



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:14 am BST

PDB ID : 6J13
Title : Redox protein from Chlamydomonas reinhardtii
Authors : Charoenwattansatien, R.; Zinzius, K.; Tanaka, H.; Hippler, M.; Kurisu, G.
Deposited on : 2018-12-27
Resolution : 2.40 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:

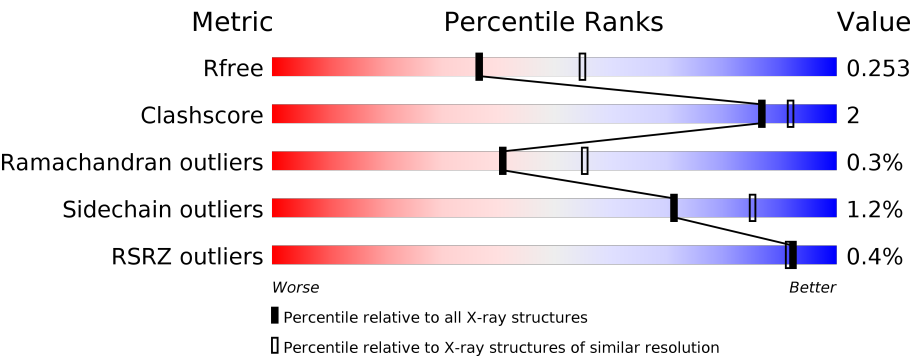
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	221	<div><div></div><div>68%6%26%</div></div>
1	B	221	<div><div></div><div>70%26%</div></div>
1	C	221	<div><div>%</div><div>66%8%26%</div></div>
1	D	221	<div><div>2%</div><div>65%9%26%</div></div>
1	E	221	<div><div></div><div>67%7%27%</div></div>
1	F	221	<div><div></div><div>69%5%26%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	221	 66%7%26%
1	H	221	 71%2%26%
1	I	221	 68%6%26%
1	J	221	 69%5%26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13006 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1297	840	210	246	1			
1	B	163	Total	C	N	O	S	0	1	0
			1302	842	211	248	1			
1	C	163	Total	C	N	O	S	0	0	0
			1287	833	209	244	1			
1	D	163	Total	C	N	O	S	0	0	0
			1274	825	204	244	1			
1	E	162	Total	C	N	O	S	0	0	0
			1278	830	204	243	1			
1	F	163	Total	C	N	O	S	0	0	0
			1295	839	209	246	1			
1	G	163	Total	C	N	O	S	0	0	0
			1288	835	206	246	1			
1	H	164	Total	C	N	O	S	0	0	0
			1293	838	209	245	1			
1	I	163	Total	C	N	O	S	0	0	0
			1297	840	210	246	1			
1	J	164	Total	C	N	O	S	0	0	0
			1302	844	210	247	1			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9FE86
A	174	SER	CYS	engineered mutation	UNP Q9FE86
A	200	GLN	-	expression tag	UNP Q9FE86
A	201	ASP	-	expression tag	UNP Q9FE86
A	202	PRO	-	expression tag	UNP Q9FE86
A	203	ASN	-	expression tag	UNP Q9FE86
A	204	SER	-	expression tag	UNP Q9FE86
A	205	SER	-	expression tag	UNP Q9FE86
A	206	SER	-	expression tag	UNP Q9FE86

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Chain	Residue	Modelled	Actual	Comment	Reference
A	207	VAL	-	expression tag	UNP Q9FE86
A	208	ASP	-	expression tag	UNP Q9FE86
A	209	LYS	-	expression tag	UNP Q9FE86
A	210	LEU	-	expression tag	UNP Q9FE86
A	211	ALA	-	expression tag	UNP Q9FE86
A	212	ALA	-	expression tag	UNP Q9FE86
A	213	ALA	-	expression tag	UNP Q9FE86
A	214	LEU	-	expression tag	UNP Q9FE86
A	215	GLU	-	expression tag	UNP Q9FE86
A	216	HIS	-	expression tag	UNP Q9FE86
A	217	HIS	-	expression tag	UNP Q9FE86
A	218	HIS	-	expression tag	UNP Q9FE86
A	219	HIS	-	expression tag	UNP Q9FE86
A	220	HIS	-	expression tag	UNP Q9FE86
A	221	HIS	-	expression tag	UNP Q9FE86
B	1	MET	-	initiating methionine	UNP Q9FE86
B	174	SER	CYS	engineered mutation	UNP Q9FE86
B	200	GLN	-	expression tag	UNP Q9FE86
B	201	ASP	-	expression tag	UNP Q9FE86
B	202	PRO	-	expression tag	UNP Q9FE86
B	203	ASN	-	expression tag	UNP Q9FE86
B	204	SER	-	expression tag	UNP Q9FE86
B	205	SER	-	expression tag	UNP Q9FE86
B	206	SER	-	expression tag	UNP Q9FE86
B	207	VAL	-	expression tag	UNP Q9FE86
B	208	ASP	-	expression tag	UNP Q9FE86
B	209	LYS	-	expression tag	UNP Q9FE86
B	210	LEU	-	expression tag	UNP Q9FE86
B	211	ALA	-	expression tag	UNP Q9FE86
B	212	ALA	-	expression tag	UNP Q9FE86
B	213	ALA	-	expression tag	UNP Q9FE86
B	214	LEU	-	expression tag	UNP Q9FE86
B	215	GLU	-	expression tag	UNP Q9FE86
B	216	HIS	-	expression tag	UNP Q9FE86
B	217	HIS	-	expression tag	UNP Q9FE86
B	218	HIS	-	expression tag	UNP Q9FE86
B	219	HIS	-	expression tag	UNP Q9FE86
B	220	HIS	-	expression tag	UNP Q9FE86
B	221	HIS	-	expression tag	UNP Q9FE86
C	1	MET	-	initiating methionine	UNP Q9FE86
C	174	SER	CYS	engineered mutation	UNP Q9FE86
C	200	GLN	-	expression tag	UNP Q9FE86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	201	ASP	-	expression tag	UNP Q9FE86
C	202	PRO	-	expression tag	UNP Q9FE86
C	203	ASN	-	expression tag	UNP Q9FE86
C	204	SER	-	expression tag	UNP Q9FE86
C	205	SER	-	expression tag	UNP Q9FE86
C	206	SER	-	expression tag	UNP Q9FE86
C	207	VAL	-	expression tag	UNP Q9FE86
C	208	ASP	-	expression tag	UNP Q9FE86
C	209	LYS	-	expression tag	UNP Q9FE86
C	210	LEU	-	expression tag	UNP Q9FE86
C	211	ALA	-	expression tag	UNP Q9FE86
C	212	ALA	-	expression tag	UNP Q9FE86
C	213	ALA	-	expression tag	UNP Q9FE86
C	214	LEU	-	expression tag	UNP Q9FE86
C	215	GLU	-	expression tag	UNP Q9FE86
C	216	HIS	-	expression tag	UNP Q9FE86
C	217	HIS	-	expression tag	UNP Q9FE86
C	218	HIS	-	expression tag	UNP Q9FE86
C	219	HIS	-	expression tag	UNP Q9FE86
C	220	HIS	-	expression tag	UNP Q9FE86
C	221	HIS	-	expression tag	UNP Q9FE86
D	1	MET	-	initiating methionine	UNP Q9FE86
D	174	SER	CYS	engineered mutation	UNP Q9FE86
D	200	GLN	-	expression tag	UNP Q9FE86
D	201	ASP	-	expression tag	UNP Q9FE86
D	202	PRO	-	expression tag	UNP Q9FE86
D	203	ASN	-	expression tag	UNP Q9FE86
D	204	SER	-	expression tag	UNP Q9FE86
D	205	SER	-	expression tag	UNP Q9FE86
D	206	SER	-	expression tag	UNP Q9FE86
D	207	VAL	-	expression tag	UNP Q9FE86
D	208	ASP	-	expression tag	UNP Q9FE86
D	209	LYS	-	expression tag	UNP Q9FE86
D	210	LEU	-	expression tag	UNP Q9FE86
D	211	ALA	-	expression tag	UNP Q9FE86
D	212	ALA	-	expression tag	UNP Q9FE86
D	213	ALA	-	expression tag	UNP Q9FE86
D	214	LEU	-	expression tag	UNP Q9FE86
D	215	GLU	-	expression tag	UNP Q9FE86
D	216	HIS	-	expression tag	UNP Q9FE86
D	217	HIS	-	expression tag	UNP Q9FE86
D	218	HIS	-	expression tag	UNP Q9FE86

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Chain	Residue	Modelled	Actual	Comment	Reference
D	219	HIS	-	expression tag	UNP Q9FE86
D	220	HIS	-	expression tag	UNP Q9FE86
D	221	HIS	-	expression tag	UNP Q9FE86
E	1	MET	-	initiating methionine	UNP Q9FE86
E	174	SER	CYS	engineered mutation	UNP Q9FE86
E	200	GLN	-	expression tag	UNP Q9FE86
E	201	ASP	-	expression tag	UNP Q9FE86
E	202	PRO	-	expression tag	UNP Q9FE86
E	203	ASN	-	expression tag	UNP Q9FE86
E	204	SER	-	expression tag	UNP Q9FE86
E	205	SER	-	expression tag	UNP Q9FE86
E	206	SER	-	expression tag	UNP Q9FE86
E	207	VAL	-	expression tag	UNP Q9FE86
E	208	ASP	-	expression tag	UNP Q9FE86
E	209	LYS	-	expression tag	UNP Q9FE86
E	210	LEU	-	expression tag	UNP Q9FE86
E	211	ALA	-	expression tag	UNP Q9FE86
E	212	ALA	-	expression tag	UNP Q9FE86
E	213	ALA	-	expression tag	UNP Q9FE86
E	214	LEU	-	expression tag	UNP Q9FE86
E	215	GLU	-	expression tag	UNP Q9FE86
E	216	HIS	-	expression tag	UNP Q9FE86
E	217	HIS	-	expression tag	UNP Q9FE86
E	218	HIS	-	expression tag	UNP Q9FE86
E	219	HIS	-	expression tag	UNP Q9FE86
E	220	HIS	-	expression tag	UNP Q9FE86
E	221	HIS	-	expression tag	UNP Q9FE86
F	1	MET	-	initiating methionine	UNP Q9FE86
F	174	SER	CYS	engineered mutation	UNP Q9FE86
F	200	GLN	-	expression tag	UNP Q9FE86
F	201	ASP	-	expression tag	UNP Q9FE86
F	202	PRO	-	expression tag	UNP Q9FE86
F	203	ASN	-	expression tag	UNP Q9FE86
F	204	SER	-	expression tag	UNP Q9FE86
F	205	SER	-	expression tag	UNP Q9FE86
F	206	SER	-	expression tag	UNP Q9FE86
F	207	VAL	-	expression tag	UNP Q9FE86
F	208	ASP	-	expression tag	UNP Q9FE86
F	209	LYS	-	expression tag	UNP Q9FE86
F	210	LEU	-	expression tag	UNP Q9FE86
F	211	ALA	-	expression tag	UNP Q9FE86
F	212	ALA	-	expression tag	UNP Q9FE86

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Chain	Residue	Modelled	Actual	Comment	Reference
F	213	ALA	-	expression tag	UNP Q9FE86
F	214	LEU	-	expression tag	UNP Q9FE86
F	215	GLU	-	expression tag	UNP Q9FE86
F	216	HIS	-	expression tag	UNP Q9FE86
F	217	HIS	-	expression tag	UNP Q9FE86
F	218	HIS	-	expression tag	UNP Q9FE86
F	219	HIS	-	expression tag	UNP Q9FE86
F	220	HIS	-	expression tag	UNP Q9FE86
F	221	HIS	-	expression tag	UNP Q9FE86
G	1	MET	-	initiating methionine	UNP Q9FE86
G	174	SER	CYS	engineered mutation	UNP Q9FE86
G	200	GLN	-	expression tag	UNP Q9FE86
G	201	ASP	-	expression tag	UNP Q9FE86
G	202	PRO	-	expression tag	UNP Q9FE86
G	203	ASN	-	expression tag	UNP Q9FE86
G	204	SER	-	expression tag	UNP Q9FE86
G	205	SER	-	expression tag	UNP Q9FE86
G	206	SER	-	expression tag	UNP Q9FE86
G	207	VAL	-	expression tag	UNP Q9FE86
G	208	ASP	-	expression tag	UNP Q9FE86
G	209	LYS	-	expression tag	UNP Q9FE86
G	210	LEU	-	expression tag	UNP Q9FE86
G	211	ALA	-	expression tag	UNP Q9FE86
G	212	ALA	-	expression tag	UNP Q9FE86
G	213	ALA	-	expression tag	UNP Q9FE86
G	214	LEU	-	expression tag	UNP Q9FE86
G	215	GLU	-	expression tag	UNP Q9FE86
G	216	HIS	-	expression tag	UNP Q9FE86
G	217	HIS	-	expression tag	UNP Q9FE86
G	218	HIS	-	expression tag	UNP Q9FE86
G	219	HIS	-	expression tag	UNP Q9FE86
G	220	HIS	-	expression tag	UNP Q9FE86
G	221	HIS	-	expression tag	UNP Q9FE86
H	1	MET	-	initiating methionine	UNP Q9FE86
H	174	SER	CYS	engineered mutation	UNP Q9FE86
H	200	GLN	-	expression tag	UNP Q9FE86
H	201	ASP	-	expression tag	UNP Q9FE86
H	202	PRO	-	expression tag	UNP Q9FE86
H	203	ASN	-	expression tag	UNP Q9FE86
H	204	SER	-	expression tag	UNP Q9FE86
H	205	SER	-	expression tag	UNP Q9FE86
H	206	SER	-	expression tag	UNP Q9FE86

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Chain	Residue	Modelled	Actual	Comment	Reference
H	207	VAL	-	expression tag	UNP Q9FE86
H	208	ASP	-	expression tag	UNP Q9FE86
H	209	LYS	-	expression tag	UNP Q9FE86
H	210	LEU	-	expression tag	UNP Q9FE86
H	211	ALA	-	expression tag	UNP Q9FE86
H	212	ALA	-	expression tag	UNP Q9FE86
H	213	ALA	-	expression tag	UNP Q9FE86
H	214	LEU	-	expression tag	UNP Q9FE86
H	215	GLU	-	expression tag	UNP Q9FE86
H	216	HIS	-	expression tag	UNP Q9FE86
H	217	HIS	-	expression tag	UNP Q9FE86
H	218	HIS	-	expression tag	UNP Q9FE86
H	219	HIS	-	expression tag	UNP Q9FE86
H	220	HIS	-	expression tag	UNP Q9FE86
H	221	HIS	-	expression tag	UNP Q9FE86
I	1	MET	-	initiating methionine	UNP Q9FE86
I	174	SER	CYS	engineered mutation	UNP Q9FE86
I	200	GLN	-	expression tag	UNP Q9FE86
I	201	ASP	-	expression tag	UNP Q9FE86
I	202	PRO	-	expression tag	UNP Q9FE86
I	203	ASN	-	expression tag	UNP Q9FE86
I	204	SER	-	expression tag	UNP Q9FE86
I	205	SER	-	expression tag	UNP Q9FE86
I	206	SER	-	expression tag	UNP Q9FE86
I	207	VAL	-	expression tag	UNP Q9FE86
I	208	ASP	-	expression tag	UNP Q9FE86
I	209	LYS	-	expression tag	UNP Q9FE86
I	210	LEU	-	expression tag	UNP Q9FE86
I	211	ALA	-	expression tag	UNP Q9FE86
I	212	ALA	-	expression tag	UNP Q9FE86
I	213	ALA	-	expression tag	UNP Q9FE86
I	214	LEU	-	expression tag	UNP Q9FE86
I	215	GLU	-	expression tag	UNP Q9FE86
I	216	HIS	-	expression tag	UNP Q9FE86
I	217	HIS	-	expression tag	UNP Q9FE86
I	218	HIS	-	expression tag	UNP Q9FE86
I	219	HIS	-	expression tag	UNP Q9FE86
I	220	HIS	-	expression tag	UNP Q9FE86
I	221	HIS	-	expression tag	UNP Q9FE86
J	1	MET	-	initiating methionine	UNP Q9FE86
J	174	SER	CYS	engineered mutation	UNP Q9FE86
J	200	GLN	-	expression tag	UNP Q9FE86

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Chain	Residue	Modelled	Actual	Comment	Reference
J	201	ASP	-	expression tag	UNP Q9FE86
J	202	PRO	-	expression tag	UNP Q9FE86
J	203	ASN	-	expression tag	UNP Q9FE86
J	204	SER	-	expression tag	UNP Q9FE86
J	205	SER	-	expression tag	UNP Q9FE86
J	206	SER	-	expression tag	UNP Q9FE86
J	207	VAL	-	expression tag	UNP Q9FE86
J	208	ASP	-	expression tag	UNP Q9FE86
J	209	LYS	-	expression tag	UNP Q9FE86
J	210	LEU	-	expression tag	UNP Q9FE86
J	211	ALA	-	expression tag	UNP Q9FE86
J	212	ALA	-	expression tag	UNP Q9FE86
J	213	ALA	-	expression tag	UNP Q9FE86
J	214	LEU	-	expression tag	UNP Q9FE86
J	215	GLU	-	expression tag	UNP Q9FE86
J	216	HIS	-	expression tag	UNP Q9FE86
J	217	HIS	-	expression tag	UNP Q9FE86
J	218	HIS	-	expression tag	UNP Q9FE86
J	219	HIS	-	expression tag	UNP Q9FE86
J	220	HIS	-	expression tag	UNP Q9FE86
J	221	HIS	-	expression tag	UNP Q9FE86

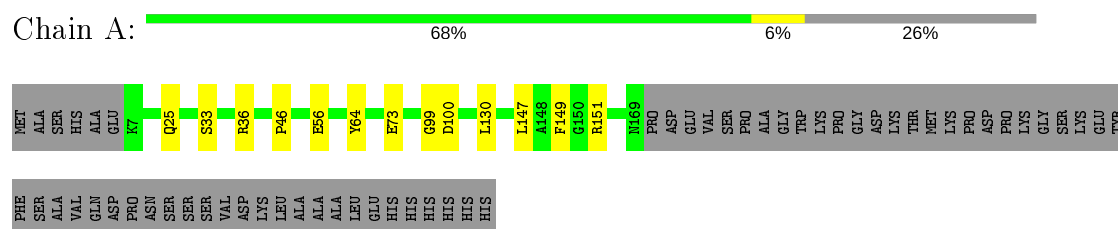
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	3	Total O 3 3	0	0
2	E	1	Total O 1 1	0	0
2	F	4	Total O 4 4	0	0
2	G	5	Total O 5 5	0	0
2	H	9	Total O 9 9	0	0
2	I	32	Total O 32 32	0	0
2	J	26	Total O 26 26	0	0

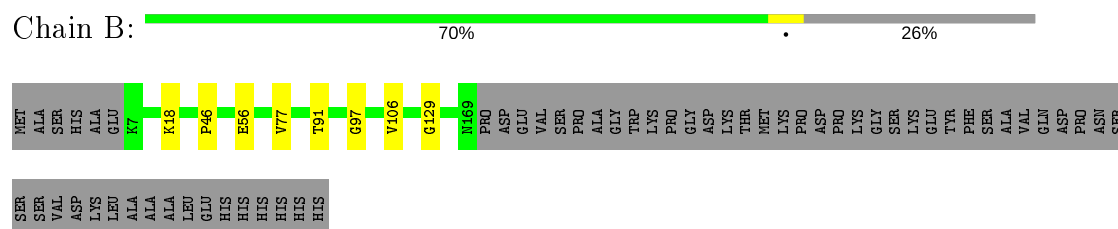
3 Residue-property plots [i](#)

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.

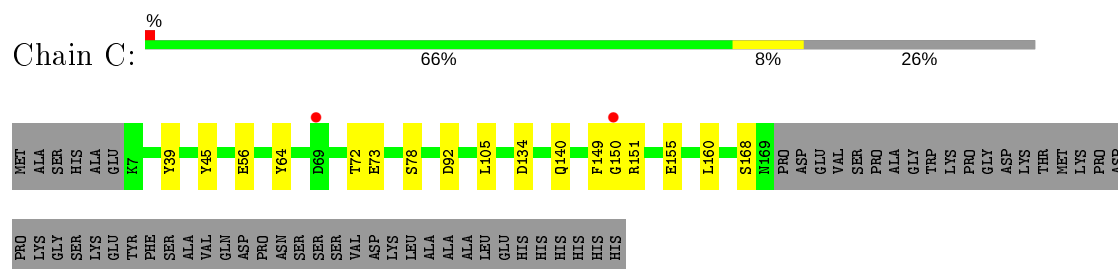
- Molecule 1: 2-cys peroxiredoxin



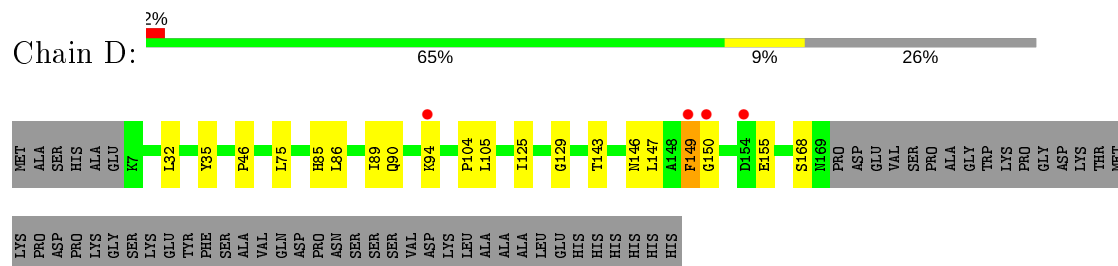
- Molecule 1: 2-cys peroxiredoxin

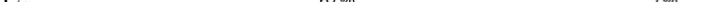


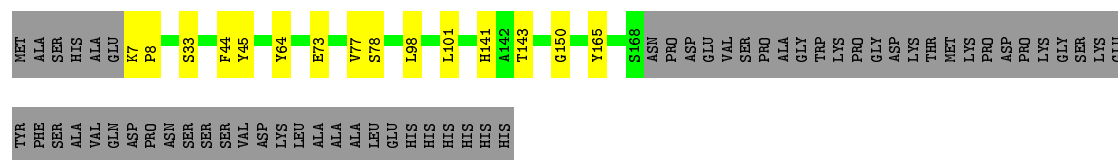
- Molecule 1: 2-cys peroxiredoxin



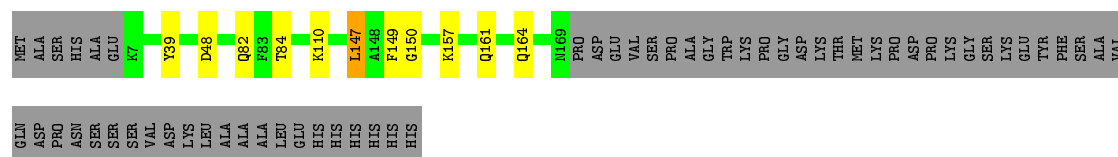
- Molecule 1: 2-cys peroxiredoxin

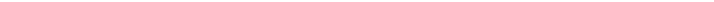


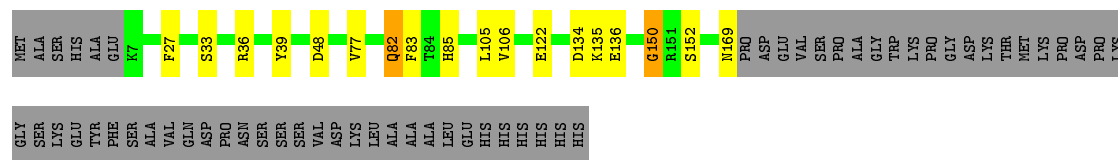
Chain E:  67% 7% 27%



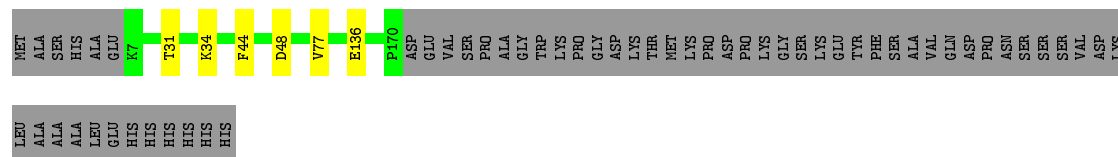
Chain F:  69% 5% 26%

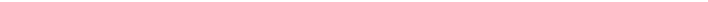


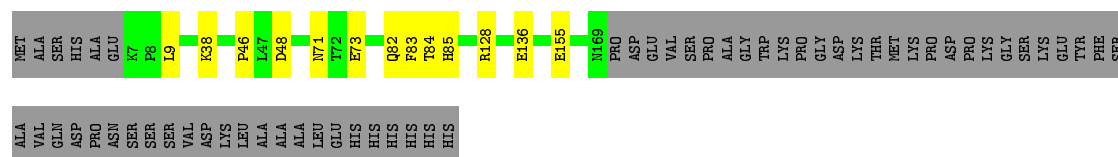
Chain G:  66% 7% • 26%



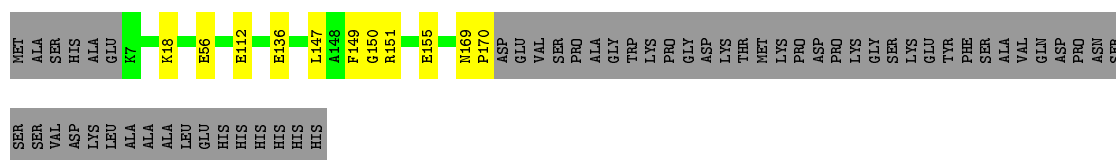
Chain H: 71% . 26%



Chain I:  68% 6% 26%



Response	Percentage
Yes, the U.S. is a democracy	69%
No, the U.S. is not a democracy	5%
Don't know	26%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.99 Å 419.23 Å 94.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.37 – 2.40 47.37 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.37-2.40) 99.0 (47.37-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.251 0.222 , 0.253	Depositor DCC
R_{free} test set	5201 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13006	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 45.92 % 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 1.2336e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.91	2/1324 (0.2%)	1.02	0/1793
1	B	0.91	2/1329 (0.2%)	1.01	0/1801
1	C	0.79	1/1314 (0.1%)	0.93	2/1782 (0.1%)
1	D	0.74	0/1301	0.89	0/1769
1	E	0.79	0/1305	0.96	0/1770
1	F	0.78	0/1322	1.01	0/1791
1	G	0.88	1/1315 (0.1%)	1.03	0/1784
1	H	0.96	2/1321 (0.2%)	1.06	0/1793
1	I	1.07	7/1324 (0.5%)	1.11	2/1793 (0.1%)
1	J	1.03	4/1330 (0.3%)	1.07	0/1803
All	All	0.89	19/13185 (0.1%)	1.01	4/17879 (0.0%)

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	C	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	J	0	1
All	All	0	5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	136	GLU	CD-OE1	12.05	1.39	1.25
1	I	136	GLU	CD-OE2	8.14	1.34	1.25
1	G	136	GLU	CD-OE1	7.76	1.34	1.25
1	C	56	GLU	CD-OE1	6.88	1.33	1.25
1	I	73	GLU	CD-OE2	6.58	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	128	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	C	151	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	C	151	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	I	128	ARG	CG-CD-NE	-5.04	101.20	111.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	150	GLY	Peptide
1	E	150	GLY	Peptide
1	F	150	GLY	Peptide
1	G	150	GLY	Peptide
1	J	150	GLY	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	1297	0	1287	7	0
1	B	1302	0	1283	2	0
1	C	1287	0	1268	7	0
1	D	1274	0	1227	11	0
1	E	1278	0	1252	5	0
1	F	1295	0	1280	5	0
1	G	1288	0	1257	10	0
1	H	1293	0	1270	2	0
1	I	1297	0	1287	3	0
1	J	1302	0	1287	4	0
2	A	13	0	0	0	0
2	B	3	0	0	0	0
2	E	1	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	9	0	0	0	0
2	I	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	26	0	0	0	0
All	All	13006	0	12698	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 53 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:F:110:LYS:HE3	1:G:122:GLU:O	1.95	0.66
1:C:64:TYR:OH	1:C:73:GLU:OE2	2.09	0.65
1:G:27:PHE:CE1	1:G:82:GLN:HG3	2.34	0.62
1:A:25:GLN:NE2	1:A:100:ASP:OD1	2.32	0.61
1:D:147:LEU:HB2	1:D:149:PHE:HE2	1.71	0.56

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	161/221 (73%)	156 (97%)	4 (2%)	1 (1%)	25	36
1	B	162/221 (73%)	158 (98%)	3 (2%)	1 (1%)	25	36
1	C	161/221 (73%)	156 (97%)	5 (3%)	0	100	100
1	D	161/221 (73%)	151 (94%)	9 (6%)	1 (1%)	25	36
1	E	160/221 (72%)	156 (98%)	4 (2%)	0	100	100
1	F	161/221 (73%)	156 (97%)	5 (3%)	0	100	100
1	G	161/221 (73%)	155 (96%)	5 (3%)	1 (1%)	25	36
1	H	162/221 (73%)	153 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	161/221 (73%)	155 (96%)	5 (3%)	1 (1%)	25	36
1	J	162/221 (73%)	153 (94%)	9 (6%)	0	100	100
All	All	1612/2210 (73%)	1549 (96%)	58 (4%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	150	GLY
1	G	150	GLY
1	B	46	PRO
1	I	46	PRO
1	A	46	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	140/189 (74%)	140 (100%)	0	100	100
1	B	140/189 (74%)	139 (99%)	1 (1%)	84	92
1	C	138/189 (73%)	135 (98%)	3 (2%)	52	71
1	D	133/189 (70%)	130 (98%)	3 (2%)	50	70
1	E	135/189 (71%)	131 (97%)	4 (3%)	41	61
1	F	139/189 (74%)	137 (99%)	2 (1%)	67	82
1	G	136/189 (72%)	133 (98%)	3 (2%)	52	71
1	H	138/189 (73%)	138 (100%)	0	100	100
1	I	140/189 (74%)	140 (100%)	0	100	100
1	J	140/189 (74%)	140 (100%)	0	100	100
All	All	1379/1890 (73%)	1363 (99%)	16 (1%)	71	85

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	33	SER
1	E	98	LEU
1	F	147	LEU
1	D	168	SER
1	G	82	GLN

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	20	GLN
1	C	82	GLN
1	F	82	GLN
1	G	28	GLN
1	I	28	GLN

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	163/221 (73%)	-0.33	0 100 100	33, 43, 62, 74	0
1	B	163/221 (73%)	-0.32	0 100 100	37, 46, 64, 87	0
1	C	163/221 (73%)	-0.12	2 (1%) 79 77	46, 63, 85, 107	0
1	D	163/221 (73%)	0.07	4 (2%) 57 55	53, 74, 97, 113	0
1	E	162/221 (73%)	-0.06	0 100 100	54, 68, 86, 102	0
1	F	163/221 (73%)	-0.19	0 100 100	43, 55, 77, 90	0
1	G	163/221 (73%)	-0.10	0 100 100	39, 53, 75, 87	0
1	H	164/221 (74%)	-0.22	0 100 100	34, 45, 65, 114	0
1	I	163/221 (73%)	-0.29	0 100 100	31, 40, 58, 76	0
1	J	164/221 (74%)	-0.25	0 100 100	31, 41, 64, 108	0
All	All	1631/2210 (73%)	-0.18	6 (0%) 92 91	31, 52, 83, 114	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	GLY	4.1
1	D	94	LYS	3.5
1	D	149	PHE	2.2
1	C	69	ASP	2.1
1	C	150	GLY	2.1

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.