



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:11 am BST

PDB ID : 3ZTL
Title : Crystal structure of decameric form of Peroxiredoxin I from *Schistosoma mansoni*
Authors : Saccoccia, F.; Angelucci, F.; Bellelli, A.; Boumis, G.; Brunori, M.; Miele, A.E.
Deposited on : 2011-07-11
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

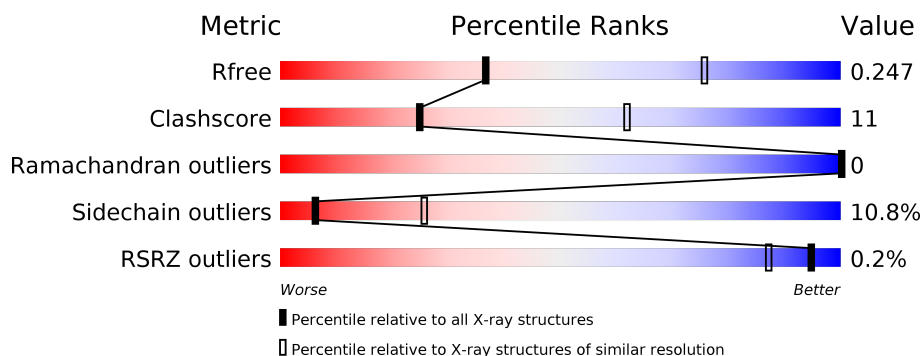
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div></div><div>57%20%19%</div></div>
1	H	222	<div><div>%</div><div></div><div>54%23%20%</div></div>
1	I	222	<div><div></div><div>56%21%20%</div></div>
1	J	222	<div><div></div><div>60%18%5%18%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14405 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 THIOREDOXIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1442	922	249	265	6			
1	B	183	Total	C	N	O	S	0	2	0
			1477	946	255	269	7			
1	C	182	Total	C	N	O	S	0	0	0
			1457	932	251	267	7			
1	D	172	Total	C	N	O	S	0	2	0
			1392	892	237	257	6			
1	E	176	Total	C	N	O	S	0	0	0
			1414	903	244	261	6			
1	F	181	Total	C	N	O	S	0	0	0
			1450	927	250	266	7			
1	G	180	Total	C	N	O	S	0	1	0
			1448	926	249	267	6			
1	H	178	Total	C	N	O	S	0	0	0
			1429	913	246	263	7			
1	I	178	Total	C	N	O	S	0	1	0
			1432	915	246	265	6			
1	J	183	Total	C	N	O	S	0	0	0
			1464	936	252	269	7			

There are 370 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
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
B	-23	SER	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
C	-19	GLY	-	expression tag	UNP O97161
C	-18	GLN	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
D	-15	GLY	-	expression tag	UNP O97161
D	-14	ARG	-	expression tag	UNP O97161
D	-13	ASP	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP O97161
F	-1	SER	-	expression tag	UNP O97161
F	0	THR	-	expression tag	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
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
H	-36	MET	-	expression tag	UNP O97161
H	-35	ARG	-	expression tag	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
J	-36	MET	-	expression tag	UNP O97161
J	-35	ARG	-	expression tag	UNP O97161
J	-34	GLY	-	expression tag	UNP O97161
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

• Molecule 1: THIOREDOXIN PEROXIDASE

[illegible]

• Molecule 1: THIOREDOXIN PEROXIDASE

V182	E51	MET
N183	I52	ARG
GLN	V59	GLY
LYS	S73	SER
	T74	HIS
	H80	HIS
	D84	HIS
	H85	GLY
	L86	GLY
	G92	MET
	L93	THR
	G94	GLY
	H95	GLY
	M96	GLN
	L100	GLN
	D103	MET
	R104	GLY
	K105	ARG
	Q106	ASP
	G113	LYS
	F123	TRP
	R124	ARG
	G125	GLY
	I128	GLY
	I129	GLY
	D130	SER
	P131	THR
	Q137	M1
	I138	V2
	T139	L3
	R147	K13
	A158	A16
	F161	V17
	V162	I18
	E163	K23
	K164	E24
	V168	C26
	K174	Y40
	R175	D43
	H178	V47
	G179	C48
	I180	P49
	F181	T50

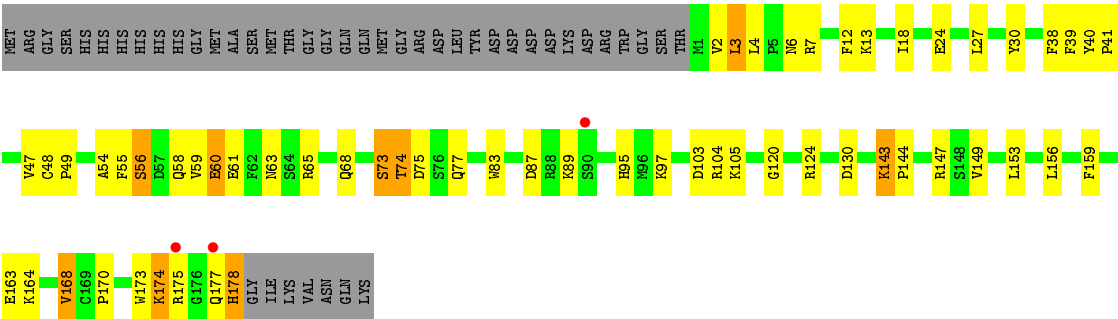
● Molecule 1: THIOREDOXIN PEROXIDASE

S73	ARG	MET
T74	GLY	
Q77	SER	
D87	HIS	
L93	HIS	
M96	HIS	
K97	HIS	
I98	GLY	
	MET	
	ALA	
D103	SER	
R104	MET	
K105	THR	
Q106	GLY	
	GLY	
S109	GLN	
F115	GLN	
D116	GLY	
	ARG	
M121	ASP	
A122	LEU	
F123	TYR	
R124	ASP	
G125	ASP	
	ASP	
D130	ASP	
	LYS	
I134	ASP	
	ARG	
T139	TRP	
	GLY	
D142	SER	
K143	THR	
P144		M1
		V2
L153		L3
L156	F12	
	K13	
F159		
Q160	C26	
	L27	
E163		
	P41	
V168	F46	
C169	V47	
P170	C48	
M173	P49	
K174		
R175	I52	
V182	Q58	
ASN		
GLN		
THR	R65	

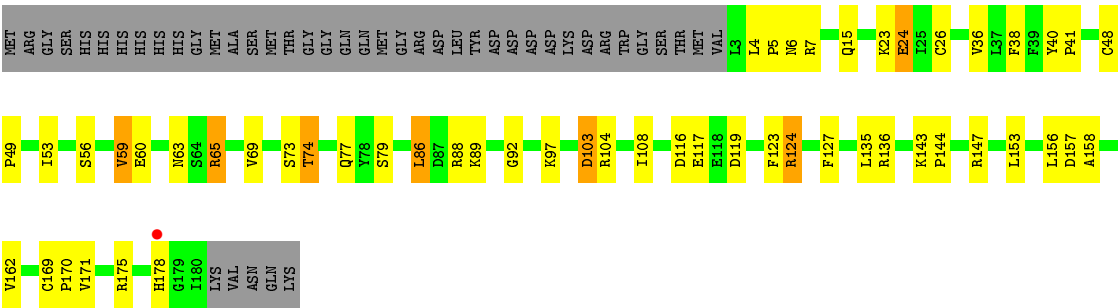
● Molecule 1: THIOREDOXIN PEROXIDASE



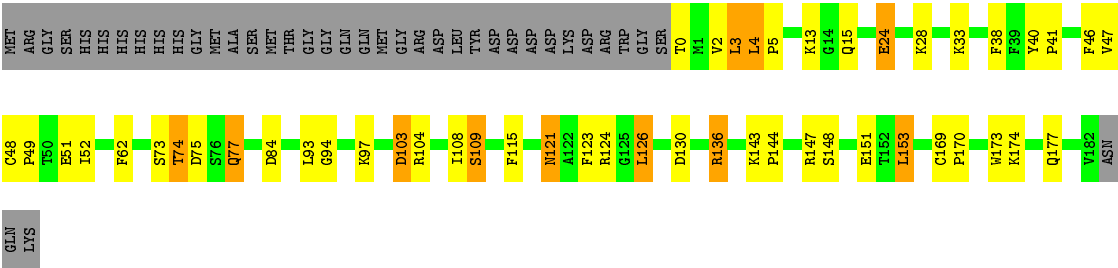
WORLD WIDE
PDB
PROTEIN DATA BANK



● Molecule 1: THIOREDOXIN PEROXIDASE



● Molecule 1: THIOREDOXIN PEROXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.51Å 116.90Å 117.35Å 69.12° 92.00° 86.93°	Depositor
Resolution (Å)	43.00 – 3.00 43.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (43.00-3.00) 99.0 (43.00-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.204 , 0.248 0.200 , 0.247	Depositor DCC
R_{free} test set	2458 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14405	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/1476	0.47	0/1994
1	B	0.30	0/1517	0.49	0/2047
1	C	0.31	0/1491	0.51	0/2014
1	D	0.31	0/1431	0.48	0/1936
1	E	0.30	0/1448	0.48	0/1957
1	F	0.29	0/1484	0.46	0/2004
1	G	0.30	0/1485	0.47	0/2006
1	H	0.30	0/1463	0.50	0/1977
1	I	0.31	0/1469	0.47	0/1985
1	J	0.30	0/1498	0.47	0/2024
All	All	0.30	0/14762	0.48	0/19944

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	143	LYS	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	1442	0	1415	26	0
1	B	1477	0	1468	29	0
1	C	1457	0	1436	36	0
1	D	1392	0	1365	42	0
1	E	1414	0	1379	50	0
1	F	1450	0	1427	22	0
1	G	1448	0	1421	35	0
1	H	1429	0	1400	37	0
1	I	1432	0	1399	33	0
1	J	1464	0	1443	36	0
All	All	14405	0	14153	307	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 11.

All (307) 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:I:86:LEU:HB3	1:I:92:GLY:HA3	1.55	0.86
1:A:41:PRO:HD2	1:A:48:CYS:SG	2.23	0.79
1:D:41:PRO:HD2	1:D:48:CYS:SG	2.23	0.79
1:E:86:LEU:HB3	1:E:92:GLY:HA3	1.64	0.79
1:E:174:LYS:HZ3	1:E:177:GLN:HG2	1.53	0.73
1:E:41:PRO:HD2	1:E:48:CYS:SG	2.29	0.72
1:I:53:ILE:HG23	1:I:88:ARG:HH21	1.54	0.72
1:E:174:LYS:HG3	1:E:177:GLN:HE21	1.55	0.71
1:D:104:ARG:HG3	1:E:120:GLY:HA3	1.73	0.70
1:G:49:PRO:HG3	1:G:83:TRP:HZ2	1.55	0.70
1:G:41:PRO:HD2	1:G:48:CYS:SG	2.31	0.69
1:C:116:ASP:HB2	1:D:7:ARG:NH2	2.08	0.68
1:D:124:ARG:HB3	1:D:147:ARG:CZ	2.24	0.67
1:C:13:LYS:HD2	1:C:26:CYS:HB3	1.75	0.67
1:J:38:PHE:HB2	1:J:147:ARG:NH1	2.10	0.66
1:B:74:THR:HA	1:B:103:ASP:HB3	1.78	0.66
1:D:74:THR:HG21	1:D:121:ASN:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:PRO:HG3	1:G:83:TRP:CZ2	2.30	0.66
1:C:41:PRO:HD2	1:C:48:CYS:SG	2.37	0.65
1:F:41:PRO:HD2	1:F:48:CYS:SG	2.36	0.64
1:H:49:PRO:HG3	1:H:83:TRP:CZ2	2.32	0.64
1:H:58:GLN:HG3	1:H:149:VAL:HG11	1.80	0.64
1:I:41:PRO:HD2	1:I:48:CYS:SG	2.38	0.64
1:B:86:LEU:HB3	1:B:92:GLY:HA3	1.78	0.64
1:C:65:ARG:HH12	1:C:175:ARG:HH11	1.45	0.63
1:H:41:PRO:HD2	1:H:48:CYS:SG	2.38	0.63
1:D:165:HIS:HB3	1:D:167:GLU:HG3	1.81	0.62
1:I:60:GLU:HA	1:I:63:ASN:HB2	1.82	0.61
1:C:74:THR:HA	1:C:103:ASP:O	2.01	0.61
1:G:46:PHE:O	1:G:49:PRO:HD2	2.00	0.61
1:D:58[B]:GLN:HG3	1:D:61:GLU:HG3	1.83	0.61
1:H:174:LYS:HE2	1:H:177:GLN:HE21	1.64	0.61
1:A:164:LYS:HD3	1:A:165:HIS:CE1	2.36	0.60
1:G:168:VAL:HG21	1:H:47:VAL:HG22	1.83	0.60
1:E:96:MET:CE	1:E:98:ILE:HG12	2.32	0.60
1:B:104:ARG:HE	1:C:121:ASN:HB3	1.67	0.59
1:C:1:MET:HA	1:D:2:VAL:HA	1.85	0.59
1:H:60:GLU:HA	1:H:63:ASN:HB2	1.85	0.58
1:C:142:ASP:O	1:C:143:LYS:HG2	2.04	0.58
1:F:124:ARG:HB3	1:F:147:ARG:CZ	2.33	0.58
1:H:177:GLN:O	1:H:178:HIS:HB2	2.03	0.58
1:E:164:LYS:HG2	1:E:165:HIS:HD2	1.67	0.58
1:D:5:PRO:O	1:D:135:LEU:O	2.21	0.58
1:I:6:ASN:HB3	1:I:7:ARG:HH11	1.69	0.58
1:G:40:TYR:CZ	1:G:73:SER:HB2	2.39	0.58
1:H:124:ARG:HB3	1:H:147:ARG:CZ	2.34	0.58
1:I:123:PHE:CE1	1:J:5:PRO:HG2	2.39	0.58
1:B:161:PHE:CZ	1:B:178:HIS:HA	2.39	0.57
1:I:74:THR:HA	1:I:103:ASP:O	2.04	0.57
1:F:84:ASP:HA	1:F:93:LEU:HB2	1.86	0.57
1:J:48:CYS:O	1:J:52:ILE:HG13	2.04	0.57
1:G:74:THR:HG21	1:G:121:ASN:HA	1.86	0.57
1:C:46:PHE:O	1:C:49:PRO:HD2	2.05	0.57
1:E:47:VAL:HG13	1:F:170:PRO:HA	1.87	0.57
1:J:4:LEU:HD12	1:J:5:PRO:HD2	1.87	0.57
1:A:170:PRO:HA	1:B:47:VAL:HG13	1.86	0.56
1:E:73:SER:HB3	1:E:80:HIS:CE1	2.39	0.56
1:J:124:ARG:HB3	1:J:147:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PRO:HB3	1:D:168:VAL:HG12	1.87	0.56
1:E:40:TYR:CZ	1:E:73:SER:HB2	2.41	0.56
1:I:15:GLN:HE21	1:I:24:GLU:HG3	1.71	0.56
1:E:18:ILE:HG12	1:E:99:PRO:HB3	1.87	0.56
1:F:104:ARG:HE	1:G:121:ASN:HB3	1.70	0.55
1:I:38:PHE:HB2	1:I:147:ARG:NH1	2.22	0.55
1:H:61:GLU:HG2	1:H:65:ARG:HH21	1.71	0.55
1:D:4:LEU:HD12	1:D:5:PRO:HD3	1.88	0.55
1:H:177:GLN:O	1:H:178:HIS:CB	2.55	0.55
1:D:170:PRO:HD2	1:D:173:TRP:CD1	2.42	0.54
1:G:144:PRO:HA	1:H:168:VAL:HG12	1.89	0.54
1:B:84:ASP:HA	1:B:93:LEU:HB2	1.90	0.54
1:E:106:GLN:O	1:E:110:LYS:HG3	2.08	0.54
1:E:73:SER:HB3	1:E:80:HIS:HE1	1.72	0.54
1:J:3:LEU:O	1:J:4:LEU:HD13	2.08	0.54
1:I:5:PRO:O	1:I:135:LEU:O	2.26	0.54
1:F:118:GLU:O	1:G:105:LYS:HE2	2.09	0.53
1:C:124:ARG:HE	1:C:143:LYS:HA	1.73	0.53
1:D:104:ARG:NH2	1:E:74:THR:HG23	2.23	0.53
1:D:41:PRO:O	1:D:121:ASN:HB2	2.09	0.53
1:D:3:LEU:O	1:D:4:LEU:HD13	2.09	0.53
1:E:5:PRO:O	1:E:135:LEU:O	2.27	0.53
1:G:86:LEU:HB3	1:G:92:GLY:HA3	1.91	0.53
1:A:30:TYR:CE1	1:A:68:GLN:HG2	2.44	0.52
1:B:93:LEU:O	1:B:96:MET:HE2	2.08	0.52
1:C:65:ARG:HH12	1:C:175:ARG:NH1	2.05	0.52
1:G:74:THR:HA	1:G:103:ASP:O	2.09	0.52
1:H:163:GLU:HG3	1:H:164:LYS:N	2.25	0.52
1:A:74:THR:HA	1:A:103:ASP:O	2.09	0.52
1:F:74:THR:HG21	1:F:121:ASN:HA	1.92	0.52
1:I:48:CYS:N	1:I:49:PRO:HD2	2.25	0.52
1:C:41:PRO:HG3	1:C:143:LYS:HD2	1.91	0.52
1:G:124:ARG:HB3	1:G:147:ARG:NH2	2.24	0.52
1:H:124:ARG:HB3	1:H:147:ARG:NH2	2.25	0.52
1:J:84:ASP:HA	1:J:93:LEU:HB2	1.92	0.52
1:A:4:LEU:HD11	1:B:113:GLY:O	2.11	0.51
1:E:84:ASP:O	1:E:94:GLY:O	2.29	0.51
1:E:164:LYS:HG2	1:E:165:HIS:CD2	2.46	0.51
1:I:143:LYS:N	1:I:144:PRO:HD2	2.26	0.51
1:J:40:TYR:HB2	1:J:48:CYS:SG	2.51	0.50
1:A:41:PRO:O	1:A:121:ASN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LYS:O	1:B:106:GLN:HB2	2.11	0.50
1:E:40:TYR:HB2	1:E:48:CYS:SG	2.51	0.50
1:H:38:PHE:HB2	1:H:147:ARG:NH1	2.27	0.50
1:I:40:TYR:HB2	1:I:48:CYS:SG	2.52	0.50
1:J:103:ASP:HB2	1:J:108:ILE:HD12	1.92	0.50
1:D:143:LYS:N	1:D:144:PRO:HD2	2.27	0.50
1:A:61:GLU:O	1:A:65:ARG:HG2	2.11	0.50
1:B:125:GLY:HA2	1:B:139:THR:O	2.11	0.50
1:F:84:ASP:O	1:F:94:GLY:O	2.30	0.50
1:G:172:ASN:HD21	1:H:149:VAL:HG23	1.75	0.50
1:B:52:ILE:HG22	1:B:96:MET:SD	2.52	0.50
1:A:12:PHE:CE2	1:A:27:LEU:HD13	2.47	0.49
1:B:13[A]:LYS:HG3	1:B:26:CYS:HB3	1.93	0.49
1:E:126:LEU:HB3	1:E:139:THR:HB	1.93	0.49
1:C:142:ASP:HA	1:D:5:PRO:HB2	1.94	0.49
1:E:74:THR:HG21	1:E:121:ASN:HA	1.94	0.49
1:I:124:ARG:HB2	1:I:147:ARG:CZ	2.42	0.49
1:E:74:THR:HA	1:E:103:ASP:O	2.12	0.49
1:F:164:LYS:HD3	1:F:165:HIS:NE2	2.28	0.49
1:G:84:ASP:OD1	1:G:96:MET:HG3	2.13	0.49
1:J:74:THR:HA	1:J:103:ASP:O	2.13	0.49
1:D:74:THR:HA	1:D:103:ASP:O	2.13	0.49
1:D:120:GLY:HA3	1:E:104:ARG:HB3	1.94	0.49
1:E:126:LEU:HD21	1:E:152:THR:HG23	1.95	0.49
1:H:6:ASN:HB3	1:H:7:ARG:NH1	2.28	0.49
1:A:124:ARG:HB2	1:A:147:ARG:CZ	2.42	0.49
1:A:40:TYR:HB2	1:A:48:CYS:SG	2.53	0.49
1:C:168:VAL:HG12	1:D:144:PRO:HB3	1.95	0.49
1:D:15:GLN:HG2	1:D:77:GLN:OE1	2.13	0.49
1:E:38:PHE:HB2	1:E:147:ARG:NH1	2.28	0.49
1:A:53:ILE:HA	1:A:96:MET:HE3	1.95	0.48
1:E:170:PRO:HD2	1:E:173:TRP:CD1	2.48	0.48
1:G:38:PHE:HB2	1:G:147:ARG:NH1	2.28	0.48
1:I:56:SER:O	1:I:59:VAL:HG22	2.13	0.48
1:A:137:GLN:HG3	1:A:155:LEU:HD13	1.96	0.48
1:F:53:ILE:HG13	1:F:96:MET:HE1	1.95	0.48
1:G:6:ASN:HB3	1:G:7:ARG:HH11	1.78	0.48
1:G:84:ASP:O	1:G:94:GLY:O	2.31	0.48
1:E:15:GLN:OE1	1:E:24:GLU:HG2	2.14	0.48
1:B:168:VAL:HG23	1:B:180:ILE:HB	1.96	0.48
1:H:55:PHE:CE1	1:H:149:VAL:HG22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ARG:HG3	1:E:120:GLY:CA	2.42	0.48
1:D:86:LEU:HB3	1:D:92:GLY:HA3	1.96	0.48
1:I:36:VAL:HB	1:I:69:VAL:HG22	1.94	0.48
1:C:144:PRO:HB2	1:D:162:VAL:HG21	1.96	0.47
1:A:105:LYS:O	1:A:106:GLN:HB2	2.15	0.47
1:D:86:LEU:O	1:D:92:GLY:HA3	2.13	0.47
1:B:43:ASP:OD2	1:B:80:HIS:HD2	1.98	0.47
1:G:87:ASP:OD2	1:G:90:SER:HB2	2.15	0.47
1:H:65:ARG:HD2	1:H:156:LEU:HD23	1.97	0.47
1:A:46:PHE:N	1:A:46:PHE:CD1	2.82	0.47
1:E:124:ARG:HB3	1:E:147:ARG:NH2	2.30	0.47
1:B:23:LYS:HE3	1:B:23:LYS:HB2	1.62	0.47
1:G:7:ARG:HD3	1:G:7:ARG:N	2.28	0.47
1:J:84:ASP:O	1:J:94:GLY:O	2.32	0.47
1:A:84:ASP:HA	1:A:93:LEU:HB2	1.97	0.47
1:A:170:PRO:HD2	1:A:173:TRP:CD1	2.50	0.46
1:C:52:ILE:HD12	1:C:93:LEU:HD21	1.96	0.46
1:D:2:VAL:HG22	1:D:4:LEU:HD22	1.97	0.46
1:A:84:ASP:O	1:A:94:GLY:O	2.33	0.46
1:E:46:PHE:N	1:E:46:PHE:CD1	2.83	0.46
1:G:73:SER:HB3	1:G:80:HIS:HE1	1.79	0.46
1:I:65:ARG:HD3	1:I:157:ASP:OD1	2.14	0.46
1:J:143:LYS:N	1:J:144:PRO:HD2	2.31	0.46
1:J:174:LYS:HB2	1:J:177:GLN:NE2	2.31	0.46
1:H:54:ALA:O	1:H:58:GLN:HG2	2.15	0.46
1:C:41:PRO:O	1:C:121:ASN:HB2	2.16	0.46
1:C:125:GLY:HA2	1:C:139:THR:O	2.15	0.46
1:C:105:LYS:O	1:C:106:GLN:HB2	2.14	0.46
1:F:65:ARG:HD3	1:F:157:ASP:OD1	2.15	0.46
1:A:58:GLN:HG3	1:A:149:VAL:HG11	1.98	0.46
1:F:41:PRO:HG3	1:F:143:LYS:HG2	1.98	0.46
1:I:170:PRO:HA	1:J:47:VAL:HG13	1.97	0.46
1:J:124:ARG:HB3	1:J:147:ARG:NH2	2.31	0.46
1:H:3:LEU:CD2	1:H:3:LEU:H	2.29	0.46
1:E:178:HIS:H	1:E:178:HIS:CD2	2.34	0.46
1:D:169:CYS:HA	1:D:170:PRO:HD3	1.75	0.45
1:J:48:CYS:N	1:J:49:PRO:HD2	2.31	0.45
1:C:170:PRO:HD2	1:C:173:TRP:CD1	2.51	0.45
1:E:15:GLN:HG3	1:E:77:GLN:OE1	2.16	0.45
1:B:124:ARG:HB3	1:B:147:ARG:CZ	2.46	0.45
1:F:162:VAL:HG13	1:F:167:GLU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:ASP:O	1:I:119:ASP:O	2.34	0.45
1:D:137:GLN:HG3	1:D:155:LEU:HD13	1.98	0.45
1:D:153:LEU:HD12	1:D:153:LEU:HA	1.79	0.45
1:G:41:PRO:O	1:G:121:ASN:HB2	2.15	0.45
1:D:23:LYS:HE2	1:D:23:LYS:HB3	1.50	0.45
1:E:161:PHE:HZ	1:E:178:HIS:HB2	1.82	0.45
1:E:84:ASP:HA	1:E:93:LEU:HB2	1.99	0.45
1:F:74:THR:HA	1:F:103:ASP:O	2.17	0.45
1:B:16:ALA:HA	1:B:100:LEU:O	2.17	0.45
1:C:109:SER:HB2	1:C:115:PHE:HB2	1.98	0.45
1:E:74:THR:HG21	1:E:120:GLY:O	2.16	0.45
1:G:12:PHE:HB2	1:G:108:ILE:HD13	1.99	0.45
1:H:39:PHE:O	1:H:124:ARG:HA	2.17	0.45
1:B:174:LYS:HE2	1:B:174:LYS:HB2	1.82	0.45
1:F:75:ASP:CG	1:G:104:ARG:HH22	2.21	0.45
1:H:56:SER:O	1:H:59:VAL:HG23	2.17	0.45
1:J:41:PRO:O	1:J:121:ASN:HB2	2.17	0.45
1:G:48:CYS:HB2	1:G:49:PRO:HD3	1.99	0.45
1:B:158:ALA:O	1:B:162:VAL:HG13	2.17	0.44
1:H:30:TYR:CE1	1:H:68:GLN:HG2	2.51	0.44
1:H:49:PRO:HG3	1:H:83:TRP:HZ2	1.77	0.44
1:C:48:CYS:O	1:C:52:ILE:HG13	2.18	0.44
1:G:153:LEU:HA	1:G:153:LEU:HD12	1.84	0.44
1:I:103:ASP:HB2	1:I:108:ILE:HD12	1.99	0.44
1:E:62:PHE:CE1	1:E:153:LEU:HD13	2.52	0.44
1:E:116:ASP:O	1:E:119:ASP:O	2.34	0.44
1:E:96:MET:HE2	1:E:98:ILE:H	1.82	0.44
1:F:127:PHE:HB3	1:F:135:LEU:HD11	2.00	0.44
1:A:5:PRO:HG2	1:B:123:PHE:CE1	2.53	0.44
1:E:130:ASP:HB2	1:E:131:PRO:CD	2.48	0.44
1:E:175:ARG:HD2	1:E:175:ARG:HA	1.63	0.44
1:J:41:PRO:HD2	1:J:48:CYS:SG	2.57	0.44
1:B:47:VAL:HB	1:B:124:ARG:NH2	2.32	0.44
1:H:143:LYS:N	1:H:144:PRO:HD2	2.33	0.44
1:G:142:ASP:HB3	1:H:159:PHE:HE1	1.83	0.43
1:B:40:TYR:CZ	1:B:73:SER:HB3	2.53	0.43
1:F:40:TYR:CZ	1:F:73:SER:HB3	2.53	0.43
1:F:75:ASP:HB2	1:F:80:HIS:CE1	2.53	0.43
1:H:13:LYS:HE2	1:H:24:GLU:OE2	2.18	0.43
1:B:1:MET:HB2	1:B:2:VAL:H	1.59	0.43
1:C:124:ARG:HE	1:C:143:LYS:CA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:GLN:HG2	1:J:77:GLN:OE1	2.19	0.43
1:B:40:TYR:HB2	1:B:48:CYS:SG	2.58	0.43
1:D:5:PRO:HB3	1:D:136:ARG:O	2.18	0.43
1:I:124:ARG:HB2	1:I:147:ARG:NH2	2.33	0.43
1:E:165:HIS:C	1:E:167:GLU:H	2.22	0.43
1:J:0:THR:HG23	1:J:3:LEU:HD13	2.01	0.43
1:J:3:LEU:HD12	1:J:3:LEU:HA	1.87	0.43
1:J:46:PHE:N	1:J:46:PHE:CD1	2.86	0.43
1:D:104:ARG:HH22	1:E:75:ASP:CG	2.21	0.43
1:G:3:LEU:HD23	1:G:3:LEU:HA	1.86	0.43
1:H:120:GLY:HA3	1:I:104:ARG:CG	2.48	0.43
1:I:169:CYS:HA	1:I:170:PRO:HD3	1.83	0.43
1:I:4:LEU:HB2	1:I:7:ARG:HD3	2.00	0.43
1:J:13:LYS:HE3	1:J:24:GLU:OE2	2.18	0.43
1:C:97:LYS:HD3	1:C:97:LYS:HA	1.57	0.43
1:E:178:HIS:N	1:E:178:HIS:CD2	2.86	0.43
1:H:74:THR:HA	1:H:103:ASP:O	2.19	0.43
1:I:123:PHE:CD1	1:J:5:PRO:HG2	2.54	0.43
1:A:121:ASN:HB3	1:J:104:ARG:HH21	1.83	0.43
1:B:48:CYS:N	1:B:49:PRO:HD2	2.34	0.43
1:C:12:PHE:CE1	1:C:27:LEU:HD13	2.54	0.43
1:C:13:LYS:HD2	1:C:26:CYS:CB	2.46	0.43
1:C:142:ASP:O	1:C:144:PRO:HD3	2.18	0.43
1:D:39:PHE:O	1:D:124:ARG:HA	2.19	0.43
1:I:5:PRO:HB3	1:I:136:ARG:O	2.19	0.43
1:A:48:CYS:N	1:A:49:PRO:HD2	2.34	0.42
1:B:128:ILE:HD12	1:B:137:GLN:HB3	2.00	0.42
1:G:109:SER:HB2	1:G:115:PHE:HB2	2.00	0.42
1:E:96:MET:HE1	1:E:98:ILE:HG12	2.00	0.42
1:G:33:LYS:O	1:G:131:PRO:HA	2.19	0.42
1:C:170:PRO:HA	1:D:47:VAL:HG13	2.01	0.42
1:E:144:PRO:HB2	1:F:162:VAL:HG11	2.02	0.42
1:H:40:TYR:HB2	1:H:48:CYS:SG	2.59	0.42
1:J:169:CYS:HA	1:J:170:PRO:HD3	1.75	0.42
1:A:104:ARG:HH22	1:J:75:ASP:CG	2.22	0.42
1:D:48:CYS:N	1:D:49:PRO:HD2	2.34	0.42
1:A:105:LYS:HB3	1:A:107:GLU:HG3	2.00	0.42
1:C:47:VAL:HB	1:C:124:ARG:NH2	2.35	0.42
1:C:156:LEU:O	1:C:160:GLN:HG3	2.20	0.42
1:E:151:GLU:HG2	1:F:151:GLU:HG2	2.00	0.42
1:H:120:GLY:HA3	1:I:104:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:HB3	1:D:147:ARG:NH2	2.34	0.42
1:J:104:ARG:HG3	1:J:104:ARG:O	2.18	0.42
1:A:125:GLY:HA2	1:A:139:THR:O	2.19	0.41
1:J:148:SER:HB3	1:J:151:GLU:HB3	2.02	0.41
1:C:142:ASP:C	1:C:143:LYS:HG2	2.39	0.41
1:J:109:SER:HB2	1:J:115:PHE:HB2	2.00	0.41
1:B:51:GLU:CD	1:B:147:ARG:HH21	2.23	0.41
1:B:84:ASP:O	1:B:94:GLY:O	2.38	0.41
1:C:159:PHE:CD1	1:D:145:VAL:HG21	2.55	0.41
1:I:158:ALA:O	1:I:162:VAL:HG13	2.20	0.41
1:J:5:PRO:HB3	1:J:136:ARG:O	2.21	0.41
1:F:105:LYS:O	1:F:106:GLN:HB2	2.20	0.41
1:F:157:ASP:CG	1:F:175:ARG:HD2	2.41	0.41
1:G:113:GLY:O	1:H:4:LEU:HD21	2.21	0.41
1:I:171:VAL:HB	1:J:51:GLU:HG3	2.03	0.41
1:J:126:LEU:HD12	1:J:147:ARG:HD2	2.02	0.41
1:H:170:PRO:HD2	1:H:173:TRP:CD1	2.55	0.41
1:C:116:ASP:HB3	1:C:123:PHE:CE2	2.56	0.41
1:C:169:CYS:HA	1:C:170:PRO:HD3	1.84	0.41
1:E:8:PRO:HA	1:E:134:ILE:HA	2.03	0.41
1:H:12:PHE:CE2	1:H:27:LEU:HD13	2.56	0.41
1:H:75:ASP:CG	1:I:104:ARG:HH12	2.24	0.41
1:J:62:PHE:CE1	1:J:153:LEU:HD13	2.56	0.41
1:J:170:PRO:HD2	1:J:173:TRP:CD1	2.55	0.41
1:A:18:ILE:O	1:A:19:ASN:HB2	2.21	0.41
1:E:48:CYS:N	1:E:49:PRO:HD2	2.35	0.41
1:G:69:VAL:O	1:G:99:PRO:HD2	2.20	0.41
1:D:101:LEU:HD21	1:D:108:ILE:HD13	2.03	0.41
1:H:47:VAL:HB	1:H:124:ARG:NH2	2.36	0.41
1:I:127:PHE:HB3	1:I:135:LEU:HD11	2.02	0.41
1:D:121:ASN:HB3	1:E:104:ARG:HH21	1.86	0.40
1:H:40:TYR:CZ	1:H:73:SER:HB3	2.56	0.40
1:D:4:LEU:HA	1:D:5:PRO:HD3	1.84	0.40
1:E:127:PHE:HB3	1:E:135:LEU:HD11	2.02	0.40
1:G:116:ASP:HB3	1:G:123:PHE:CE2	2.57	0.40
1:G:40:TYR:HA	1:G:41:PRO:HD3	1.91	0.40
1:G:73:SER:HB3	1:G:80:HIS:CE1	2.55	0.40
1:I:6:ASN:HB2	1:J:123:PHE:CZ	2.56	0.40
1:D:105:LYS:O	1:D:106:GLN:HB2	2.21	0.40
1:D:4:LEU:HA	1:D:4:LEU:HD12	1.90	0.40
1:C:52:ILE:HG13	1:C:52:ILE:H	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LEU:HA	1:E:5:PRO:HD3	1.82	0.40
1:I:41:PRO:HG3	1:I:143:LYS:HG2	2.03	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	178/222 (80%)	171 (96%)	7 (4%)	0	100	100
1	B	183/222 (82%)	179 (98%)	4 (2%)	0	100	100
1	C	180/222 (81%)	176 (98%)	4 (2%)	0	100	100
1	D	172/222 (78%)	167 (97%)	5 (3%)	0	100	100
1	E	174/222 (78%)	167 (96%)	7 (4%)	0	100	100
1	F	179/222 (81%)	175 (98%)	4 (2%)	0	100	100
1	G	179/222 (81%)	172 (96%)	7 (4%)	0	100	100
1	H	176/222 (79%)	169 (96%)	7 (4%)	0	100	100
1	I	177/222 (80%)	174 (98%)	3 (2%)	0	100	100
1	J	181/222 (82%)	175 (97%)	6 (3%)	0	100	100
All	All	1779/2220 (80%)	1725 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	156/191 (82%)	140 (90%)	16 (10%)	7	28
1	B	161/191 (84%)	143 (89%)	18 (11%)	6	24
1	C	158/191 (83%)	143 (90%)	15 (10%)	8	32
1	D	152/191 (80%)	143 (94%)	9 (6%)	19	54
1	E	153/191 (80%)	135 (88%)	18 (12%)	5	22
1	F	157/191 (82%)	140 (89%)	17 (11%)	6	26
1	G	157/191 (82%)	138 (88%)	19 (12%)	5	21
1	H	155/191 (81%)	134 (86%)	21 (14%)	4	17
1	I	155/191 (81%)	135 (87%)	20 (13%)	4	19
1	J	159/191 (83%)	142 (89%)	17 (11%)	6	26
All	All	1563/1910 (82%)	1393 (89%)	170 (11%)	6	25

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	ARG
1	A	64	SER
1	A	73	SER
1	A	74	THR
1	A	90	SER
1	A	96	MET
1	A	97	LYS
1	A	98	ILE
1	A	105	LYS
1	A	119	ASP
1	A	124	ARG
1	A	130	ASP
1	A	136	ARG
1	A	153	LEU
1	A	180	ILE
1	B	1	MET
1	B	3	LEU
1	B	13[A]	LYS
1	B	13[B]	LYS
1	B	18	ILE
1	B	24	GLU

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Mol	Chain	Res	Type
1	B	59	VAL
1	B	73	SER
1	B	74	THR
1	B	104	ARG
1	B	130	ASP
1	B	162	VAL
1	B	164	LYS
1	B	174	LYS
1	B	175	ARG
1	B	178	HIS
1	B	180	ILE
1	B	182	VAL
1	C	1	MET
1	C	3	LEU
1	C	58	GLN
1	C	73	SER
1	C	77	GLN
1	C	87	ASP
1	C	96	MET
1	C	97	LYS
1	C	98	ILE
1	C	105	LYS
1	C	124	ARG
1	C	130	ASP
1	C	134	ILE
1	C	153	LEU
1	C	163	GLU
1	D	4	LEU
1	D	24	GLU
1	D	28	LYS
1	D	45	THR
1	D	74	THR
1	D	89	LYS
1	D	126	LEU
1	D	130	ASP
1	D	153	LEU
1	E	3	LEU
1	E	4	LEU
1	E	23	LYS
1	E	24	GLU
1	E	59	VAL
1	E	65	ARG

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Mol	Chain	Res	Type
1	E	77	GLN
1	E	86	LEU
1	E	87	ASP
1	E	104	ARG
1	E	105	LYS
1	E	124	ARG
1	E	126	LEU
1	E	137	GLN
1	E	148	SER
1	E	153	LEU
1	E	174	LYS
1	E	175	ARG
1	F	1	MET
1	F	18	ILE
1	F	23	LYS
1	F	31	ARG
1	F	45	THR
1	F	56	SER
1	F	65	ARG
1	F	74	THR
1	F	77	GLN
1	F	80	HIS
1	F	87	ASP
1	F	89	LYS
1	F	96	MET
1	F	98	ILE
1	F	130	ASP
1	F	153	LEU
1	F	175	ARG
1	G	3	LEU
1	G	4	LEU
1	G	23	LYS
1	G	28	LYS
1	G	45	THR
1	G	65	ARG
1	G	74	THR
1	G	77	GLN
1	G	79	SER
1	G	90	SER
1	G	98	ILE
1	G	105	LYS
1	G	109	SER

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Mol	Chain	Res	Type
1	G	121	ASN
1	G	124	ARG
1	G	130	ASP
1	G	134	ILE
1	G	136	ARG
1	G	153	LEU
1	H	2	VAL
1	H	3	LEU
1	H	18	ILE
1	H	56	SER
1	H	60	GLU
1	H	73	SER
1	H	74	THR
1	H	77	GLN
1	H	87	ASP
1	H	89	LYS
1	H	95	HIS
1	H	97	LYS
1	H	104	ARG
1	H	105	LYS
1	H	130	ASP
1	H	143	LYS
1	H	153	LEU
1	H	168	VAL
1	H	174	LYS
1	H	175	ARG
1	H	178	HIS
1	I	23	LYS
1	I	24	GLU
1	I	26	CYS
1	I	59	VAL
1	I	65	ARG
1	I	73	SER
1	I	74	THR
1	I	77	GLN
1	I	79	SER
1	I	86	LEU
1	I	89	LYS
1	I	97	LYS
1	I	103	ASP
1	I	117[A]	GLU
1	I	117[B]	GLU

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Mol	Chain	Res	Type
1	I	124	ARG
1	I	153	LEU
1	I	156	LEU
1	I	175	ARG
1	I	178	HIS
1	J	2	VAL
1	J	3	LEU
1	J	4	LEU
1	J	24	GLU
1	J	28	LYS
1	J	33	LYS
1	J	73	SER
1	J	74	THR
1	J	77	GLN
1	J	97	LYS
1	J	103	ASP
1	J	109	SER
1	J	121	ASN
1	J	126	LEU
1	J	130	ASP
1	J	136	ARG
1	J	153	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	B	80	HIS
1	E	165	HIS
1	E	177	GLN
1	G	121	ASN
1	H	177	GLN
1	I	15	GLN
1	I	137	GLN
1	J	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	180/222 (81%)	-0.47	0	100 100	16, 23, 45, 52	0
1	B	183/222 (82%)	-0.58	0	100 100	15, 24, 39, 50	0
1	C	182/222 (81%)	-0.47	0	100 100	17, 27, 46, 55	0
1	D	172/222 (77%)	-0.52	0	100 100	18, 26, 44, 54	0
1	E	176/222 (79%)	-0.52	0	100 100	17, 24, 40, 54	0
1	F	181/222 (81%)	-0.48	0	100 100	19, 28, 41, 53	0
1	G	180/222 (81%)	-0.45	0	100 100	20, 28, 49, 61	0
1	H	178/222 (80%)	-0.28	3 (1%)	70 41	22, 34, 51, 56	0
1	I	178/222 (80%)	-0.48	1 (0%)	89 72	18, 29, 41, 52	0
1	J	183/222 (82%)	-0.59	0	100 100	17, 24, 34, 42	0
All	All	1793/2220 (80%)	-0.48	4 (0%)	95 87	15, 26, 44, 61	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	175	ARG	2.5
1	I	178	HIS	2.3
1	H	177	GLN	2.3
1	H	90	SER	2.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.