER	-	EXPRESSION TAG	UNP O08807
C	39	HIS	-	EXPRESSION TAG	UNP O08807
C	40	MET	-	EXPRESSION TAG	UNP O08807
C	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
D	20	MET	-	EXPRESSION TAG	UNP O08807
D	21	GLY	-	EXPRESSION TAG	UNP O08807
D	22	SER	-	EXPRESSION TAG	UNP O08807
D	23	SER	-	EXPRESSION TAG	UNP O08807
D	24	HIS	-	EXPRESSION TAG	UNP O08807
D	25	HIS	-	EXPRESSION TAG	UNP O08807
D	26	HIS	-	EXPRESSION TAG	UNP O08807
D	27	HIS	-	EXPRESSION TAG	UNP O08807
D	28	HIS	-	EXPRESSION TAG	UNP O08807
D	29	HIS	-	EXPRESSION TAG	UNP O08807
D	30	SER	-	EXPRESSION TAG	UNP O08807
D	31	SER	-	EXPRESSION TAG	UNP O08807
D	32	GLY	-	EXPRESSION TAG	UNP O08807
D	33	LEU	-	EXPRESSION TAG	UNP O08807
D	34	VAL	-	EXPRESSION TAG	UNP O08807
D	35	PRO	-	EXPRESSION TAG	UNP O08807
D	36	ARG	-	EXPRESSION TAG	UNP O08807
D	37	GLY	-	EXPRESSION TAG	UNP O08807
D	38	SER	-	EXPRESSION TAG	UNP O08807
D	39	HIS	-	EXPRESSION TAG	UNP O08807
D	40	MET	-	EXPRESSION TAG	UNP O08807
D	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
E	20	MET	-	EXPRESSION TAG	UNP O08807
E	21	GLY	-	EXPRESSION TAG	UNP O08807
E	22	SER	-	EXPRESSION TAG	UNP O08807
E	23	SER	-	EXPRESSION TAG	UNP O08807
E	24	HIS	-	EXPRESSION TAG	UNP O08807

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Chain	Residue	Modelled	Actual	Comment	Reference
E	25	HIS	-	EXPRESSION TAG	UNP O08807
E	26	HIS	-	EXPRESSION TAG	UNP O08807
E	27	HIS	-	EXPRESSION TAG	UNP O08807
E	28	HIS	-	EXPRESSION TAG	UNP O08807
E	29	HIS	-	EXPRESSION TAG	UNP O08807
E	30	SER	-	EXPRESSION TAG	UNP O08807
E	31	SER	-	EXPRESSION TAG	UNP O08807
E	32	GLY	-	EXPRESSION TAG	UNP O08807
E	33	LEU	-	EXPRESSION TAG	UNP O08807
E	34	VAL	-	EXPRESSION TAG	UNP O08807
E	35	PRO	-	EXPRESSION TAG	UNP O08807
E	36	ARG	-	EXPRESSION TAG	UNP O08807
E	37	GLY	-	EXPRESSION TAG	UNP O08807
E	38	SER	-	EXPRESSION TAG	UNP O08807
E	39	HIS	-	EXPRESSION TAG	UNP O08807
E	40	MET	-	EXPRESSION TAG	UNP O08807
E	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
F	20	MET	-	EXPRESSION TAG	UNP O08807
F	21	GLY	-	EXPRESSION TAG	UNP O08807
F	22	SER	-	EXPRESSION TAG	UNP O08807
F	23	SER	-	EXPRESSION TAG	UNP O08807
F	24	HIS	-	EXPRESSION TAG	UNP O08807
F	25	HIS	-	EXPRESSION TAG	UNP O08807
F	26	HIS	-	EXPRESSION TAG	UNP O08807
F	27	HIS	-	EXPRESSION TAG	UNP O08807
F	28	HIS	-	EXPRESSION TAG	UNP O08807
F	29	HIS	-	EXPRESSION TAG	UNP O08807
F	30	SER	-	EXPRESSION TAG	UNP O08807
F	31	SER	-	EXPRESSION TAG	UNP O08807
F	32	GLY	-	EXPRESSION TAG	UNP O08807
F	33	LEU	-	EXPRESSION TAG	UNP O08807
F	34	VAL	-	EXPRESSION TAG	UNP O08807
F	35	PRO	-	EXPRESSION TAG	UNP O08807
F	36	ARG	-	EXPRESSION TAG	UNP O08807
F	37	GLY	-	EXPRESSION TAG	UNP O08807
F	38	SER	-	EXPRESSION TAG	UNP O08807
F	39	HIS	-	EXPRESSION TAG	UNP O08807
F	40	MET	-	EXPRESSION TAG	UNP O08807
F	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
G	20	MET	-	EXPRESSION TAG	UNP O08807
G	21	GLY	-	EXPRESSION TAG	UNP O08807
G	22	SER	-	EXPRESSION TAG	UNP O08807

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Chain	Residue	Modelled	Actual	Comment	Reference
G	23	SER	-	EXPRESSION TAG	UNP O08807
G	24	HIS	-	EXPRESSION TAG	UNP O08807
G	25	HIS	-	EXPRESSION TAG	UNP O08807
G	26	HIS	-	EXPRESSION TAG	UNP O08807
G	27	HIS	-	EXPRESSION TAG	UNP O08807
G	28	HIS	-	EXPRESSION TAG	UNP O08807
G	29	HIS	-	EXPRESSION TAG	UNP O08807
G	30	SER	-	EXPRESSION TAG	UNP O08807
G	31	SER	-	EXPRESSION TAG	UNP O08807
G	32	GLY	-	EXPRESSION TAG	UNP O08807
G	33	LEU	-	EXPRESSION TAG	UNP O08807
G	34	VAL	-	EXPRESSION TAG	UNP O08807
G	35	PRO	-	EXPRESSION TAG	UNP O08807
G	36	ARG	-	EXPRESSION TAG	UNP O08807
G	37	GLY	-	EXPRESSION TAG	UNP O08807
G	38	SER	-	EXPRESSION TAG	UNP O08807
G	39	HIS	-	EXPRESSION TAG	UNP O08807
G	40	MET	-	EXPRESSION TAG	UNP O08807
G	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
H	20	MET	-	EXPRESSION TAG	UNP O08807
H	21	GLY	-	EXPRESSION TAG	UNP O08807
H	22	SER	-	EXPRESSION TAG	UNP O08807
H	23	SER	-	EXPRESSION TAG	UNP O08807
H	24	HIS	-	EXPRESSION TAG	UNP O08807
H	25	HIS	-	EXPRESSION TAG	UNP O08807
H	26	HIS	-	EXPRESSION TAG	UNP O08807
H	27	HIS	-	EXPRESSION TAG	UNP O08807
H	28	HIS	-	EXPRESSION TAG	UNP O08807
H	29	HIS	-	EXPRESSION TAG	UNP O08807
H	30	SER	-	EXPRESSION TAG	UNP O08807
H	31	SER	-	EXPRESSION TAG	UNP O08807
H	32	GLY	-	EXPRESSION TAG	UNP O08807
H	33	LEU	-	EXPRESSION TAG	UNP O08807
H	34	VAL	-	EXPRESSION TAG	UNP O08807
H	35	PRO	-	EXPRESSION TAG	UNP O08807
H	36	ARG	-	EXPRESSION TAG	UNP O08807
H	37	GLY	-	EXPRESSION TAG	UNP O08807
H	38	SER	-	EXPRESSION TAG	UNP O08807
H	39	HIS	-	EXPRESSION TAG	UNP O08807
H	40	MET	-	EXPRESSION TAG	UNP O08807
H	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
I	20	MET	-	EXPRESSION TAG	UNP O08807

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Chain	Residue	Modelled	Actual	Comment	Reference
I	21	GLY	-	EXPRESSION TAG	UNP O08807
I	22	SER	-	EXPRESSION TAG	UNP O08807
I	23	SER	-	EXPRESSION TAG	UNP O08807
I	24	HIS	-	EXPRESSION TAG	UNP O08807
I	25	HIS	-	EXPRESSION TAG	UNP O08807
I	26	HIS	-	EXPRESSION TAG	UNP O08807
I	27	HIS	-	EXPRESSION TAG	UNP O08807
I	28	HIS	-	EXPRESSION TAG	UNP O08807
I	29	HIS	-	EXPRESSION TAG	UNP O08807
I	30	SER	-	EXPRESSION TAG	UNP O08807
I	31	SER	-	EXPRESSION TAG	UNP O08807
I	32	GLY	-	EXPRESSION TAG	UNP O08807
I	33	LEU	-	EXPRESSION TAG	UNP O08807
I	34	VAL	-	EXPRESSION TAG	UNP O08807
I	35	PRO	-	EXPRESSION TAG	UNP O08807
I	36	ARG	-	EXPRESSION TAG	UNP O08807
I	37	GLY	-	EXPRESSION TAG	UNP O08807
I	38	SER	-	EXPRESSION TAG	UNP O08807
I	39	HIS	-	EXPRESSION TAG	UNP O08807
I	40	MET	-	EXPRESSION TAG	UNP O08807
I	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807
J	20	MET	-	EXPRESSION TAG	UNP O08807
J	21	GLY	-	EXPRESSION TAG	UNP O08807
J	22	SER	-	EXPRESSION TAG	UNP O08807
J	23	SER	-	EXPRESSION TAG	UNP O08807
J	24	HIS	-	EXPRESSION TAG	UNP O08807
J	25	HIS	-	EXPRESSION TAG	UNP O08807
J	26	HIS	-	EXPRESSION TAG	UNP O08807
J	27	HIS	-	EXPRESSION TAG	UNP O08807
J	28	HIS	-	EXPRESSION TAG	UNP O08807
J	29	HIS	-	EXPRESSION TAG	UNP O08807
J	30	SER	-	EXPRESSION TAG	UNP O08807
J	31	SER	-	EXPRESSION TAG	UNP O08807
J	32	GLY	-	EXPRESSION TAG	UNP O08807
J	33	LEU	-	EXPRESSION TAG	UNP O08807
J	34	VAL	-	EXPRESSION TAG	UNP O08807
J	35	PRO	-	EXPRESSION TAG	UNP O08807
J	36	ARG	-	EXPRESSION TAG	UNP O08807
J	37	GLY	-	EXPRESSION TAG	UNP O08807
J	38	SER	-	EXPRESSION TAG	UNP O08807
J	39	HIS	-	EXPRESSION TAG	UNP O08807
J	40	MET	-	EXPRESSION TAG	UNP O08807

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| Chain	Residue	Modelled	Actual	Comment	Reference
J	54	ALA	CYS	ENGINEERED MUTATION	UNP O08807

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.
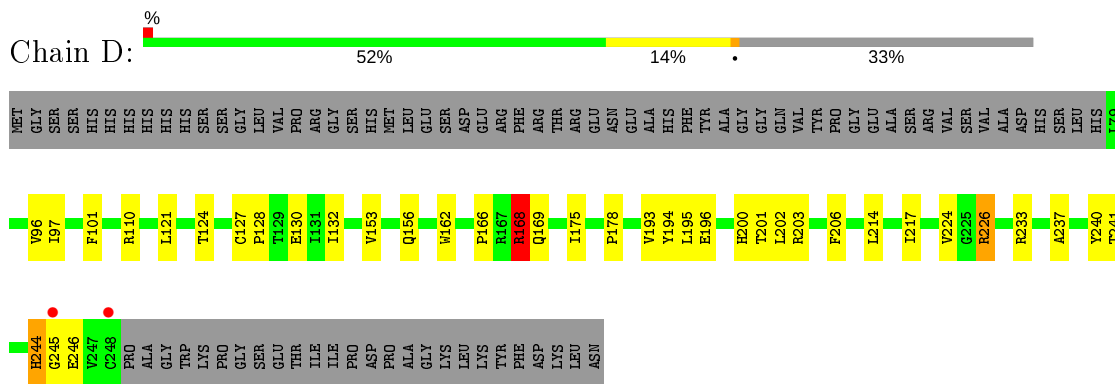
- Molecule 1: Peroxiredoxin-4
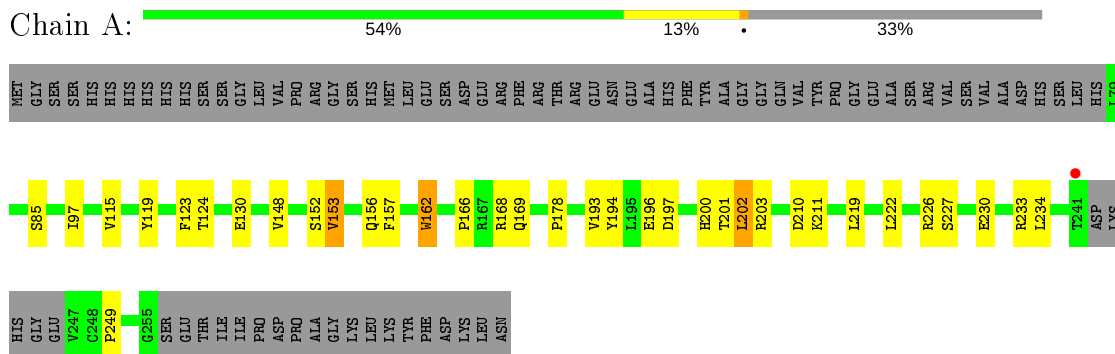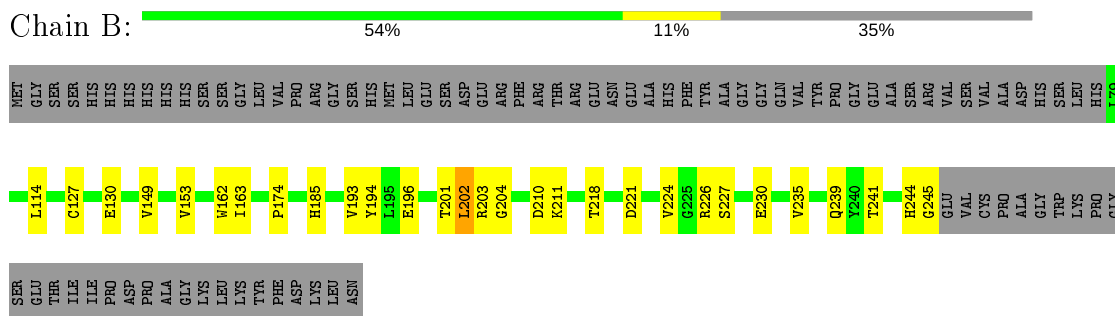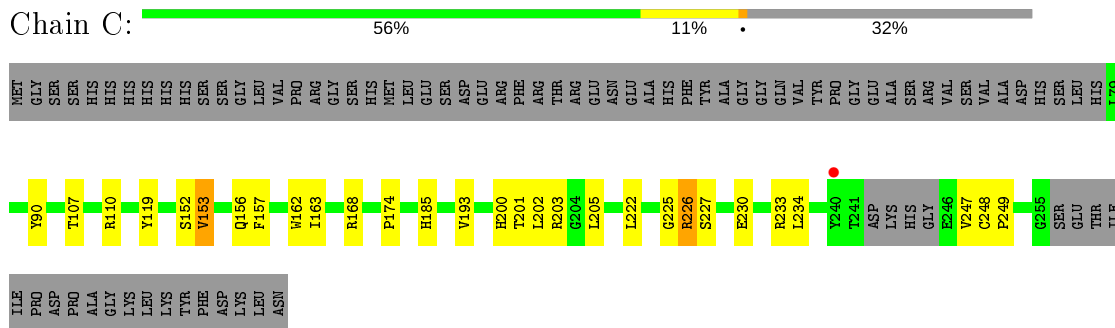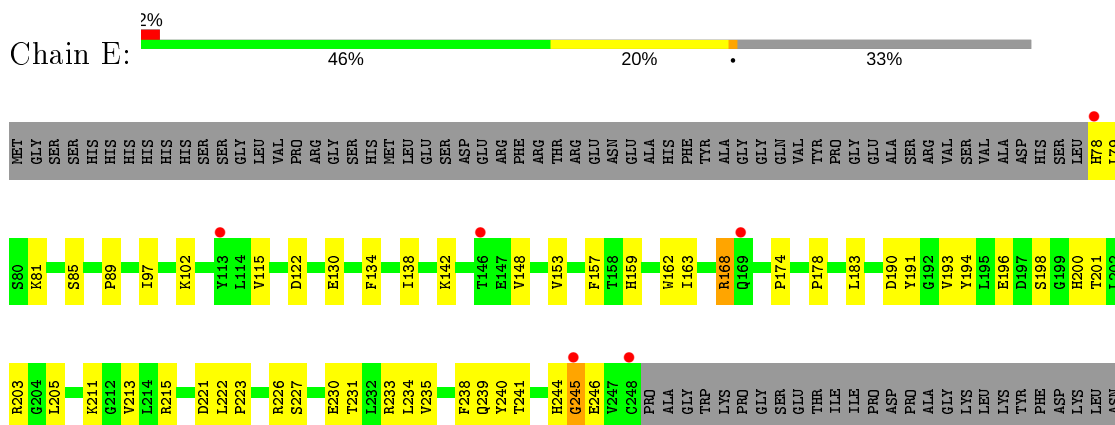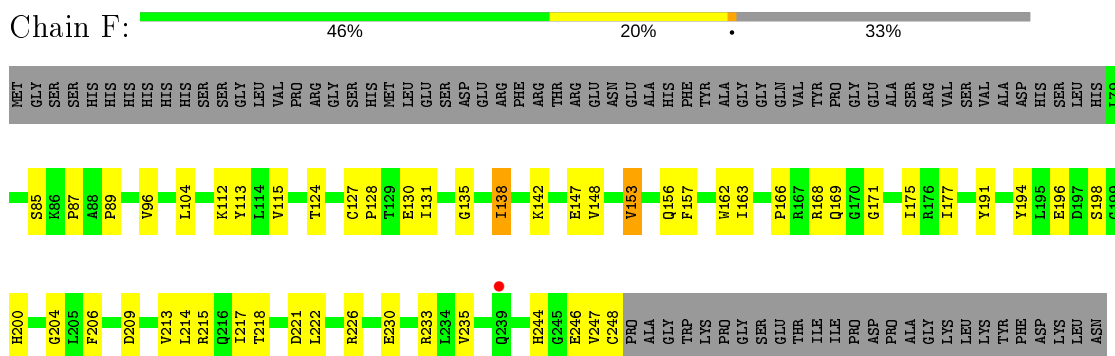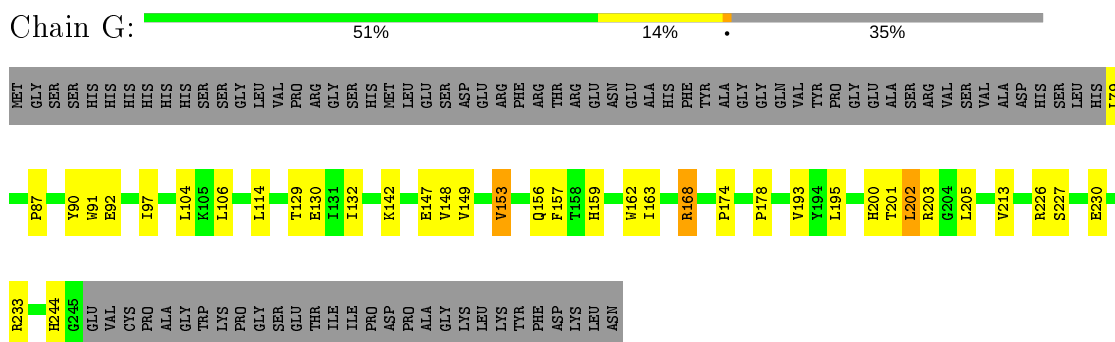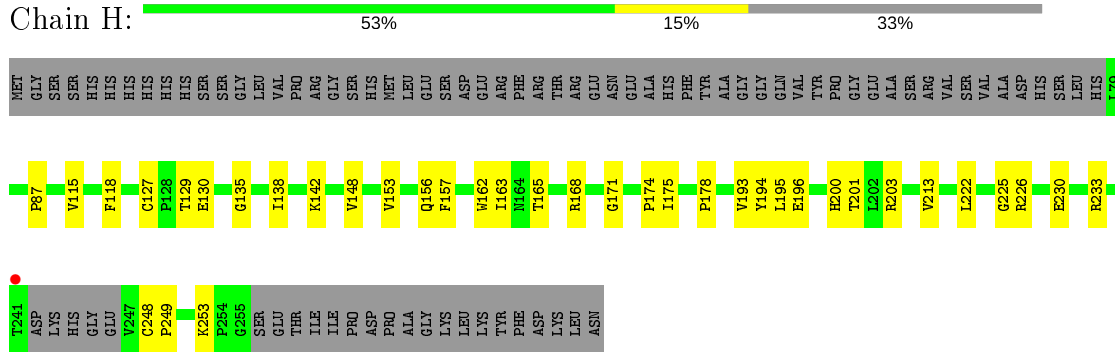

- Molecule 1: Peroxiredoxin-4

- Molecule 1: Peroxiredoxin-4

- Molecule 1: Peroxiredoxin-4

Chain D:

• Molecule 1: Peroxiredoxin-4

Chain E:

• Molecule 1: Peroxiredoxin-4

Chain F:

• Molecule 1: Peroxiredoxin-4

Chain G:

• Molecule 1: Peroxiredoxin-4

Chain H:

53%   15%   33%

• Molecule 1: Peroxiredoxin-4

Chain I:

48%   17%   35%

• Molecule 1: Peroxiredoxin-4

Chain J:

49%   16%   35%
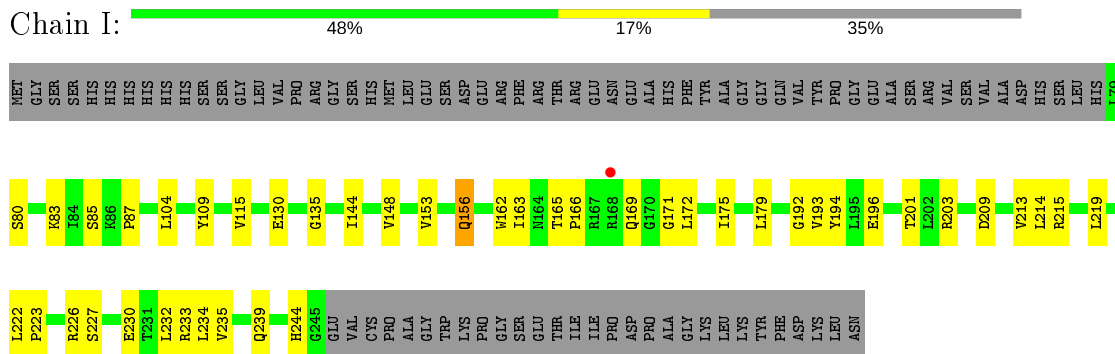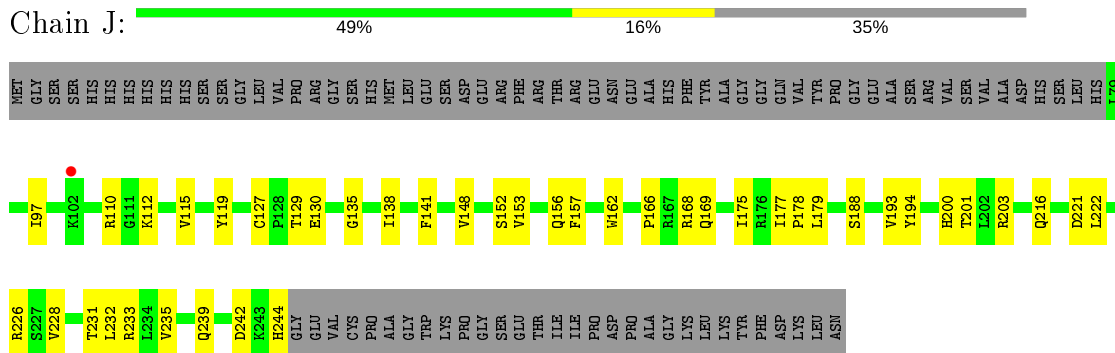
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.47Å 118.66Å 255.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.11 – 3.30 43.73 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.4 (43.11-3.30) 94.4 (43.73-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.203 , 0.255 0.188 , 0.245	Depositor DCC
R_{free} test set	1936 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.0	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13617	wwPDB-VP
Average B, all atoms (Å^2)	67.0	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 28.39 % 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 1.8583e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (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	0.67	0/1411	0.83	2/1915 (0.1%)
1	B	0.67	0/1377	0.87	1/1867 (0.1%)
1	C	0.64	0/1420	0.88	3/1927 (0.2%)
1	D	0.64	0/1399	0.88	2/1897 (0.1%)
1	E	0.73	0/1410	0.90	2/1912 (0.1%)
1	F	0.71	0/1399	0.89	0/1897
1	G	0.64	0/1377	0.89	4/1867 (0.2%)
1	H	0.65	0/1411	0.85	0/1915
1	I	0.68	0/1377	0.84	1/1867 (0.1%)
1	J	0.68	0/1373	0.84	1/1862 (0.1%)
All	All	0.67	0/13954	0.87	16/18926 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	ARG	CA-CB-CG	8.33	131.72	113.40
1	E	245	GLY	N-CA-C	7.99	133.07	113.10
1	D	168	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	202	LEU	CA-CB-CG	7.16	131.77	115.30
1	C	226	ARG	NE-CZ-NH1	6.92	123.76	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	1376	0	1371	23	0
1	B	1344	0	1337	17	0
1	C	1385	0	1376	25	0
1	D	1366	0	1356	30	0
1	E	1376	0	1363	37	0
1	F	1366	0	1356	35	0
1	G	1344	0	1337	24	0
1	H	1376	0	1371	24	0
1	I	1344	0	1338	28	0
1	J	1340	0	1335	25	0
All	All	13617	0	13540	238	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 9.

The worst 5 of 238 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:168:ARG:HG2	1:D:168:ARG:HH11	1.28	0.94
1:F:138:ILE:HD11	1:F:142:LYS:HE3	1.61	0.81
1:H:118:PHE:O	1:H:226:ARG:NH2	2.13	0.80
1:A:130:GLU:OE1	1:A:203:ARG:NH1	2.15	0.78
1:I:166:PRO:HG2	1:I:169:GLN:HG3	1.67	0.77

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	168/255 (66%)	163 (97%)	5 (3%)	0	100	100
1	B	165/255 (65%)	160 (97%)	5 (3%)	0	100	100

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	169/255 (66%)	164 (97%)	5 (3%)	0	100	100
1	D	168/255 (66%)	163 (97%)	5 (3%)	0	100	100
1	E	169/255 (66%)	163 (96%)	6 (4%)	0	100	100
1	F	168/255 (66%)	162 (96%)	6 (4%)	0	100	100
1	G	165/255 (65%)	160 (97%)	5 (3%)	0	100	100
1	H	168/255 (66%)	164 (98%)	4 (2%)	0	100	100
1	I	165/255 (65%)	160 (97%)	5 (3%)	0	100	100
1	J	164/255 (64%)	158 (96%)	6 (4%)	0	100	100
All	All	1669/2550 (66%)	1617 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	150/220 (68%)	148 (99%)	2 (1%)	69	82
1	B	147/220 (67%)	144 (98%)	3 (2%)	55	76
1	C	151/220 (69%)	148 (98%)	3 (2%)	55	76
1	D	150/220 (68%)	146 (97%)	4 (3%)	44	71
1	E	151/220 (69%)	145 (96%)	6 (4%)	31	61
1	F	150/220 (68%)	145 (97%)	5 (3%)	38	66
1	G	147/220 (67%)	142 (97%)	5 (3%)	37	65
1	H	150/220 (68%)	147 (98%)	3 (2%)	55	76
1	I	147/220 (67%)	143 (97%)	4 (3%)	44	71
1	J	147/220 (67%)	142 (97%)	5 (3%)	37	65
All	All	1490/2200 (68%)	1450 (97%)	40 (3%)	44	71

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	138	ILE
1	F	248	CYS
1	J	153	VAL
1	F	244	HIS
1	G	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	159	HIS
1	D	244	HIS
1	F	236	GLN
1	I	156	GLN
1	J	159	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 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	172/255 (67%)	-0.25	1 (0%)	89	90	44, 62, 89, 109	0
1	B	167/255 (65%)	-0.30	0	100	100	42, 60, 86, 106	0
1	C	173/255 (67%)	-0.21	1 (0%)	89	90	43, 63, 89, 112	0
1	D	170/255 (66%)	-0.19	2 (1%)	79	78	46, 63, 92, 116	0
1	E	171/255 (67%)	-0.04	6 (3%)	44	42	46, 65, 108, 133	0
1	F	170/255 (66%)	-0.04	1 (0%)	89	90	47, 67, 104, 144	0
1	G	167/255 (65%)	-0.39	0	100	100	44, 61, 90, 112	0
1	H	172/255 (67%)	-0.28	1 (0%)	89	90	46, 65, 90, 109	0
1	I	167/255 (65%)	-0.17	1 (0%)	89	90	49, 66, 96, 110	0
1	J	166/255 (65%)	-0.18	1 (0%)	89	90	49, 66, 94, 116	0
All	All	1695/2550 (66%)	-0.20	14 (0%)	86	86	42, 64, 95, 144	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	113	TYR	3.5
1	E	78	HIS	3.3
1	A	241	THR	2.9
1	H	241	THR	2.9
1	E	146	THR	2.7

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.