



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:18 PM UTC

PDB ID : 6J13 / pdb_00006j13
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

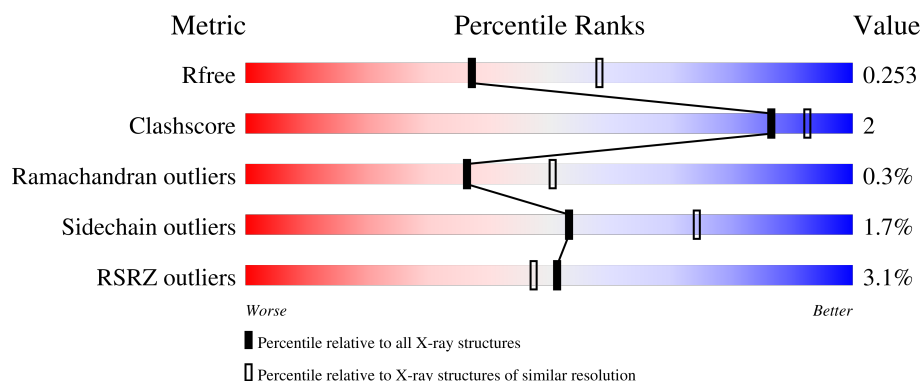
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	221	0% 65% 9% 26%
1	B	221	67% 6% 26%
1	C	221	4% 66% 8% 26%
1	D	221	4% 63% 10% 26%
1	E	221	3% 67% 5% 27%

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Mol	Chain	Length	Quality of chain
1	F	221	2% 67% 6% 26%
1	G	221	2% 65% 8% 26%
1	H	221	4% 64% 10% 26%
1	I	221	% 62% 12% 26%
1	J	221	2% 63% 11% 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
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J	221	HIS	-	expression tag	UNP Q9FE86

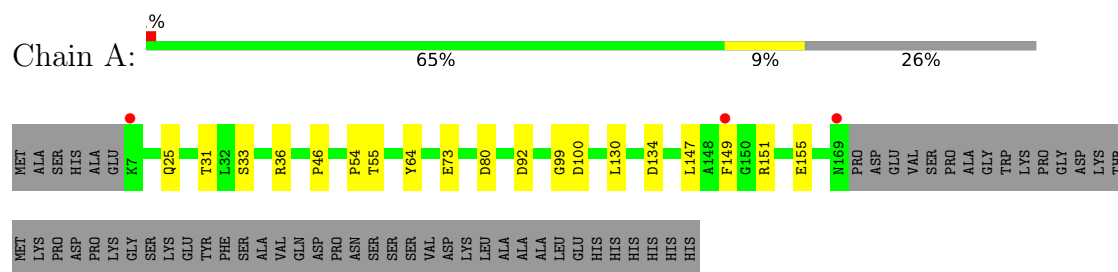
- Molecule 2 is water.

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

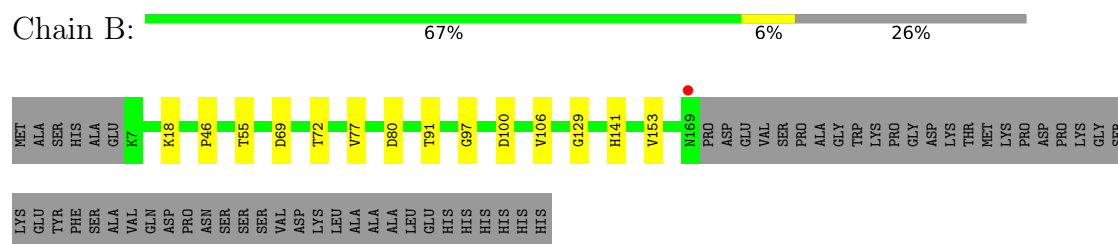
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

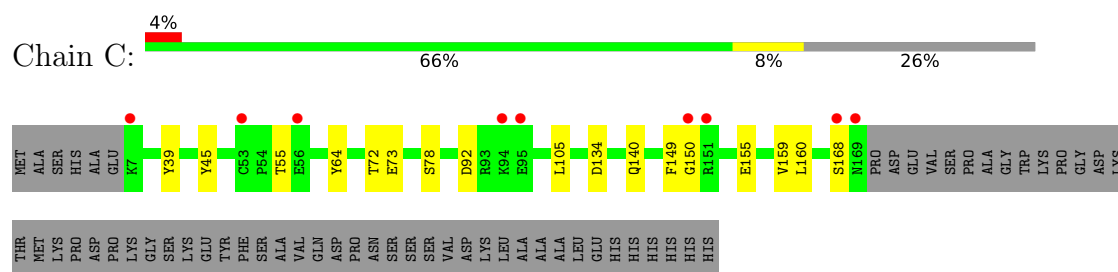
• Molecule 1: 2-cys peroxiredoxin



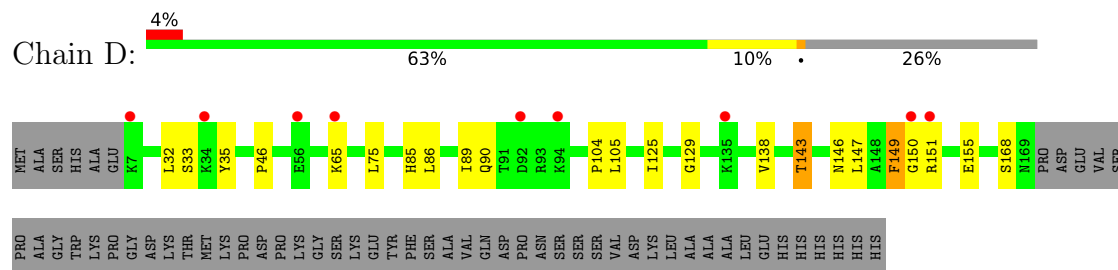
• Molecule 1: 2-cys peroxiredoxin



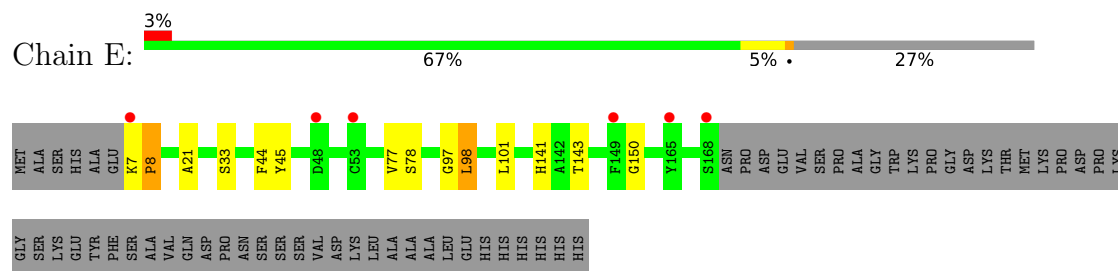
• Molecule 1: 2-cys peroxiredoxin



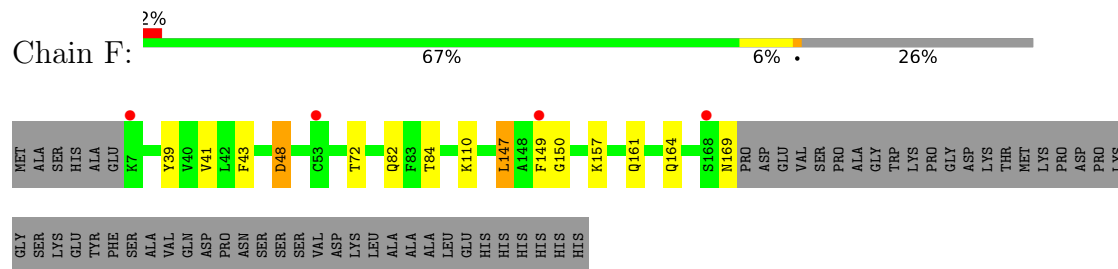
• Molecule 1: 2-cys peroxiredoxin



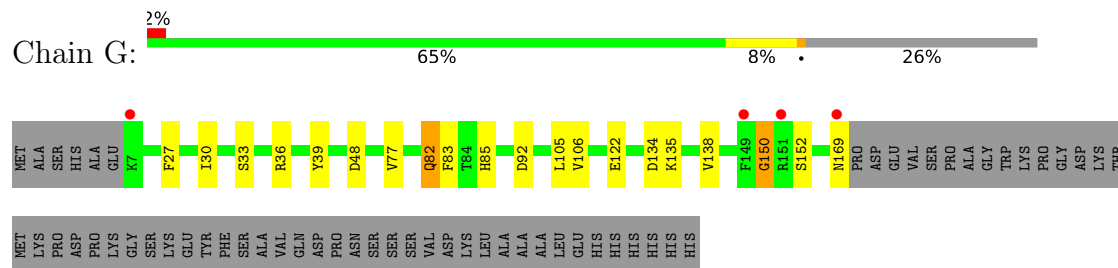
- Molecule 1: 2-cys peroxiredoxin



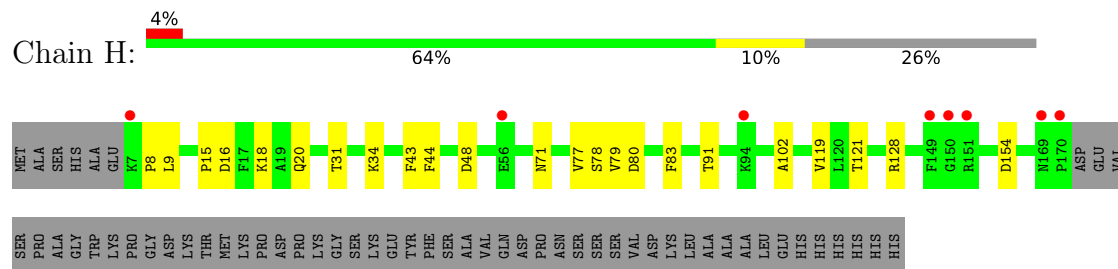
- Molecule 1: 2-cys peroxiredoxin



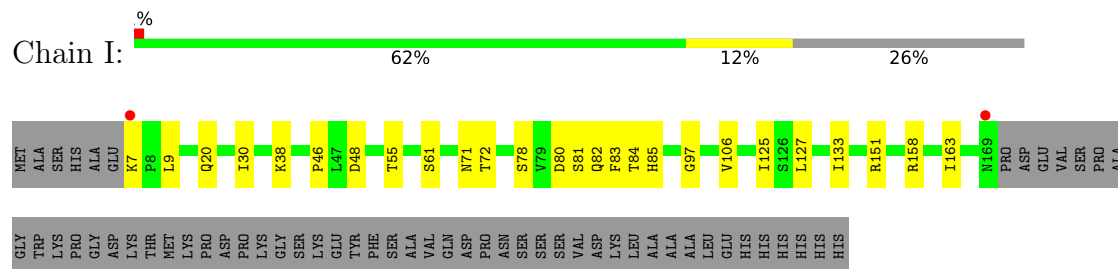
- Molecule 1: 2-cys peroxiredoxin



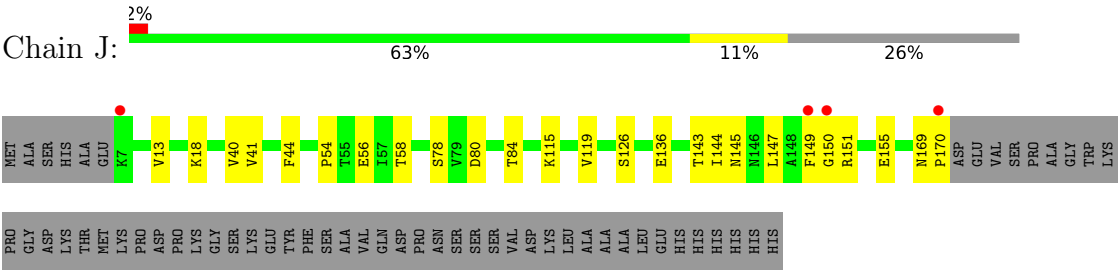
- Molecule 1: 2-cys peroxiredoxin



- Molecule 1: 2-cys peroxiredoxin



- Molecule 1: 2-cys peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 419.23Å 94.53Å 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 2.39Å)	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 , 28.2	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	0.95	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	1.25	3/1324 (0.2%)	1.54	7/1793 (0.4%)
1	B	1.27	3/1329 (0.2%)	1.49	6/1801 (0.3%)
1	C	1.13	0/1314	1.45	1/1782 (0.1%)
1	D	1.12	1/1301 (0.1%)	1.48	2/1769 (0.1%)
1	E	1.14	2/1305 (0.2%)	1.50	2/1770 (0.1%)
1	F	1.13	0/1322	1.52	3/1791 (0.2%)
1	G	1.23	1/1315 (0.1%)	1.54	1/1784 (0.1%)
1	H	1.36	11/1321 (0.8%)	1.61	10/1793 (0.6%)
1	I	1.42	9/1324 (0.7%)	1.58	8/1793 (0.4%)
1	J	1.35	6/1330 (0.5%)	1.60	11/1803 (0.6%)
All	All	1.25	36/13185 (0.3%)	1.53	51/17879 (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	C	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	J	0	1
All	All	0	5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	48	ASP	C-O	-9.21	1.12	1.23
1	I	9	LEU	C-O	9.09	1.34	1.24
1	I	84	THR	C-O	8.06	1.33	1.24
1	B	129	GLY	C-O	7.83	1.32	1.23
1	A	155	GLU	C-O	-7.24	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	136	GLU	CD-OE1	7.14	1.39	1.25
1	I	20	GLN	C-O	6.71	1.32	1.23
1	I	106	VAL	C-O	-6.66	1.16	1.24
1	H	78	SER	C-O	6.55	1.32	1.23
1	A	92	ASP	C-O	6.49	1.31	1.23
1	I	80	ASP	C-O	6.46	1.32	1.23
1	H	20	GLN	C-O	6.33	1.31	1.23
1	J	155	GLU	C-O	-6.31	1.16	1.24
1	I	78	SER	C-O	6.14	1.31	1.24
1	H	15	PRO	C-O	5.78	1.31	1.24
1	I	127	LEU	C-O	5.77	1.31	1.23
1	H	80	ASP	C-O	5.73	1.31	1.23
1	A	80	ASP	C-O	5.69	1.31	1.23
1	J	80	ASP	C-O	5.68	1.31	1.23
1	H	102	ALA	C-O	5.63	1.31	1.24
1	J	78	SER	C-O	5.63	1.31	1.23
1	B	153	VAL	C-O	-5.61	1.17	1.24
1	H	121	THR	C-O	5.55	1.31	1.23
1	B	80	ASP	C-O	5.40	1.31	1.23
1	H	8	PRO	C-O	5.36	1.29	1.23
1	J	84	THR	C-O	5.35	1.30	1.24
1	D	143	THR	C-O	5.32	1.30	1.24
1	H	9	LEU	C-O	5.29	1.30	1.24
1	I	81	SER	C-O	5.26	1.31	1.23
1	H	83	PHE	C-O	5.26	1.30	1.24
1	J	13	VAL	C-O	-5.17	1.19	1.24
1	E	98	LEU	C-O	5.11	1.31	1.23
1	I	97	GLY	C-O	-5.09	1.19	1.23
1	H	119	VAL	C-O	5.04	1.30	1.23
1	E	97	GLY	C-O	5.03	1.28	1.24
1	G	138	VAL	C-O	5.03	1.30	1.24

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	72	THR	CA-CB-OG1	-6.81	99.38	109.60
1	B	55	THR	CA-CB-OG1	-6.79	99.42	109.60
1	I	151	ARG	N-CA-C	-6.72	99.08	109.76
1	J	54	PRO	N-CA-CB	-6.71	98.31	102.81
1	A	54	PRO	N-CA-CB	-6.68	98.38	102.79
1	I	55	THR	CA-CB-OG1	-6.53	99.81	109.60
1	A	134	ASP	CA-C-N	6.31	129.37	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ASP	C-N-CA	6.31	129.37	120.28
1	F	72	THR	CA-CB-OG1	-6.09	100.46	109.60
1	B	72	THR	CA-CB-OG1	-6.06	100.50	109.60
1	H	16	ASP	CA-C-O	-6.02	114.88	121.87
1	H	91	THR	CA-CB-OG1	-5.96	100.67	109.60
1	G	92	ASP	CA-CB-CG	5.93	118.53	112.60
1	J	44	PHE	CA-C-O	-5.60	114.22	120.66
1	A	80	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	55	THR	CA-CB-OG1	-5.57	101.25	109.60
1	B	80	ASP	CA-CB-CG	5.54	118.14	112.60
1	H	43	PHE	CA-C-N	5.54	130.80	122.99
1	H	43	PHE	C-N-CA	5.54	130.80	122.99
1	I	61	SER	CA-C-N	5.48	128.39	120.38
1	I	61	SER	C-N-CA	5.48	128.39	120.38
1	C	159	VAL	N-CA-C	-5.46	105.21	110.72
1	I	158	ARG	N-CA-C	-5.38	105.33	111.14
1	J	145	ASN	CB-CA-C	5.37	119.63	109.37
1	A	31	THR	CA-CB-OG1	-5.37	101.55	109.60
1	H	128	ARG	CA-C-N	5.37	127.92	121.38
1	H	128	ARG	C-N-CA	5.37	127.92	121.38
1	J	58	THR	CA-CB-OG1	-5.36	101.57	109.60
1	E	21	ALA	CA-C-O	-5.35	115.36	121.40
1	H	18	LYS	CA-C-O	-5.33	114.58	120.33
1	B	141	HIS	CA-C-O	-5.30	114.02	120.54
1	B	100	ASP	CA-CB-CG	5.30	117.90	112.60
1	F	43	PHE	CA-CB-CG	5.30	119.10	113.80
1	F	48	ASP	CA-CB-CG	5.27	117.87	112.60
1	J	155	GLU	N-CA-C	-5.27	105.62	111.36
1	J	119	VAL	CA-C-O	-5.25	115.19	119.97
1	D	65	LYS	CA-C-N	5.22	127.80	120.28
1	D	65	LYS	C-N-CA	5.22	127.80	120.28
1	I	133	ILE	CA-C-O	-5.20	114.93	120.39
1	I	163	ILE	N-CA-C	-5.16	105.35	110.62
1	H	154	ASP	CA-CB-CG	5.16	117.76	112.60
1	J	115	LYS	CA-C-N	5.15	127.18	120.28
1	J	115	LYS	C-N-CA	5.15	127.18	120.28
1	J	126	SER	CA-C-O	-5.11	115.22	121.36
1	E	8	PRO	CB-CA-C	-5.10	105.29	111.46
1	A	155	GLU	N-CA-C	-5.08	105.65	111.14
1	H	79	VAL	CA-C-O	-5.08	114.43	120.78
1	B	69	ASP	CA-CB-CG	5.08	117.68	112.60
1	H	71	ASN	CA-CB-CG	-5.07	107.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	40	VAL	CA-C-N	-5.00	116.37	122.93
1	J	40	VAL	C-N-CA	-5.00	116.37	122.93

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	12	0
1	E	1278	0	1252	4	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	5	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
2	J	26	0	0	0	0
All	All	13006	0	12698	54	0

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

All (54) 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
1:J:169:ASN:HB3	1:J:170:PRO:HD2	1.88	0.56
1:A:147:LEU:HB2	1:A:149:PHE:CE1	2.41	0.55
1:D:85:HIS:O	1:D:89:ILE:HG13	2.07	0.55
1:D:86:LEU:HD11	1:D:90:GLN:NE2	2.23	0.54
1:J:147:LEU:HB2	1:J:149:PHE:CZ	2.44	0.52
1:D:147:LEU:HB2	1:D:149:PHE:CE2	2.46	0.51
1:D:75:LEU:HD23	1:D:104:PRO:HB2	1.92	0.50
1:G:48:ASP:OD2	1:G:85:HIS:ND1	2.41	0.49
1:H:31:THR:HB	1:H:34:LYS:HG3	1.95	0.49
1:A:130:LEU:HD13	1:A:151:ARG:HD2	1.95	0.48
1:I:38:LYS:HG2	1:I:71:ASN:OD1	2.14	0.48
1:A:64:TYR:OH	1:A:73:GLU:OE2	2.21	0.48
1:C:39:TYR:CD2	1:C:134:ASP:HA	2.49	0.48
1:B:77:VAL:HG22	1:B:106:VAL:HB	1.95	0.48
1:F:147:LEU:HB2	1:F:149:PHE:CE1	2.48	0.47
1:F:157:LYS:O	1:F:161:GLN:HG3	2.14	0.47
1:A:33:SER:O	1:A:36:ARG:HG2	2.14	0.47
1:C:45:TYR:CZ	1:C:78:SER:HB3	2.50	0.47
1:A:147:LEU:HB2	1:A:149:PHE:CZ	2.50	0.46
1:I:82:GLN:HG2	1:I:83:PHE:N	2.29	0.46
1:F:48:ASP:OD2	1:F:84:THR:HG22	2.16	0.45
1:C:155:GLU:HG2	1:D:155:GLU:HG2	1.99	0.45
1:G:27:PHE:CD1	1:G:82:GLN:HG3	2.51	0.45
1:G:82:GLN:HG2	1:G:83:PHE:N	2.31	0.45
1:A:99:GLY:O	1:A:100:ASP:C	2.58	0.44
1:F:39:TYR:CE1	1:F:164:GLN:HG2	2.53	0.44
1:C:105:LEU:HD12	1:C:105:LEU:HA	1.88	0.44
1:D:46:PRO:HB3	1:D:125:ILE:HD12	2.00	0.44
1:G:135:LYS:HB2	1:G:135:LYS:HE2	1.67	0.43
1:B:91:THR:O	1:B:97:GLY:HA3	2.18	0.43
1:E:44:PHE:HA	1:E:77:VAL:O	2.19	0.43
1:D:33:SER:C	1:D:35:TYR:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:GLY:HA2	1:D:143:THR:O	2.19	0.42
1:G:77:VAL:HG22	1:G:106:VAL:HB	2.01	0.42
1:J:56:GLU:HB2	1:J:151:ARG:NH1	2.34	0.42
1:D:32:LEU:O	1:D:35:TYR:HB2	2.20	0.42
1:E:45:TYR:CZ	1:E:78:SER:HB3	2.55	0.42
1:G:105:LEU:HD12	1:G:105:LEU:HA	1.86	0.42
1:H:44:PHE:HA	1:H:77:VAL:O	2.19	0.42
1:E:141:HIS:NE2	1:E:143:THR:OG1	2.51	0.42
1:G:33:SER:O	1:G:36:ARG:HG2	2.20	0.42
1:D:105:LEU:HD12	1:D:105:LEU:HA	1.91	0.42
1:I:48:ASP:OD2	1:I:85:HIS:ND1	2.42	0.41
1:C:72:THR:HG21	1:C:160:LEU:HD21	2.02	0.41
1:E:7:LYS:N	1:E:8:PRO:CD	2.84	0.41
1:J:18:LYS:HB2	1:J:18:LYS:HE3	1.92	0.41
1:C:140:GLN:OE1	1:D:146:ASN:HB3	2.21	0.41
1:J:143:THR:C	1:J:144:ILE:HG13	2.46	0.41
1:G:39:TYR:CD1	1:G:134:ASP:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	21	32
1	B	162/221 (73%)	158 (98%)	3 (2%)	1 (1%)	21	32
1	C	161/221 (73%)	156 (97%)	5 (3%)	0	100	100
1	D	161/221 (73%)	151 (94%)	9 (6%)	1 (1%)	21	32
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%)	21	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	162/221 (73%)	153 (94%)	9 (6%)	0	100	100
1	I	161/221 (73%)	155 (96%)	5 (3%)	1 (1%)	21	32
1	J	162/221 (73%)	153 (94%)	9 (6%)	0	100	100
All	All	1612/2210 (73%)	1549 (96%)	58 (4%)	5 (0%)	36	50

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%)	76	88
1	C	138/189 (73%)	134 (97%)	4 (3%)	37	60
1	D	133/189 (70%)	129 (97%)	4 (3%)	36	58
1	E	135/189 (71%)	132 (98%)	3 (2%)	45	67
1	F	139/189 (74%)	135 (97%)	4 (3%)	37	60
1	G	136/189 (72%)	132 (97%)	4 (3%)	37	60
1	H	138/189 (73%)	138 (100%)	0	100	100
1	I	140/189 (74%)	137 (98%)	3 (2%)	47	69
1	J	140/189 (74%)	139 (99%)	1 (1%)	76	88
All	All	1379/1890 (73%)	1355 (98%)	24 (2%)	53	74

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	LYS
1	C	55	THR
1	C	92	ASP
1	C	149	PHE
1	C	168	SER
1	D	138	VAL
1	D	149	PHE
1	D	151	ARG
1	D	168	SER
1	E	33	SER
1	E	98	LEU
1	E	101	LEU
1	F	41	VAL
1	F	82	GLN
1	F	147	LEU
1	F	169	ASN
1	G	30	ILE
1	G	82	GLN
1	G	152	SER
1	G	169	ASN
1	I	7	LYS
1	I	30	ILE
1	I	125	ILE
1	J	41	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	B	20	GLN
1	B	25	GLN
1	B	90	GLN
1	B	146	ASN
1	C	25	GLN
1	C	90	GLN
1	C	169	ASN
1	D	20	GLN
1	E	20	GLN
1	F	20	GLN
1	F	82	GLN
1	F	90	GLN
1	F	169	ASN
1	G	28	GLN

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Mol	Chain	Res	Type
1	G	146	ASN
1	I	28	GLN
1	J	20	GLN
1	J	90	GLN
1	J	146	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 oligosaccharides 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, 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%)	-0.26	3 (1%) 67 63	33, 43, 62, 74	0
1	B	163/221 (73%)	-0.22	1 (0%) 85 83	22, 46, 64, 87	1 (0%)
1	C	163/221 (73%)	0.18	9 (5%) 30 27	46, 63, 85, 107	0
1	D	163/221 (73%)	0.52	9 (5%) 30 27	53, 74, 97, 113	0
1	E	162/221 (73%)	0.39	6 (3%) 45 41	54, 68, 86, 102	0
1	F	163/221 (73%)	0.08	4 (2%) 58 54	43, 55, 77, 90	0
1	G	163/221 (73%)	0.05	4 (2%) 58 54	39, 53, 75, 87	0
1	H	164/221 (74%)	-0.02	8 (4%) 35 31	34, 45, 65, 114	0
1	I	163/221 (73%)	-0.22	2 (1%) 76 73	31, 40, 58, 76	0
1	J	164/221 (74%)	-0.20	4 (2%) 59 55	31, 41, 64, 108	0
All	All	1631/2210 (73%)	0.03	50 (3%) 51 47	22, 52, 83, 114	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	170	PRO	6.4
1	J	170	PRO	5.0
1	D	7	LYS	4.2
1	G	7	LYS	4.1
1	E	168	SER	4.1
1	E	149	PHE	3.9
1	A	7	LYS	3.6
1	H	7	LYS	3.5
1	J	149	PHE	3.4
1	D	92	ASP	3.3
1	E	7	LYS	3.2
1	E	165	TYR	3.2
1	J	150	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	151	ARG	3.1
1	F	7	LYS	3.0
1	D	150	GLY	3.0
1	C	7	LYS	2.9
1	D	135	LYS	2.9
1	C	95	GLU	2.9
1	C	150	GLY	2.9
1	F	149	PHE	2.8
1	I	169	ASN	2.7
1	I	7	LYS	2.6
1	B	169	ASN	2.6
1	H	150	GLY	2.6
1	F	53	CYS	2.6
1	F	168	SER	2.5
1	E	53	CYS	2.5
1	J	7	LYS	2.5
1	H	151	ARG	2.4
1	H	149	PHE	2.4
1	C	169	ASN	2.4
1	D	151	ARG	2.3
1	H	56	GLU	2.3
1	G	151	ARG	2.3
1	A	149	PHE	2.3
1	G	149	PHE	2.3
1	D	56	GLU	2.3
1	C	168	SER	2.3
1	C	53	CYS	2.3
1	D	34	LYS	2.2
1	E	48	ASP	2.2
1	D	65	LYS	2.2
1	A	169	ASN	2.1
1	D	94	LYS	2.1
1	H	94	LYS	2.1
1	C	56	GLU	2.1
1	G	169	ASN	2.0
1	C	94	LYS	2.0
1	H	169	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.