Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 04:19 AM EDT

PDB ID	:	4MH2
Title	:	Crystal structure of Bovine Mitochondrial Peroxiredoxin III
Authors	:	Cao, Z.; McGow, D.P.; Shepherd, C.; Lindsay, J.G.
Deposited on	:	2013-08-29
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

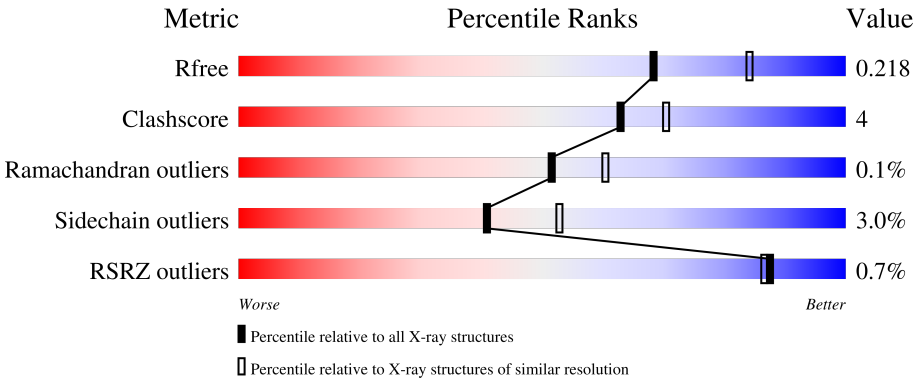
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	220	70% 5% 25%
1	B	220	65% 10% 25%
1	C	220	64% 10% 25%
1	D	220	69% 6% 25%
1	E	220	.% 65% 8% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	220	68% 7% 25%
1	G	220	61% 12% 25%
1	H	220	65% 9% 26%
1	I	220	65% 8% 25%
1	J	220	66% 7% 26%
1	K	220	% 65% 10% 25%
1	L	220	67% 8% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16330 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-dependent peroxide reductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	5	0
			1317	858	218	238	3			
1	B	165	Total	C	N	O	S	0	3	0
			1310	856	217	234	3			
1	C	164	Total	C	N	O	S	0	6	0
			1318	859	218	238	3			
1	D	165	Total	C	N	O	S	0	3	0
			1307	852	216	236	3			
1	E	163	Total	C	N	O	S	0	4	0
			1301	847	213	238	3			
1	F	165	Total	C	N	O	S	0	8	0
			1346	878	222	242	4			
1	G	164	Total	C	N	O	S	0	9	0
			1345	877	221	243	4			
1	H	163	Total	C	N	O	S	0	3	0
			1295	843	214	235	3			
1	I	165	Total	C	N	O	S	0	6	0
			1330	864	220	243	3			
1	J	163	Total	C	N	O	S	0	2	0
			1284	836	212	233	3			
1	K	164	Total	C	N	O	S	0	3	0
			1304	848	218	235	3			
1	L	165	Total	C	N	O	S	0	5	0
			1319	861	217	238	3			

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP P35705
A	-23	GLY	-	expression tag	UNP P35705
A	-22	SER	-	expression tag	UNP P35705
A	-21	SER	-	expression tag	UNP P35705
A	-20	HIS	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	HIS	-	expression tag	UNP P35705
A	-18	HIS	-	expression tag	UNP P35705
A	-17	HIS	-	expression tag	UNP P35705
A	-16	HIS	-	expression tag	UNP P35705
A	-15	HIS	-	expression tag	UNP P35705
A	-14	SER	-	expression tag	UNP P35705
A	-13	SER	-	expression tag	UNP P35705
A	-12	GLY	-	expression tag	UNP P35705
A	-11	LEU	-	expression tag	UNP P35705
A	-10	VAL	-	expression tag	UNP P35705
A	-9	PRO	-	expression tag	UNP P35705
A	-8	ARG	-	expression tag	UNP P35705
A	-7	GLY	-	expression tag	UNP P35705
A	-6	SER	-	expression tag	UNP P35705
A	-5	HIS	-	expression tag	UNP P35705
A	-4	MET	-	expression tag	UNP P35705
A	-3	LEU	-	expression tag	UNP P35705
A	-2	GLU	-	expression tag	UNP P35705
A	-1	ASP	-	expression tag	UNP P35705
A	0	PRO	-	expression tag	UNP P35705
A	190	LEU	PHE	engineered mutation	UNP P35705
B	-24	MET	-	expression tag	UNP P35705
B	-23	GLY	-	expression tag	UNP P35705
B	-22	SER	-	expression tag	UNP P35705
B	-21	SER	-	expression tag	UNP P35705
B	-20	HIS	-	expression tag	UNP P35705
B	-19	HIS	-	expression tag	UNP P35705
B	-18	HIS	-	expression tag	UNP P35705
B	-17	HIS	-	expression tag	UNP P35705
B	-16	HIS	-	expression tag	UNP P35705
B	-15	HIS	-	expression tag	UNP P35705
B	-14	SER	-	expression tag	UNP P35705
B	-13	SER	-	expression tag	UNP P35705
B	-12	GLY	-	expression tag	UNP P35705
B	-11	LEU	-	expression tag	UNP P35705
B	-10	VAL	-	expression tag	UNP P35705
B	-9	PRO	-	expression tag	UNP P35705
B	-8	ARG	-	expression tag	UNP P35705
B	-7	GLY	-	expression tag	UNP P35705
B	-6	SER	-	expression tag	UNP P35705
B	-5	HIS	-	expression tag	UNP P35705
B	-4	MET	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	LEU	-	expression tag	UNP P35705
B	-2	GLU	-	expression tag	UNP P35705
B	-1	ASP	-	expression tag	UNP P35705
B	0	PRO	-	expression tag	UNP P35705
B	190	LEU	PHE	engineered mutation	UNP P35705
C	-24	MET	-	expression tag	UNP P35705
C	-23	GLY	-	expression tag	UNP P35705
C	-22	SER	-	expression tag	UNP P35705
C	-21	SER	-	expression tag	UNP P35705
C	-20	HIS	-	expression tag	UNP P35705
C	-19	HIS	-	expression tag	UNP P35705
C	-18	HIS	-	expression tag	UNP P35705
C	-17	HIS	-	expression tag	UNP P35705
C	-16	HIS	-	expression tag	UNP P35705
C	-15	HIS	-	expression tag	UNP P35705
C	-14	SER	-	expression tag	UNP P35705
C	-13	SER	-	expression tag	UNP P35705
C	-12	GLY	-	expression tag	UNP P35705
C	-11	LEU	-	expression tag	UNP P35705
C	-10	VAL	-	expression tag	UNP P35705
C	-9	PRO	-	expression tag	UNP P35705
C	-8	ARG	-	expression tag	UNP P35705
C	-7	GLY	-	expression tag	UNP P35705
C	-6	SER	-	expression tag	UNP P35705
C	-5	HIS	-	expression tag	UNP P35705
C	-4	MET	-	expression tag	UNP P35705
C	-3	LEU	-	expression tag	UNP P35705
C	-2	GLU	-	expression tag	UNP P35705
C	-1	ASP	-	expression tag	UNP P35705
C	0	PRO	-	expression tag	UNP P35705
C	190	LEU	PHE	engineered mutation	UNP P35705
D	-24	MET	-	expression tag	UNP P35705
D	-23	GLY	-	expression tag	UNP P35705
D	-22	SER	-	expression tag	UNP P35705
D	-21	SER	-	expression tag	UNP P35705
D	-20	HIS	-	expression tag	UNP P35705
D	-19	HIS	-	expression tag	UNP P35705
D	-18	HIS	-	expression tag	UNP P35705
D	-17	HIS	-	expression tag	UNP P35705
D	-16	HIS	-	expression tag	UNP P35705
D	-15	HIS	-	expression tag	UNP P35705
D	-14	SER	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	SER	-	expression tag	UNP P35705
D	-12	GLY	-	expression tag	UNP P35705
D	-11	LEU	-	expression tag	UNP P35705
D	-10	VAL	-	expression tag	UNP P35705
D	-9	PRO	-	expression tag	UNP P35705
D	-8	ARG	-	expression tag	UNP P35705
D	-7	GLY	-	expression tag	UNP P35705
D	-6	SER	-	expression tag	UNP P35705
D	-5	HIS	-	expression tag	UNP P35705
D	-4	MET	-	expression tag	UNP P35705
D	-3	LEU	-	expression tag	UNP P35705
D	-2	GLU	-	expression tag	UNP P35705
D	-1	ASP	-	expression tag	UNP P35705
D	0	PRO	-	expression tag	UNP P35705
D	190	LEU	PHE	engineered mutation	UNP P35705
E	-24	MET	-	expression tag	UNP P35705
E	-23	GLY	-	expression tag	UNP P35705
E	-22	SER	-	expression tag	UNP P35705
E	-21	SER	-	expression tag	UNP P35705
E	-20	HIS	-	expression tag	UNP P35705
E	-19	HIS	-	expression tag	UNP P35705
E	-18	HIS	-	expression tag	UNP P35705
E	-17	HIS	-	expression tag	UNP P35705
E	-16	HIS	-	expression tag	UNP P35705
E	-15	HIS	-	expression tag	UNP P35705
E	-14	SER	-	expression tag	UNP P35705
E	-13	SER	-	expression tag	UNP P35705
E	-12	GLY	-	expression tag	UNP P35705
E	-11	LEU	-	expression tag	UNP P35705
E	-10	VAL	-	expression tag	UNP P35705
E	-9	PRO	-	expression tag	UNP P35705
E	-8	ARG	-	expression tag	UNP P35705
E	-7	GLY	-	expression tag	UNP P35705
E	-6	SER	-	expression tag	UNP P35705
E	-5	HIS	-	expression tag	UNP P35705
E	-4	MET	-	expression tag	UNP P35705
E	-3	LEU	-	expression tag	UNP P35705
E	-2	GLU	-	expression tag	UNP P35705
E	-1	ASP	-	expression tag	UNP P35705
E	0	PRO	-	expression tag	UNP P35705
E	190	LEU	PHE	engineered mutation	UNP P35705
F	-24	MET	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-23	GLY	-	expression tag	UNP P35705
F	-22	SER	-	expression tag	UNP P35705
F	-21	SER	-	expression tag	UNP P35705
F	-20	HIS	-	expression tag	UNP P35705
F	-19	HIS	-	expression tag	UNP P35705
F	-18	HIS	-	expression tag	UNP P35705
F	-17	HIS	-	expression tag	UNP P35705
F	-16	HIS	-	expression tag	UNP P35705
F	-15	HIS	-	expression tag	UNP P35705
F	-14	SER	-	expression tag	UNP P35705
F	-13	SER	-	expression tag	UNP P35705
F	-12	GLY	-	expression tag	UNP P35705
F	-11	LEU	-	expression tag	UNP P35705
F	-10	VAL	-	expression tag	UNP P35705
F	-9	PRO	-	expression tag	UNP P35705
F	-8	ARG	-	expression tag	UNP P35705
F	-7	GLY	-	expression tag	UNP P35705
F	-6	SER	-	expression tag	UNP P35705
F	-5	HIS	-	expression tag	UNP P35705
F	-4	MET	-	expression tag	UNP P35705
F	-3	LEU	-	expression tag	UNP P35705
F	-2	GLU	-	expression tag	UNP P35705
F	-1	ASP	-	expression tag	UNP P35705
F	0	PRO	-	expression tag	UNP P35705
F	190	LEU	PHE	engineered mutation	UNP P35705
G	-24	MET	-	expression tag	UNP P35705
G	-23	GLY	-	expression tag	UNP P35705
G	-22	SER	-	expression tag	UNP P35705
G	-21	SER	-	expression tag	UNP P35705
G	-20	HIS	-	expression tag	UNP P35705
G	-19	HIS	-	expression tag	UNP P35705
G	-18	HIS	-	expression tag	UNP P35705
G	-17	HIS	-	expression tag	UNP P35705
G	-16	HIS	-	expression tag	UNP P35705
G	-15	HIS	-	expression tag	UNP P35705
G	-14	SER	-	expression tag	UNP P35705
G	-13	SER	-	expression tag	UNP P35705
G	-12	GLY	-	expression tag	UNP P35705
G	-11	LEU	-	expression tag	UNP P35705
G	-10	VAL	-	expression tag	UNP P35705
G	-9	PRO	-	expression tag	UNP P35705
G	-8	ARG	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLY	-	expression tag	UNP P35705
G	-6	SER	-	expression tag	UNP P35705
G	-5	HIS	-	expression tag	UNP P35705
G	-4	MET	-	expression tag	UNP P35705
G	-3	LEU	-	expression tag	UNP P35705
G	-2	GLU	-	expression tag	UNP P35705
G	-1	ASP	-	expression tag	UNP P35705
G	0	PRO	-	expression tag	UNP P35705
G	190	LEU	PHE	engineered mutation	UNP P35705
H	-24	MET	-	expression tag	UNP P35705
H	-23	GLY	-	expression tag	UNP P35705
H	-22	SER	-	expression tag	UNP P35705
H	-21	SER	-	expression tag	UNP P35705
H	-20	HIS	-	expression tag	UNP P35705
H	-19	HIS	-	expression tag	UNP P35705
H	-18	HIS	-	expression tag	UNP P35705
H	-17	HIS	-	expression tag	UNP P35705
H	-16	HIS	-	expression tag	UNP P35705
H	-15	HIS	-	expression tag	UNP P35705
H	-14	SER	-	expression tag	UNP P35705
H	-13	SER	-	expression tag	UNP P35705
H	-12	GLY	-	expression tag	UNP P35705
H	-11	LEU	-	expression tag	UNP P35705
H	-10	VAL	-	expression tag	UNP P35705
H	-9	PRO	-	expression tag	UNP P35705
H	-8	ARG	-	expression tag	UNP P35705
H	-7	GLY	-	expression tag	UNP P35705
H	-6	SER	-	expression tag	UNP P35705
H	-5	HIS	-	expression tag	UNP P35705
H	-4	MET	-	expression tag	UNP P35705
H	-3	LEU	-	expression tag	UNP P35705
H	-2	GLU	-	expression tag	UNP P35705
H	-1	ASP	-	expression tag	UNP P35705
H	0	PRO	-	expression tag	UNP P35705
H	190	LEU	PHE	engineered mutation	UNP P35705
I	-24	MET	-	expression tag	UNP P35705
I	-23	GLY	-	expression tag	UNP P35705
I	-22	SER	-	expression tag	UNP P35705
I	-21	SER	-	expression tag	UNP P35705
I	-20	HIS	-	expression tag	UNP P35705
I	-19	HIS	-	expression tag	UNP P35705
I	-18	HIS	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-17	HIS	-	expression tag	UNP P35705
I	-16	HIS	-	expression tag	UNP P35705
I	-15	HIS	-	expression tag	UNP P35705
I	-14	SER	-	expression tag	UNP P35705
I	-13	SER	-	expression tag	UNP P35705
I	-12	GLY	-	expression tag	UNP P35705
I	-11	LEU	-	expression tag	UNP P35705
I	-10	VAL	-	expression tag	UNP P35705
I	-9	PRO	-	expression tag	UNP P35705
I	-8	ARG	-	expression tag	UNP P35705
I	-7	GLY	-	expression tag	UNP P35705
I	-6	SER	-	expression tag	UNP P35705
I	-5	HIS	-	expression tag	UNP P35705
I	-4	MET	-	expression tag	UNP P35705
I	-3	LEU	-	expression tag	UNP P35705
I	-2	GLU	-	expression tag	UNP P35705
I	-1	ASP	-	expression tag	UNP P35705
I	0	PRO	-	expression tag	UNP P35705
I	190	LEU	PHE	engineered mutation	UNP P35705
J	-24	MET	-	expression tag	UNP P35705
J	-23	GLY	-	expression tag	UNP P35705
J	-22	SER	-	expression tag	UNP P35705
J	-21	SER	-	expression tag	UNP P35705
J	-20	HIS	-	expression tag	UNP P35705
J	-19	HIS	-	expression tag	UNP P35705
J	-18	HIS	-	expression tag	UNP P35705
J	-17	HIS	-	expression tag	UNP P35705
J	-16	HIS	-	expression tag	UNP P35705
J	-15	HIS	-	expression tag	UNP P35705
J	-14	SER	-	expression tag	UNP P35705
J	-13	SER	-	expression tag	UNP P35705
J	-12	GLY	-	expression tag	UNP P35705
J	-11	LEU	-	expression tag	UNP P35705
J	-10	VAL	-	expression tag	UNP P35705
J	-9	PRO	-	expression tag	UNP P35705
J	-8	ARG	-	expression tag	UNP P35705
J	-7	GLY	-	expression tag	UNP P35705
J	-6	SER	-	expression tag	UNP P35705
J	-5	HIS	-	expression tag	UNP P35705
J	-4	MET	-	expression tag	UNP P35705
J	-3	LEU	-	expression tag	UNP P35705
J	-2	GLU	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

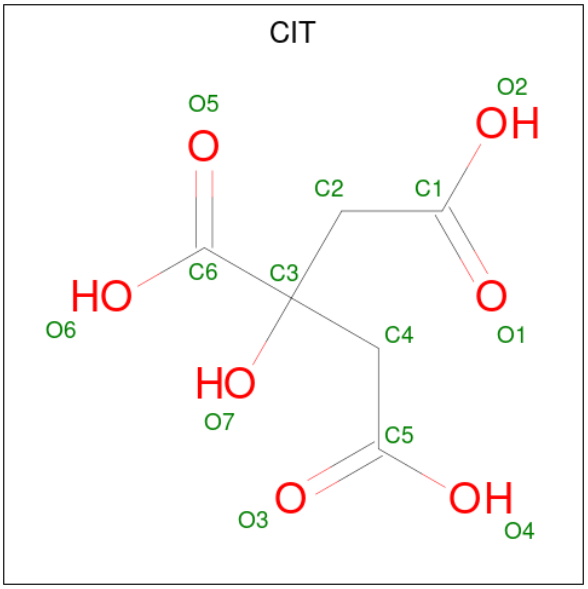
Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	ASP	-	expression tag	UNP P35705
J	0	PRO	-	expression tag	UNP P35705
J	190	LEU	PHE	engineered mutation	UNP P35705
K	-24	MET	-	expression tag	UNP P35705
K	-23	GLY	-	expression tag	UNP P35705
K	-22	SER	-	expression tag	UNP P35705
K	-21	SER	-	expression tag	UNP P35705
K	-20	HIS	-	expression tag	UNP P35705
K	-19	HIS	-	expression tag	UNP P35705
K	-18	HIS	-	expression tag	UNP P35705
K	-17	HIS	-	expression tag	UNP P35705
K	-16	HIS	-	expression tag	UNP P35705
K	-15	HIS	-	expression tag	UNP P35705
K	-14	SER	-	expression tag	UNP P35705
K	-13	SER	-	expression tag	UNP P35705
K	-12	GLY	-	expression tag	UNP P35705
K	-11	LEU	-	expression tag	UNP P35705
K	-10	VAL	-	expression tag	UNP P35705
K	-9	PRO	-	expression tag	UNP P35705
K	-8	ARG	-	expression tag	UNP P35705
K	-7	GLY	-	expression tag	UNP P35705
K	-6	SER	-	expression tag	UNP P35705
K	-5	HIS	-	expression tag	UNP P35705
K	-4	MET	-	expression tag	UNP P35705
K	-3	LEU	-	expression tag	UNP P35705
K	-2	GLU	-	expression tag	UNP P35705
K	-1	ASP	-	expression tag	UNP P35705
K	0	PRO	-	expression tag	UNP P35705
K	190	LEU	PHE	engineered mutation	UNP P35705
L	-24	MET	-	expression tag	UNP P35705
L	-23	GLY	-	expression tag	UNP P35705
L	-22	SER	-	expression tag	UNP P35705
L	-21	SER	-	expression tag	UNP P35705
L	-20	HIS	-	expression tag	UNP P35705
L	-19	HIS	-	expression tag	UNP P35705
L	-18	HIS	-	expression tag	UNP P35705
L	-17	HIS	-	expression tag	UNP P35705
L	-16	HIS	-	expression tag	UNP P35705
L	-15	HIS	-	expression tag	UNP P35705
L	-14	SER	-	expression tag	UNP P35705
L	-13	SER	-	expression tag	UNP P35705
L	-12	GLY	-	expression tag	UNP P35705

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-11	LEU	-	expression tag	UNP P35705
L	-10	VAL	-	expression tag	UNP P35705
L	-9	PRO	-	expression tag	UNP P35705
L	-8	ARG	-	expression tag	UNP P35705
L	-7	GLY	-	expression tag	UNP P35705
L	-6	SER	-	expression tag	UNP P35705
L	-5	HIS	-	expression tag	UNP P35705
L	-4	MET	-	expression tag	UNP P35705
L	-3	LEU	-	expression tag	UNP P35705
L	-2	GLU	-	expression tag	UNP P35705
L	-1	ASP	-	expression tag	UNP P35705
L	0	PRO	-	expression tag	UNP P35705
L	190	LEU	PHE	engineered mutation	UNP P35705

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0
2	J	1	Total C O 13 6 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total O 77 77	0	0
3	B	40	Total O 40 40	0	0
3	C	27	Total O 27 27	0	0
3	D	35	Total O 35 35	0	0
3	E	27	Total O 27 27	0	0
3	F	19	Total O 19 19	0	0
3	G	42	Total O 42 42	0	0
3	H	35	Total O 35 35	0	0
3	I	57	Total O 57 57	0	0
3	J	23	Total O 23 23	0	0
3	K	28	Total O 28 28	0	0
3	L	66	Total O 66 66	0	0

3 Residue-property plots (i)

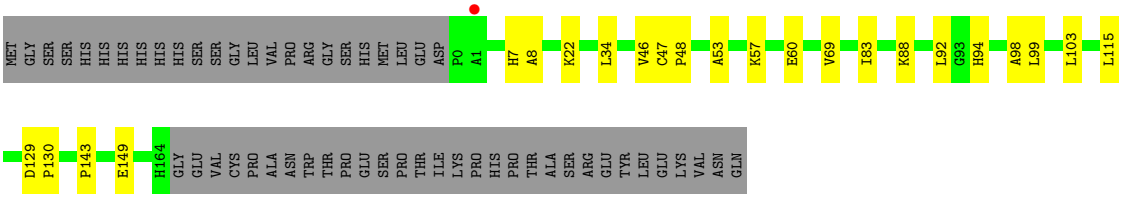
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-dependent peroxide reductase, mitochondrial

Chain A:

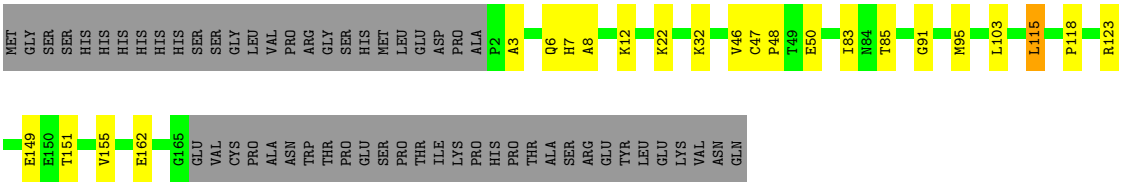
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain B:



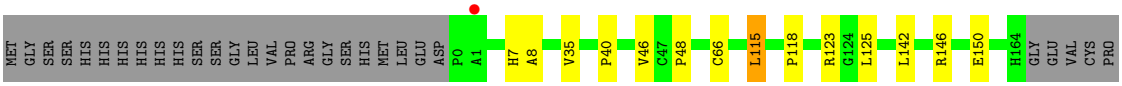
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain C:



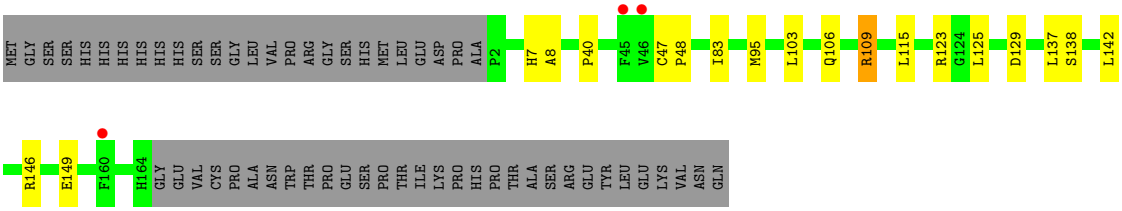
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain D:



• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain E:

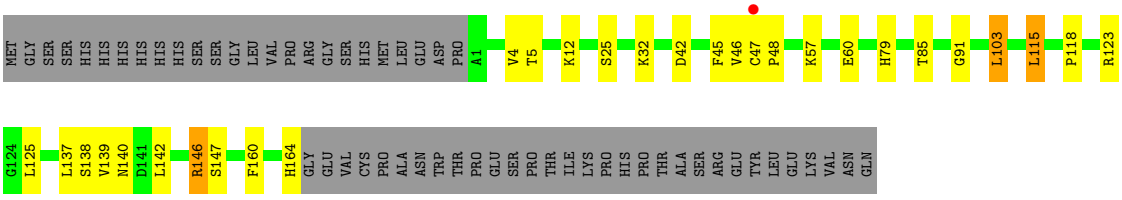


• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain F:

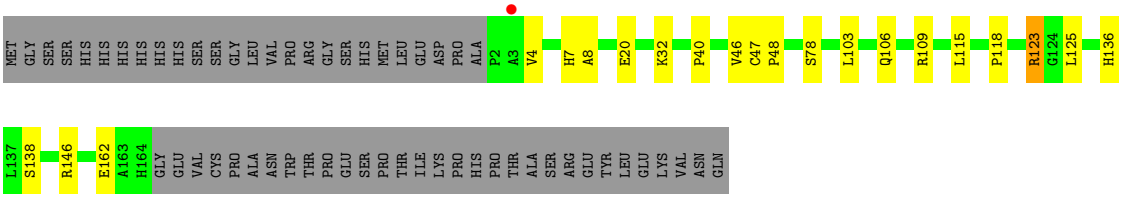
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain G:



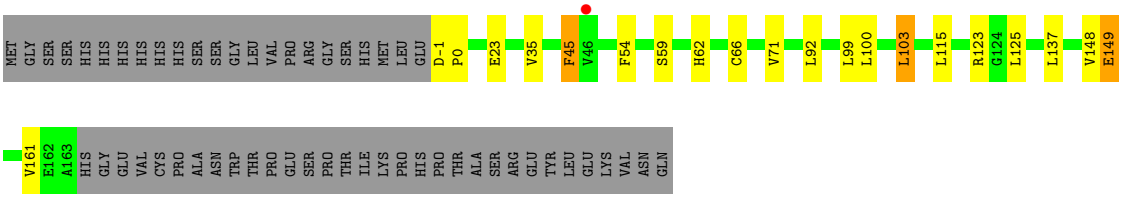
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain H:



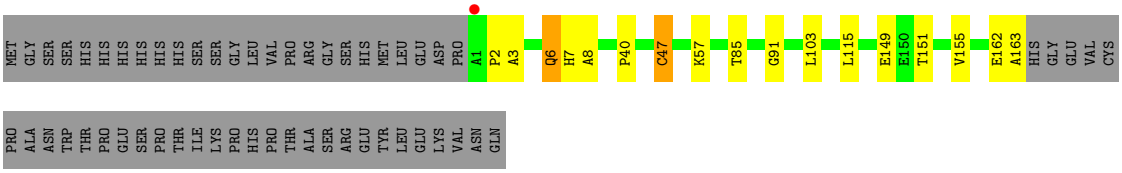
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain I:



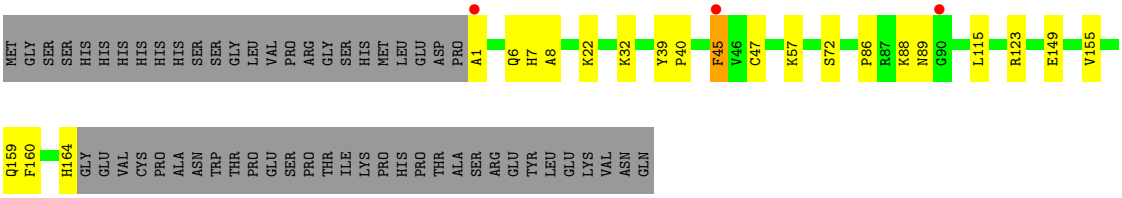
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain J:



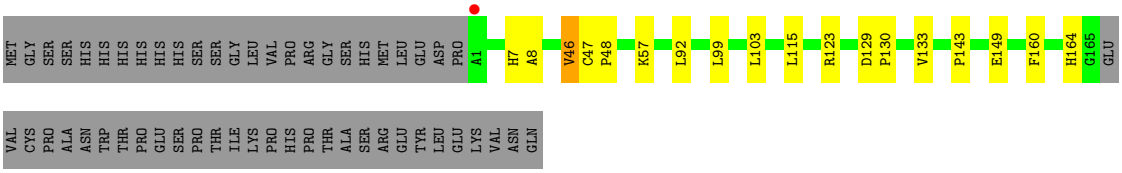
• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain K:



• Molecule 1: Thioredoxin-dependent peroxide reductase, mitochondrial

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.57Å 260.82Å 81.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.47 – 2.20 95.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (95.47-2.20) 98.6 (95.29-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.180 , 0.219 0.180 , 0.218	Depositor DCC
R_{free} test set	7516 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16330	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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

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

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	0.71	0/1367	0.77	0/1855
1	B	0.67	0/1356	0.75	0/1842
1	C	0.57	0/1371	0.67	0/1859
1	D	0.59	0/1351	0.71	0/1834
1	E	0.57	0/1347	0.67	0/1828
1	F	0.51	0/1393	0.63	0/1894
1	G	0.61	0/1394	0.70	1/1895 (0.1%)
1	H	0.62	0/1338	0.69	1/1816 (0.1%)
1	I	0.71	0/1378	0.78	0/1873
1	J	0.60	0/1323	0.70	0/1797
1	K	0.62	0/1345	0.69	0/1827
1	L	0.67	0/1370	0.74	0/1860
All	All	0.62	0/16333	0.71	2/22180 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	123	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	103	LEU	CB-CG-CD2	5.05	119.59	111.00

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	1317	0	1317	6	0
1	B	1310	0	1305	14	0
1	C	1318	0	1318	11	0
1	D	1307	0	1308	11	0
1	E	1301	0	1293	12	0
1	F	1346	0	1338	10	0
1	G	1345	0	1337	23	0
1	H	1295	0	1289	14	0
1	I	1330	0	1316	12	0
1	J	1284	0	1283	8	0
1	K	1304	0	1296	12	0
1	L	1319	0	1313	10	0
2	A	13	0	5	0	0
2	D	13	0	5	2	0
2	F	13	0	5	2	0
2	H	13	0	5	0	0
2	J	13	0	5	0	0
2	L	13	0	5	0	0
3	A	77	0	0	2	0
3	B	40	0	0	0	0
3	C	27	0	0	1	0
3	D	35	0	0	0	0
3	E	27	0	0	0	0
3	F	19	0	0	0	0
3	G	42	0	0	0	0
3	H	35	0	0	0	0
3	I	57	0	0	1	0
3	J	23	0	0	0	0
3	K	28	0	0	0	0
3	L	66	0	0	1	0
All	All	16330	0	15743	137	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 4.

All (137) 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:G:47[A]:CYS:N	1:G:48[A]:PRO:HD2	1.73	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47[A]:CYS:HA	1:F:123:ARG:HH22	1.32	0.93
1:K:1:ALA:HB3	1:K:6[B]:GLN:OE1	1.68	0.93
1:G:47[A]:CYS:HA	1:G:123:ARG:HH22	1.36	0.88
1:H:106:GLN:HE22	1:H:109:ARG:HH11	1.19	0.85
1:G:47[A]:CYS:N	1:G:48[A]:PRO:CD	2.42	0.83
1:D:125:LEU:HD13	1:D:146:ARG:HD2	1.57	0.83
1:F:47[A]:CYS:N	1:F:48[A]:PRO:HD2	1.98	0.78
1:I:149[A]:GLU:H	1:I:149[A]:GLU:CD	1.88	0.76
1:L:7[B]:HIS:HD2	1:L:8:ALA:O	1.69	0.74
1:L:57:LYS:HE3	1:L:149[A]:GLU:OE1	1.88	0.73
1:F:47[A]:CYS:N	1:F:48[A]:PRO:CD	2.54	0.71
1:A:123:ARG:HD3	3:A:304:HOH:O	1.92	0.69
1:K:57:LYS:NZ	1:K:149:GLU:OE2	2.26	0.68
1:B:57:LYS:HE2	1:B:149:GLU:OE2	1.93	0.67
1:E:106:GLN:HE22	1:E:109:ARG:HH21	1.44	0.66
1:C:3:ALA:O	1:C:6[B]:GLN:HB2	1.96	0.66
1:E:7[B]:HIS:HD2	1:E:8:ALA:O	1.80	0.64
1:L:129:ASP:OD1	1:L:133:VAL:N	2.25	0.63
1:H:106:GLN:NE2	1:H:109:ARG:HH11	1.95	0.62
1:E:125:LEU:HD13	1:E:146:ARG:HD2	1.79	0.62
1:G:47[A]:CYS:CA	1:G:123:ARG:HH22	2.11	0.61
1:G:57:LYS:HD3	1:G:60:GLU:OE2	2.01	0.61
1:E:40:PRO:HG3	1:E:142:LEU:HD22	1.82	0.59
1:B:7[B]:HIS:HD2	1:B:8:ALA:O	1.84	0.59
1:G:47[A]:CYS:H	1:G:48[A]:PRO:HD2	1.63	0.59
1:I:45:PHE:CD1	1:I:45:PHE:N	2.71	0.59
1:J:7[B]:HIS:HD2	1:J:8:ALA:O	1.86	0.58
1:L:129:ASP:HB2	1:L:130:PRO:CD	2.34	0.57
1:B:46:VAL:HG21	1:B:143:PRO:HA	1.87	0.57
1:L:129:ASP:HB2	1:L:130:PRO:HD2	1.87	0.56
1:J:2:PRO:HA	1:J:6[A]:GLN:OE1	2.06	0.56
1:K:160:PHE:O	1:K:164:HIS:HD2	1.89	0.55
1:B:57:LYS:CE	1:B:149:GLU:OE2	2.54	0.55
1:G:140:ASN:OD1	1:H:136:HIS:ND1	2.37	0.55
1:C:162:GLU:HA	1:C:162:GLU:OE1	2.07	0.54
1:D:40:PRO:HG3	1:D:142:LEU:HD22	1.89	0.54
1:E:47:CYS:N	1:E:48:PRO:HD2	2.23	0.54
1:A:7[B]:HIS:HD2	1:A:8:ALA:O	1.91	0.54
1:G:46[A]:VAL:C	1:G:48[A]:PRO:HD2	2.28	0.54
1:B:34:LEU:HD11	1:B:69:VAL:HG13	1.90	0.53
1:H:40:PRO:HD2	1:H:47:CYS:SG	2.49	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47[A]:CYS:CA	1:F:123:ARG:HH22	2.14	0.53
1:I:45:PHE:HD1	1:I:45:PHE:H	1.56	0.53
1:K:47:CYS:HA	1:K:123:ARG:HH22	1.74	0.53
1:F:46[A]:VAL:C	1:F:48[A]:PRO:HD2	2.28	0.53
1:B:83:ILE:HD11	1:B:99:LEU:HD22	1.91	0.52
1:B:57:LYS:NZ	1:B:60:GLU:OE2	2.27	0.51
1:D:35:VAL:HG23	1:D:66:CYS:SG	2.51	0.51
1:D:46:VAL:C	1:D:48:PRO:HD2	2.31	0.51
1:D:123:ARG:HB3	1:D:146:ARG:HH22	1.76	0.51
1:K:45:PHE:H	1:K:45:PHE:HD1	1.58	0.50
1:K:45:PHE:N	1:K:45:PHE:CD1	2.79	0.50
1:D:125:LEU:CD1	1:D:146:ARG:HD2	2.35	0.50
1:E:149[B]:GLU:CD	1:E:149[B]:GLU:H	2.15	0.50
1:H:125:LEU:HD13	1:H:146:ARG:CD	2.42	0.50
1:D:7[B]:HIS:HD2	1:D:8:ALA:O	1.95	0.50
1:A:94[A]:HIS:CE1	3:A:318:HOH:O	2.64	0.49
1:G:139:VAL:O	1:H:4:VAL:HG21	2.12	0.49
1:K:47:CYS:HA	1:K:123:ARG:NH2	2.27	0.49
1:H:47:CYS:N	1:H:48:PRO:HD2	2.28	0.48
1:J:3:ALA:O	1:J:6[A]:GLN:HB3	2.14	0.48
1:B:47:CYS:N	1:B:48:PRO:HD2	2.29	0.48
1:F:150:GLU:HG2	2:F:201:CIT:H41	1.96	0.48
1:H:7[A]:HIS:HD2	1:H:8:ALA:O	1.97	0.47
1:I:92:LEU:CD1	1:I:99:LEU:HD21	2.44	0.47
1:J:162:GLU:O	1:J:163:ALA:CB	2.62	0.47
1:C:7[B]:HIS:HD2	1:C:8:ALA:O	1.96	0.47
1:I:123:ARG:HD3	3:I:217:HOH:O	2.15	0.47
1:G:85:THR:HB	1:G:91:GLY:HA3	1.97	0.47
1:L:123:ARG:HD3	3:L:333:HOH:O	2.13	0.47
1:K:39:TYR:CZ	1:K:72:SER:HB3	2.50	0.46
1:G:146:ARG:HG2	1:G:147:SER:N	2.30	0.46
1:C:115:LEU:HB3	1:C:118:PRO:HD2	1.97	0.46
1:I:125:LEU:O	1:I:137:LEU:HA	2.16	0.46
1:B:129:ASP:HB2	1:B:130:PRO:CD	2.45	0.46
1:C:123:ARG:HD2	3:C:213:HOH:O	2.15	0.46
1:J:57:LYS:NZ	1:J:149:GLU:OE2	2.41	0.45
1:E:129:ASP:OD1	1:E:129:ASP:C	2.55	0.45
1:G:42:ASP:OD2	1:G:79:HIS:ND1	2.45	0.45
1:I:35:VAL:HG23	1:I:66:CYS:SG	2.57	0.45
1:I:59:SER:HA	1:I:62[A]:HIS:HB2	1.98	0.45
1:A:129:ASP:HB2	1:A:130:PRO:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:CYS:N	1:C:48:PRO:HD2	2.32	0.45
1:K:155:VAL:O	1:K:159:GLN:HG3	2.16	0.45
1:B:57:LYS:NZ	1:B:149:GLU:OE2	2.50	0.44
1:D:46:VAL:HG12	1:D:123:ARG:HH22	1.82	0.44
1:G:123:ARG:NE	1:G:142:LEU:O	2.43	0.44
1:B:53:ALA:O	1:B:57:LYS:HG2	2.18	0.43
1:J:85:THR:HB	1:J:91:GLY:HA3	2.00	0.43
1:E:47:CYS:N	1:E:48:PRO:CD	2.81	0.43
1:G:125:LEU:HD13	1:G:146:ARG:HD3	2.00	0.43
1:E:125:LEU:O	1:E:137:LEU:HA	2.18	0.43
1:G:115:LEU:HB3	1:G:118:PRO:HD2	1.99	0.43
1:I:71:VAL:HG22	1:I:100:LEU:HB3	2.00	0.43
1:G:125:LEU:O	1:G:137:LEU:HA	2.19	0.43
1:H:46:VAL:O	1:H:123:ARG:NH2	2.51	0.43
1:K:86:PRO:HD2	1:K:89:ASN:HD22	1.84	0.43
1:K:88:LYS:H	1:K:88:LYS:HG3	1.46	0.43
1:L:46:VAL:HG21	1:L:143:PRO:HA	2.00	0.43
1:G:12:LYS:HG3	1:G:25:SER:HB3	2.01	0.43
1:A:50:GLU:CD	1:A:146:ARG:HG2	2.39	0.43
1:D:150:GLU:HG3	2:D:201:CIT:H41	2.00	0.43
1:J:151:THR:O	1:J:155:VAL:HG23	2.19	0.43
1:G:146:ARG:CG	1:G:147:SER:N	2.82	0.42
1:C:85:THR:O	1:C:91:GLY:HA3	2.19	0.42
1:D:115:LEU:HB3	1:D:118:PRO:HG2	2.01	0.42
1:B:47:CYS:N	1:B:48:PRO:CD	2.82	0.42
1:B:69:VAL:HB	1:B:98:ALA:HB3	2.02	0.42
1:C:83:ILE:HG12	1:C:95:MET:HG3	2.00	0.42
1:E:123:ARG:NE	1:E:142:LEU:O	2.45	0.42
1:G:138:SER:HB3	1:H:138:SER:HB3	2.01	0.42
1:C:12:LYS:HE3	1:C:12:LYS:HB3	1.74	0.42
1:F:146:ARG:HG2	2:F:201:CIT:O4	2.20	0.42
1:G:160:PHE:CE1	1:G:164:HIS:HD2	2.37	0.42
1:H:106:GLN:HE22	1:H:109:ARG:NH1	2.01	0.41
1:H:118:PRO:O	1:I:103:LEU:HD13	2.20	0.41
1:H:47:CYS:N	1:H:48:PRO:CD	2.83	0.41
1:F:47[B]:CYS:SG	1:F:48[B]:PRO:HD2	2.60	0.41
1:D:150:GLU:CG	2:D:201:CIT:H41	2.50	0.41
1:G:138:SER:HB3	1:H:138:SER:CB	2.50	0.41
1:L:47:CYS:N	1:L:48:PRO:HD2	2.35	0.41
1:L:160:PHE:CE2	1:L:164:HIS:HD2	2.39	0.41
1:C:50[B]:GLU:H	1:C:50[B]:GLU:CD	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:VAL:HG12	1:G:5:THR:HG23	2.03	0.41
1:C:151:THR:O	1:C:155:VAL:HG23	2.20	0.41
1:E:83:ILE:HG12	1:E:95:MET:HG3	2.03	0.41
1:E:138:SER:HB2	1:F:138:SER:HB3	2.03	0.41
1:G:47[A]:CYS:HA	1:G:123:ARG:NH2	2.19	0.41
1:B:92:LEU:CD1	1:B:99:LEU:HD21	2.51	0.40
1:I:-1:ASP:N	1:I:0:PRO:CD	2.84	0.40
1:J:40:PRO:HD2	1:J:47:CYS:SG	2.62	0.40
1:F:129:ASP:HB2	1:F:130:PRO:CD	2.51	0.40
1:I:54:PHE:CE2	1:I:148:VAL:HG22	2.57	0.40
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.91	0.40
1:K:7[B]:HIS:HD2	1:K:8:ALA:O	2.04	0.40
1:L:92:LEU:CD1	1:L:99:LEU:HD21	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	168/220 (76%)	159 (95%)	9 (5%)	0	100	100
1	B	166/220 (76%)	159 (96%)	7 (4%)	0	100	100
1	C	168/220 (76%)	161 (96%)	7 (4%)	0	100	100
1	D	166/220 (76%)	160 (96%)	6 (4%)	0	100	100
1	E	165/220 (75%)	160 (97%)	5 (3%)	0	100	100
1	F	171/220 (78%)	162 (95%)	8 (5%)	1 (1%)	25	26
1	G	171/220 (78%)	164 (96%)	7 (4%)	0	100	100
1	H	164/220 (74%)	158 (96%)	6 (4%)	0	100	100
1	I	169/220 (77%)	161 (95%)	8 (5%)	0	100	100
1	J	163/220 (74%)	157 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	165/220 (75%)	158 (96%)	6 (4%)	1 (1%)	25 26
1	L	168/220 (76%)	160 (95%)	8 (5%)	0	100 100
All	All	2004/2640 (76%)	1919 (96%)	83 (4%)	2 (0%)	51 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	40	PRO
1	K	40	PRO

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	145/190 (76%)	143 (99%)	2 (1%)	67 80
1	B	144/190 (76%)	139 (96%)	5 (4%)	36 46
1	C	146/190 (77%)	140 (96%)	6 (4%)	30 39
1	D	144/190 (76%)	143 (99%)	1 (1%)	84 91
1	E	144/190 (76%)	141 (98%)	3 (2%)	53 67
1	F	149/190 (78%)	144 (97%)	5 (3%)	37 47
1	G	149/190 (78%)	143 (96%)	6 (4%)	31 40
1	H	143/190 (75%)	137 (96%)	6 (4%)	30 38
1	I	147/190 (77%)	139 (95%)	8 (5%)	22 26
1	J	141/190 (74%)	136 (96%)	5 (4%)	36 46
1	K	143/190 (75%)	139 (97%)	4 (3%)	43 56
1	L	145/190 (76%)	142 (98%)	3 (2%)	53 67
All	All	1740/2280 (76%)	1686 (97%)	54 (3%)	41 51

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	147	SER
1	B	22	LYS
1	B	88	LYS
1	B	94	HIS
1	B	103	LEU
1	B	115	LEU
1	C	22	LYS
1	C	32	LYS
1	C	46	VAL
1	C	103	LEU
1	C	115	LEU
1	C	149	GLU
1	D	115	LEU
1	E	103	LEU
1	E	109	ARG
1	E	115	LEU
1	F	12	LYS
1	F	23	GLU
1	F	88	LYS
1	F	103	LEU
1	F	115	LEU
1	G	32	LYS
1	G	45[A]	PHE
1	G	45[B]	PHE
1	G	103	LEU
1	G	115	LEU
1	G	146	ARG
1	H	20	GLU
1	H	32	LYS
1	H	78	SER
1	H	103	LEU
1	H	115	LEU
1	H	162	GLU
1	I	23[A]	GLU
1	I	23[B]	GLU
1	I	45	PHE
1	I	103	LEU
1	I	115	LEU
1	I	149[A]	GLU
1	I	149[B]	GLU
1	I	161	VAL
1	J	6[A]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	6[B]	GLN
1	J	47	CYS
1	J	103	LEU
1	J	115	LEU
1	K	22	LYS
1	K	32	LYS
1	K	45	PHE
1	K	115	LEU
1	L	46	VAL
1	L	103	LEU
1	L	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	HIS
1	C	89	ASN
1	C	164	HIS
1	E	89	ASN
1	E	106	GLN
1	E	164	HIS
1	F	76	HIS
1	G	164	HIS
1	H	106	GLN
1	I	65	ASN
1	I	89	ASN
1	J	89	ASN
1	K	89	ASN
1	K	164	HIS
1	L	6	GLN
1	L	164	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	CIT	H	201	-	12,12,12	1.02	0	17,17,17	1.74	3 (17%)
2	CIT	D	201	-	12,12,12	1.29	1 (8%)	17,17,17	1.93	3 (17%)
2	CIT	F	201	-	12,12,12	1.13	0	17,17,17	1.76	4 (23%)
2	CIT	A	201	-	12,12,12	1.02	0	17,17,17	1.52	3 (17%)
2	CIT	L	201	-	12,12,12	1.26	0	17,17,17	1.92	3 (17%)
2	CIT	J	201	-	12,12,12	1.38	1 (8%)	17,17,17	2.02	4 (23%)

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	CIT	H	201	-	-	3/16/16/16	-
2	CIT	D	201	-	-	5/16/16/16	-
2	CIT	F	201	-	-	5/16/16/16	-
2	CIT	A	201	-	-	2/16/16/16	-
2	CIT	L	201	-	-	3/16/16/16	-
2	CIT	J	201	-	-	6/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201	CIT	C3-C6	2.51	1.56	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	CIT	C3-C6	2.10	1.55	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	201	CIT	O6-C6-C3	5.62	122.82	113.05
2	H	201	CIT	O6-C6-C3	4.90	121.57	113.05
2	F	201	CIT	O6-C6-C3	4.88	121.53	113.05
2	J	201	CIT	O6-C6-C3	4.45	120.78	113.05
2	D	201	CIT	C3-C4-C5	4.40	124.47	113.81
2	J	201	CIT	C3-C4-C5	4.34	124.31	113.81
2	D	201	CIT	O6-C6-C3	3.98	119.95	113.05
2	D	201	CIT	O7-C3-C6	3.77	114.15	108.86
2	L	201	CIT	O5-C6-C3	-3.30	117.57	122.25
2	J	201	CIT	C4-C3-C6	3.21	117.00	110.11
2	H	201	CIT	O5-C6-C3	-3.20	117.73	122.25
2	L	201	CIT	C4-C3-C6	3.13	116.84	110.11
2	F	201	CIT	C3-C4-C5	3.03	121.16	113.81
2	A	201	CIT	O6-C6-C3	3.03	118.31	113.05
2	A	201	CIT	O2-C1-C2	2.78	123.29	114.35
2	A	201	CIT	O5-C6-C3	-2.76	118.35	122.25
2	J	201	CIT	C3-C2-C1	2.32	119.43	113.81
2	F	201	CIT	O5-C6-C3	-2.15	119.21	122.25
2	H	201	CIT	C3-C4-C5	2.07	118.83	113.81
2	F	201	CIT	O2-C1-C2	2.01	120.80	114.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	201	CIT	C2-C3-C4-C5
2	D	201	CIT	O7-C3-C4-C5
2	D	201	CIT	C6-C3-C4-C5
2	F	201	CIT	C2-C3-C4-C5
2	F	201	CIT	O7-C3-C4-C5
2	F	201	CIT	C6-C3-C4-C5
2	H	201	CIT	C2-C3-C4-C5
2	H	201	CIT	O7-C3-C4-C5
2	H	201	CIT	C6-C3-C4-C5
2	J	201	CIT	C1-C2-C3-O7
2	J	201	CIT	C1-C2-C3-C6
2	L	201	CIT	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	L	201	CIT	C6-C3-C4-C5
2	L	201	CIT	O7-C3-C4-C5
2	J	201	CIT	C1-C2-C3-C4
2	J	201	CIT	C6-C3-C4-C5
2	A	201	CIT	O2-C1-C2-C3
2	A	201	CIT	O1-C1-C2-C3
2	D	201	CIT	C1-C2-C3-O7
2	J	201	CIT	C2-C3-C4-C5
2	J	201	CIT	O7-C3-C4-C5
2	D	201	CIT	C1-C2-C3-C6
2	F	201	CIT	C1-C2-C3-C6
2	F	201	CIT	C1-C2-C3-O7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	CIT	2	0
2	F	201	CIT	2	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

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	165/220 (75%)	-0.22	1 (0%) 89 88	23, 29, 47, 72	3 (1%)
1	B	165/220 (75%)	-0.24	1 (0%) 89 88	23, 33, 54, 83	0
1	C	164/220 (74%)	-0.27	0 100 100	26, 41, 61, 109	1 (0%)
1	D	165/220 (75%)	-0.21	1 (0%) 89 88	27, 43, 67, 93	0
1	E	163/220 (74%)	-0.20	3 (1%) 68 66	27, 44, 64, 97	0
1	F	165/220 (75%)	-0.22	0 100 100	28, 49, 76, 96	0
1	G	164/220 (74%)	-0.27	1 (0%) 89 88	27, 40, 61, 86	0
1	H	163/220 (74%)	-0.29	1 (0%) 89 88	23, 38, 62, 92	0
1	I	165/220 (75%)	-0.27	1 (0%) 89 88	23, 31, 49, 89	0
1	J	163/220 (74%)	-0.25	1 (0%) 89 88	27, 43, 64, 81	0
1	K	164/220 (74%)	-0.17	3 (1%) 68 66	30, 42, 69, 95	0
1	L	165/220 (75%)	-0.21	1 (0%) 89 88	23, 30, 47, 79	0
All	All	1971/2640 (74%)	-0.23	14 (0%) 87 86	23, 38, 65, 109	4 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	90	GLY	4.3
1	K	1	ALA	3.7
1	E	45	PHE	3.0
1	I	46	VAL	3.0
1	J	1	ALA	2.9
1	E	46	VAL	2.8
1	E	160	PHE	2.7
1	B	1	ALA	2.7
1	G	47[A]	CYS	2.6
1	A	1	ALA	2.6
1	D	1	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	3	ALA	2.2
1	K	45	PHE	2.1
1	L	1	ALA	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	J	201	13/13	0.57	0.24	69,85,97,101	0
2	CIT	F	201	13/13	0.58	0.33	87,99,106,106	0
2	CIT	D	201	13/13	0.62	0.30	66,85,96,98	0
2	CIT	L	201	13/13	0.69	0.25	58,80,86,96	0
2	CIT	H	201	13/13	0.73	0.28	87,101,109,113	0
2	CIT	A	201	13/13	0.87	0.23	67,79,88,89	0

6.5 Other polymers (i)

There are no such residues in this entry.