



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:23 am GMT

PDB ID : 3ZL5  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

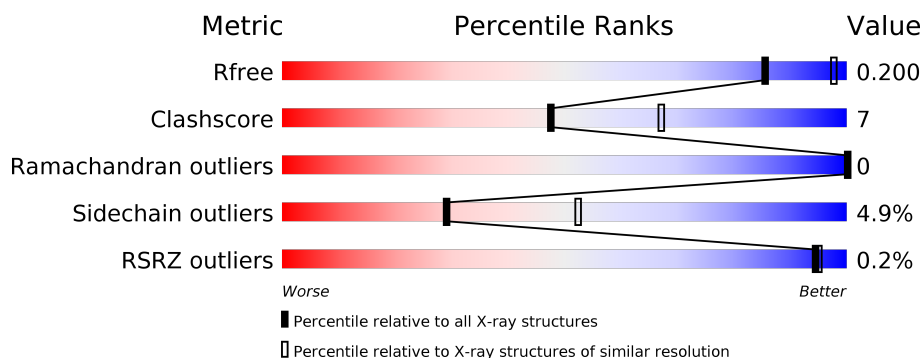
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	222	
1	B	222	
1	C	222	
1	D	222	
1	E	222	
1	F	222	

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Mol	Chain	Length	Quality of chain
1	G	222	
1	H	222	
1	I	222	
1	J	222	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	G	1164	-	-	-	X
3	PEG	F	1165	-	-	-	X
3	PEG	I	1167	-	-	-	X

## 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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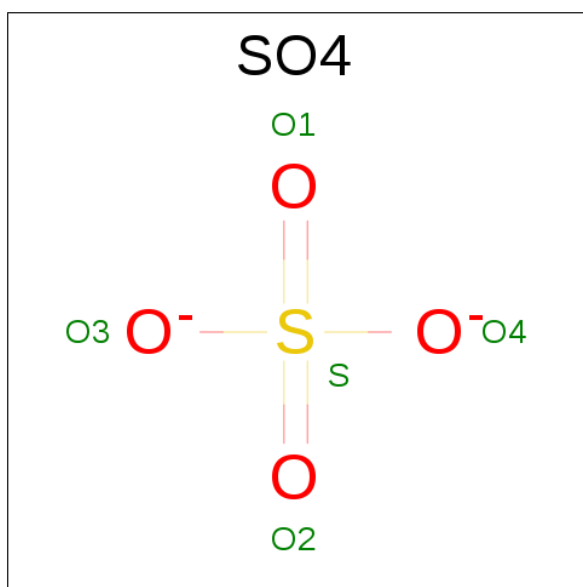
Chain	Residue	Modelled	Actual	Comment	Reference
H	48	SER	CYS	ENGINEERED MUTATION	UNP O97161
I	-36	MET	-	EXPRESSION TAG	UNP O97161
I	-35	ARG	-	EXPRESSION TAG	UNP O97161
I	-34	GLY	-	EXPRESSION TAG	UNP O97161
I	-33	SER	-	EXPRESSION TAG	UNP O97161
I	-32	HIS	-	EXPRESSION TAG	UNP O97161
I	-31	HIS	-	EXPRESSION 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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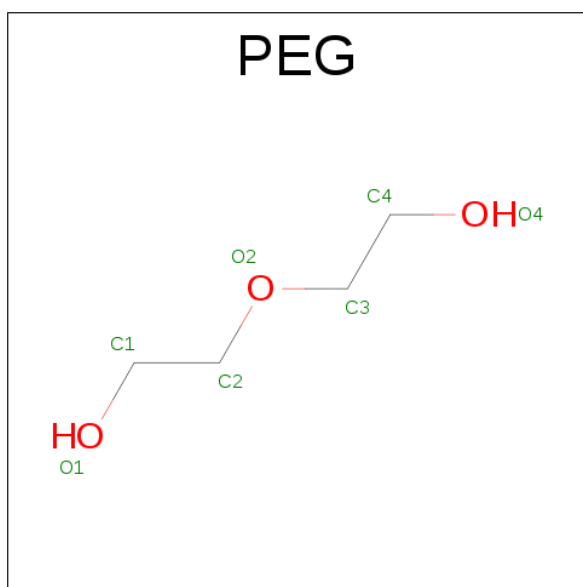
Chain	Residue	Modelled	Actual	Comment	Reference
J	-33	SER	-	EXPRESSION TAG	UNP O97161
J	-32	HIS	-	EXPRESSION TAG	UNP O97161
J	-31	HIS	-	EXPRESSION TAG	UNP O97161
J	-30	HIS	-	EXPRESSION TAG	UNP O97161
J	-29	HIS	-	EXPRESSION TAG	UNP O97161
J	-28	HIS	-	EXPRESSION TAG	UNP O97161
J	-27	HIS	-	EXPRESSION TAG	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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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.

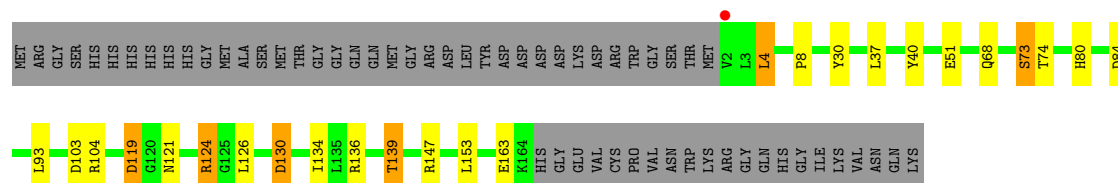
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	14	Total	O	0	0
			14	14		
4	C	7	Total	O	0	0
			7	7		
4	D	11	Total	O	0	0
			11	11		
4	E	9	Total	O	0	0
			9	9		
4	F	14	Total	O	0	0
			14	14		
4	G	9	Total	O	0	0
			9	9		
4	H	12	Total	O	0	0
			12	12		

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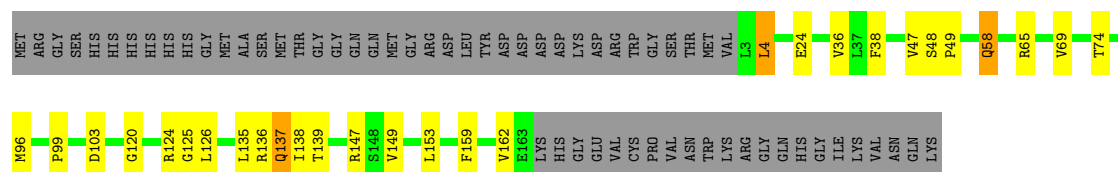
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	24	Total 24	O 24	0	0
4	J	5	Total 5	O 5	0	0





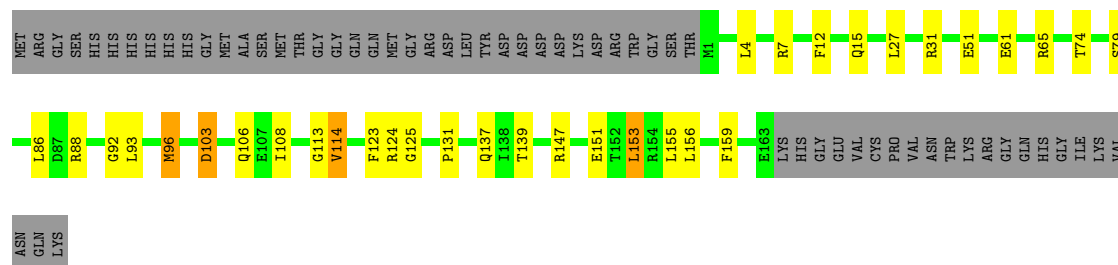
• Molecule 1: PEROXIREDOXIN I

Chain E: 60% 11% 27%



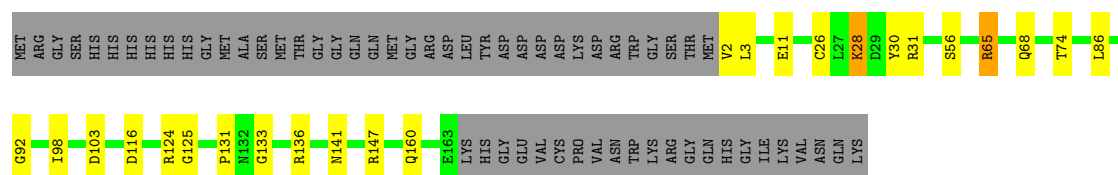
• Molecule 1: PEROXIREDOXIN I

Chain F: 59% 13% 27%



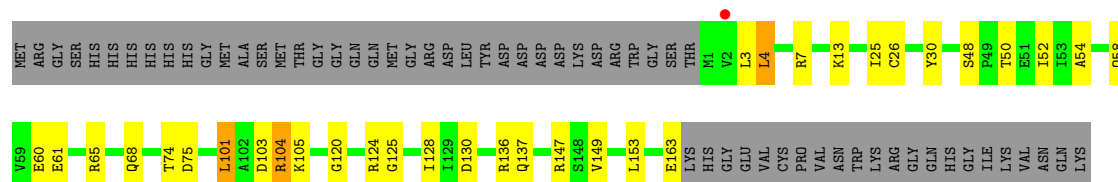
• Molecule 1: PEROXIREDOXIN I

Chain G: 62% 10% 27%



• Molecule 1: PEROXIREDOXIN I

Chain H: 59% 14% 27%



• Molecule 1: PEROXIREDOXIN I

Chain I: 59% 13% 27%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.188 , 0.203 0.187 , 0.200	Depositor DCC
$R_{free}$ test set	4042 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 13.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	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	0.93	EDS
Total number of atoms	13287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: PEG, SO4

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	0.26	0/1328	0.50	0/1794
1	B	0.25	0/1371	0.49	0/1851
1	C	0.27	0/1343	0.49	0/1814
1	D	0.27	0/1346	0.51	0/1818
1	E	0.27	0/1319	0.50	0/1783
1	F	0.26	0/1343	0.49	0/1814
1	G	0.25	0/1326	0.51	0/1793
1	H	0.27	0/1345	0.50	0/1817
1	I	0.26	0/1326	0.48	0/1793
1	J	0.26	0/1343	0.49	0/1814
All	All	0.26	0/13390	0.50	0/18091

There are no bond length outliers.

There are no bond angle outliers.

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	24	0
1	B	1333	0	1317	21	0
1	C	1314	0	1294	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1314	0	1295	15	0
1	E	1290	0	1260	16	0
1	F	1311	0	1294	23	0
1	G	1297	0	1269	15	0
1	H	1313	0	1294	22	0
1	I	1297	0	1269	23	0
1	J	1314	0	1294	22	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	183	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 (183) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:126:LEU:HB3	1:D:139:THR:HG22	1.74	0.69
1:C:124:ARG:NH2	2:C:1165:SO4:O2	2.25	0.69
1:F:65:ARG:HH21	1:F:153:LEU:HG	1.58	0.69
1:G:11:GLU:OE1	1:G:28:LYS:NZ	2.22	0.67
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:142:ASP:OD2	1:D:136:ARG:NH1	2.31	0.63
1:C:65:ARG:O	1:C:160:GLN:NE2	2.29	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:130:ASP:OD2	1:H:136:ARG:NH1	2.38	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:I:2:VAL:N	1:J:1:MET:H2	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:119:ASP:OD2	1:B:143:LYS:NZ	2.37	0.53
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: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: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: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:F:103:ASP:HB2	1:F:108:ILE:HD12	1.93	0.50
1:F:61:GLU:O	1:F:65:ARG:HG3	2.11	0.50
1:C:74:THR:HA	1:C:103:ASP:O	2.12	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:57:ASP:CG	1:A:88:ARG:HH22	2.17	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: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: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
1:C:51:GLU:CD	1:C:147:ARG:HH21	2.19	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:E:136:ARG:HA	1:E:136:ARG:HD3	1.75	0.44
1:H:136:ARG:HD2	1:H:163:GLU:OE2	2.17	0.44
1:H:30:TYR:CE1	1:H:68:GLN:HG2	2.52	0.44
1:C:52:ILE:HG22	1:C:96:MET:HE1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:73:SER:OG	1:I:75:ASP:OD2	2.26	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:H:75:ASP:CG	1:I:104:ARG:HH22	2.23	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:A:52:ILE:HG22	1:A:96:MET:SD	2.60	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:3:LEU:HA	1:C:3:LEU:HD12	1.85	0.41
1:A:28:LYS:HB3	1:A:28:LYS:HE3	1.86	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:F:51:GLU:CD	1:F:147:ARG:HH21	2.23	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

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	160/222 (72%)	159 (99%)	1 (1%)	0	100	100
1	B	165/222 (74%)	162 (98%)	3 (2%)	0	100	100
1	C	162/222 (73%)	157 (97%)	5 (3%)	0	100	100
1	D	162/222 (73%)	158 (98%)	4 (2%)	0	100	100
1	E	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
1	F	162/222 (73%)	159 (98%)	3 (2%)	0	100	100
1	G	160/222 (72%)	156 (98%)	4 (2%)	0	100	100
1	H	162/222 (73%)	158 (98%)	4 (2%)	0	100	100
1	I	160/222 (72%)	156 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	162/222 (73%)	159 (98%)	3 (2%)	0	100	100
All	All	1614/2220 (73%)	1582 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/191 (74%)	134 (95%)	7 (5%)	28	51
1	B	146/191 (76%)	138 (94%)	8 (6%)	25	46
1	C	143/191 (75%)	134 (94%)	9 (6%)	21	38
1	D	143/191 (75%)	133 (93%)	10 (7%)	18	33
1	E	140/191 (73%)	133 (95%)	7 (5%)	28	51
1	F	143/191 (75%)	136 (95%)	7 (5%)	29	52
1	G	141/191 (74%)	137 (97%)	4 (3%)	49	76
1	H	143/191 (75%)	137 (96%)	6 (4%)	34	59
1	I	141/191 (74%)	135 (96%)	6 (4%)	33	58
1	J	143/191 (75%)	136 (95%)	7 (5%)	29	52
All	All	1424/1910 (75%)	1353 (95%)	71 (5%)	29	51

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	89	LYS
1	A	105	LYS
1	A	114	VAL
1	A	130	ASP
1	A	136	ARG
1	A	153	LEU
1	B	2	VAL

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Mol	Chain	Res	Type
1	B	3	LEU
1	B	24	GLU
1	B	31[A]	ARG
1	B	31[B]	ARG
1	B	47	VAL
1	B	52	ILE
1	B	130	ASP
1	C	1	MET
1	C	3	LEU
1	C	47	VAL
1	C	63	ASN
1	C	65	ARG
1	C	80	HIS
1	C	105	LYS
1	C	116	ASP
1	C	153	LEU
1	D	4	LEU
1	D	37	LEU
1	D	73	SER
1	D	80	HIS
1	D	119	ASP
1	D	124	ARG
1	D	130	ASP
1	D	139	THR
1	D	153	LEU
1	D	163	GLU
1	E	4	LEU
1	E	24	GLU
1	E	58	GLN
1	E	65	ARG
1	E	96	MET
1	E	137	GLN
1	E	153	LEU
1	F	15	GLN
1	F	79	SER
1	F	88	ARG
1	F	96	MET
1	F	103	ASP
1	F	114	VAL
1	F	153	LEU
1	G	3	LEU
1	G	28	LYS

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Mol	Chain	Res	Type
1	G	65	ARG
1	G	136	ARG
1	H	4	LEU
1	H	50	THR
1	H	60	GLU
1	H	101	LEU
1	H	104	ARG
1	H	153	LEU
1	I	65	ARG
1	I	80	HIS
1	I	90	SER
1	I	100	LEU
1	I	109	SER
1	I	153	LEU
1	J	2	VAL
1	J	47	VAL
1	J	58	GLN
1	J	80	HIS
1	J	93	LEU
1	J	136	ARG
1	J	153	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	141	ASN
1	J	66	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	1165	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	C	1165	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	D	1165	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	E	1164	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	F	1164	-	4,4,4	0.16	0	6,6,6	0.09	0
3	PEG	F	1165	-	6,6,6	0.63	0	5,5,5	1.52	0
3	PEG	F	1166	-	6,6,6	0.66	0	5,5,5	1.31	0
2	SO4	G	1164	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	H	1164	-	4,4,4	0.15	0	6,6,6	0.06	0
3	PEG	H	1165	-	6,6,6	0.62	0	5,5,5	1.45	0
2	SO4	I	1164	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	I	1165	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	I	1166	-	4,4,4	0.12	0	6,6,6	0.13	0
3	PEG	I	1167	-	6,6,6	0.65	0	5,5,5	1.38	0
2	SO4	J	1165	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	J	1166	-	4,4,4	0.15	0	6,6,6	0.04	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
2	SO4	A	1165	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1165	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1165	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1164	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1164	-	-	0/0/0/0	0/0/0/0
3	PEG	F	1165	-	-	0/4/4/4	0/0/0/0
3	PEG	F	1166	-	-	0/4/4/4	0/0/0/0
2	SO4	G	1164	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1164	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	H	1165	-	-	0/4/4/4	0/0/0/0
2	SO4	I	1164	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1165	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1166	-	-	0/0/0/0	0/0/0/0
3	PEG	I	1167	-	-	0/4/4/4	0/0/0/0
2	SO4	J	1165	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1166	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	162/222 (72%)	-0.09	0 100 100	22, 25, 29, 34	0
1	B	164/222 (73%)	-0.00	0 100 100	25, 28, 34, 37	0
1	C	164/222 (73%)	-0.03	1 (0%) 89 89	25, 29, 34, 36	0
1	D	163/222 (73%)	-0.07	1 (0%) 89 89	24, 27, 32, 37	0
1	E	161/222 (72%)	0.01	0 100 100	25, 28, 32, 34	0
1	F	163/222 (73%)	-0.08	0 100 100	23, 27, 30, 32	0
1	G	162/222 (72%)	-0.10	0 100 100	24, 28, 32, 34	0
1	H	163/222 (73%)	-0.07	1 (0%) 89 89	24, 27, 31, 40	0
1	I	162/222 (72%)	-0.12	0 100 100	23, 25, 29, 32	0
1	J	164/222 (73%)	-0.09	0 100 100	24, 27, 32, 36	0
All	All	1628/2220 (73%)	-0.06	3 (0%) 94 95	22, 27, 32, 40	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	VAL	2.9
1	H	2	VAL	2.4
1	C	47	VAL	2.4

### 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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	F	1165	7/7	0.90	0.25	5.20	26,26,27,28	0
3	PEG	I	1167	7/7	0.91	0.20	3.37	25,26,27,28	0
2	SO4	G	1164	5/5	0.94	0.24	2.63	27,28,29,29	5
3	PEG	H	1165	7/7	0.91	0.28	1.96	28,29,32,35	0
2	SO4	J	1166	5/5	0.96	0.14	-0.18	26,27,28,28	5
2	SO4	H	1164	5/5	0.98	0.15	-0.30	29,30,31,32	0
2	SO4	C	1165	5/5	0.97	0.17	-0.30	29,30,31,32	5
2	SO4	E	1164	5/5	0.98	0.15	-0.45	28,29,29,30	5
2	SO4	J	1165	5/5	0.97	0.14	-0.68	27,29,30,30	0
2	SO4	A	1165	5/5	0.99	0.12	-1.24	23,25,25,25	0
2	SO4	F	1164	5/5	0.99	0.12	-1.59	23,24,25,26	0
2	SO4	I	1164	5/5	0.99	0.10	-1.87	25,26,27,28	0
2	SO4	D	1165	5/5	0.99	0.11	-3.88	25,26,26,27	0
3	PEG	F	1166	7/7	0.94	0.22	-	28,31,33,35	0
2	SO4	I	1166	5/5	0.95	0.20	-	26,28,28,28	5
2	SO4	I	1165	5/5	0.95	0.20	-	30,30,31,31	5

## 6.5 Other polymers

There are no such residues in this entry.