



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:25 PM UTC

PDB ID : 3ZL5 / pdb_00003zl5
Title : Crystal structure of Schistosoma mansoni Peroxiredoxin I C48S mutant with one decamer in the ASU
Authors : Saccoccia, F.; Angelucci, F.; Ardini, M.; Boumis, G.; Brunori, M.; DiLeandro, L.; Ippoliti, R.; Miele, A.E.; Natoli, G.; Scotti, S.; Bellelli, A.
Deposited on : 2013-01-28
Resolution : 2.49 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
Mogul : 2022.3.0, CSD as543be (2022)
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

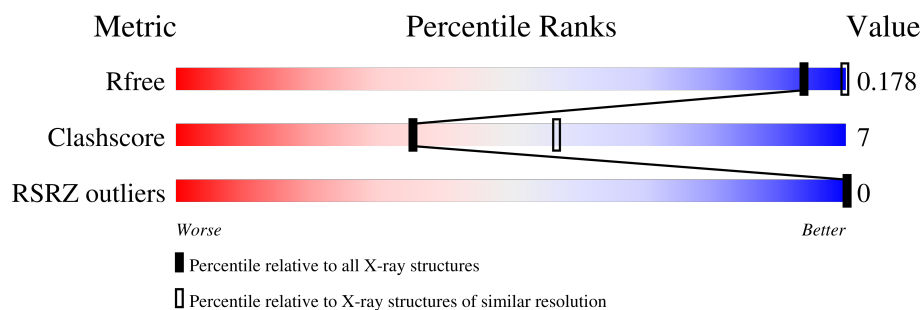
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	222	
1	B	222	
1	C	222	
1	D	222	
1	E	222	
1	F	222	
1	G	222	

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Mol	Chain	Length	Quality of chain
1	H	222	 59% 15% 27%
1	I	222	 59% 14% 27%
1	J	222	 59% 15% 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13287 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 I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1299	832	219	244	4			
1	B	164	Total	C	N	O	S	0	3	0
			1333	854	224	250	5			
1	C	164	Total	C	N	O	S	0	0	0
			1314	842	221	246	5			
1	D	163	Total	C	N	O	S	0	1	0
			1314	842	223	245	4			
1	E	161	Total	C	N	O	S	0	0	0
			1290	826	217	243	4			
1	F	163	Total	C	N	O	S	0	1	0
			1311	841	220	245	5			
1	G	162	Total	C	N	O	S	0	0	0
			1297	831	218	244	4			
1	H	163	Total	C	N	O	S	0	1	0
			1313	841	222	245	5			
1	I	162	Total	C	N	O	S	0	0	0
			1297	831	218	244	4			
1	J	164	Total	C	N	O	S	0	0	0
			1314	842	221	246	5			

There are 380 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	MET	-	expression tag	UNP O97161
A	-35	ARG	-	expression tag	UNP O97161
A	-34	GLY	-	expression tag	UNP O97161
A	-33	SER	-	expression tag	UNP O97161
A	-32	HIS	-	expression tag	UNP O97161
A	-31	HIS	-	expression tag	UNP O97161
A	-30	HIS	-	expression tag	UNP O97161
A	-29	HIS	-	expression tag	UNP O97161
A	-28	HIS	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	HIS	-	expression tag	UNP O97161
A	-26	GLY	-	expression tag	UNP O97161
A	-25	MET	-	expression tag	UNP O97161
A	-24	ALA	-	expression tag	UNP O97161
A	-23	SER	-	expression tag	UNP O97161
A	-22	MET	-	expression tag	UNP O97161
A	-21	THR	-	expression tag	UNP O97161
A	-20	GLY	-	expression tag	UNP O97161
A	-19	GLY	-	expression tag	UNP O97161
A	-18	GLN	-	expression tag	UNP O97161
A	-17	GLN	-	expression tag	UNP O97161
A	-16	MET	-	expression tag	UNP O97161
A	-15	GLY	-	expression tag	UNP O97161
A	-14	ARG	-	expression tag	UNP O97161
A	-13	ASP	-	expression tag	UNP O97161
A	-12	LEU	-	expression tag	UNP O97161
A	-11	TYR	-	expression tag	UNP O97161
A	-10	ASP	-	expression tag	UNP O97161
A	-9	ASP	-	expression tag	UNP O97161
A	-8	ASP	-	expression tag	UNP O97161
A	-7	ASP	-	expression tag	UNP O97161
A	-6	LYS	-	expression tag	UNP O97161
A	-5	ASP	-	expression tag	UNP O97161
A	-4	ARG	-	expression tag	UNP O97161
A	-3	TRP	-	expression tag	UNP O97161
A	-2	GLY	-	expression tag	UNP O97161
A	-1	SER	-	expression tag	UNP O97161
A	0	THR	-	expression tag	UNP O97161
A	48	SER	CYS	engineered mutation	UNP O97161
B	-36	MET	-	expression tag	UNP O97161
B	-35	ARG	-	expression tag	UNP O97161
B	-34	GLY	-	expression tag	UNP O97161
B	-33	SER	-	expression tag	UNP O97161
B	-32	HIS	-	expression tag	UNP O97161
B	-31	HIS	-	expression tag	UNP O97161
B	-30	HIS	-	expression tag	UNP O97161
B	-29	HIS	-	expression tag	UNP O97161
B	-28	HIS	-	expression tag	UNP O97161
B	-27	HIS	-	expression tag	UNP O97161
B	-26	GLY	-	expression tag	UNP O97161
B	-25	MET	-	expression tag	UNP O97161
B	-24	ALA	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	SER	-	expression tag	UNP O97161
B	-22	MET	-	expression tag	UNP O97161
B	-21	THR	-	expression tag	UNP O97161
B	-20	GLY	-	expression tag	UNP O97161
B	-19	GLY	-	expression tag	UNP O97161
B	-18	GLN	-	expression tag	UNP O97161
B	-17	GLN	-	expression tag	UNP O97161
B	-16	MET	-	expression tag	UNP O97161
B	-15	GLY	-	expression tag	UNP O97161
B	-14	ARG	-	expression tag	UNP O97161
B	-13	ASP	-	expression tag	UNP O97161
B	-12	LEU	-	expression tag	UNP O97161
B	-11	TYR	-	expression tag	UNP O97161
B	-10	ASP	-	expression tag	UNP O97161
B	-9	ASP	-	expression tag	UNP O97161
B	-8	ASP	-	expression tag	UNP O97161
B	-7	ASP	-	expression tag	UNP O97161
B	-6	LYS	-	expression tag	UNP O97161
B	-5	ASP	-	expression tag	UNP O97161
B	-4	ARG	-	expression tag	UNP O97161
B	-3	TRP	-	expression tag	UNP O97161
B	-2	GLY	-	expression tag	UNP O97161
B	-1	SER	-	expression tag	UNP O97161
B	0	THR	-	expression tag	UNP O97161
B	48	SER	CYS	engineered mutation	UNP O97161
C	-36	MET	-	expression tag	UNP O97161
C	-35	ARG	-	expression tag	UNP O97161
C	-34	GLY	-	expression tag	UNP O97161
C	-33	SER	-	expression tag	UNP O97161
C	-32	HIS	-	expression tag	UNP O97161
C	-31	HIS	-	expression tag	UNP O97161
C	-30	HIS	-	expression tag	UNP O97161
C	-29	HIS	-	expression tag	UNP O97161
C	-28	HIS	-	expression tag	UNP O97161
C	-27	HIS	-	expression tag	UNP O97161
C	-26	GLY	-	expression tag	UNP O97161
C	-25	MET	-	expression tag	UNP O97161
C	-24	ALA	-	expression tag	UNP O97161
C	-23	SER	-	expression tag	UNP O97161
C	-22	MET	-	expression tag	UNP O97161
C	-21	THR	-	expression tag	UNP O97161
C	-20	GLY	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	GLY	-	expression tag	UNP O97161
C	-18	GLN	-	expression tag	UNP O97161
C	-17	GLN	-	expression tag	UNP O97161
C	-16	MET	-	expression tag	UNP O97161
C	-15	GLY	-	expression tag	UNP O97161
C	-14	ARG	-	expression tag	UNP O97161
C	-13	ASP	-	expression tag	UNP O97161
C	-12	LEU	-	expression tag	UNP O97161
C	-11	TYR	-	expression tag	UNP O97161
C	-10	ASP	-	expression tag	UNP O97161
C	-9	ASP	-	expression tag	UNP O97161
C	-8	ASP	-	expression tag	UNP O97161
C	-7	ASP	-	expression tag	UNP O97161
C	-6	LYS	-	expression tag	UNP O97161
C	-5	ASP	-	expression tag	UNP O97161
C	-4	ARG	-	expression tag	UNP O97161
C	-3	TRP	-	expression tag	UNP O97161
C	-2	GLY	-	expression tag	UNP O97161
C	-1	SER	-	expression tag	UNP O97161
C	0	THR	-	expression tag	UNP O97161
C	48	SER	CYS	engineered mutation	UNP O97161
D	-36	MET	-	expression tag	UNP O97161
D	-35	ARG	-	expression tag	UNP O97161
D	-34	GLY	-	expression tag	UNP O97161
D	-33	SER	-	expression tag	UNP O97161
D	-32	HIS	-	expression tag	UNP O97161
D	-31	HIS	-	expression tag	UNP O97161
D	-30	HIS	-	expression tag	UNP O97161
D	-29	HIS	-	expression tag	UNP O97161
D	-28	HIS	-	expression tag	UNP O97161
D	-27	HIS	-	expression tag	UNP O97161
D	-26	GLY	-	expression tag	UNP O97161
D	-25	MET	-	expression tag	UNP O97161
D	-24	ALA	-	expression tag	UNP O97161
D	-23	SER	-	expression tag	UNP O97161
D	-22	MET	-	expression tag	UNP O97161
D	-21	THR	-	expression tag	UNP O97161
D	-20	GLY	-	expression tag	UNP O97161
D	-19	GLY	-	expression tag	UNP O97161
D	-18	GLN	-	expression tag	UNP O97161
D	-17	GLN	-	expression tag	UNP O97161
D	-16	MET	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	expression tag	UNP O97161
D	-14	ARG	-	expression tag	UNP O97161
D	-13	ASP	-	expression tag	UNP O97161
D	-12	LEU	-	expression tag	UNP O97161
D	-11	TYR	-	expression tag	UNP O97161
D	-10	ASP	-	expression tag	UNP O97161
D	-9	ASP	-	expression tag	UNP O97161
D	-8	ASP	-	expression tag	UNP O97161
D	-7	ASP	-	expression tag	UNP O97161
D	-6	LYS	-	expression tag	UNP O97161
D	-5	ASP	-	expression tag	UNP O97161
D	-4	ARG	-	expression tag	UNP O97161
D	-3	TRP	-	expression tag	UNP O97161
D	-2	GLY	-	expression tag	UNP O97161
D	-1	SER	-	expression tag	UNP O97161
D	0	THR	-	expression tag	UNP O97161
D	48	SER	CYS	engineered mutation	UNP O97161
E	-36	MET	-	expression tag	UNP O97161
E	-35	ARG	-	expression tag	UNP O97161
E	-34	GLY	-	expression tag	UNP O97161
E	-33	SER	-	expression tag	UNP O97161
E	-32	HIS	-	expression tag	UNP O97161
E	-31	HIS	-	expression tag	UNP O97161
E	-30	HIS	-	expression tag	UNP O97161
E	-29	HIS	-	expression tag	UNP O97161
E	-28	HIS	-	expression tag	UNP O97161
E	-27	HIS	-	expression tag	UNP O97161
E	-26	GLY	-	expression tag	UNP O97161
E	-25	MET	-	expression tag	UNP O97161
E	-24	ALA	-	expression tag	UNP O97161
E	-23	SER	-	expression tag	UNP O97161
E	-22	MET	-	expression tag	UNP O97161
E	-21	THR	-	expression tag	UNP O97161
E	-20	GLY	-	expression tag	UNP O97161
E	-19	GLY	-	expression tag	UNP O97161
E	-18	GLN	-	expression tag	UNP O97161
E	-17	GLN	-	expression tag	UNP O97161
E	-16	MET	-	expression tag	UNP O97161
E	-15	GLY	-	expression tag	UNP O97161
E	-14	ARG	-	expression tag	UNP O97161
E	-13	ASP	-	expression tag	UNP O97161
E	-12	LEU	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	TYR	-	expression tag	UNP O97161
E	-10	ASP	-	expression tag	UNP O97161
E	-9	ASP	-	expression tag	UNP O97161
E	-8	ASP	-	expression tag	UNP O97161
E	-7	ASP	-	expression tag	UNP O97161
E	-6	LYS	-	expression tag	UNP O97161
E	-5	ASP	-	expression tag	UNP O97161
E	-4	ARG	-	expression tag	UNP O97161
E	-3	TRP	-	expression tag	UNP O97161
E	-2	GLY	-	expression tag	UNP O97161
E	-1	SER	-	expression tag	UNP O97161
E	0	THR	-	expression tag	UNP O97161
E	48	SER	CYS	engineered mutation	UNP O97161
F	-36	MET	-	expression tag	UNP O97161
F	-35	ARG	-	expression tag	UNP O97161
F	-34	GLY	-	expression tag	UNP O97161
F	-33	SER	-	expression tag	UNP O97161
F	-32	HIS	-	expression tag	UNP O97161
F	-31	HIS	-	expression tag	UNP O97161
F	-30	HIS	-	expression tag	UNP O97161
F	-29	HIS	-	expression tag	UNP O97161
F	-28	HIS	-	expression tag	UNP O97161
F	-27	HIS	-	expression tag	UNP O97161
F	-26	GLY	-	expression tag	UNP O97161
F	-25	MET	-	expression tag	UNP O97161
F	-24	ALA	-	expression tag	UNP O97161
F	-23	SER	-	expression tag	UNP O97161
F	-22	MET	-	expression tag	UNP O97161
F	-21	THR	-	expression tag	UNP O97161
F	-20	GLY	-	expression tag	UNP O97161
F	-19	GLY	-	expression tag	UNP O97161
F	-18	GLN	-	expression tag	UNP O97161
F	-17	GLN	-	expression tag	UNP O97161
F	-16	MET	-	expression tag	UNP O97161
F	-15	GLY	-	expression tag	UNP O97161
F	-14	ARG	-	expression tag	UNP O97161
F	-13	ASP	-	expression tag	UNP O97161
F	-12	LEU	-	expression tag	UNP O97161
F	-11	TYR	-	expression tag	UNP O97161
F	-10	ASP	-	expression tag	UNP O97161
F	-9	ASP	-	expression tag	UNP O97161
F	-8	ASP	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	ASP	-	expression tag	UNP O97161
F	-6	LYS	-	expression tag	UNP O97161
F	-5	ASP	-	expression tag	UNP O97161
F	-4	ARG	-	expression tag	UNP O97161
F	-3	TRP	-	expression tag	UNP O97161
F	-2	GLY	-	expression tag	UNP O97161
F	-1	SER	-	expression tag	UNP O97161
F	0	THR	-	expression tag	UNP O97161
F	48	SER	CYS	engineered mutation	UNP O97161
G	-36	MET	-	expression tag	UNP O97161
G	-35	ARG	-	expression tag	UNP O97161
G	-34	GLY	-	expression tag	UNP O97161
G	-33	SER	-	expression tag	UNP O97161
G	-32	HIS	-	expression tag	UNP O97161
G	-31	HIS	-	expression tag	UNP O97161
G	-30	HIS	-	expression tag	UNP O97161
G	-29	HIS	-	expression tag	UNP O97161
G	-28	HIS	-	expression tag	UNP O97161
G	-27	HIS	-	expression tag	UNP O97161
G	-26	GLY	-	expression tag	UNP O97161
G	-25	MET	-	expression tag	UNP O97161
G	-24	ALA	-	expression tag	UNP O97161
G	-23	SER	-	expression tag	UNP O97161
G	-22	MET	-	expression tag	UNP O97161
G	-21	THR	-	expression tag	UNP O97161
G	-20	GLY	-	expression tag	UNP O97161
G	-19	GLY	-	expression tag	UNP O97161
G	-18	GLN	-	expression tag	UNP O97161
G	-17	GLN	-	expression tag	UNP O97161
G	-16	MET	-	expression tag	UNP O97161
G	-15	GLY	-	expression tag	UNP O97161
G	-14	ARG	-	expression tag	UNP O97161
G	-13	ASP	-	expression tag	UNP O97161
G	-12	LEU	-	expression tag	UNP O97161
G	-11	TYR	-	expression tag	UNP O97161
G	-10	ASP	-	expression tag	UNP O97161
G	-9	ASP	-	expression tag	UNP O97161
G	-8	ASP	-	expression tag	UNP O97161
G	-7	ASP	-	expression tag	UNP O97161
G	-6	LYS	-	expression tag	UNP O97161
G	-5	ASP	-	expression tag	UNP O97161
G	-4	ARG	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	TRP	-	expression tag	UNP O97161
G	-2	GLY	-	expression tag	UNP O97161
G	-1	SER	-	expression tag	UNP O97161
G	0	THR	-	expression tag	UNP O97161
G	48	SER	CYS	engineered mutation	UNP O97161
H	-36	MET	-	expression tag	UNP O97161
H	-35	ARG	-	expression tag	UNP O97161
H	-34	GLY	-	expression tag	UNP O97161
H	-33	SER	-	expression tag	UNP O97161
H	-32	HIS	-	expression tag	UNP O97161
H	-31	HIS	-	expression tag	UNP O97161
H	-30	HIS	-	expression tag	UNP O97161
H	-29	HIS	-	expression tag	UNP O97161
H	-28	HIS	-	expression tag	UNP O97161
H	-27	HIS	-	expression tag	UNP O97161
H	-26	GLY	-	expression tag	UNP O97161
H	-25	MET	-	expression tag	UNP O97161
H	-24	ALA	-	expression tag	UNP O97161
H	-23	SER	-	expression tag	UNP O97161
H	-22	MET	-	expression tag	UNP O97161
H	-21	THR	-	expression tag	UNP O97161
H	-20	GLY	-	expression tag	UNP O97161
H	-19	GLY	-	expression tag	UNP O97161
H	-18	GLN	-	expression tag	UNP O97161
H	-17	GLN	-	expression tag	UNP O97161
H	-16	MET	-	expression tag	UNP O97161
H	-15	GLY	-	expression tag	UNP O97161
H	-14	ARG	-	expression tag	UNP O97161
H	-13	ASP	-	expression tag	UNP O97161
H	-12	LEU	-	expression tag	UNP O97161
H	-11	TYR	-	expression tag	UNP O97161
H	-10	ASP	-	expression tag	UNP O97161
H	-9	ASP	-	expression tag	UNP O97161
H	-8	ASP	-	expression tag	UNP O97161
H	-7	ASP	-	expression tag	UNP O97161
H	-6	LYS	-	expression tag	UNP O97161
H	-5	ASP	-	expression tag	UNP O97161
H	-4	ARG	-	expression tag	UNP O97161
H	-3	TRP	-	expression tag	UNP O97161
H	-2	GLY	-	expression tag	UNP O97161
H	-1	SER	-	expression tag	UNP O97161
H	0	THR	-	expression tag	UNP O97161

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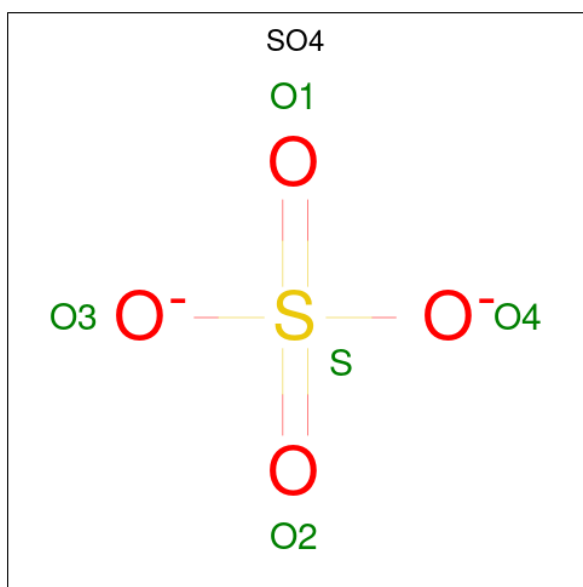
Chain	Residue	Modelled	Actual	Comment	Reference
H	48	SER	CYS	engineered mutation	UNP O97161
I	-36	MET	-	expression tag	UNP O97161
I	-35	ARG	-	expression tag	UNP O97161
I	-34	GLY	-	expression tag	UNP O97161
I	-33	SER	-	expression tag	UNP O97161
I	-32	HIS	-	expression tag	UNP O97161
I	-31	HIS	-	expression tag	UNP O97161
I	-30	HIS	-	expression tag	UNP O97161
I	-29	HIS	-	expression tag	UNP O97161
I	-28	HIS	-	expression tag	UNP O97161
I	-27	HIS	-	expression tag	UNP O97161
I	-26	GLY	-	expression tag	UNP O97161
I	-25	MET	-	expression tag	UNP O97161
I	-24	ALA	-	expression tag	UNP O97161
I	-23	SER	-	expression tag	UNP O97161
I	-22	MET	-	expression tag	UNP O97161
I	-21	THR	-	expression tag	UNP O97161
I	-20	GLY	-	expression tag	UNP O97161
I	-19	GLY	-	expression tag	UNP O97161
I	-18	GLN	-	expression tag	UNP O97161
I	-17	GLN	-	expression tag	UNP O97161
I	-16	MET	-	expression tag	UNP O97161
I	-15	GLY	-	expression tag	UNP O97161
I	-14	ARG	-	expression tag	UNP O97161
I	-13	ASP	-	expression tag	UNP O97161
I	-12	LEU	-	expression tag	UNP O97161
I	-11	TYR	-	expression tag	UNP O97161
I	-10	ASP	-	expression tag	UNP O97161
I	-9	ASP	-	expression tag	UNP O97161
I	-8	ASP	-	expression tag	UNP O97161
I	-7	ASP	-	expression tag	UNP O97161
I	-6	LYS	-	expression tag	UNP O97161
I	-5	ASP	-	expression tag	UNP O97161
I	-4	ARG	-	expression tag	UNP O97161
I	-3	TRP	-	expression tag	UNP O97161
I	-2	GLY	-	expression tag	UNP O97161
I	-1	SER	-	expression tag	UNP O97161
I	0	THR	-	expression tag	UNP O97161
I	48	SER	CYS	engineered mutation	UNP O97161
J	-36	MET	-	expression tag	UNP O97161
J	-35	ARG	-	expression tag	UNP O97161
J	-34	GLY	-	expression tag	UNP O97161

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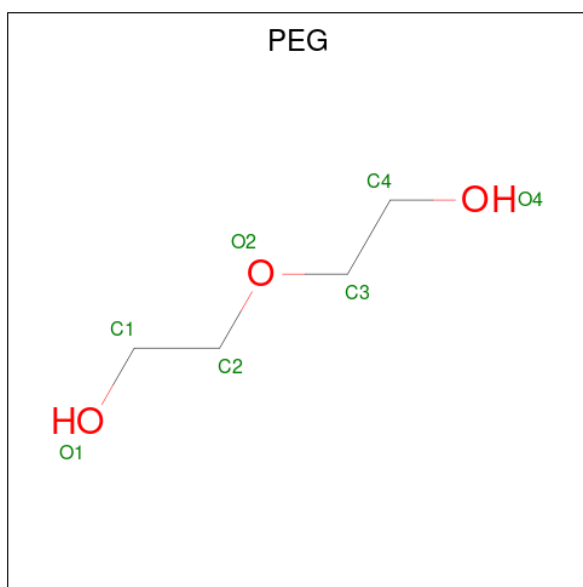
Chain	Residue	Modelled	Actual	Comment	Reference
J	-33	SER	-	expression tag	UNP O97161
J	-32	HIS	-	expression tag	UNP O97161
J	-31	HIS	-	expression tag	UNP O97161
J	-30	HIS	-	expression tag	UNP O97161
J	-29	HIS	-	expression tag	UNP O97161
J	-28	HIS	-	expression tag	UNP O97161
J	-27	HIS	-	expression tag	UNP O97161
J	-26	GLY	-	expression tag	UNP O97161
J	-25	MET	-	expression tag	UNP O97161
J	-24	ALA	-	expression tag	UNP O97161
J	-23	SER	-	expression tag	UNP O97161
J	-22	MET	-	expression tag	UNP O97161
J	-21	THR	-	expression tag	UNP O97161
J	-20	GLY	-	expression tag	UNP O97161
J	-19	GLY	-	expression tag	UNP O97161
J	-18	GLN	-	expression tag	UNP O97161
J	-17	GLN	-	expression tag	UNP O97161
J	-16	MET	-	expression tag	UNP O97161
J	-15	GLY	-	expression tag	UNP O97161
J	-14	ARG	-	expression tag	UNP O97161
J	-13	ASP	-	expression tag	UNP O97161
J	-12	LEU	-	expression tag	UNP O97161
J	-11	TYR	-	expression tag	UNP O97161
J	-10	ASP	-	expression tag	UNP O97161
J	-9	ASP	-	expression tag	UNP O97161
J	-8	ASP	-	expression tag	UNP O97161
J	-7	ASP	-	expression tag	UNP O97161
J	-6	LYS	-	expression tag	UNP O97161
J	-5	ASP	-	expression tag	UNP O97161
J	-4	ARG	-	expression tag	UNP O97161
J	-3	TRP	-	expression tag	UNP O97161
J	-2	GLY	-	expression tag	UNP O97161
J	-1	SER	-	expression tag	UNP O97161
J	0	THR	-	expression tag	UNP O97161
J	48	SER	CYS	engineered mutation	UNP O97161

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	H	1	Total	C	O	0	0
			7	4	3		
3	I	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	14	Total	O	0	0
			14	14		
4	C	7	Total	O	0	0
			7	7		
4	D	11	Total	O	0	0
			11	11		
4	E	9	Total	O	0	0
			9	9		
4	F	14	Total	O	0	0
			14	14		
4	G	9	Total	O	0	0
			9	9		
4	H	12	Total	O	0	0
			12	12		

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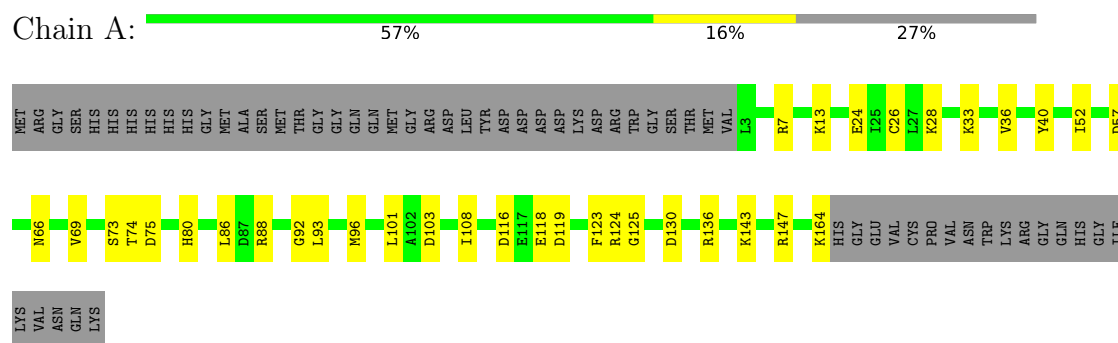
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	24	Total 24	O 24	0	0
4	J	5	Total 5	O 5	0	0

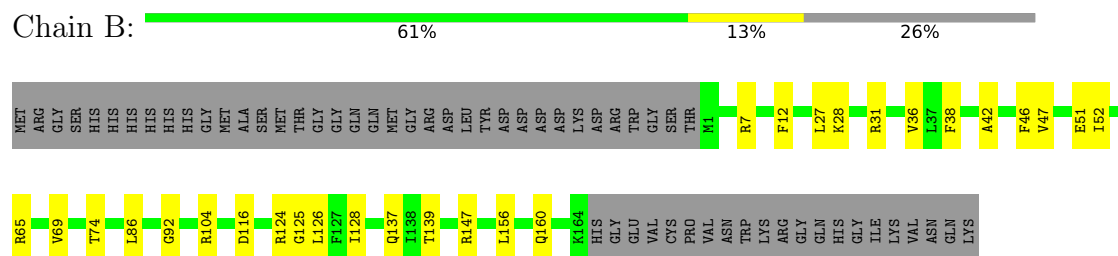
3 Residue-property plots

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.

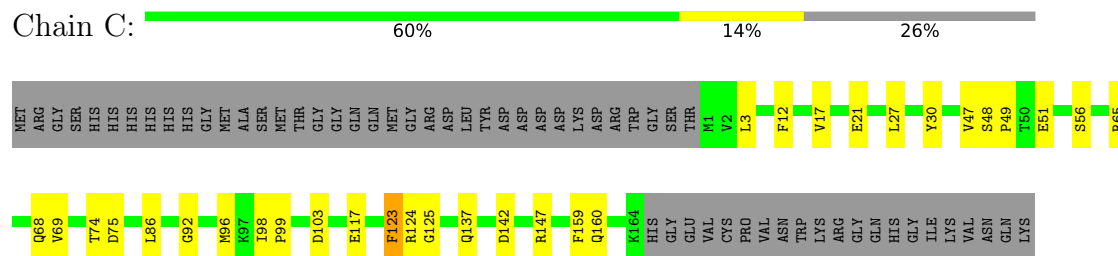
• Molecule 1: PEROXIREDOXIN I



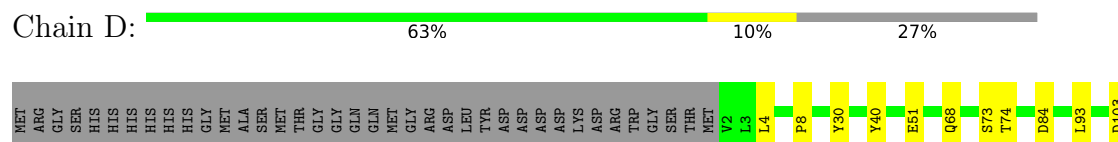
• Molecule 1: PEROXIREDOXIN I

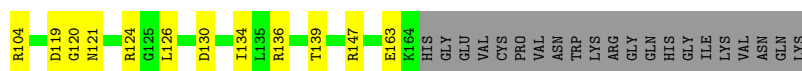


• Molecule 1: PEROXIREDOXIN I

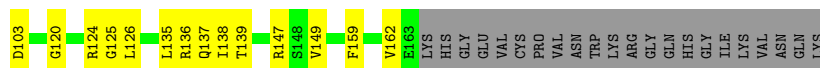
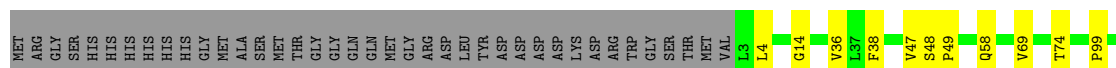


• Molecule 1: PEROXIREDOXIN I

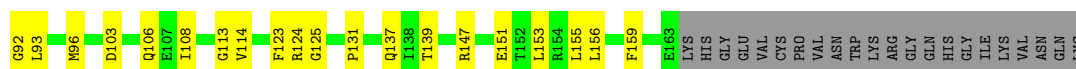




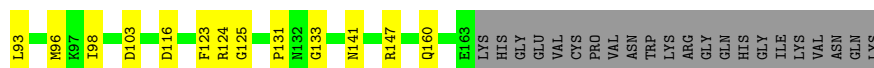
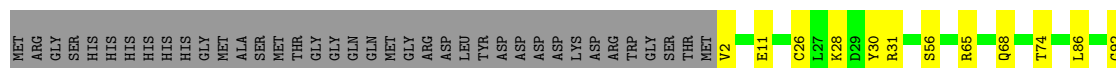
• Molecule 1: PEROXIREDOXIN I



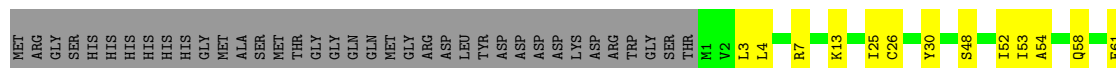
• Molecule 1: PEROXIREDOXIN I



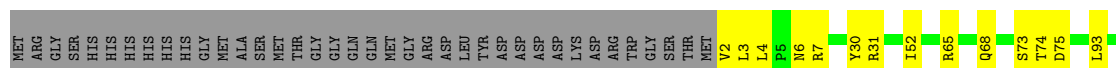
• Molecule 1: PEROXIREDOXIN I



• Molecule 1: PEROXIREDOXIN I

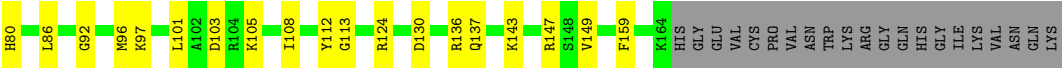


• Molecule 1: PEROXIREDOXIN I





● Molecule 1: PEROXIREDOXIN I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.44Å 94.98Å 114.42Å 90.00° 108.51° 90.00°	Depositor
Resolution (Å)	29.43 – 2.49 29.43 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.43-2.49) 99.4 (29.43-2.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.203 (Not available) , 0.178	Depositor DCC
R_{free} test set	4044 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 13.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.429 for l,-k,h	Xtriage
Reported twinning fraction	0.440 for L,-K,H	Depositor
Outliers	0 of 80696 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13287	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PEG

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	0.34	0/1328	0.82	2/1794 (0.1%)
1	B	0.33	0/1371	0.79	1/1851 (0.1%)
1	C	0.35	0/1343	0.81	3/1814 (0.2%)
1	D	0.35	0/1346	0.84	2/1818 (0.1%)
1	E	0.35	0/1319	0.80	1/1783 (0.1%)
1	F	0.34	0/1343	0.78	0/1814
1	G	0.35	0/1326	0.84	2/1793 (0.1%)
1	H	0.35	0/1345	0.80	0/1817
1	I	0.34	0/1326	0.78	0/1793
1	J	0.34	0/1343	0.77	0/1814
All	All	0.34	0/13390	0.80	11/18091 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	GLU	N-CA-C	5.50	118.11	111.40
1	B	42	ALA	N-CA-C	5.39	117.04	108.79
1	D	120	GLY	N-CA-C	-5.31	107.35	115.00
1	A	123	PHE	CA-C-N	-5.19	114.78	122.41
1	A	123	PHE	C-N-CA	-5.19	114.78	122.41
1	C	123	PHE	CA-C-N	-5.17	114.81	122.41
1	C	123	PHE	C-N-CA	-5.17	114.81	122.41
1	E	14	GLY	N-CA-C	5.15	118.10	110.63
1	C	47	VAL	N-CA-C	5.08	118.97	113.43
1	G	123	PHE	CA-C-N	-5.02	115.03	122.41
1	G	123	PHE	C-N-CA	-5.02	115.03	122.41

There are no chirality outliers.

There are no planarity outliers.

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	1299	0	1273	26	0
1	B	1333	0	1317	21	0
1	C	1314	0	1294	22	0
1	D	1314	0	1295	15	0
1	E	1290	0	1260	16	0
1	F	1311	0	1294	24	0
1	G	1297	0	1269	16	0
1	H	1313	0	1294	25	0
1	I	1297	0	1269	25	0
1	J	1314	0	1294	23	0
2	A	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	1	0
2	H	5	0	0	1	0
2	I	15	0	0	0	0
2	J	10	0	0	1	0
3	F	14	0	20	3	0
3	H	7	0	10	1	0
3	I	7	0	10	0	0
4	A	12	0	0	0	0
4	B	14	0	0	0	0
4	C	7	0	0	0	0
4	D	11	0	0	0	0
4	E	9	0	0	0	0
4	F	14	0	0	0	0
4	G	9	0	0	2	0
4	H	12	0	0	0	0
4	I	24	0	0	0	0
4	J	5	0	0	0	0
All	All	13287	0	12899	194	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 7.

All (194) 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:H:104:ARG:HB3	1:I:120:GLY:HA3	1.58	0.84
1:B:46:PHE:H	1:B:47:VAL:HA	1.46	0.80
1:J:13:LYS:HG3	1:J:26:CYS:HB3	1.66	0.78
1:H:125:GLY:O	1:H:147:ARG:NH1	2.17	0.77
1:G:11:GLU:OE1	1:G:28:LYS:NZ	2.22	0.73
1:G:56:SER:HA	1:G:98:ILE:HD13	1.74	0.69
1:C:86:LEU:HB3	1:C:92:GLY:HA3	1.74	0.69
1:C:124:ARG:NH2	2:C:1165:SO4:O2	2.25	0.69
1:D:126:LEU:HB3	1:D:139:THR:HG22	1.74	0.69
1:F:65:ARG:HH21	1:F:153:LEU:HG	1.58	0.69
1:B:125:GLY:O	1:B:147:ARG:NH1	2.29	0.65
1:E:137:GLN:OE1	1:E:139:THR:OG1	2.13	0.64
1:H:128:ILE:HB	1:H:137:GLN:HB3	1.80	0.64
1:I:128:ILE:HB	1:I:137:GLN:HB3	1.79	0.64
1:A:125:GLY:O	1:A:147:ARG:NH1	2.31	0.64
1:E:125:GLY:O	1:E:147:ARG:NH1	2.30	0.64
1:C:65:ARG:O	1:C:160:GLN:NE2	2.29	0.63
1:C:142:ASP:OD2	1:D:136:ARG:NH1	2.31	0.63
1:H:120:GLY:HA3	1:I:104:ARG:HG3	1.81	0.63
1:D:51:GLU:OE1	1:D:124:ARG:NH1	2.31	0.63
1:G:124:ARG:NH2	2:G:1164:SO4:O4	2.33	0.62
1:J:13:LYS:NZ	1:J:26:CYS:SG	2.73	0.61
1:H:25:ILE:HD11	1:H:101:LEU:HD12	1.83	0.61
1:J:74:THR:HA	1:J:103:ASP:O	2.02	0.60
1:F:74:THR:HA	1:F:103:ASP:O	2.02	0.60
1:D:104:ARG:HG3	1:E:120:GLY:HA3	1.82	0.59
1:F:125:GLY:O	1:F:147:ARG:NH1	2.35	0.59
1:G:74:THR:HA	1:G:103:ASP:O	2.02	0.59
1:J:86:LEU:HB3	1:J:92:GLY:HA3	1.84	0.59
1:I:116:ASP:HB3	1:I:123:PHE:HE2	1.67	0.58
1:A:74:THR:HA	1:A:103:ASP:O	2.04	0.58
1:E:135:LEU:HD21	1:E:138:ILE:HG13	1.86	0.57
1:A:86:LEU:HB3	1:A:92:GLY:HA3	1.86	0.57
1:H:93:LEU:HB3	1:H:96:MET:HE2	1.87	0.57
1:H:130:ASP:OD2	1:H:136:ARG:NH1	2.38	0.57
1:I:2:VAL:N	1:J:1:MET:H2	2.03	0.57
1:F:86:LEU:HB3	1:F:92:GLY:HA3	1.87	0.56
1:B:46:PHE:N	1:B:47:VAL:HA	2.12	0.56
1:F:52:ILE:HG22	1:F:96:MET:HE2	1.88	0.56
1:A:57:ASP:OD1	1:A:88:ARG:NH2	2.38	0.56
1:C:48:SER:HB2	1:C:124:ARG:HH22	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:PRO:HA	1:D:134:ILE:HA	1.88	0.55
1:G:31:ARG:HH21	1:G:133:GLY:HA3	1.71	0.55
1:G:116:ASP:OD1	1:H:7:ARG:NH2	2.38	0.55
1:D:74:THR:HA	1:D:103:ASP:O	2.06	0.55
1:C:56:SER:HA	1:C:98:ILE:HD13	1.87	0.55
1:F:4:LEU:HB3	1:F:7:ARG:HD2	1.89	0.54
1:E:74:THR:HA	1:E:103:ASP:O	2.06	0.54
1:H:4:LEU:HB2	1:H:7:ARG:HD3	1.90	0.54
1:H:13:LYS:HG3	1:H:26:CYS:HB3	1.88	0.54
1:I:93:LEU:HB3	1:I:96:MET:HE2	1.89	0.54
1:I:3:LEU:HD23	1:J:2:VAL:HG21	1.91	0.53
1:B:86:LEU:HB3	1:B:92:GLY:HA3	1.91	0.53
1:G:26:CYS:SG	4:G:2003:HOH:O	2.59	0.53
1:A:57:ASP:CG	1:A:88:ARG:HH22	2.17	0.52
1:H:58:GLN:HG3	1:H:149:VAL:HG11	1.90	0.52
1:I:6:ASN:HB3	1:I:7:ARG:NH1	2.25	0.52
1:B:36:VAL:HB	1:B:69:VAL:HG22	1.91	0.52
1:B:51:GLU:OE2	1:B:147:ARG:N	2.43	0.52
1:F:93:LEU:HB3	1:F:96:MET:SD	2.50	0.52
1:H:53:ILE:HG13	1:H:96:MET:HE1	1.92	0.52
1:D:30:TYR:CE1	1:D:68:GLN:HG2	2.45	0.51
1:A:13:LYS:HD2	1:A:24:GLU:HG2	1.92	0.51
1:I:109:SER:HB2	1:I:115:PHE:HB2	1.91	0.51
1:I:74:THR:HA	1:I:103:ASP:O	2.10	0.51
1:G:125:GLY:O	1:G:147:ARG:NH1	2.43	0.51
1:H:74:THR:HA	1:H:103:ASP:O	2.10	0.51
1:A:118:GLU:O	1:J:105:LYS:HD3	2.10	0.51
1:B:128:ILE:HB	1:B:137:GLN:HB3	1.92	0.51
1:A:7:ARG:NH2	1:B:116:ASP:OD1	2.34	0.51
1:F:151:GLU:HG2	3:F:1165:PEG:H41	1.93	0.51
1:G:141:ASN:OD1	1:H:137:GLN:NE2	2.30	0.51
1:A:119:ASP:OD2	1:A:143:LYS:NZ	2.43	0.50
1:C:30:TYR:CE1	1:C:68:GLN:HG2	2.47	0.50
1:A:93:LEU:O	1:A:96:MET:HE3	2.11	0.50
1:H:61:GLU:HB3	1:H:65:ARG:HH21	1.77	0.50
1:B:137:GLN:NE2	1:B:139:THR:OG1	2.40	0.50
1:C:48:SER:N	1:C:49:PRO:HD2	2.26	0.50
1:C:51:GLU:CD	1:C:147:ARG:HH21	2.19	0.50
1:F:61:GLU:O	1:F:65:ARG:HG3	2.11	0.50
1:F:103:ASP:HB2	1:F:108:ILE:HD12	1.93	0.50
1:C:74:THR:HA	1:C:103:ASP:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:ARG:O	1:I:160:GLN:NE2	2.38	0.50
1:F:65:ARG:HE	1:F:153:LEU:HD12	1.76	0.49
1:G:86:LEU:HB3	1:G:92:GLY:HA3	1.92	0.49
1:F:139:THR:HG21	3:F:1165:PEG:H32	1.93	0.49
1:I:116:ASP:HB3	1:I:123:PHE:CE2	2.46	0.49
1:E:36:VAL:HG13	1:E:69:VAL:HA	1.94	0.49
1:I:124:ARG:HB3	1:I:147:ARG:CZ	2.42	0.49
1:F:124:ARG:HB3	1:F:147:ARG:CZ	2.43	0.48
1:G:30:TYR:CE1	1:G:68:GLN:HG2	2.48	0.48
1:F:31:ARG:HG3	1:F:131:PRO:O	2.12	0.48
1:J:124:ARG:HB3	1:J:147:ARG:CZ	2.43	0.48
1:F:65:ARG:HD2	1:F:156:LEU:HD23	1.96	0.48
1:E:47:VAL:HG22	1:E:124:ARG:NH2	2.28	0.48
1:J:130:ASP:OD2	1:J:136:ARG:NH1	2.46	0.48
1:F:51:GLU:OE1	1:F:124:ARG:NH1	2.47	0.48
1:B:126:LEU:HB3	1:B:139:THR:HB	1.96	0.47
1:A:124:ARG:HB3	1:A:147:ARG:CZ	2.44	0.47
1:H:124:ARG:NH2	2:H:1164:SO4:O1	2.47	0.47
1:A:116:ASP:OD1	1:B:7:ARG:NH2	2.47	0.47
1:E:48:SER:N	1:E:49:PRO:HD2	2.29	0.47
1:H:75:ASP:CG	1:I:104:ARG:HH22	2.23	0.47
1:C:123:PHE:CE2	1:D:4:LEU:HG	2.50	0.47
1:I:4:LEU:HD21	1:J:113:GLY:O	2.15	0.47
1:H:54:ALA:O	1:H:58:GLN:HG2	2.13	0.47
1:E:124:ARG:HB3	1:E:147:ARG:CZ	2.45	0.47
1:E:126:LEU:HB3	1:E:139:THR:HB	1.97	0.47
1:D:40:TYR:CZ	1:D:73:SER:HB3	2.50	0.46
1:F:51:GLU:CD	1:F:147:ARG:HH21	2.23	0.46
1:I:52:ILE:HG22	1:I:96:MET:HE3	1.97	0.46
1:D:124:ARG:HB3	1:D:147:ARG:CZ	2.46	0.46
1:B:38:PHE:CZ	1:B:52:ILE:HG23	2.51	0.46
1:A:13:LYS:HD3	1:A:26:CYS:HB3	1.98	0.46
1:F:114:VAL:HG12	1:F:123:PHE:HB2	1.97	0.46
1:E:38:PHE:HB2	1:E:147:ARG:NH1	2.31	0.46
1:A:36:VAL:HB	1:A:69:VAL:HG22	1.97	0.46
1:C:137:GLN:HB2	1:C:159:PHE:CE2	2.51	0.46
1:G:124:ARG:HB3	1:G:147:ARG:CZ	2.45	0.46
1:D:136:ARG:HA	1:D:136:ARG:HD3	1.72	0.46
1:A:33:LYS:HB2	1:A:66:ASN:O	2.16	0.45
1:B:38:PHE:HZ	1:B:52:ILE:HG23	1.80	0.45
1:J:3:LEU:HD11	1:J:112:TYR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:73:SER:OG	1:I:75:ASP:OD2	2.26	0.45
1:J:101:LEU:HD21	1:J:108:ILE:HD13	1.99	0.45
1:J:73:SER:HB3	1:J:80:HIS:CE1	2.52	0.45
1:B:28:LYS:O	1:B:31[A]:ARG:NH1	2.44	0.45
1:A:96:MET:HA	1:A:96:MET:HE2	1.99	0.45
1:E:136:ARG:HA	1:E:136:ARG:HD3	1.75	0.44
1:H:30:TYR:CE1	1:H:68:GLN:HG2	2.52	0.44
1:H:136:ARG:HD2	1:H:163:GLU:OE2	2.17	0.44
1:J:73:SER:HB3	1:J:80:HIS:HE1	1.82	0.44
1:E:4:LEU:HD11	1:F:113:GLY:O	2.17	0.44
1:C:51:GLU:OE1	1:C:124:ARG:NH1	2.50	0.44
1:C:125:GLY:O	1:C:147:ARG:NH1	2.50	0.44
1:I:30:TYR:CE1	1:I:68:GLN:HG2	2.52	0.44
1:B:65:ARG:HD2	1:B:156:LEU:HD23	2.00	0.44
1:F:151:GLU:O	1:F:155:LEU:HD13	2.18	0.44
1:H:105:LYS:HD2	1:I:119:ASP:HA	1.99	0.44
1:I:124:ARG:NE	1:I:143:LYS:O	2.34	0.44
1:A:73:SER:HB3	1:A:80:HIS:HE1	1.81	0.44
1:F:147:ARG:HB3	3:F:1165:PEG:H12	2.00	0.44
1:G:31:ARG:HG3	1:G:131:PRO:O	2.17	0.43
1:D:130:ASP:OD1	1:D:134:ILE:N	2.41	0.43
1:H:3:LEU:HB2	3:H:1165:PEG:H12	1.99	0.43
1:A:116:ASP:OD2	1:A:143:LYS:NZ	2.42	0.43
1:I:116:ASP:HB2	1:J:7:ARG:NH2	2.33	0.43
1:E:159:PHE:HA	1:E:162:VAL:HG22	2.01	0.43
1:C:96:MET:HE3	1:C:96:MET:HB3	1.92	0.43
1:J:73:SER:OG	1:J:75:ASP:OD1	2.29	0.43
1:E:69:VAL:O	1:E:99:PRO:HD2	2.19	0.43
1:F:137:GLN:HB2	1:F:159:PHE:CZ	2.54	0.43
1:I:153:LEU:HD12	1:I:153:LEU:HA	1.90	0.43
1:A:164:LYS:HA	1:A:164:LYS:HD3	1.78	0.43
1:C:12:PHE:CE2	1:C:27:LEU:HD13	2.54	0.43
1:I:31:ARG:HA	1:I:31:ARG:HD3	1.78	0.43
1:C:123:PHE:HE2	1:D:4:LEU:HG	1.84	0.42
1:A:40:TYR:CZ	1:A:73:SER:HB2	2.54	0.42
1:B:65:ARG:O	1:B:160:GLN:NE2	2.52	0.42
1:J:124:ARG:NH2	2:J:1165:SO4:O3	2.52	0.42
1:E:58:GLN:OE1	1:E:149:VAL:HG11	2.19	0.42
1:J:18:ILE:HD12	1:J:23:LYS:HB2	2.01	0.42
1:C:117:GLU:H	1:C:117:GLU:CD	2.28	0.42
1:A:52:ILE:HG22	1:A:96:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:OG	1:A:75:ASP:OD1	2.28	0.42
1:H:48:SER:O	1:H:52:ILE:HG13	2.19	0.42
1:F:103:ASP:OD2	1:F:106:GLN:HA	2.20	0.42
1:B:12:PHE:CE2	1:B:27:LEU:HD13	2.55	0.42
1:B:124:ARG:HB3	1:B:147:ARG:CZ	2.49	0.41
1:H:136:ARG:NH1	1:H:163:GLU:OE2	2.43	0.41
1:J:59:VAL:HG11	1:J:97:LYS:HE3	2.01	0.41
1:G:65:ARG:O	1:G:160:GLN:NE2	2.49	0.41
1:J:52:ILE:HG22	1:J:96:MET:SD	2.60	0.41
1:B:104:ARG:HH22	1:C:75:ASP:CG	2.28	0.41
1:D:119:ASP:HB3	1:D:121:ASN:H	1.85	0.41
1:J:137:GLN:HB2	1:J:159:PHE:CE2	2.55	0.41
1:I:6:ASN:HB3	1:I:7:ARG:HH11	1.84	0.41
1:J:124:ARG:NE	1:J:143:LYS:O	2.51	0.41
1:C:17:VAL:HA	1:C:21:GLU:O	2.21	0.41
1:D:84:ASP:HA	1:D:93:LEU:HB2	2.02	0.41
1:C:69:VAL:O	1:C:99:PRO:HD2	2.21	0.41
1:A:101:LEU:HD21	1:A:108:ILE:HD13	2.03	0.41
1:J:58:GLN:HG2	1:J:149:VAL:HG11	2.03	0.41
1:A:28:LYS:HE3	1:A:28:LYS:HB3	1.86	0.41
1:C:3:LEU:HD12	1:C:3:LEU:HA	1.85	0.41
1:I:105:LYS:HB3	1:I:107:GLU:HG3	2.01	0.41
1:G:2:VAL:N	4:G:2001:HOH:O	2.54	0.41
1:B:126:LEU:N	1:B:139:THR:O	2.46	0.40
1:H:52:ILE:HG22	1:H:96:MET:HE3	2.03	0.40
1:A:130:ASP:HB3	1:A:136:ARG:HD3	2.04	0.40
1:F:12:PHE:CE2	1:F:27:LEU:HB2	2.56	0.40
1:A:86:LEU:HB3	1:A:92:GLY:CA	2.52	0.40
1:G:93:LEU:O	1:G:96:MET:HE3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	F	1164	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	H	1164	-	4,4,4	0.24	0	6,6,6	0.05	0
3	PEG	F	1166	-	6,6,6	0.67	0	5,5,5	1.34	0
2	SO4	J	1166	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	1165	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	A	1165	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	I	1166	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	J	1165	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	E	1164	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	D	1165	-	4,4,4	0.26	0	6,6,6	0.04	0
3	PEG	I	1167	-	6,6,6	0.66	0	5,5,5	1.42	0
3	PEG	F	1165	-	6,6,6	0.64	0	5,5,5	1.56	0
2	SO4	I	1165	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	G	1164	-	4,4,4	0.22	0	6,6,6	0.11	0
3	PEG	H	1165	-	6,6,6	0.63	0	5,5,5	1.49	0
2	SO4	I	1164	-	4,4,4	0.22	0	6,6,6	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	F	1166	-	-	0/4/4/4	-
3	PEG	I	1167	-	-	3/4/4/4	-
3	PEG	H	1165	-	-	3/4/4/4	-
3	PEG	F	1165	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1165	PEG	O2-C3-C4-O4
3	H	1165	PEG	O1-C1-C2-O2
3	I	1167	PEG	C4-C3-O2-C2
3	I	1167	PEG	C1-C2-O2-C3
3	I	1167	PEG	O2-C3-C4-O4
3	H	1165	PEG	C4-C3-O2-C2
3	F	1165	PEG	C4-C3-O2-C2
3	H	1165	PEG	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1164	SO4	1	0
2	C	1165	SO4	1	0
2	J	1165	SO4	1	0
3	F	1165	PEG	3	0
2	G	1164	SO4	1	0
3	H	1165	PEG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	162/222 (72%)	-1.69	0 100 100	22, 25, 29, 34	0
1	B	164/222 (73%)	-1.65	0 100 100	15, 28, 34, 37	3 (1%)
1	C	164/222 (73%)	-1.64	0 100 100	25, 29, 34, 36	0
1	D	163/222 (73%)	-1.64	0 100 100	16, 27, 32, 37	1 (0%)
1	E	161/222 (72%)	-1.63	0 100 100	25, 28, 32, 34	0
1	F	163/222 (73%)	-1.67	0 100 100	18, 27, 30, 32	1 (0%)
1	G	162/222 (72%)	-1.65	0 100 100	24, 28, 32, 34	0
1	H	163/222 (73%)	-1.66	0 100 100	16, 27, 31, 40	1 (0%)
1	I	162/222 (72%)	-1.69	0 100 100	23, 25, 29, 32	0
1	J	164/222 (73%)	-1.64	0 100 100	24, 27, 32, 36	0
All	All	1628/2220 (73%)	-1.66	0 100 100	15, 27, 32, 40	6 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	F	1166	7/7	0.98	0.04	28,31,33,35	0
2	SO4	G	1164	5/5	0.99	0.04	27,28,29,29	5
2	SO4	H	1164	5/5	0.99	0.05	29,30,31,32	0
2	SO4	I	1165	5/5	0.99	0.04	30,30,31,31	5
2	SO4	J	1166	5/5	0.99	0.03	26,27,28,28	5
3	PEG	F	1165	7/7	0.99	0.05	26,26,27,28	0
2	SO4	C	1165	5/5	0.99	0.04	29,30,31,32	5
3	PEG	H	1165	7/7	0.99	0.04	28,29,32,35	0
3	PEG	I	1167	7/7	0.99	0.03	25,26,27,28	0
2	SO4	I	1166	5/5	1.00	0.03	26,28,28,28	5
2	SO4	J	1165	5/5	1.00	0.04	27,29,30,30	0
2	SO4	F	1164	5/5	1.00	0.03	23,24,25,26	0
2	SO4	A	1165	5/5	1.00	0.02	23,25,25,25	0
2	SO4	D	1165	5/5	1.00	0.03	25,26,26,27	0
2	SO4	I	1164	5/5	1.00	0.03	25,26,27,28	0
2	SO4	E	1164	5/5	1.00	0.02	28,29,29,30	5

6.5 Other polymers [i](#)

There are no such residues in this entry.