



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:19 PM GMT

PDB ID : 3TKR  
Title : Crystal structure of full-length human peroxiredoxin 4 with T118E mutation  
Authors : Wang, X.; Wang, L.; Wang, X.; Sun, F.; Wang, C.-C.  
Deposited on : 2011-08-28  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

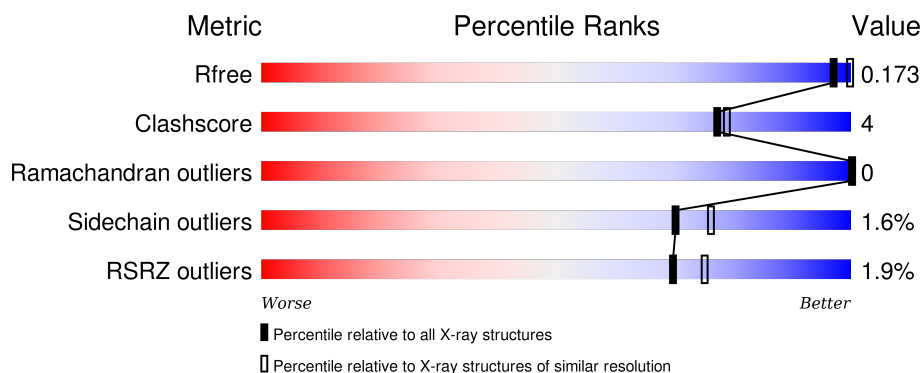
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 74%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>74%</span> <span>6% •</span> <span>20%</span> </div> </div>
1	B	246	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 76%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>76%</span> <span>•</span> <span>20%</span> </div> </div>
1	C	246	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">2%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 72%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>72%</span> <span>7% •</span> <span>20%</span> </div> </div>
1	D	246	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">2%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 74%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>74%</span> <span>5%</span> <span>20%</span> </div> </div>
1	E	246	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -5px; left: 0;">2%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 72%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>72%</span> <span>7%</span> <span>20%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	246	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>72%</div><div>7%</div><div>20%</div></div></div>
1	G	246	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>73%</div><div>7%</div><div>21%</div></div></div>
1	H	246	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>74%</div><div>6%</div><div>20%</div></div></div>
1	I	246	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>74%</div><div>5%</div><div>20%</div></div></div>
1	J	246	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>73%</div><div>7%</div><div>20%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18082 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	197	Total	C	N	O	S	0	7	0
			1624	1054	269	298	3			
1	I	197	Total	C	N	O	S	0	2	0
			1593	1031	264	295	3			
1	G	195	Total	C	N	O	S	0	0	0
			1564	1012	259	290	3			
1	C	197	Total	C	N	O	S	0	6	0
			1615	1047	269	296	3			
1	F	197	Total	C	N	O	S	0	3	0
			1597	1035	264	295	3			
1	D	197	Total	C	N	O	S	0	1	0
			1588	1028	264	293	3			
1	B	197	Total	C	N	O	S	0	2	0
			1593	1033	264	293	3			
1	H	197	Total	C	N	O	S	0	2	0
			1592	1031	263	295	3			
1	E	197	Total	C	N	O	S	0	1	0
			1587	1029	263	292	3			
1	J	197	Total	C	N	O	S	0	2	0
			1594	1032	263	296	3			

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q13162
A	-10	ARG	-	EXPRESSION TAG	UNP Q13162
A	-9	GLY	-	EXPRESSION TAG	UNP Q13162
A	-8	SER	-	EXPRESSION TAG	UNP Q13162
A	-7	HIS	-	EXPRESSION TAG	UNP Q13162
A	-6	HIS	-	EXPRESSION TAG	UNP Q13162
A	-5	HIS	-	EXPRESSION TAG	UNP Q13162
A	-4	HIS	-	EXPRESSION TAG	UNP Q13162
A	-3	HIS	-	EXPRESSION TAG	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	EXPRESSION TAG	UNP Q13162
A	-1	GLY	-	EXPRESSION TAG	UNP Q13162
A	0	SER	-	EXPRESSION TAG	UNP Q13162
A	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
I	-11	MET	-	EXPRESSION TAG	UNP Q13162
I	-10	ARG	-	EXPRESSION TAG	UNP Q13162
I	-9	GLY	-	EXPRESSION TAG	UNP Q13162
I	-8	SER	-	EXPRESSION TAG	UNP Q13162
I	-7	HIS	-	EXPRESSION TAG	UNP Q13162
I	-6	HIS	-	EXPRESSION TAG	UNP Q13162
I	-5	HIS	-	EXPRESSION TAG	UNP Q13162
I	-4	HIS	-	EXPRESSION TAG	UNP Q13162
I	-3	HIS	-	EXPRESSION TAG	UNP Q13162
I	-2	HIS	-	EXPRESSION TAG	UNP Q13162
I	-1	GLY	-	EXPRESSION TAG	UNP Q13162
I	0	SER	-	EXPRESSION TAG	UNP Q13162
I	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
G	-11	MET	-	EXPRESSION TAG	UNP Q13162
G	-10	ARG	-	EXPRESSION TAG	UNP Q13162
G	-9	GLY	-	EXPRESSION TAG	UNP Q13162
G	-8	SER	-	EXPRESSION TAG	UNP Q13162
G	-7	HIS	-	EXPRESSION TAG	UNP Q13162
G	-6	HIS	-	EXPRESSION TAG	UNP Q13162
G	-5	HIS	-	EXPRESSION TAG	UNP Q13162
G	-4	HIS	-	EXPRESSION TAG	UNP Q13162
G	-3	HIS	-	EXPRESSION TAG	UNP Q13162
G	-2	HIS	-	EXPRESSION TAG	UNP Q13162
G	-1	GLY	-	EXPRESSION TAG	UNP Q13162
G	0	SER	-	EXPRESSION TAG	UNP Q13162
G	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
C	-11	MET	-	EXPRESSION TAG	UNP Q13162
C	-10	ARG	-	EXPRESSION TAG	UNP Q13162
C	-9	GLY	-	EXPRESSION TAG	UNP Q13162
C	-8	SER	-	EXPRESSION TAG	UNP Q13162
C	-7	HIS	-	EXPRESSION TAG	UNP Q13162
C	-6	HIS	-	EXPRESSION TAG	UNP Q13162
C	-5	HIS	-	EXPRESSION TAG	UNP Q13162
C	-4	HIS	-	EXPRESSION TAG	UNP Q13162
C	-3	HIS	-	EXPRESSION TAG	UNP Q13162
C	-2	HIS	-	EXPRESSION TAG	UNP Q13162
C	-1	GLY	-	EXPRESSION TAG	UNP Q13162
C	0	SER	-	EXPRESSION TAG	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
C	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
F	-11	MET	-	EXPRESSION TAG	UNP Q13162
F	-10	ARG	-	EXPRESSION TAG	UNP Q13162
F	-9	GLY	-	EXPRESSION TAG	UNP Q13162
F	-8	SER	-	EXPRESSION TAG	UNP Q13162
F	-7	HIS	-	EXPRESSION TAG	UNP Q13162
F	-6	HIS	-	EXPRESSION TAG	UNP Q13162
F	-5	HIS	-	EXPRESSION TAG	UNP Q13162
F	-4	HIS	-	EXPRESSION TAG	UNP Q13162
F	-3	HIS	-	EXPRESSION TAG	UNP Q13162
F	-2	HIS	-	EXPRESSION TAG	UNP Q13162
F	-1	GLY	-	EXPRESSION TAG	UNP Q13162
F	0	SER	-	EXPRESSION TAG	UNP Q13162
F	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
D	-11	MET	-	EXPRESSION TAG	UNP Q13162
D	-10	ARG	-	EXPRESSION TAG	UNP Q13162
D	-9	GLY	-	EXPRESSION TAG	UNP Q13162
D	-8	SER	-	EXPRESSION TAG	UNP Q13162
D	-7	HIS	-	EXPRESSION TAG	UNP Q13162
D	-6	HIS	-	EXPRESSION TAG	UNP Q13162
D	-5	HIS	-	EXPRESSION TAG	UNP Q13162
D	-4	HIS	-	EXPRESSION TAG	UNP Q13162
D	-3	HIS	-	EXPRESSION TAG	UNP Q13162
D	-2	HIS	-	EXPRESSION TAG	UNP Q13162
D	-1	GLY	-	EXPRESSION TAG	UNP Q13162
D	0	SER	-	EXPRESSION TAG	UNP Q13162
D	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
B	-11	MET	-	EXPRESSION TAG	UNP Q13162
B	-10	ARG	-	EXPRESSION TAG	UNP Q13162
B	-9	GLY	-	EXPRESSION TAG	UNP Q13162
B	-8	SER	-	EXPRESSION TAG	UNP Q13162
B	-7	HIS	-	EXPRESSION TAG	UNP Q13162
B	-6	HIS	-	EXPRESSION TAG	UNP Q13162
B	-5	HIS	-	EXPRESSION TAG	UNP Q13162
B	-4	HIS	-	EXPRESSION TAG	UNP Q13162
B	-3	HIS	-	EXPRESSION TAG	UNP Q13162
B	-2	HIS	-	EXPRESSION TAG	UNP Q13162
B	-1	GLY	-	EXPRESSION TAG	UNP Q13162
B	0	SER	-	EXPRESSION TAG	UNP Q13162
B	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
H	-11	MET	-	EXPRESSION TAG	UNP Q13162
H	-10	ARG	-	EXPRESSION TAG	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	GLY	-	EXPRESSION TAG	UNP Q13162
H	-8	SER	-	EXPRESSION TAG	UNP Q13162
H	-7	HIS	-	EXPRESSION TAG	UNP Q13162
H	-6	HIS	-	EXPRESSION TAG	UNP Q13162
H	-5	HIS	-	EXPRESSION TAG	UNP Q13162
H	-4	HIS	-	EXPRESSION TAG	UNP Q13162
H	-3	HIS	-	EXPRESSION TAG	UNP Q13162
H	-2	HIS	-	EXPRESSION TAG	UNP Q13162
H	-1	GLY	-	EXPRESSION TAG	UNP Q13162
H	0	SER	-	EXPRESSION TAG	UNP Q13162
H	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
E	-11	MET	-	EXPRESSION TAG	UNP Q13162
E	-10	ARG	-	EXPRESSION TAG	UNP Q13162
E	-9	GLY	-	EXPRESSION TAG	UNP Q13162
E	-8	SER	-	EXPRESSION TAG	UNP Q13162
E	-7	HIS	-	EXPRESSION TAG	UNP Q13162
E	-6	HIS	-	EXPRESSION TAG	UNP Q13162
E	-5	HIS	-	EXPRESSION TAG	UNP Q13162
E	-4	HIS	-	EXPRESSION TAG	UNP Q13162
E	-3	HIS	-	EXPRESSION TAG	UNP Q13162
E	-2	HIS	-	EXPRESSION TAG	UNP Q13162
E	-1	GLY	-	EXPRESSION TAG	UNP Q13162
E	0	SER	-	EXPRESSION TAG	UNP Q13162
E	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162
J	-11	MET	-	EXPRESSION TAG	UNP Q13162
J	-10	ARG	-	EXPRESSION TAG	UNP Q13162
J	-9	GLY	-	EXPRESSION TAG	UNP Q13162
J	-8	SER	-	EXPRESSION TAG	UNP Q13162
J	-7	HIS	-	EXPRESSION TAG	UNP Q13162
J	-6	HIS	-	EXPRESSION TAG	UNP Q13162
J	-5	HIS	-	EXPRESSION TAG	UNP Q13162
J	-4	HIS	-	EXPRESSION TAG	UNP Q13162
J	-3	HIS	-	EXPRESSION TAG	UNP Q13162
J	-2	HIS	-	EXPRESSION TAG	UNP Q13162
J	-1	GLY	-	EXPRESSION TAG	UNP Q13162
J	0	SER	-	EXPRESSION TAG	UNP Q13162
J	118	GLU	THR	ENGINEERED MUTATION	UNP Q13162

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	232	Total O 232 232	0	0

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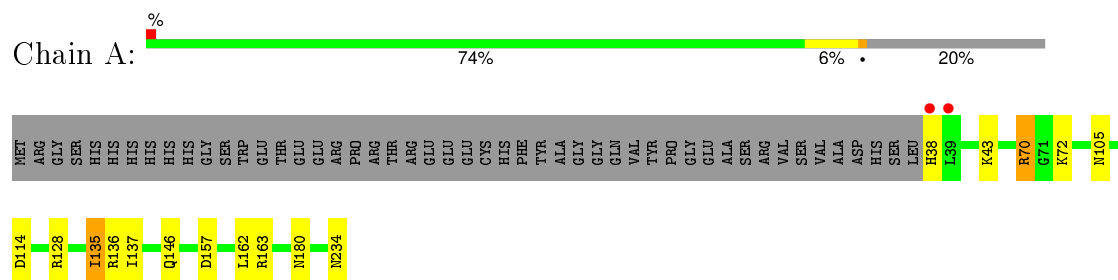
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	216	Total 216	O 216	0	0
2	G	226	Total 226	O 226	0	0
2	C	228	Total 228	O 228	0	0
2	F	215	Total 215	O 215	0	0
2	D	220	Total 220	O 220	0	0
2	B	226	Total 226	O 226	0	0
2	H	233	Total 233	O 233	0	0
2	E	176	Total 176	O 176	0	0
2	J	163	Total 163	O 163	0	0



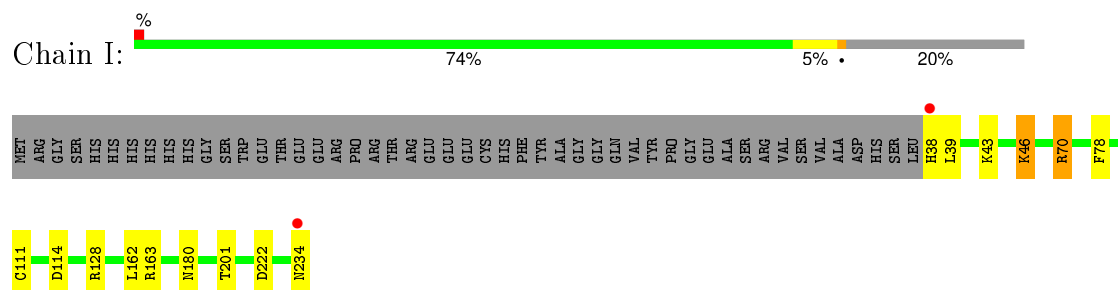
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

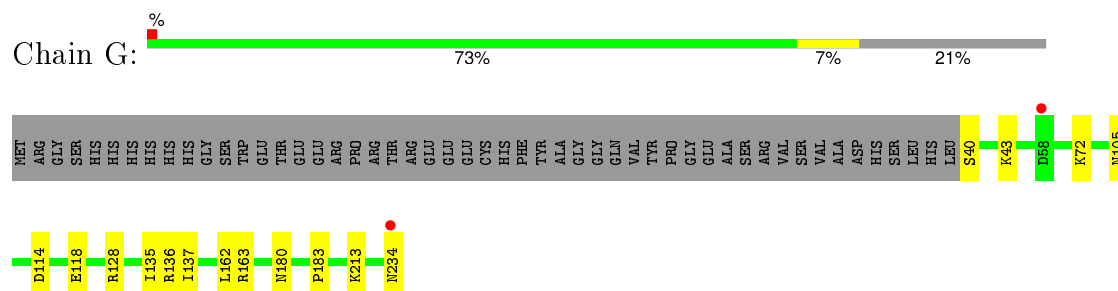
- Molecule 1: Peroxiredoxin-4



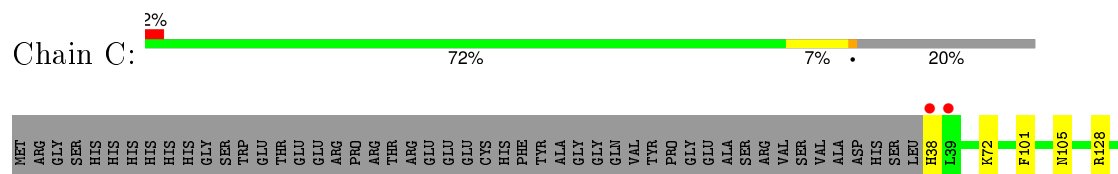
- Molecule 1: Peroxiredoxin-4

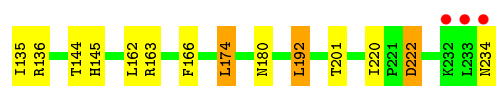


- Molecule 1: Peroxiredoxin-4

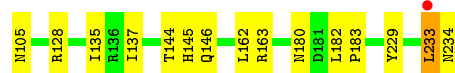
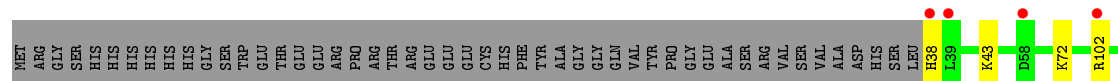


- Molecule 1: Peroxiredoxin-4

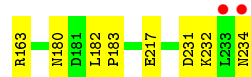
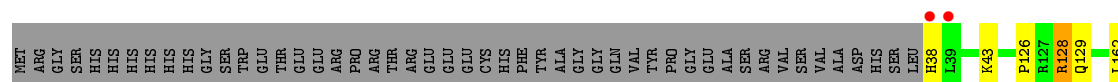
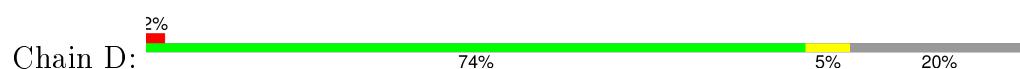




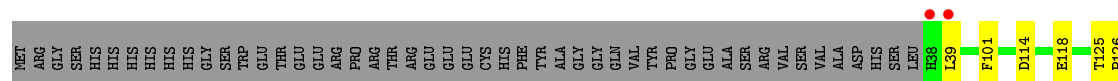
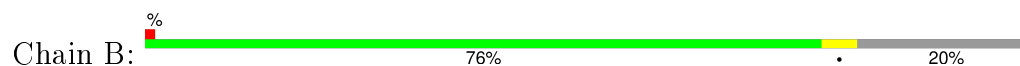
• Molecule 1: Peroxiredoxin-4



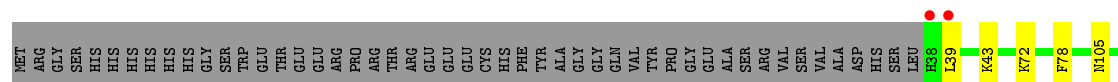
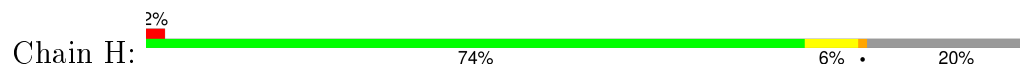
• Molecule 1: Peroxiredoxin-4



• Molecule 1: Peroxiredoxin-4

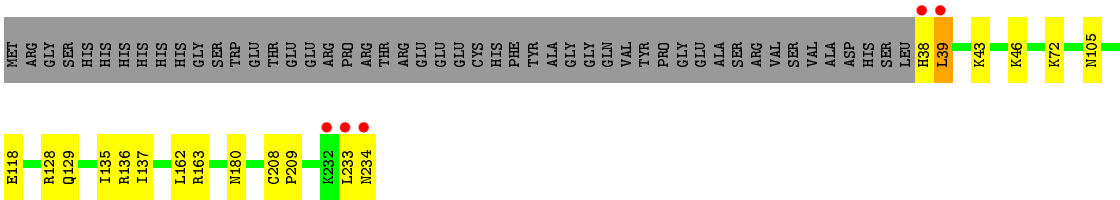


• Molecule 1: Peroxiredoxin-4

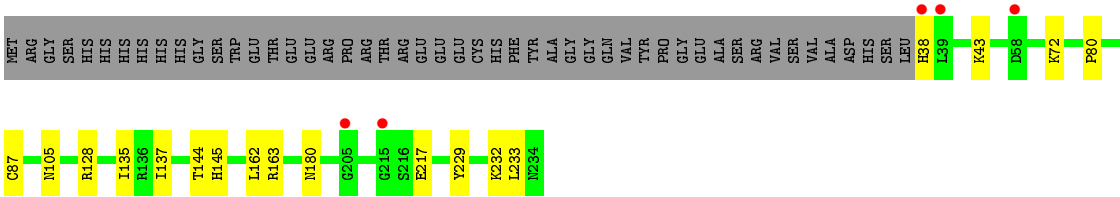


• Molecule 1: Peroxiredoxin-4





● Molecule 1: Peroxiredoxin-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.71Å 139.12Å 178.97Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	46.00 – 2.10 49.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.00-2.10) 98.0 (49.78-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.150 , 0.178 0.145 , 0.173	Depositor DCC
$R_{free}$ test set	8537 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 171197 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 34.49 % 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 6.7729e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/1687	0.53	0/2285
1	B	0.37	0/1641	0.52	0/2226
1	C	0.38	0/1675	0.54	0/2271
1	D	0.37	0/1633	0.52	0/2214
1	E	0.35	0/1632	0.51	0/2213
1	F	0.42	0/1648	0.55	1/2233 (0.0%)
1	G	0.38	0/1605	0.52	0/2176
1	H	0.40	0/1640	0.56	0/2224
1	I	0.39	0/1641	0.52	0/2226
1	J	0.34	0/1642	0.50	0/2226
All	All	0.38	0/16444	0.53	1/22294 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	102	ARG	NE-CZ-NH1	-8.26	116.17	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	1624	0	1631	23	0
1	B	1593	0	1587	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1615	0	1621	15	0
1	D	1588	0	1576	14	0
1	E	1587	0	1579	12	0
1	F	1597	0	1592	14	0
1	G	1564	0	1550	13	0
1	H	1592	0	1581	16	0
1	I	1593	0	1580	21	0
1	J	1594	0	1580	10	0
2	A	232	0	0	4	0
2	B	226	0	0	1	0
2	C	228	0	0	4	0
2	D	220	0	0	2	0
2	E	176	0	0	2	0
2	F	215	0	0	1	0
2	G	226	0	0	2	0
2	H	233	0	0	4	0
2	I	216	0	0	3	0
2	J	163	0	0	0	0
All	All	18082	0	15877	119	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 4.

All (119) 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:128:ARG:HG2	1:D:128:ARG:HH11	1.32	0.95
1:I:39:LEU:HB3	2:I:1749:HOH:O	1.69	0.93
1:G:43:LYS:HE3	1:C:38:HIS:HB2	1.50	0.92
1:H:201[B]:THR:HG23	2:H:454:HOH:O	1.69	0.90
1:A:43:LYS:HE3	1:I:38:HIS:HB2	1.52	0.90
1:H:128:ARG:HH12	1:H:129:GLN:HE21	1.20	0.87
1:E:43:LYS:HE3	1:J:38:HIS:HB2	1.57	0.86
1:F:38:HIS:HB2	1:D:43:LYS:HE2	1.57	0.84
1:I:128:ARG:HH11	1:I:128:ARG:HG3	1.46	0.80
1:H:128:ARG:NH1	1:H:129:GLN:HE21	1.79	0.79
1:I:201:THR:HG23	2:I:271:HOH:O	1.83	0.77
1:H:161:THR:HG23	1:H:162:LEU:O	1.84	0.76
1:D:128:ARG:CG	1:D:128:ARG:HH11	1.99	0.75
1:G:234:ASN:HB2	1:C:128:ARG:HG2	1.74	0.69
1:H:78:PHE:HB3	1:H:161:THR:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201[B]:THR:HG23	2:C:862:HOH:O	1.96	0.65
1:I:128:ARG:NH1	1:I:128:ARG:HG3	2.11	0.64
1:C:128:ARG:HG3	2:C:261:HOH:O	1.96	0.64
1:D:128:ARG:NH1	1:D:128:ARG:HG2	2.10	0.63
1:H:128:ARG:NE	2:H:1698:HOH:O	2.33	0.61
1:G:234:ASN:CB	1:C:128:ARG:HG2	2.31	0.61
1:D:128:ARG:CZ	2:D:1908:HOH:O	2.48	0.61
1:A:234:ASN:HB2	1:I:128:ARG:HG2	1.83	0.60
1:B:101:PHE:CE2	1:B:192:LEU:HD13	2.35	0.60
1:G:40:SER:N	2:G:2070:HOH:O	2.36	0.58
1:H:161:THR:HB	2:H:235:HOH:O	2.04	0.58
1:C:101:PHE:CE2	1:C:192:LEU:HD13	2.39	0.58
1:H:39:LEU:HD23	1:H:39:LEU:H	1.67	0.57
1:F:233:LEU:HD13	1:F:234:ASN:ND2	2.19	0.57
1:A:136:ARG:NE	2:A:1918:HOH:O	2.38	0.56
1:D:128:ARG:NH2	2:D:1908:HOH:O	2.39	0.56
1:H:39:LEU:N	1:H:39:LEU:HD23	2.23	0.54
1:A:38:HIS:HB2	1:I:43:LYS:HD2	1.90	0.54
1:A:135:ILE:HG13	1:A:137:ILE:H	1.73	0.54
1:A:72[B]:LYS:HG2	1:A:105:ASN:OD1	2.08	0.54
1:A:136:ARG:NH2	2:A:1918:HOH:O	2.40	0.54
1:E:39:LEU:HD12	2:E:2053:HOH:O	2.08	0.54
1:F:146:GLN:HG3	2:F:1889:HOH:O	2.08	0.53
1:A:72[A]:LYS:HG2	1:A:105:ASN:OD1	2.09	0.53
1:F:128:ARG:HG2	1:D:234:ASN:HB2	1.90	0.52
1:E:128:ARG:HH12	1:E:129:GLN:HE21	1.58	0.52
1:A:234:ASN:HB2	1:I:128:ARG:CG	2.40	0.52
1:J:135:ILE:HG13	1:J:137:ILE:H	1.75	0.51
1:A:146[A]:GLN:NE2	2:A:1338:HOH:O	2.43	0.51
1:E:234:ASN:HB2	1:J:128:ARG:HG2	1.92	0.50
1:C:135:ILE:HD12	2:C:371:HOH:O	2.11	0.50
1:E:72:LYS:HG2	1:E:105:ASN:OD1	2.11	0.50
1:A:234:ASN:OXT	1:I:128:ARG:NH1	2.45	0.49
1:H:72:LYS:HG2	1:H:105:ASN:OD1	2.12	0.49
1:F:135:ILE:HG13	1:F:137:ILE:H	1.78	0.49
1:F:38:HIS:CB	1:D:43:LYS:HE2	2.37	0.48
1:F:72[B]:LYS:HG2	1:F:105:ASN:OD1	2.13	0.48
1:J:72:LYS:HG2	1:J:105:ASN:OD1	2.13	0.48
1:J:229:TYR:CZ	1:J:233:LEU:HD22	2.49	0.48
1:A:128[A]:ARG:HD2	1:I:234:ASN:O	2.14	0.48
1:H:128:ARG:HH12	1:H:129:GLN:NE2	2.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:ARG:HB2	1:G:180:ASN:HB2	1.96	0.48
1:C:144:THR:O	1:C:145:HIS:HB2	2.14	0.48
1:G:128:ARG:HE	1:C:234:ASN:C	2.18	0.47
1:A:72[B]:LYS:HB2	1:A:72[B]:LYS:HE2	1.38	0.47
1:C:136[A]:ARG:NH1	2:C:2116:HOH:O	2.48	0.47
1:A:128[A]:ARG:HH11	1:I:234:ASN:C	2.18	0.47
1:B:101:PHE:CZ	1:B:192:LEU:HD13	2.50	0.46
1:G:118:GLU:OE2	1:B:114:ASP:OD1	2.34	0.46
1:C:163:ARG:HB2	1:C:180:ASN:HB2	1.98	0.46
1:I:70:ARG:NH1	2:I:834:HOH:O	2.25	0.45
1:G:72:LYS:HG2	1:G:105:ASN:OD1	2.16	0.45
1:A:114:ASP:OD1	1:H:118:GLU:OE1	2.35	0.45
1:H:43:LYS:NZ	2:H:2163:HOH:O	2.49	0.45
1:F:233:LEU:H	1:F:233:LEU:HD12	1.82	0.45
1:E:136:ARG:NH1	2:E:1798:HOH:O	2.25	0.45
1:I:46:LYS:HD2	1:I:46:LYS:HA	1.85	0.45
1:A:136:ARG:CZ	2:A:1918:HOH:O	2.64	0.44
1:D:182:LEU:N	1:D:183:PRO:CD	2.80	0.44
1:H:163:ARG:HB2	1:H:180:ASN:HB2	1.98	0.44
1:G:135:ILE:HG12	1:G:137:ILE:H	1.82	0.44
1:G:114:ASP:OD1	1:B:118:GLU:OE1	2.36	0.44
1:E:38:HIS:HB2	1:J:43:LYS:HD2	1.99	0.44
1:G:183:PRO:HB2	1:C:201[B]:THR:HG21	2.00	0.44
1:F:72[A]:LYS:HG2	1:F:105:ASN:OD1	2.17	0.44
1:A:70:ARG:HH11	1:A:70:ARG:HG3	1.82	0.44
1:F:144:THR:O	1:F:145:HIS:HB2	2.18	0.43
1:D:163:ARG:HB2	1:D:180:ASN:HB2	1.99	0.43
1:E:135:ILE:HG12	1:E:137:ILE:H	1.83	0.43
1:E:163:ARG:HB2	1:E:180:ASN:HB2	2.00	0.43
1:B:163:ARG:HB2	1:B:180:ASN:HB2	2.01	0.43
1:D:126:PRO:HG2	1:D:129[B]:GLN:NE2	2.34	0.43
1:J:80:PRO:HD2	1:J:87:CYS:SG	2.59	0.43
1:A:163:ARG:HB2	1:A:180:ASN:HB2	2.01	0.42
1:D:128:ARG:CG	1:D:128:ARG:NH1	2.68	0.42
1:C:220:ILE:HG22	1:C:222[B]:ASP:OD1	2.20	0.42
1:J:144:THR:O	1:J:145:HIS:HB2	2.20	0.42
1:G:135:ILE:HG12	1:G:136:ARG:N	2.35	0.42
1:J:163:ARG:HB2	1:J:180:ASN:HB2	2.00	0.42
1:F:43:LYS:HE2	1:D:38:HIS:HB2	2.01	0.42
1:C:166:PHE:HB3	1:C:174[A]:LEU:HD21	2.02	0.42
1:I:43:LYS:HB3	1:I:43:LYS:HE3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:ARG:HB2	1:F:180:ASN:HB2	2.02	0.42
1:H:169:ASP:OD2	1:H:175:ARG:HD3	2.19	0.42
1:G:213:LYS:NZ	2:G:1486:HOH:O	2.46	0.41
1:B:125:THR:HA	1:B:126:PRO:HD3	1.95	0.41
1:I:114:ASP:OD1	1:E:118:GLU:OE1	2.37	0.41
1:I:70:ARG:HB3	1:I:70:ARG:HH11	1.85	0.41
1:D:217:GLU:OE2	1:D:232:LYS:HE3	2.20	0.41
1:B:39:LEU:HD12	2:B:1289:HOH:O	2.20	0.41
1:I:163:ARG:HB2	1:I:180:ASN:HB2	2.02	0.41
1:A:234:ASN:OXT	1:I:128:ARG:HD3	2.21	0.41
1:F:229:TYR:O	1:F:233:LEU:HD12	2.19	0.41
1:A:70:ARG:CG	1:A:70:ARG:HH11	2.33	0.41
1:F:182:LEU:N	1:F:183:PRO:CD	2.84	0.41
1:C:72:LYS:HG2	1:C:105:ASN:OD1	2.20	0.41
1:A:128[A]:ARG:CG	1:I:234:ASN:HB2	2.51	0.41
1:H:78:PHE:HA	1:H:111:CYS:O	2.21	0.40
1:I:78:PHE:HA	1:I:111:CYS:O	2.21	0.40
1:J:217[B]:GLU:OE1	1:J:232:LYS:HD2	2.22	0.40
1:E:208:CYS:HA	1:E:209:PRO:HD3	1.86	0.40
1:E:128:ARG:NH1	1:E:129:GLN:HE21	2.17	0.40
1:A:128[A]:ARG:HG2	1:I:234:ASN:HB2	2.03	0.40
1:A:70:ARG:CG	1:A:70:ARG:NH1	2.84	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	202/246 (82%)	195 (96%)	7 (4%)	0	100	100
1	B	197/246 (80%)	189 (96%)	8 (4%)	0	100	100
1	C	201/246 (82%)	193 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	196/246 (80%)	188 (96%)	8 (4%)	0	100	100
1	E	196/246 (80%)	188 (96%)	8 (4%)	0	100	100
1	F	198/246 (80%)	189 (96%)	9 (4%)	0	100	100
1	G	193/246 (78%)	185 (96%)	8 (4%)	0	100	100
1	H	197/246 (80%)	188 (95%)	9 (5%)	0	100	100
1	I	197/246 (80%)	190 (96%)	7 (4%)	0	100	100
1	J	197/246 (80%)	189 (96%)	8 (4%)	0	100	100
All	All	1974/2460 (80%)	1894 (96%)	80 (4%)	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	179/213 (84%)	174 (97%)	5 (3%)	51	55
1	B	174/213 (82%)	172 (99%)	2 (1%)	80	85
1	C	178/213 (84%)	172 (97%)	6 (3%)	44	45
1	D	173/213 (81%)	170 (98%)	3 (2%)	68	74
1	E	173/213 (81%)	169 (98%)	4 (2%)	58	62
1	F	175/213 (82%)	173 (99%)	2 (1%)	80	85
1	G	170/213 (80%)	169 (99%)	1 (1%)	90	94
1	H	174/213 (82%)	172 (99%)	2 (1%)	80	85
1	I	174/213 (82%)	169 (97%)	5 (3%)	50	53
1	J	174/213 (82%)	173 (99%)	1 (1%)	90	94
All	All	1744/2130 (82%)	1713 (98%)	31 (2%)	70	72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	135	ILE
1	A	157[A]	ASP
1	A	157[B]	ASP
1	A	162	LEU
1	I	46	LYS
1	I	70	ARG
1	I	162	LEU
1	I	222[A]	ASP
1	I	222[B]	ASP
1	G	162	LEU
1	C	162	LEU
1	C	174[A]	LEU
1	C	174[B]	LEU
1	C	192	LEU
1	C	222[A]	ASP
1	C	222[B]	ASP
1	F	162	LEU
1	F	233	LEU
1	D	128	ARG
1	D	162	LEU
1	D	231	ASP
1	B	162	LEU
1	B	192	LEU
1	H	161	THR
1	H	162	LEU
1	E	39	LEU
1	E	46	LYS
1	E	162	LEU
1	E	233	LEU
1	J	162	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	38	HIS
1	F	124	ASN
1	H	129	GLN
1	E	129	GLN
1	E	204	HIS
1	J	234	ASN

### 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 ⓘ

### 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	197/246 (80%)	-0.44	2 (1%) 84 87	11, 17, 35, 65	0
1	B	197/246 (80%)	-0.42	3 (1%) 76 81	11, 18, 38, 56	0
1	C	197/246 (80%)	-0.31	5 (2%) 61 67	11, 17, 37, 64	0
1	D	197/246 (80%)	-0.31	4 (2%) 68 73	12, 18, 36, 64	0
1	E	197/246 (80%)	-0.21	5 (2%) 61 67	14, 23, 46, 62	0
1	F	197/246 (80%)	-0.45	5 (2%) 61 67	12, 18, 35, 64	0
1	G	195/246 (79%)	-0.49	2 (1%) 84 87	11, 18, 35, 49	0
1	H	197/246 (80%)	-0.30	4 (2%) 68 73	11, 16, 35, 64	0
1	I	197/246 (80%)	-0.37	2 (1%) 84 87	12, 17, 37, 60	0
1	J	197/246 (80%)	-0.27	5 (2%) 61 67	14, 23, 43, 58	0
All	All	1968/2460 (80%)	-0.36	37 (1%) 70 75	11, 19, 38, 65	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	233	LEU	7.5
1	D	233	LEU	7.1
1	C	233	LEU	5.5
1	B	39	LEU	5.5
1	D	39	LEU	4.9
1	A	39	LEU	4.6
1	I	38	HIS	4.4
1	J	205	GLY	4.3
1	D	234	ASN	4.1
1	A	38	HIS	4.0
1	E	234	ASN	4.0
1	C	234	ASN	3.7
1	E	232	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	233	LEU	3.3
1	E	39	LEU	3.2
1	J	38	HIS	3.1
1	F	39	LEU	2.9
1	F	38	HIS	2.7
1	G	234	ASN	2.6
1	J	215	GLY	2.5
1	B	233	LEU	2.5
1	F	102	ARG	2.5
1	D	38	HIS	2.5
1	E	38	HIS	2.5
1	I	234	ASN	2.5
1	C	38	HIS	2.5
1	B	38	HIS	2.5
1	J	39	LEU	2.4
1	F	233	LEU	2.4
1	J	58	ASP	2.3
1	C	232	LYS	2.3
1	H	38	HIS	2.3
1	G	58	ASP	2.3
1	H	39	LEU	2.2
1	H	234	ASN	2.2
1	C	39	LEU	2.1
1	F	58	ASP	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 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.