Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 02:19 PM JST

PDB ID	:	6J7G
Title	:	Human H-ferritin mutant-C90A/C102A/C130A/D144C
Authors	:	Zang, J.; Chen, H.; Zhang, X.; Zhao, G.
Deposited on	:	2019-01-18
Resolution	:	3.87 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 (1)) were used in the production of this report:

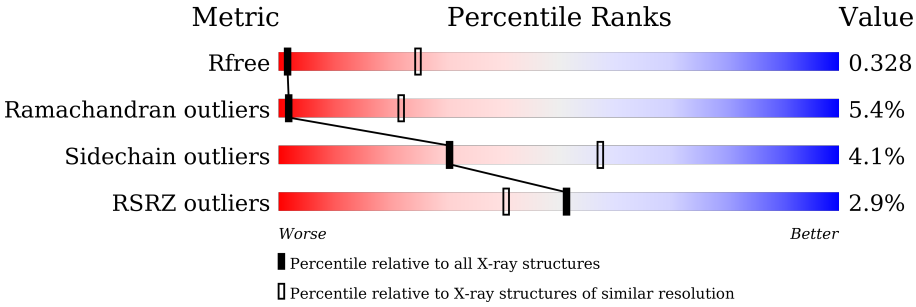
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.87 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	1048 (4.10-3.62)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)

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	176	3% 86% 7% • 6%
1	B	176	2% 80% 13% • 6%
1	C	176	2% 78% 15% • 6%
1	D	176	3% 81% 11% • • 6%
1	G	176	3% 86% 8% • 6%
1	H	176	3% 89% 5% 6%
1	I	176	3% 86% 7% • 6%

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Mol	Chain	Length	Quality of chain
1	J	176	3% 82% 13% 6%
1	M	176	3% 85% 9% 6%
1	N	176	2% 88% 6% 6%
1	O	176	2% 86% 7% 6%
1	P	176	2% 84% 11% 6%
1	Q	176	2% 88% 7% 6%
1	R	176	4% 83% 11% 6%
1	S	176	3% 85% 8% 6%
1	T	176	2% 81% 11% 6%
1	W	176	2% 87% 7% 6%
1	X	176	2% 88% 6% 6%
1	Y	176	3% 85% 9% 6%
1	Z	176	2% 82% 12% 6%
1	a	176	5% 89% 5% 6%
1	b	176	2% 86% 7% 6%
1	e	176	3% 86% 8% 6%
1	f	176	% 87% 7% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32524 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	166	1356	854	238	259	5	0	0	0
1	B	166	1356	854	238	259	5	0	0	0
1	C	166	1356	854	238	259	5	0	0	0
1	D	166	1356	854	238	259	5	0	0	0
1	G	166	1352	852	238	257	5	0	0	0
1	H	166	1356	854	238	259	5	0	0	0
1	I	166	1352	852	237	258	5	0	0	0
1	J	166	1356	854	238	259	5	0	0	0
1	M	166	1352	852	238	257	5	0	0	0
1	N	166	1356	854	238	259	5	0	0	0
1	O	166	1356	854	238	259	5	0	0	0
1	P	166	1356	854	238	259	5	0	0	0
1	Q	166	1356	854	238	259	5	0	0	0
1	R	166	1356	854	238	259	5	0	0	0
1	S	166	1352	852	237	258	5	0	0	0
1	T	166	1356	854	238	259	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	W	166	1352	852	238	257	5	0	0	0
			Total	C	N	O	S			
1	X	166	1356	854	238	259	5	0	0	0
			Total	C	N	O	S			
1	Y	166	1356	854	238	259	5	0	0	0
			Total	C	N	O	S			
1	Z	166	1356	854	238	259	5	0	0	0
			Total	C	N	O	S			
1	a	166	1352	852	237	258	5	0	0	0
			Total	C	N	O	S			
1	b	166	1356	854	238	259	5	0	0	0
			Total	C	N	O	S			
1	e	166	1352	852	238	257	5	0	0	0
			Total	C	N	O	S			
1	f	166	1356	854	238	259	5	0	0	0

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLN	LYS	conflict	UNP P02794
A	90	ALA	CYS	engineered mutation	UNP P02794
A	102	ALA	CYS	engineered mutation	UNP P02794
A	130	ALA	CYS	engineered mutation	UNP P02794
A	?	-	ASN	deletion	UNP P02794
A	?	-	GLU	deletion	UNP P02794
A	?	-	GLN	deletion	UNP P02794
A	?	-	VAL	deletion	UNP P02794
A	?	-	LYS	deletion	UNP P02794
A	?	-	ALA	deletion	UNP P02794
A	144	CYS	ASP	engineered mutation	UNP P02794
B	86	GLN	LYS	conflict	UNP P02794
B	90	ALA	CYS	engineered mutation	UNP P02794
B	102	ALA	CYS	engineered mutation	UNP P02794
B	130	ALA	CYS	engineered mutation	UNP P02794
B	?	-	ASN	deletion	UNP P02794
B	?	-	GLU	deletion	UNP P02794
B	?	-	GLN	deletion	UNP P02794
B	?	-	VAL	deletion	UNP P02794
B	?	-	LYS	deletion	UNP P02794
B	?	-	ALA	deletion	UNP P02794
B	144	CYS	ASP	engineered mutation	UNP P02794
C	86	GLN	LYS	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
C	90	ALA	CYS	engineered mutation	UNP P02794
C	102	ALA	CYS	engineered mutation	UNP P02794
C	130	ALA	CYS	engineered mutation	UNP P02794
C	?	-	ASN	deletion	UNP P02794
C	?	-	GLU	deletion	UNP P02794
C	?	-	GLN	deletion	UNP P02794
C	?	-	VAL	deletion	UNP P02794
C	?	-	LYS	deletion	UNP P02794
C	?	-	ALA	deletion	UNP P02794
C	144	CYS	ASP	engineered mutation	UNP P02794
D	86	GLN	LYS	conflict	UNP P02794
D	90	ALA	CYS	engineered mutation	UNP P02794
D	102	ALA	CYS	engineered mutation	UNP P02794
D	130	ALA	CYS	engineered mutation	UNP P02794
D	?	-	ASN	deletion	UNP P02794
D	?	-	GLU	deletion	UNP P02794
D	?	-	GLN	deletion	UNP P02794
D	?	-	VAL	deletion	UNP P02794
D	?	-	LYS	deletion	UNP P02794
D	?	-	ALA	deletion	UNP P02794
D	144	CYS	ASP	engineered mutation	UNP P02794
G	86	GLN	LYS	conflict	UNP P02794
G	90	ALA	CYS	engineered mutation	UNP P02794
G	102	ALA	CYS	engineered mutation	UNP P02794
G	130	ALA	CYS	engineered mutation	UNP P02794
G	?	-	ASN	deletion	UNP P02794
G	?	-	GLU	deletion	UNP P02794
G	?	-	GLN	deletion	UNP P02794
G	?	-	VAL	deletion	UNP P02794
G	?	-	LYS	deletion	UNP P02794
G	?	-	ALA	deletion	UNP P02794
G	144	CYS	ASP	engineered mutation	UNP P02794
H	86	GLN	LYS	conflict	UNP P02794
H	90	ALA	CYS	engineered mutation	UNP P02794
H	102	ALA	CYS	engineered mutation	UNP P02794
H	130	ALA	CYS	engineered mutation	UNP P02794
H	?	-	ASN	deletion	UNP P02794
H	?	-	GLU	deletion	UNP P02794
H	?	-	GLN	deletion	UNP P02794
H	?	-	VAL	deletion	UNP P02794
H	?	-	LYS	deletion	UNP P02794
H	?	-	ALA	deletion	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
H	144	CYS	ASP	engineered mutation	UNP P02794
I	86	GLN	LYS	conflict	UNP P02794
I	90	ALA	CYS	engineered mutation	UNP P02794
I	102	ALA	CYS	engineered mutation	UNP P02794
I	130	ALA	CYS	engineered mutation	UNP P02794
I	?	-	ASN	deletion	UNP P02794
I	?	-	GLU	deletion	UNP P02794
I	?	-	GLN	deletion	UNP P02794
I	?	-	VAL	deletion	UNP P02794
I	?	-	LYS	deletion	UNP P02794
I	?	-	ALA	deletion	UNP P02794
I	144	CYS	ASP	engineered mutation	UNP P02794
J	86	GLN	LYS	conflict	UNP P02794
J	90	ALA	CYS	engineered mutation	UNP P02794
J	102	ALA	CYS	engineered mutation	UNP P02794
J	130	ALA	CYS	engineered mutation	UNP P02794
J	?	-	ASN	deletion	UNP P02794
J	?	-	GLU	deletion	UNP P02794
J	?	-	GLN	deletion	UNP P02794
J	?	-	VAL	deletion	UNP P02794
J	?	-	LYS	deletion	UNP P02794
J	?	-	ALA	deletion	UNP P02794
J	144	CYS	ASP	engineered mutation	UNP P02794
M	86	GLN	LYS	conflict	UNP P02794
M	90	ALA	CYS	engineered mutation	UNP P02794
M	102	ALA	CYS	engineered mutation	UNP P02794
M	130	ALA	CYS	engineered mutation	UNP P02794
M	?	-	ASN	deletion	UNP P02794
M	?	-	GLU	deletion	UNP P02794
M	?	-	GLN	deletion	UNP P02794
M	?	-	VAL	deletion	UNP P02794
M	?	-	LYS	deletion	UNP P02794
M	?	-	ALA	deletion	UNP P02794
M	144	CYS	ASP	engineered mutation	UNP P02794
N	86	GLN	LYS	conflict	UNP P02794
N	90	ALA	CYS	engineered mutation	UNP P02794
N	102	ALA	CYS	engineered mutation	UNP P02794
N	130	ALA	CYS	engineered mutation	UNP P02794
N	?	-	ASN	deletion	UNP P02794
N	?	-	GLU	deletion	UNP P02794
N	?	-	GLN	deletion	UNP P02794
N	?	-	VAL	deletion	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P02794
N	?	-	ALA	deletion	UNP P02794
N	144	CYS	ASP	engineered mutation	UNP P02794
O	86	GLN	LYS	conflict	UNP P02794
O	90	ALA	CYS	engineered mutation	UNP P02794
O	102	ALA	CYS	engineered mutation	UNP P02794
O	130	ALA	CYS	engineered mutation	UNP P02794
O	?	-	ASN	deletion	UNP P02794
O	?	-	GLU	deletion	UNP P02794
O	?	-	GLN	deletion	UNP P02794
O	?	-	VAL	deletion	UNP P02794
O	?	-	LYS	deletion	UNP P02794
O	?	-	ALA	deletion	UNP P02794
O	144	CYS	ASP	engineered mutation	UNP P02794
P	86	GLN	LYS	conflict	UNP P02794
P	90	ALA	CYS	engineered mutation	UNP P02794
P	102	ALA	CYS	engineered mutation	UNP P02794
P	130	ALA	CYS	engineered mutation	UNP P02794
P	?	-	ASN	deletion	UNP P02794
P	?	-	GLU	deletion	UNP P02794
P	?	-	GLN	deletion	UNP P02794
P	?	-	VAL	deletion	UNP P02794
P	?	-	LYS	deletion	UNP P02794
P	?	-	ALA	deletion	UNP P02794
P	144	CYS	ASP	engineered mutation	UNP P02794
Q	86	GLN	LYS	conflict	UNP P02794
Q	90	ALA	CYS	engineered mutation	UNP P02794
Q	102	ALA	CYS	engineered mutation	UNP P02794
Q	130	ALA	CYS	engineered mutation	UNP P02794
Q	?	-	ASN	deletion	UNP P02794
Q	?	-	GLU	deletion	UNP P02794
Q	?	-	GLN	deletion	UNP P02794
Q	?	-	VAL	deletion	UNP P02794
Q	?	-	LYS	deletion	UNP P02794
Q	?	-	ALA	deletion	UNP P02794
Q	144	CYS	ASP	engineered mutation	UNP P02794
R	86	GLN	LYS	conflict	UNP P02794
R	90	ALA	CYS	engineered mutation	UNP P02794
R	102	ALA	CYS	engineered mutation	UNP P02794
R	130	ALA	CYS	engineered mutation	UNP P02794
R	?	-	ASN	deletion	UNP P02794
R	?	-	GLU	deletion	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	GLN	deletion	UNP P02794
R	?	-	VAL	deletion	UNP P02794
R	?	-	LYS	deletion	UNP P02794
R	?	-	ALA	deletion	UNP P02794
R	144	CYS	ASP	engineered mutation	UNP P02794
S	86	GLN	LYS	conflict	UNP P02794
S	90	ALA	CYS	engineered mutation	UNP P02794
S	102	ALA	CYS	engineered mutation	UNP P02794
S	130	ALA	CYS	engineered mutation	UNP P02794
S	?	-	ASN	deletion	UNP P02794
S	?	-	GLU	deletion	UNP P02794
S	?	-	GLN	deletion	UNP P02794
S	?	-	VAL	deletion	UNP P02794
S	?	-	LYS	deletion	UNP P02794
S	?	-	ALA	deletion	UNP P02794
S	144	CYS	ASP	engineered mutation	UNP P02794
T	86	GLN	LYS	conflict	UNP P02794
T	90	ALA	CYS	engineered mutation	UNP P02794
T	102	ALA	CYS	engineered mutation	UNP P02794
T	130	ALA	CYS	engineered mutation	UNP P02794
T	?	-	ASN	deletion	UNP P02794
T	?	-	GLU	deletion	UNP P02794
T	?	-	GLN	deletion	UNP P02794
T	?	-	VAL	deletion	UNP P02794
T	?	-	LYS	deletion	UNP P02794
T	?	-	ALA	deletion	UNP P02794
T	144	CYS	ASP	engineered mutation	UNP P02794
W	86	GLN	LYS	conflict	UNP P02794
W	90	ALA	CYS	engineered mutation	UNP P02794
W	102	ALA	CYS	engineered mutation	UNP P02794
W	130	ALA	CYS	engineered mutation	UNP P02794
W	?	-	ASN	deletion	UNP P02794
W	?	-	GLU	deletion	UNP P02794
W	?	-	GLN	deletion	UNP P02794
W	?	-	VAL	deletion	UNP P02794
W	?	-	LYS	deletion	UNP P02794
W	?	-	ALA	deletion	UNP P02794
W	144	CYS	ASP	engineered mutation	UNP P02794
X	86	GLN	LYS	conflict	UNP P02794
X	90	ALA	CYS	engineered mutation	UNP P02794
X	102	ALA	CYS	engineered mutation	UNP P02794
X	130	ALA	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
X	?	-	ASN	deletion	UNP P02794
X	?	-	GLU	deletion	UNP P02794
X	?	-	GLN	deletion	UNP P02794
X	?	-	VAL	deletion	UNP P02794
X	?	-	LYS	deletion	UNP P02794
X	?	-	ALA	deletion	UNP P02794
X	144	CYS	ASP	engineered mutation	UNP P02794
Y	86	GLN	LYS	conflict	UNP P02794
Y	90	ALA	CYS	engineered mutation	UNP P02794
Y	102	ALA	CYS	engineered mutation	UNP P02794
Y	130	ALA	CYS	engineered mutation	UNP P02794
Y	?	-	ASN	deletion	UNP P02794
Y	?	-	GLU	deletion	UNP P02794
Y	?	-	GLN	deletion	UNP P02794
Y	?	-	VAL	deletion	UNP P02794
Y	?	-	LYS	deletion	UNP P02794
Y	?	-	ALA	deletion	UNP P02794
Y	144	CYS	ASP	engineered mutation	UNP P02794
Z	86	GLN	LYS	conflict	UNP P02794
Z	90	ALA	CYS	engineered mutation	UNP P02794
Z	102	ALA	CYS	engineered mutation	UNP P02794
Z	130	ALA	CYS	engineered mutation	UNP P02794
Z	?	-	ASN	deletion	UNP P02794
Z	?	-	GLU	deletion	UNP P02794
Z	?	-	GLN	deletion	UNP P02794
Z	?	-	VAL	deletion	UNP P02794
Z	?	-	LYS	deletion	UNP P02794
Z	?	-	ALA	deletion	UNP P02794
Z	144	CYS	ASP	engineered mutation	UNP P02794
a	86	GLN	LYS	conflict	UNP P02794
a	90	ALA	CYS	engineered mutation	UNP P02794
a	102	ALA	CYS	engineered mutation	UNP P02794
a	130	ALA	CYS	engineered mutation	UNP P02794
a	?	-	ASN	deletion	UNP P02794
a	?	-	GLU	deletion	UNP P02794
a	?	-	GLN	deletion	UNP P02794
a	?	-	VAL	deletion	UNP P02794
a	?	-	LYS	deletion	UNP P02794
a	?	-	ALA	deletion	UNP P02794
a	144	CYS	ASP	engineered mutation	UNP P02794
b	86	GLN	LYS	conflict	UNP P02794
b	90	ALA	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
b	102	ALA	CYS	engineered mutation	UNP P02794
b	130	ALA	CYS	engineered mutation	UNP P02794
b	?	-	ASN	deletion	UNP P02794
b	?	-	GLU	deletion	UNP P02794
b	?	-	GLN	deletion	UNP P02794
b	?	-	VAL	deletion	UNP P02794
b	?	-	LYS	deletion	UNP P02794
b	?	-	ALA	deletion	UNP P02794
b	144	CYS	ASP	engineered mutation	UNP P02794
e	86	GLN	LYS	conflict	UNP P02794
e	90	ALA	CYS	engineered mutation	UNP P02794
e	102	ALA	CYS	engineered mutation	UNP P02794
e	130	ALA	CYS	engineered mutation	UNP P02794
e	?	-	ASN	deletion	UNP P02794
e	?	-	GLU	deletion	UNP P02794
e	?	-	GLN	deletion	UNP P02794
e	?	-	VAL	deletion	UNP P02794
e	?	-	LYS	deletion	UNP P02794
e	?	-	ALA	deletion	UNP P02794
e	144	CYS	ASP	engineered mutation	UNP P02794
f	86	GLN	LYS	conflict	UNP P02794
f	90	ALA	CYS	engineered mutation	UNP P02794
f	102	ALA	CYS	engineered mutation	UNP P02794
f	130	ALA	CYS	engineered mutation	UNP P02794
f	?	-	ASN	deletion	UNP P02794
f	?	-	GLU	deletion	UNP P02794
f	?	-	GLN	deletion	UNP P02794
f	?	-	VAL	deletion	UNP P02794
f	?	-	LYS	deletion	UNP P02794
f	?	-	ALA	deletion	UNP P02794
f	144	CYS	ASP	engineered mutation	UNP P02794

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	D	1	1	1	0	0
			Total	O		
2	H	2	2	2	0	0
			Total	O		
2	I	1	1	1	0	0
			Total	O		
2	N	1	1	1	0	0

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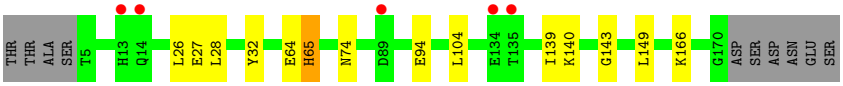
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	T	1	Total O 1 1	0	0
2	W	1	Total O 1 1	0	0
2	X	1	Total O 1 1	0	0

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.

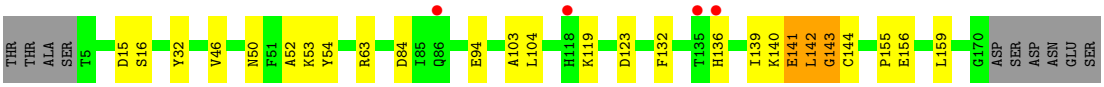
• Molecule 1: Ferritin heavy chain

Chain A:



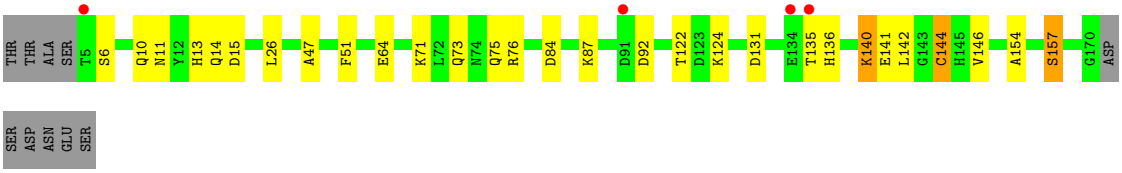
• Molecule 1: Ferritin heavy chain

Chain B:



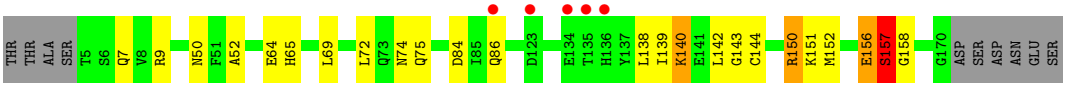
• Molecule 1: Ferritin heavy chain

Chain C:



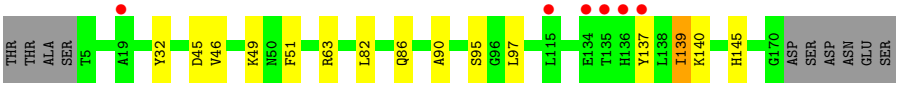
• Molecule 1: Ferritin heavy chain

Chain D:



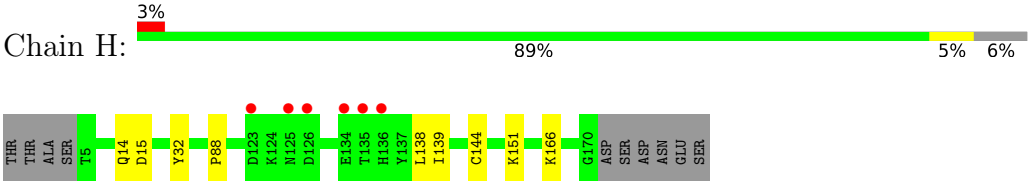
• Molecule 1: Ferritin heavy chain

Chain G:



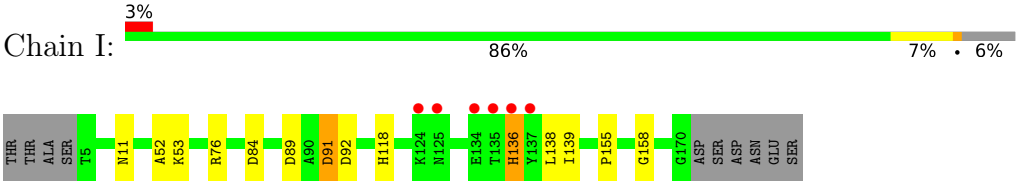
• Molecule 1: Ferritin heavy chain

Chain H:



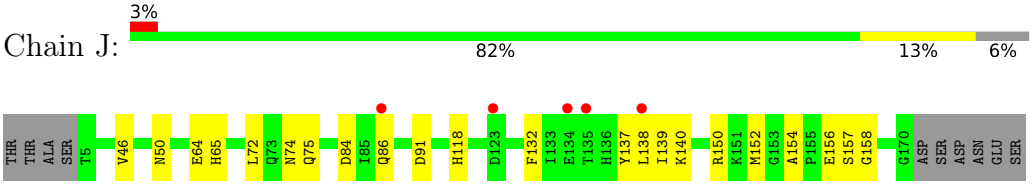
• Molecule 1: Ferritin heavy chain

Chain I:



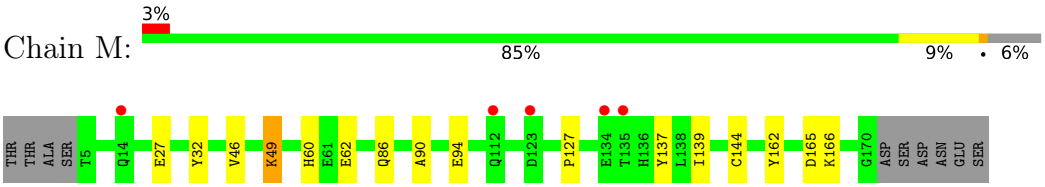
• Molecule 1: Ferritin heavy chain

Chain J:



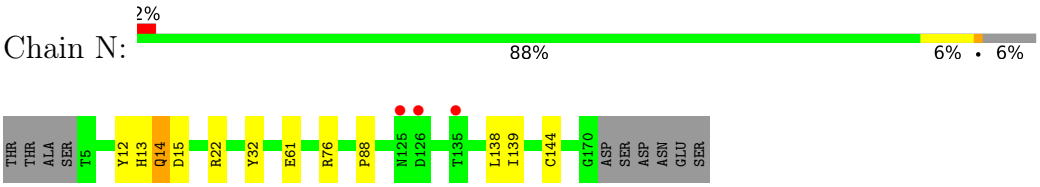
• Molecule 1: Ferritin heavy chain

Chain M:



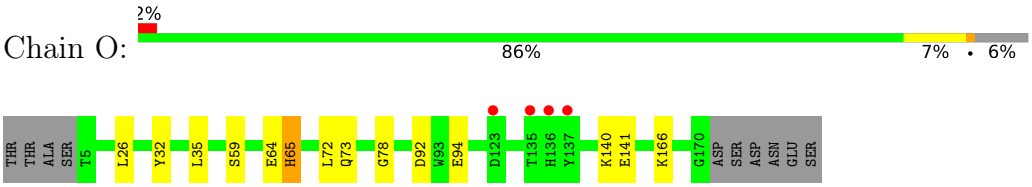
• Molecule 1: Ferritin heavy chain

Chain N:



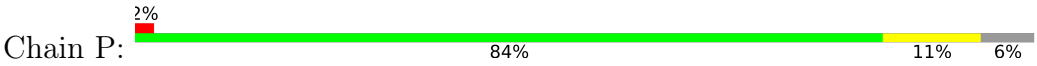
• Molecule 1: Ferritin heavy chain

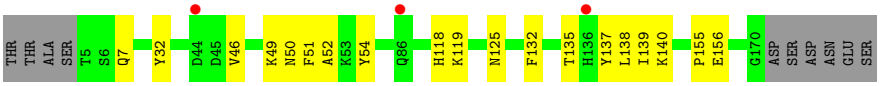
Chain O:



• Molecule 1: Ferritin heavy chain

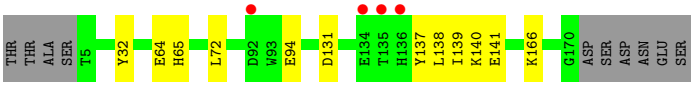
Chain P:





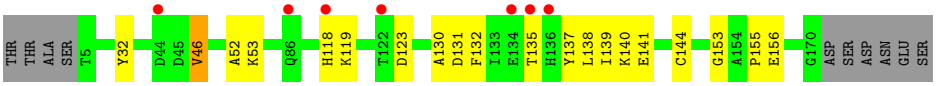
• Molecule 1: Ferritin heavy chain

Chain Q:



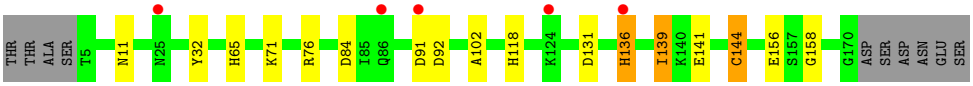
• Molecule 1: Ferritin heavy chain

Chain R:



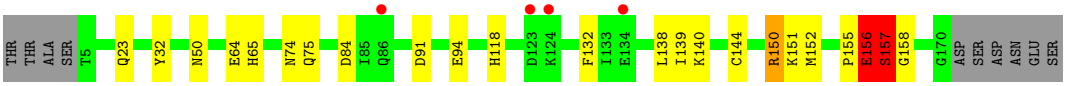
• Molecule 1: Ferritin heavy chain

Chain S:



• Molecule 1: Ferritin heavy chain

Chain T:

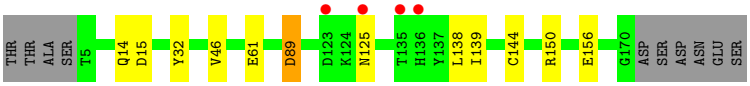


• Molecule 1: Ferritin heavy chain

Chain W:

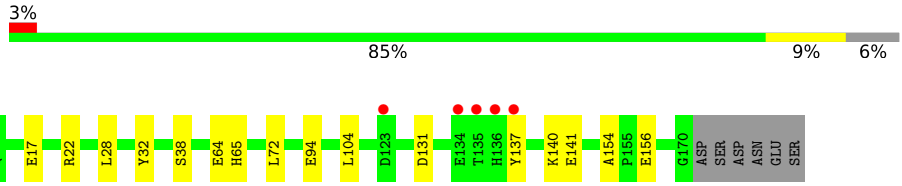
• Molecule 1: Ferritin heavy chain

Chain X:



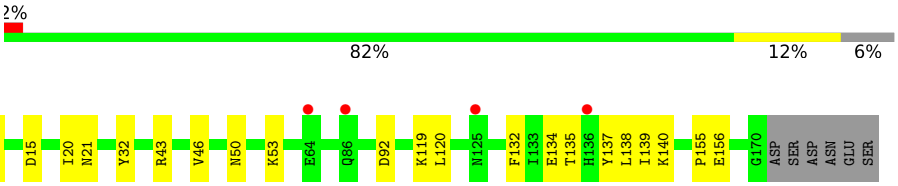
• Molecule 1: Ferritin heavy chain

Chain Y:



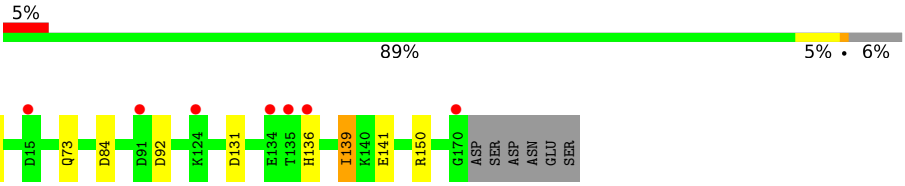
• Molecule 1: Ferritin heavy chain

Chain Z:



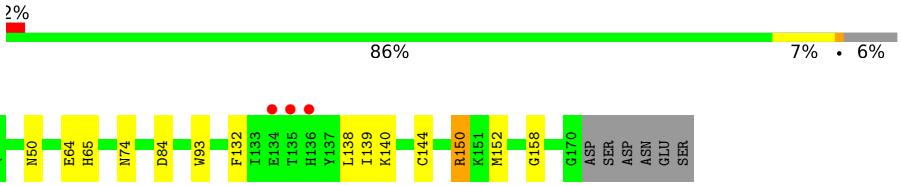
• Molecule 1: Ferritin heavy chain

Chain a:



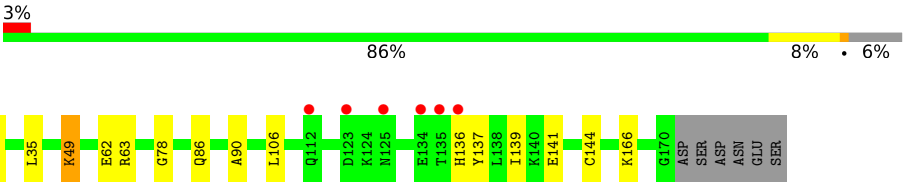
• Molecule 1: Ferritin heavy chain

Chain b:



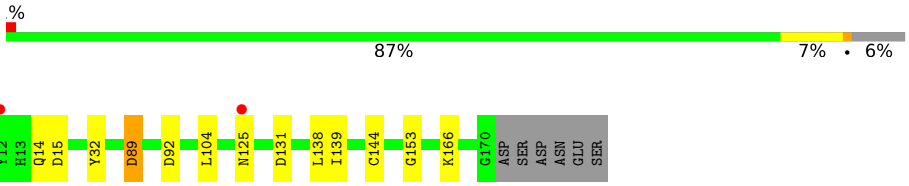
• Molecule 1: Ferritin heavy chain

Chain e:



• Molecule 1: Ferritin heavy chain

Chain f:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.38Å 165.36Å 164.87Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	40.87 – 3.87 49.87 – 3.87	Depositor EDS
% Data completeness (in resolution range)	92.4 (40.87-3.87) 92.4 (49.87-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 3.88Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.243 , 0.328 0.244 , 0.328	Depositor DCC
R_{free} test set	2730 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 77.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	32524	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.03% 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 (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	0.76	4/1385 (0.3%)	0.76	2/1867 (0.1%)
1	B	1.03	5/1385 (0.4%)	0.99	6/1867 (0.3%)
1	C	0.78	4/1385 (0.3%)	0.85	2/1867 (0.1%)
1	D	0.71	0/1385	0.89	4/1867 (0.2%)
1	G	0.68	0/1380	0.73	1/1859 (0.1%)
1	H	0.63	1/1385 (0.1%)	0.78	1/1867 (0.1%)
1	I	0.65	0/1381	0.79	2/1862 (0.1%)
1	J	0.68	0/1385	0.85	2/1867 (0.1%)
1	M	0.73	3/1380 (0.2%)	0.74	1/1859 (0.1%)
1	N	0.67	1/1385 (0.1%)	0.81	1/1867 (0.1%)
1	O	0.64	0/1385	0.72	1/1867 (0.1%)
1	P	0.62	0/1385	0.78	0/1867
1	Q	0.69	0/1385	0.77	0/1867
1	R	0.67	1/1385 (0.1%)	0.80	3/1867 (0.2%)
1	S	0.69	0/1381	0.80	1/1862 (0.1%)
1	T	0.67	1/1385 (0.1%)	0.80	1/1867 (0.1%)
1	W	0.69	1/1380 (0.1%)	0.73	0/1859
1	X	0.67	1/1385 (0.1%)	0.81	1/1867 (0.1%)
1	Y	0.71	0/1385	0.75	1/1867 (0.1%)
1	Z	0.63	0/1385	0.80	0/1867
1	a	0.67	0/1380	0.76	0/1859
1	b	0.69	1/1384 (0.1%)	0.83	1/1864 (0.1%)
1	e	0.71	3/1380 (0.2%)	0.83	2/1859 (0.1%)
1	f	0.68	1/1385 (0.1%)	0.81	2/1867 (0.1%)
All	All	0.70	27/33206 (0.1%)	0.80	35/44755 (0.1%)

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	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
1	H	0	1
1	I	0	2
1	J	0	2
1	M	0	1
1	N	0	1
1	P	0	1
1	R	0	2
1	S	0	2
1	T	0	1
1	W	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	e	0	1
All	All	0	22

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	CYS	CB-SG	22.73	2.20	1.82
1	B	141	GLU	CB-CG	10.82	1.72	1.52
1	T	144	CYS	CB-SG	9.82	1.99	1.82
1	b	144	CYS	CB-SG	9.52	1.98	1.82
1	f	144	CYS	CB-SG	-8.28	1.68	1.82
1	X	144	CYS	CB-SG	-8.14	1.68	1.82
1	B	141	GLU	CD-OE1	8.02	1.34	1.25
1	C	144	CYS	CB-SG	-7.38	1.69	1.82
1	B	140	LYS	C-N	-7.20	1.17	1.34
1	e	144	CYS	CB-SG	6.79	1.93	1.82
1	H	144	CYS	CB-SG	-6.64	1.71	1.82
1	W	27	GLU	CB-CG	6.56	1.64	1.52
1	B	141	GLU	CG-CD	6.51	1.61	1.51
1	N	144	CYS	CB-SG	-6.35	1.71	1.82
1	R	144	CYS	CB-SG	6.26	1.92	1.82
1	A	27	GLU	CB-CG	5.87	1.63	1.52
1	A	65	HIS	CG-ND1	-5.64	1.26	1.38
1	M	27	GLU	CB-CG	5.48	1.62	1.52
1	C	64	GLU	CD-OE1	-5.20	1.20	1.25
1	C	64	GLU	CD-OE2	-5.19	1.20	1.25
1	A	65	HIS	CE1-NE2	-5.18	1.20	1.32
1	e	27	GLU	CB-CG	5.16	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	162	TYR	CD2-CE2	-5.11	1.31	1.39
1	A	27	GLU	CG-CD	5.07	1.59	1.51
1	e	27	GLU	CG-CD	5.05	1.59	1.51
1	C	135	THR	CA-CB	5.05	1.66	1.53
1	M	27	GLU	CG-CD	5.01	1.59	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	142	LEU	CB-CG-CD2	-12.24	90.19	111.00
1	B	144	CYS	CA-CB-SG	10.18	132.32	114.00
1	D	157	SER	C-N-CA	-9.91	101.48	122.30
1	e	144	CYS	CA-CB-SG	9.27	130.69	114.00
1	B	140	LYS	CA-C-O	8.89	138.76	120.10
1	J	154	ALA	N-CA-C	-7.78	90.00	111.00
1	S	144	CYS	CA-CB-SG	7.75	127.96	114.00
1	b	144	CYS	CA-CB-SG	7.61	127.70	114.00
1	f	14	GLN	C-N-CA	6.63	138.28	121.70
1	B	52	ALA	C-N-CA	6.44	137.81	121.70
1	N	14	GLN	C-N-CA	6.39	137.68	121.70
1	e	35	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	R	52	ALA	C-N-CA	6.38	137.66	121.70
1	D	142	LEU	CB-CG-CD1	-6.21	100.45	111.00
1	A	28	LEU	CA-CB-CG	6.08	129.28	115.30
1	O	35	LEU	CB-CG-CD1	-6.07	100.68	111.00
1	X	14	GLN	C-N-CA	5.96	136.61	121.70
1	H	14	GLN	C-N-CA	5.93	136.53	121.70
1	T	144	CYS	CA-CB-SG	5.89	124.60	114.00
1	B	143	GLY	C-N-CA	-5.82	107.14	121.70
1	C	154	ALA	N-CA-C	-5.63	95.80	111.00
1	A	149	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	R	144	CYS	CA-CB-SG	5.59	124.07	114.00
1	G	97	LEU	CA-CB-CG	5.50	127.96	115.30
1	D	143	GLY	C-N-CA	-5.49	107.98	121.70
1	J	86	GLN	C-N-CA	5.47	135.37	121.70
1	B	140	LYS	CA-C-N	-5.45	105.20	117.20
1	M	144	CYS	CA-CB-SG	5.39	123.71	114.00
1	I	138	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	69	LEU	CA-CB-CG	-5.29	103.13	115.30
1	C	140	LYS	C-N-CA	5.19	134.68	121.70
1	Y	28	LEU	CA-CB-CG	5.18	127.22	115.30
1	R	144	CYS	CB-CA-C	5.18	120.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	155	PRO	CA-N-CD	-5.13	104.32	111.50
1	f	104	LEU	CB-CG-CD1	-5.11	102.31	111.00

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	119	LYS	Peptide
1	B	141	GLU	Mainchain
1	G	139	ILE	Peptide
1	G	45	ASP	Peptide
1	H	88	PRO	Peptide
1	I	118	HIS	Peptide
1	I	139	ILE	Peptide
1	J	137	TYR	Peptide
1	J	138	LEU	Peptide
1	M	139	ILE	Peptide
1	N	88	PRO	Peptide
1	P	119	LYS	Peptide
1	R	119	LYS	Peptide
1	R	46	VAL	Peptide
1	S	118	HIS	Peptide
1	S	139	ILE	Peptide
1	T	138	LEU	Peptide
1	W	139	ILE	Peptide
1	Z	119	LYS	Peptide
1	a	139	ILE	Peptide
1	b	138	LEU	Peptide
1	e	139	ILE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	164/176 (93%)	133 (81%)	25 (15%)	6 (4%)	3	28
1	B	164/176 (93%)	128 (78%)	22 (13%)	14 (8%)	1	13
1	C	164/176 (93%)	122 (74%)	27 (16%)	15 (9%)	1	12
1	D	164/176 (93%)	121 (74%)	27 (16%)	16 (10%)	0	10
1	G	162/176 (92%)	129 (80%)	27 (17%)	6 (4%)	3	28
1	H	164/176 (93%)	137 (84%)	23 (14%)	4 (2%)	6	36
1	I	164/176 (93%)	136 (83%)	22 (13%)	6 (4%)	3	28
1	J	164/176 (93%)	128 (78%)	22 (13%)	14 (8%)	1	13
1	M	162/176 (92%)	130 (80%)	26 (16%)	6 (4%)	3	28
1	N	164/176 (93%)	134 (82%)	26 (16%)	4 (2%)	6	36
1	O	164/176 (93%)	132 (80%)	25 (15%)	7 (4%)	2	25
1	P	164/176 (93%)	138 (84%)	16 (10%)	10 (6%)	1	19
1	Q	164/176 (93%)	134 (82%)	23 (14%)	7 (4%)	2	25
1	R	164/176 (93%)	132 (80%)	20 (12%)	12 (7%)	1	16
1	S	164/176 (93%)	131 (80%)	25 (15%)	8 (5%)	2	23
1	T	164/176 (93%)	126 (77%)	23 (14%)	15 (9%)	1	12
1	W	162/176 (92%)	135 (83%)	21 (13%)	6 (4%)	3	28
1	X	164/176 (93%)	142 (87%)	16 (10%)	6 (4%)	3	28
1	Y	164/176 (93%)	133 (81%)	22 (13%)	9 (6%)	2	21
1	Z	164/176 (93%)	129 (79%)	21 (13%)	14 (8%)	1	13
1	a	162/176 (92%)	137 (85%)	19 (12%)	6 (4%)	3	28
1	b	162/176 (92%)	130 (80%)	21 (13%)	11 (7%)	1	17
1	e	162/176 (92%)	129 (80%)	27 (17%)	6 (4%)	3	28
1	f	164/176 (93%)	142 (87%)	17 (10%)	5 (3%)	4	32
All	All	3924/4224 (93%)	3168 (81%)	543 (14%)	213 (5%)	2	22

All (213) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	94	GLU
1	A	139	ILE

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Mol	Chain	Res	Type
1	A	140	LYS
1	B	16	SER
1	B	53	LYS
1	B	103	ALA
1	B	104	LEU
1	B	136	HIS
1	B	155	PRO
1	B	156	GLU
1	C	13	HIS
1	C	14	GLN
1	C	92	ASP
1	C	136	HIS
1	C	141	GLU
1	C	142	LEU
1	C	157	SER
1	D	50	ASN
1	D	64	GLU
1	D	65	HIS
1	D	74	ASN
1	D	152	MET
1	D	157	SER
1	D	158	GLY
1	H	138	LEU
1	I	91	ASP
1	I	136	HIS
1	I	158	GLY
1	J	50	ASN
1	J	74	ASN
1	J	132	PHE
1	J	140	LYS
1	J	157	SER
1	J	158	GLY
1	M	94	GLU
1	N	15	ASP
1	N	138	LEU
1	N	139	ILE
1	O	94	GLU
1	O	141	GLU
1	P	135	THR
1	P	140	LYS
1	P	156	GLU
1	Q	94	GLU

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Mol	Chain	Res	Type
1	Q	141	GLU
1	R	140	LYS
1	R	155	PRO
1	R	156	GLU
1	S	92	ASP
1	S	158	GLY
1	T	50	ASN
1	T	64	GLU
1	T	65	HIS
1	T	74	ASN
1	T	140	LYS
1	T	152	MET
1	T	156	GLU
1	T	157	SER
1	T	158	GLY
1	X	138	LEU
1	Y	65	HIS
1	Y	94	GLU
1	Y	141	GLU
1	Y	156	GLU
1	Z	46	VAL
1	Z	135	THR
1	Z	155	PRO
1	Z	156	GLU
1	a	136	HIS
1	b	50	ASN
1	b	65	HIS
1	b	140	LYS
1	e	49	LYS
1	f	15	ASP
1	f	138	LEU
1	A	64	GLU
1	A	143	GLY
1	B	15	ASP
1	B	46	VAL
1	B	139	ILE
1	C	140	LYS
1	G	140	LYS
1	H	15	ASP
1	H	139	ILE
1	J	64	GLU
1	J	65	HIS

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Mol	Chain	Res	Type
1	J	75	GLN
1	J	139	ILE
1	J	152	MET
1	M	49	LYS
1	M	62	GLU
1	M	90	ALA
1	O	64	GLU
1	O	65	HIS
1	Q	139	ILE
1	R	46	VAL
1	R	53	LYS
1	R	130	ALA
1	S	136	HIS
1	S	144	CYS
1	T	139	ILE
1	T	150	ARG
1	W	90	ALA
1	X	15	ASP
1	X	139	ILE
1	Y	38	SER
1	Y	64	GLU
1	Z	21	ASN
1	Z	139	ILE
1	Z	140	LYS
1	a	73	GLN
1	b	64	GLU
1	b	74	ASN
1	b	132	PHE
1	b	139	ILE
1	b	150	ARG
1	b	152	MET
1	b	158	GLY
1	e	141	GLU
1	f	139	ILE
1	C	10	GLN
1	C	124	LYS
1	D	75	GLN
1	D	139	ILE
1	D	150	ARG
1	G	51	PHE
1	G	90	ALA
1	J	46	VAL

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Mol	Chain	Res	Type
1	J	91	ASP
1	P	125	ASN
1	P	138	LEU
1	Q	64	GLU
1	Q	65	HIS
1	R	135	THR
1	R	138	LEU
1	S	139	ILE
1	S	141	GLU
1	T	132	PHE
1	T	151	LYS
1	W	94	GLU
1	W	127	PRO
1	X	89	ASP
1	Z	138	LEU
1	a	10	GLN
1	a	141	GLU
1	b	93	TRP
1	e	62	GLU
1	e	78	GLY
1	C	47	ALA
1	C	73	GLN
1	D	52	ALA
1	D	138	LEU
1	D	144	CYS
1	D	151	LYS
1	H	151	LYS
1	I	53	LYS
1	I	92	ASP
1	O	78	GLY
1	O	140	LYS
1	P	137	TYR
1	P	139	ILE
1	Q	138	LEU
1	Q	140	LYS
1	R	137	TYR
1	R	139	ILE
1	S	102	ALA
1	T	75	GLN
1	T	94	GLU
1	W	62	GLU
1	W	86	GLN

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Mol	Chain	Res	Type
1	X	125	ASN
1	Y	104	LEU
1	Y	140	LYS
1	Y	154	ALA
1	Z	120	LEU
1	Z	134	GLU
1	Z	137	TYR
1	a	92	ASP
1	e	86	GLN
1	B	142	LEU
1	B	143	GLY
1	B	159	LEU
1	C	122	THR
1	I	52	ALA
1	J	150	ARG
1	M	127	PRO
1	N	14	GLN
1	P	46	VAL
1	P	52	ALA
1	P	155	PRO
1	R	118	HIS
1	R	153	GLY
1	S	91	ASP
1	Z	53	LYS
1	e	90	ALA
1	f	89	ASP
1	B	94	GLU
1	D	140	LYS
1	D	156	GLU
1	G	95	SER
1	G	139	ILE
1	M	46	VAL
1	O	59	SER
1	f	153	GLY
1	C	87	LYS
1	W	46	VAL
1	X	46	VAL
1	G	46	VAL
1	a	139	ILE
1	C	146	VAL
1	Z	8	VAL
1	Z	20	ILE

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	144/154 (94%)	139 (96%)	5 (4%)	36	61
1	B	144/154 (94%)	137 (95%)	7 (5%)	25	53
1	C	144/154 (94%)	132 (92%)	12 (8%)	11	39
1	D	144/154 (94%)	135 (94%)	9 (6%)	18	47
1	G	143/154 (93%)	136 (95%)	7 (5%)	25	53
1	H	144/154 (94%)	142 (99%)	2 (1%)	67	81
1	I	143/154 (93%)	137 (96%)	6 (4%)	30	57
1	J	144/154 (94%)	140 (97%)	4 (3%)	43	66
1	M	143/154 (93%)	136 (95%)	7 (5%)	25	53
1	N	144/154 (94%)	138 (96%)	6 (4%)	30	57
1	O	144/154 (94%)	137 (95%)	7 (5%)	25	53
1	P	144/154 (94%)	136 (94%)	8 (6%)	21	50
1	Q	144/154 (94%)	139 (96%)	5 (4%)	36	61
1	R	144/154 (94%)	139 (96%)	5 (4%)	36	61
1	S	143/154 (93%)	135 (94%)	8 (6%)	21	50
1	T	144/154 (94%)	135 (94%)	9 (6%)	18	47
1	W	143/154 (93%)	138 (96%)	5 (4%)	36	61
1	X	144/154 (94%)	141 (98%)	3 (2%)	53	73
1	Y	144/154 (94%)	138 (96%)	6 (4%)	30	57
1	Z	144/154 (94%)	138 (96%)	6 (4%)	30	57
1	a	143/154 (93%)	141 (99%)	2 (1%)	67	81
1	b	144/154 (94%)	142 (99%)	2 (1%)	67	81
1	e	143/154 (93%)	137 (96%)	6 (4%)	30	57
1	f	144/154 (94%)	138 (96%)	6 (4%)	30	57
All	All	3449/3696 (93%)	3306 (96%)	143 (4%)	30	57

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	TYR
1	A	74	ASN
1	A	104	LEU
1	A	166	LYS
1	B	32	TYR
1	B	50	ASN
1	B	54	TYR
1	B	63	ARG
1	B	84	ASP
1	B	123	ASP
1	B	132	PHE
1	C	6	SER
1	C	11	ASN
1	C	15	ASP
1	C	26	LEU
1	C	51	PHE
1	C	71	LYS
1	C	75	GLN
1	C	76	ARG
1	C	84	ASP
1	C	131	ASP
1	C	144	CYS
1	C	157	SER
1	D	7	GLN
1	D	9	ARG
1	D	72	LEU
1	D	84	ASP
1	D	86	GLN
1	D	140	LYS
1	D	150	ARG
1	D	156	GLU
1	D	157	SER
1	G	32	TYR
1	G	49	LYS
1	G	63	ARG
1	G	82	LEU
1	G	86	GLN
1	G	137	TYR
1	G	145	HIS
1	H	32	TYR
1	H	166	LYS
1	I	11	ASN

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Mol	Chain	Res	Type
1	I	76	ARG
1	I	84	ASP
1	I	89	ASP
1	I	91	ASP
1	I	136	HIS
1	J	72	LEU
1	J	84	ASP
1	J	118	HIS
1	J	156	GLU
1	M	32	TYR
1	M	49	LYS
1	M	60	HIS
1	M	86	GLN
1	M	137	TYR
1	M	165	ASP
1	M	166	LYS
1	N	12	TYR
1	N	13	HIS
1	N	22	ARG
1	N	32	TYR
1	N	61	GLU
1	N	76	ARG
1	O	26	LEU
1	O	32	TYR
1	O	65	HIS
1	O	72	LEU
1	O	73	GLN
1	O	92	ASP
1	O	166	LYS
1	P	7	GLN
1	P	32	TYR
1	P	49	LYS
1	P	50	ASN
1	P	51	PHE
1	P	54	TYR
1	P	118	HIS
1	P	132	PHE
1	Q	32	TYR
1	Q	72	LEU
1	Q	131	ASP
1	Q	137	TYR
1	Q	166	LYS

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Mol	Chain	Res	Type
1	R	32	TYR
1	R	123	ASP
1	R	131	ASP
1	R	132	PHE
1	R	141	GLU
1	S	11	ASN
1	S	32	TYR
1	S	65	HIS
1	S	71	LYS
1	S	76	ARG
1	S	84	ASP
1	S	131	ASP
1	S	136	HIS
1	T	23	GLN
1	T	32	TYR
1	T	84	ASP
1	T	91	ASP
1	T	118	HIS
1	T	150	ARG
1	T	155	PRO
1	T	156	GLU
1	T	157	SER
1	W	26	LEU
1	W	49	LYS
1	W	63	ARG
1	W	81	PHE
1	W	137	TYR
1	X	32	TYR
1	X	61	GLU
1	X	89	ASP
1	Y	17	GLU
1	Y	22	ARG
1	Y	32	TYR
1	Y	72	LEU
1	Y	131	ASP
1	Y	137	TYR
1	Z	15	ASP
1	Z	32	TYR
1	Z	43	ARG
1	Z	50	ASN
1	Z	92	ASP
1	Z	132	PHE

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Mol	Chain	Res	Type
1	a	84	ASP
1	a	131	ASP
1	b	84	ASP
1	b	150	ARG
1	e	49	LYS
1	e	63	ARG
1	e	106	LEU
1	e	136	HIS
1	e	137	TYR
1	e	166	LYS
1	f	32	TYR
1	f	89	ASP
1	f	92	ASP
1	f	125	ASN
1	f	131	ASP
1	f	166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	B	13	HIS
1	B	14	GLN
1	B	73	GLN
1	D	10	GLN
1	G	118	HIS
1	H	73	GLN
1	I	128	HIS
1	J	98	ASN
1	J	105	HIS
1	J	109	ASN
1	M	167	HIS
1	N	73	GLN
1	O	25	ASN
1	O	65	HIS
1	O	73	GLN
1	O	74	ASN
1	O	167	HIS
1	P	60	HIS
1	P	128	HIS
1	Q	167	HIS
1	R	10	GLN

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Mol	Chain	Res	Type
1	R	128	HIS
1	T	7	GLN
1	T	23	GLN
1	T	136	HIS
1	W	167	HIS
1	X	57	HIS
1	X	125	ASN
1	Y	148	ASN
1	Z	73	GLN
1	Z	167	HIS
1	b	50	ASN
1	e	11	ASN
1	f	112	GLN

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)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	W	1
1	M	1
1	G	1
1	e	1
1	b	1
1	a	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	155:PRO	C	156:GLU	N	4.10
1	M	155:PRO	C	156:GLU	N	4.08
1	G	155:PRO	C	156:GLU	N	3.99
1	e	155:PRO	C	156:GLU	N	3.87
1	b	155:PRO	C	156:GLU	N	3.07
1	a	155:PRO	C	156:GLU	N	2.89
1	B	140:LYS	C	141:GLU	N	1.17

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	166/176 (94%)	0.15	5 (3%)	50	39	33, 55, 77, 102	0
1	B	166/176 (94%)	0.07	4 (2%)	59	49	36, 53, 79, 145	0
1	C	166/176 (94%)	0.15	4 (2%)	59	49	33, 50, 81, 109	0
1	D	166/176 (94%)	0.02	5 (3%)	50	39	29, 47, 86, 119	0
1	G	166/176 (94%)	0.11	6 (3%)	42	34	24, 50, 69, 106	0
1	H	166/176 (94%)	0.06	6 (3%)	42	34	32, 47, 77, 98	0
1	I	166/176 (94%)	0.09	6 (3%)	42	34	34, 51, 69, 108	0
1	J	166/176 (94%)	-0.02	5 (3%)	50	39	30, 50, 80, 111	0
1	M	166/176 (94%)	0.18	5 (3%)	50	39	26, 52, 74, 104	0
1	N	166/176 (94%)	0.07	3 (1%)	68	60	34, 53, 76, 86	0
1	O	166/176 (94%)	0.11	4 (2%)	59	49	32, 52, 75, 101	0
1	P	166/176 (94%)	-0.02	3 (1%)	68	60	37, 49, 72, 114	0
1	Q	166/176 (94%)	0.08	4 (2%)	59	49	30, 50, 70, 106	0
1	R	166/176 (94%)	0.00	7 (4%)	36	30	29, 49, 77, 125	0
1	S	166/176 (94%)	0.13	5 (3%)	50	39	34, 50, 76, 105	0
1	T	166/176 (94%)	-0.02	4 (2%)	59	49	32, 52, 81, 115	0
1	W	166/176 (94%)	0.13	4 (2%)	59	49	36, 53, 75, 114	0
1	X	166/176 (94%)	0.05	4 (2%)	59	49	36, 52, 75, 100	0
1	Y	166/176 (94%)	0.15	6 (3%)	42	34	29, 53, 72, 113	0
1	Z	166/176 (94%)	0.01	4 (2%)	59	49	31, 50, 76, 119	0
1	a	166/176 (94%)	0.18	8 (4%)	30	26	35, 53, 73, 120	0
1	b	166/176 (94%)	0.03	4 (2%)	59	49	27, 52, 79, 119	0
1	e	166/176 (94%)	0.04	6 (3%)	42	34	28, 50, 75, 112	0
1	f	166/176 (94%)	-0.01	2 (1%)	79	71	29, 49, 74, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3984/4224 (94%)	0.07	114 (2%) 51 40	24, 51, 78, 145	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	125	ASN	6.3
1	Y	135	THR	5.8
1	M	134	GLU	5.5
1	a	135	THR	4.8
1	Y	134	GLU	4.8
1	C	135	THR	4.6
1	W	134	GLU	4.6
1	G	134	GLU	4.5
1	C	134	GLU	4.5
1	N	125	ASN	4.4
1	Q	135	THR	4.4
1	H	135	THR	4.2
1	D	135	THR	4.0
1	a	136	HIS	4.0
1	W	135	THR	3.8
1	Q	136	HIS	3.8
1	Z	136	HIS	3.7
1	R	136	HIS	3.7
1	H	134	GLU	3.7
1	P	86	GLN	3.7
1	e	134	GLU	3.7
1	Q	134	GLU	3.6
1	b	136	HIS	3.6
1	J	134	GLU	3.6
1	I	135	THR	3.5
1	X	135	THR	3.5
1	I	134	GLU	3.4
1	T	123	ASP	3.4
1	M	112	GLN	3.4
1	a	91	ASP	3.4
1	A	135	THR	3.3
1	G	136	HIS	3.3
1	M	135	THR	3.2
1	D	136	HIS	3.2
1	X	125	ASN	3.1
1	G	135	THR	3.1
1	X	123	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	124	LYS	3.0
1	A	134	GLU	3.0
1	S	91	ASP	3.0
1	S	86	GLN	2.9
1	e	135	THR	2.9
1	A	14	GLN	2.9
1	A	89	ASP	2.8
1	Y	14	GLN	2.8
1	Y	136	HIS	2.8
1	b	134	GLU	2.8
1	T	134	GLU	2.8
1	T	124	LYS	2.8
1	b	135	THR	2.8
1	R	44	ASP	2.8
1	Z	86	GLN	2.7
1	C	5	THR	2.7
1	I	137	TYR	2.7
1	Y	123	ASP	2.7
1	N	135	THR	2.6
1	a	15	ASP	2.6
1	W	14	GLN	2.6
1	G	115	LEU	2.5
1	O	137	TYR	2.5
1	R	86	GLN	2.5
1	J	123	ASP	2.5
1	C	91	ASP	2.5
1	a	5	THR	2.5
1	I	136	HIS	2.5
1	Z	125	ASN	2.5
1	R	134	GLU	2.4
1	O	136	HIS	2.4
1	e	136	HIS	2.4
1	M	14	GLN	2.4
1	J	138	LEU	2.4
1	R	135	THR	2.4
1	D	123	ASP	2.4
1	N	126	ASP	2.4
1	W	112	GLN	2.4
1	a	124	LYS	2.4
1	H	123	ASP	2.4
1	Q	92	ASP	2.4
1	I	125	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	T	86	GLN	2.3
1	f	125	ASN	2.3
1	D	134	GLU	2.3
1	R	122	THR	2.3
1	G	137	TYR	2.3
1	B	86	GLN	2.2
1	H	126	ASP	2.2
1	A	13	HIS	2.2
1	X	136	HIS	2.2
1	B	136	HIS	2.2
1	S	136	HIS	2.2
1	O	123	ASP	2.2
1	J	86	GLN	2.2
1	e	125	ASN	2.2
1	Y	137	TYR	2.2
1	J	135	THR	2.1
1	e	123	ASP	2.1
1	H	136	HIS	2.1
1	a	134	GLU	2.1
1	P	44	ASP	2.1
1	O	135	THR	2.1
1	P	136	HIS	2.1
1	S	25	ASN	2.1
1	b	14	GLN	2.1
1	e	112	GLN	2.1
1	D	86	GLN	2.1
1	B	118	HIS	2.0
1	B	135	THR	2.0
1	M	123	ASP	2.0
1	R	118	HIS	2.0
1	a	170	GLY	2.0
1	S	124	LYS	2.0
1	G	19	ALA	2.0
1	f	12	TYR	2.0
1	Z	64	GLU	2.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.