Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 12:06 am GMT

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 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:

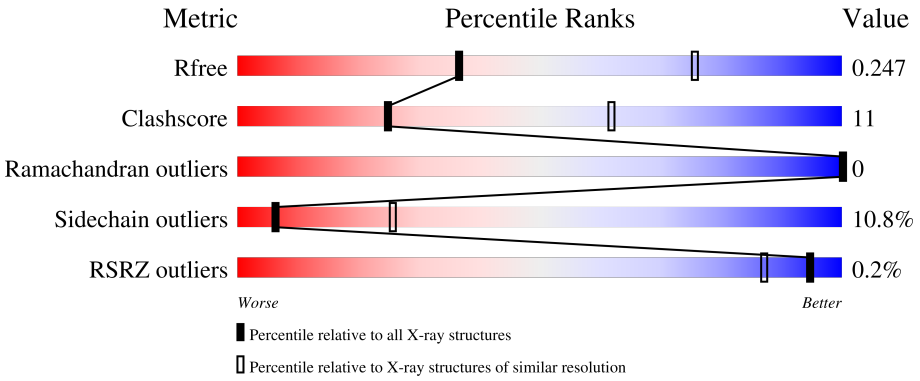
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 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 <=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	58% 21% • 19%
1	B	222	59% 19% • 18%
1	C	222	60% 19% • 18%
1	D	222	55% 21% • 23%
1	E	222	50% 25% 5% 21%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

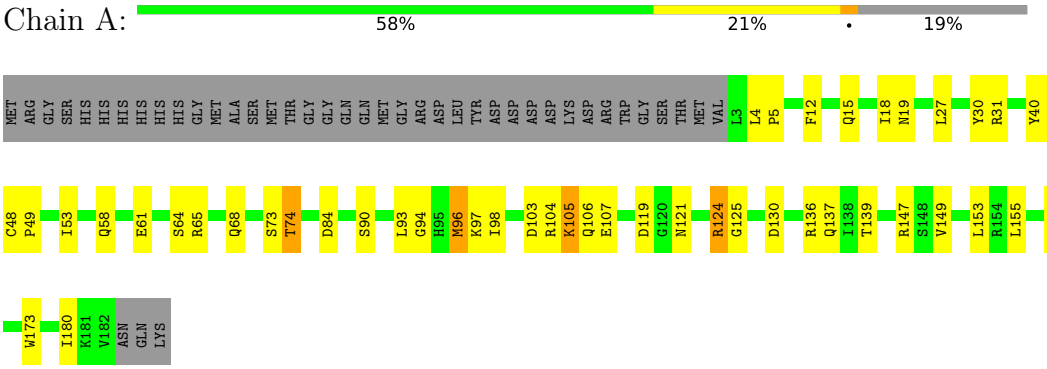
Chain	Residue	Modelled	Actual	Comment	Reference
J	-24	ALA	-	expression tag	UNP O97161
J	-23	SER	-	expression tag	UNP O97161
J	-22	MET	-	expression tag	UNP O97161
J	-21	THR	-	expression tag	UNP O97161
J	-20	GLY	-	expression tag	UNP O97161
J	-19	GLY	-	expression tag	UNP O97161
J	-18	GLN	-	expression tag	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

3 Residue-property plots (i)

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.

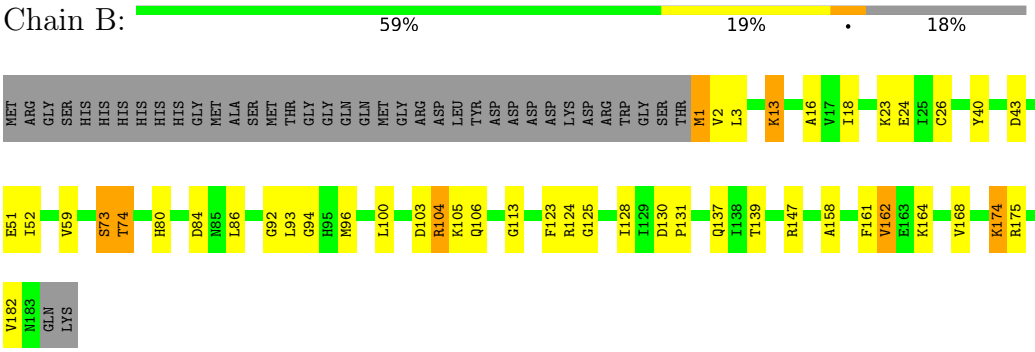
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain A:



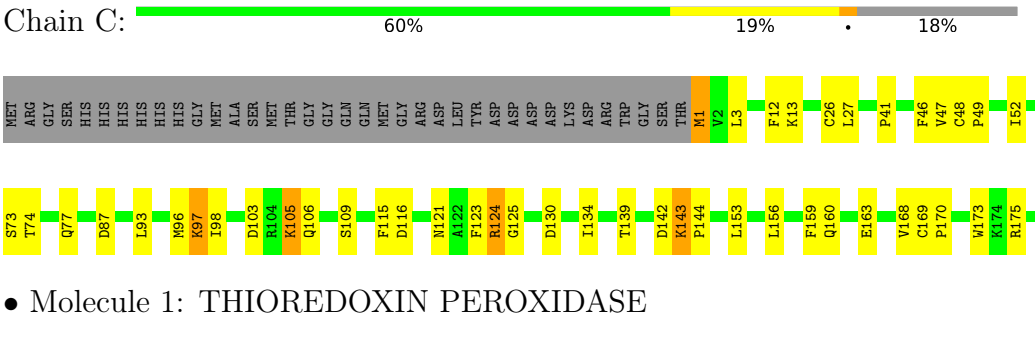
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain B:



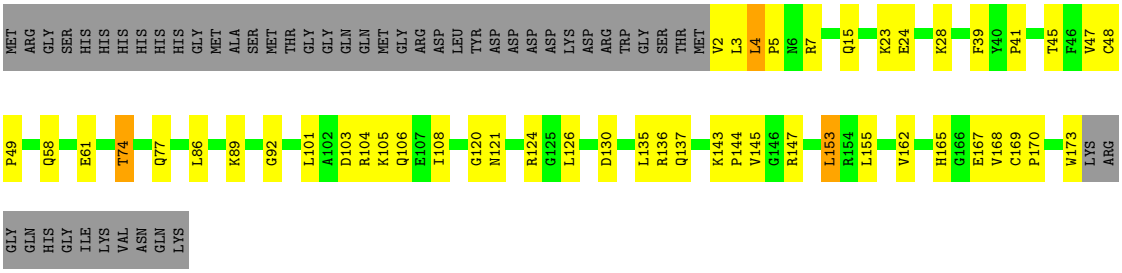
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain C:



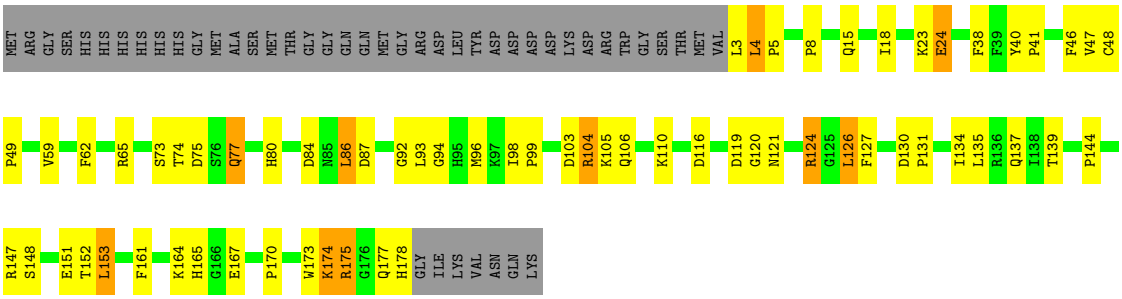
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain D:



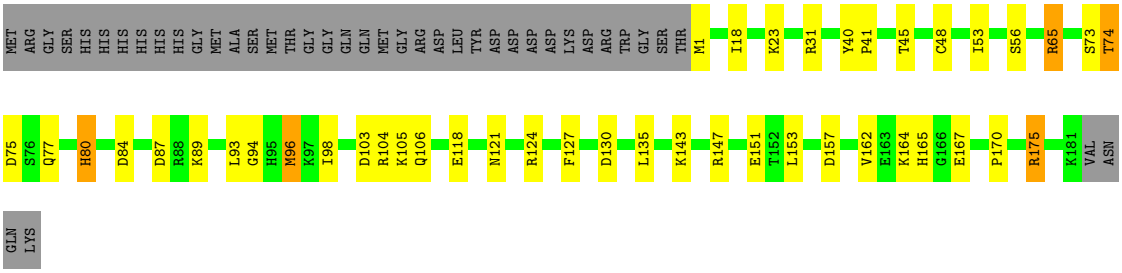
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain E:



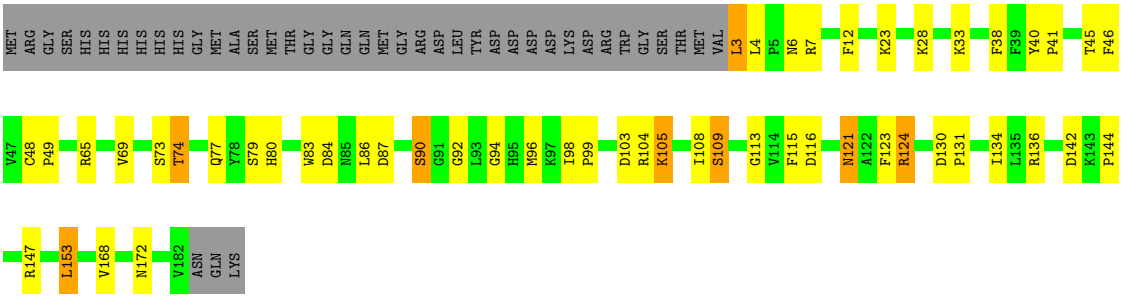
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain F:



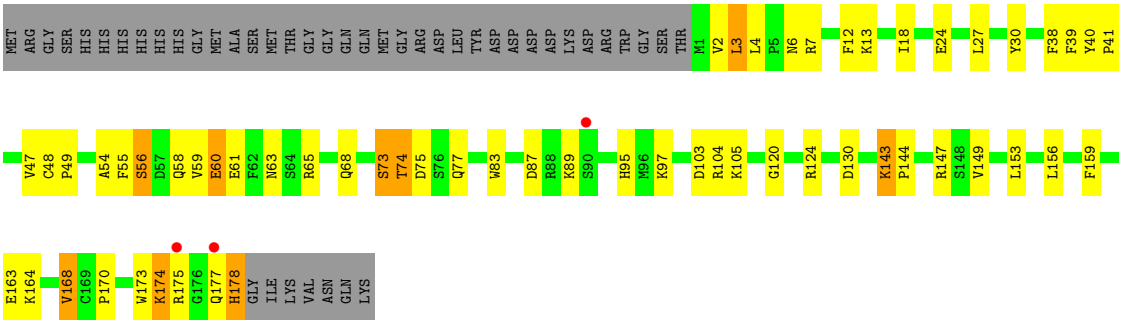
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain G:



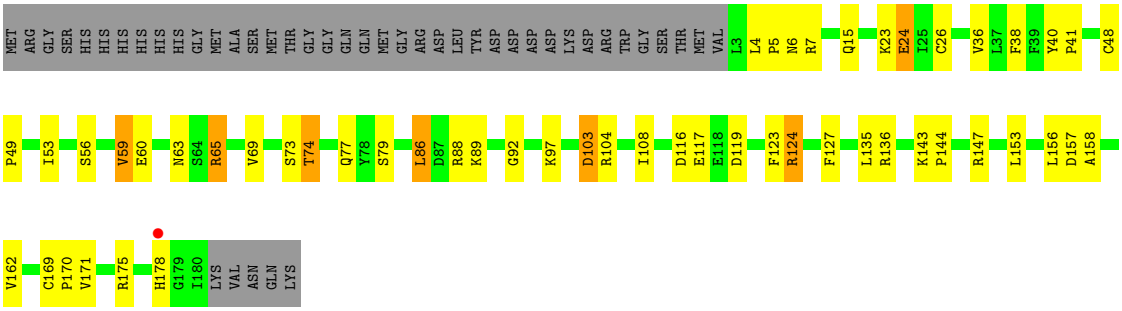
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain H:



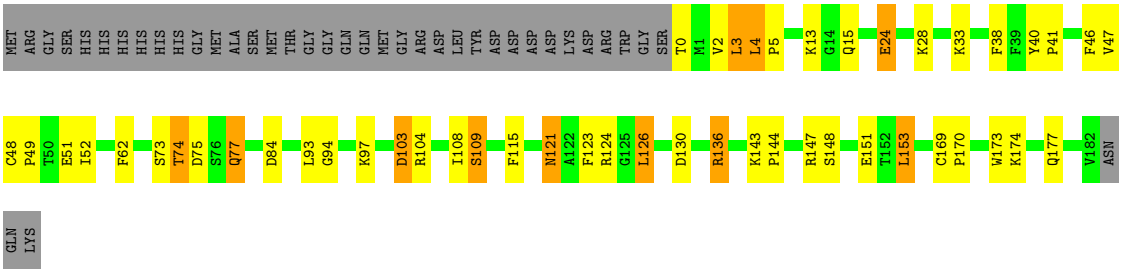
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain I:



• Molecule 1: THIOREDOXIN PEROXIDASE

Chain J:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	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 (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:3:LEU:O	1:D:4:LEU:HD13	2.09	0.53
1:D:41:PRO:O	1:D:121:ASN:HB2	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

Continued on next page...

Continued from previous page...

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:40:TYR:HB2	1:A:48:CYS:SG	2.53	0.49
1:A:124:ARG:HB2	1:A:147:ARG:CZ	2.42	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

Continued on next page...

Continued from previous page...

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:A:46:PHE:CD1	1:A:46:PHE:N	2.82	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:E:124:ARG:HB3	1:E:147:ARG:NH2	2.30	0.47
1:B:23:LYS:HB2	1:B:23:LYS:HE3	1.62	0.47
1:G:7:ARG:N	1:G:7:ARG:HD3	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:CD1	1:E:46:PHE:N	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:H	1:H:3:LEU:CD2	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

Continued on next page...

Continued from previous page...

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:84:ASP:HA	1:E:93:LEU:HB2	1.99	0.45
1:E:161:PHE:HZ	1:E:178:HIS:HB2	1.82	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:HB2	1:B:174:LYS:HE2	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:HD12	1:G:153:LEU:HA	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

Continued on next page...

Continued from previous page...

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:CD1	1:J:46:PHE:N	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:4:LEU:HB2	1:I:7:ARG:HD3	2.00	0.43
1:I:169:CYS:HA	1:I:170:PRO:HD3	1.83	0.43
1:J:13:LYS:HE3	1:J:24:GLU:OE2	2.18	0.43
1:C:97:LYS:HA	1:C:97:LYS:HD3	1.57	0.43
1:E:178:HIS:CD2	1:E:178:HIS:N	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:A:104:ARG:HH22	1:J:75:ASP:CG	2.22	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: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

Continued on next page...

Continued from previous page...

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:D:101:LEU:HD21	1:D:108:ILE:HD13	2.03	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: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: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:G:116:ASP:HB3	1:G:123:PHE:CE2	2.57	0.40
1:I:6:ASN:HB2	1:J:123:PHE:CZ	2.56	0.40
1:D:4:LEU:HD12	1:D:4:LEU:HA	1.90	0.40
1:D:105:LYS:O	1:D:106:GLN:HB2	2.21	0.40
1:C:52:ILE:HG13	1:C:52:ILE:H	1.64	0.40

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Sometimes 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 monosaccharides 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, 95^{th} 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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.