



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:44 PM UTC

PDB ID : 6J7G / pdb_00006j7g
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

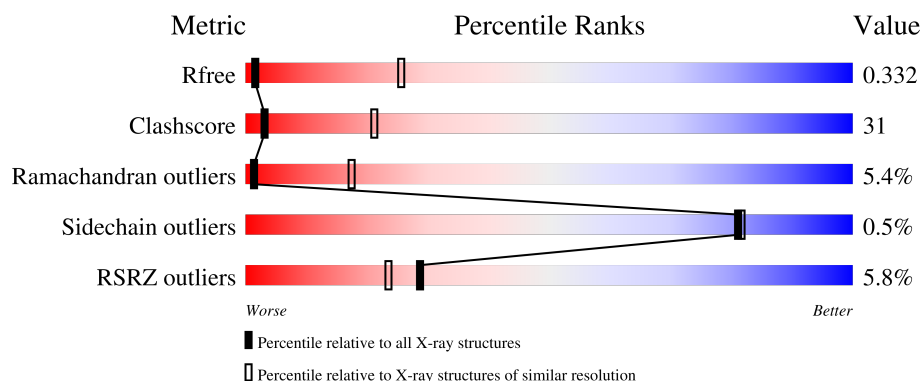
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.87 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}	180053	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	176	7% 43% 49% 6%
1	B	176	3% 39% 46% 8% 6%
1	C	176	7% 40% 46% 7% 6%
1	D	176	6% 33% 52% 7% 6%
1	G	176	7% 43% 48% 6%

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Mol	Chain	Length	Quality of chain
1	H	176	
1	I	176	
1	J	176	
1	M	176	
1	N	176	
1	O	176	
1	P	176	
1	Q	176	
1	R	176	
1	S	176	
1	T	176	
1	W	176	
1	X	176	
1	Y	176	
1	Z	176	
1	a	176	
1	b	176	
1	e	176	
1	f	176	

2 Entry composition

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

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

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
2	D	1	Total O 1 1	0	0
2	H	2	Total O 2 2	0	0
2	I	1	Total O 1 1	0	0
2	N	1	Total O 1 1	0	0

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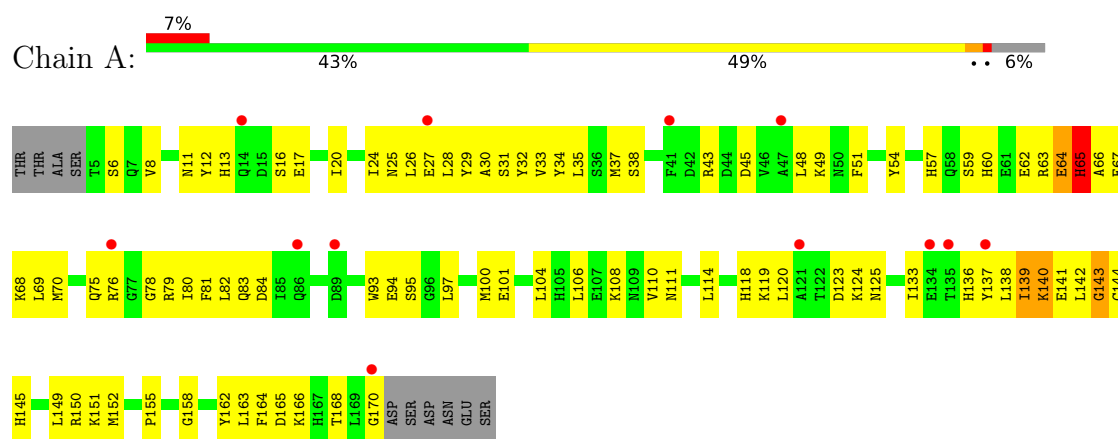
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	1	Total 1	O 1	0	0
2	W	1	Total 1	O 1	0	0
2	X	1	Total 1	O 1	0	0

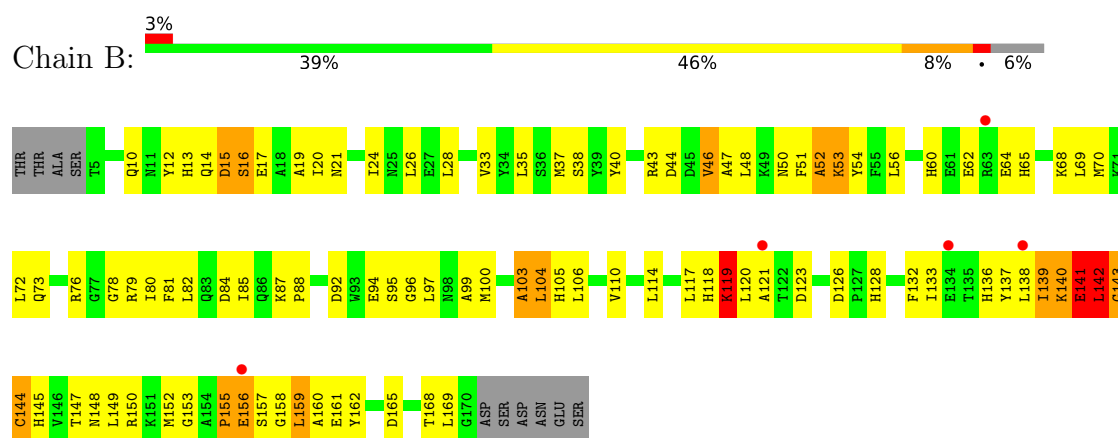
3 Residue-property plots [i](#)

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.

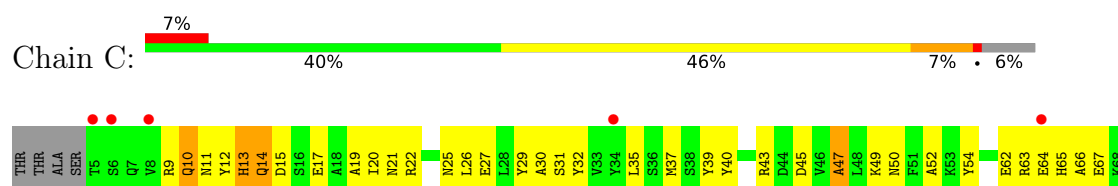
• Molecule 1: Ferritin heavy chain

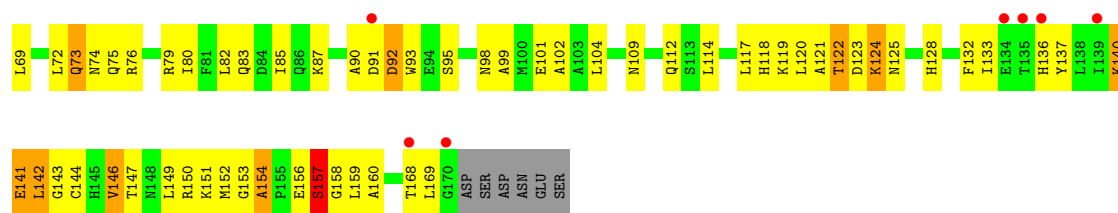


• Molecule 1: Ferritin heavy chain

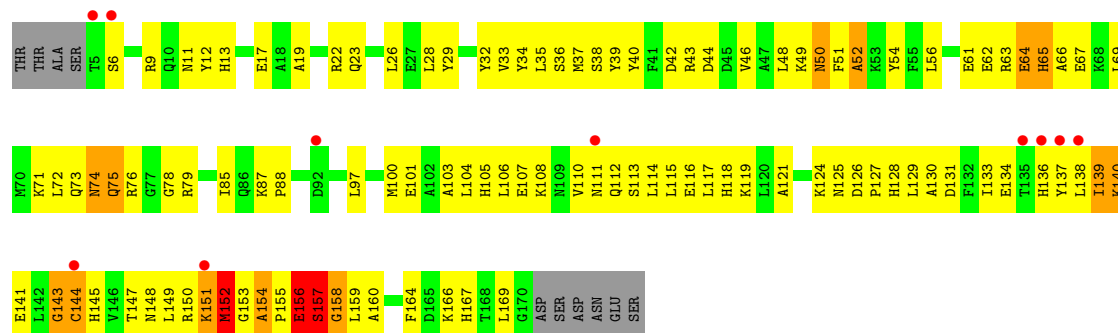


• Molecule 1: Ferritin heavy chain

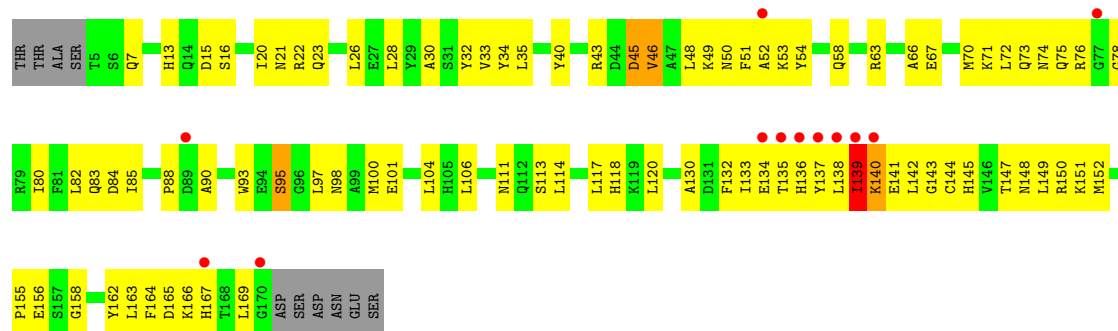
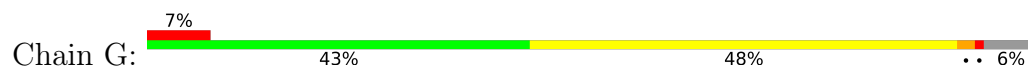




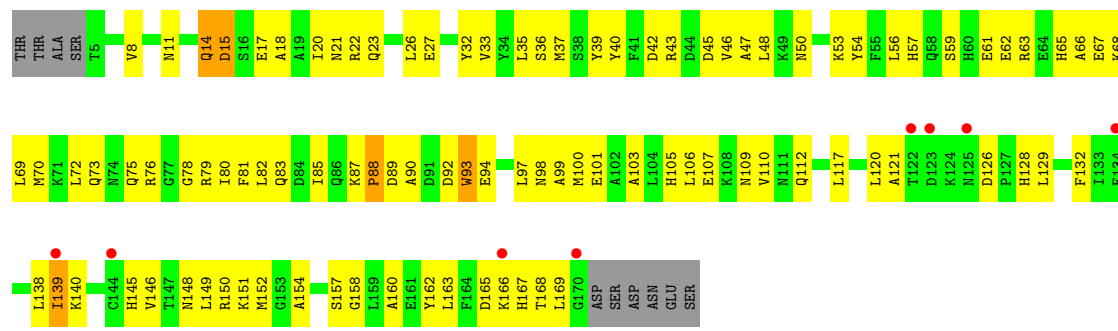
● Molecule 1: Ferritin heavy chain



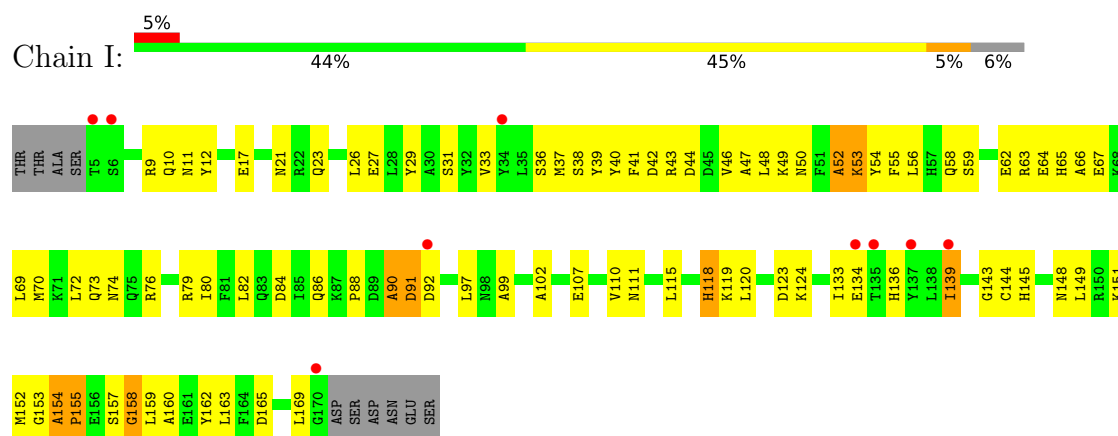
● Molecule 1: Ferritin heavy chain



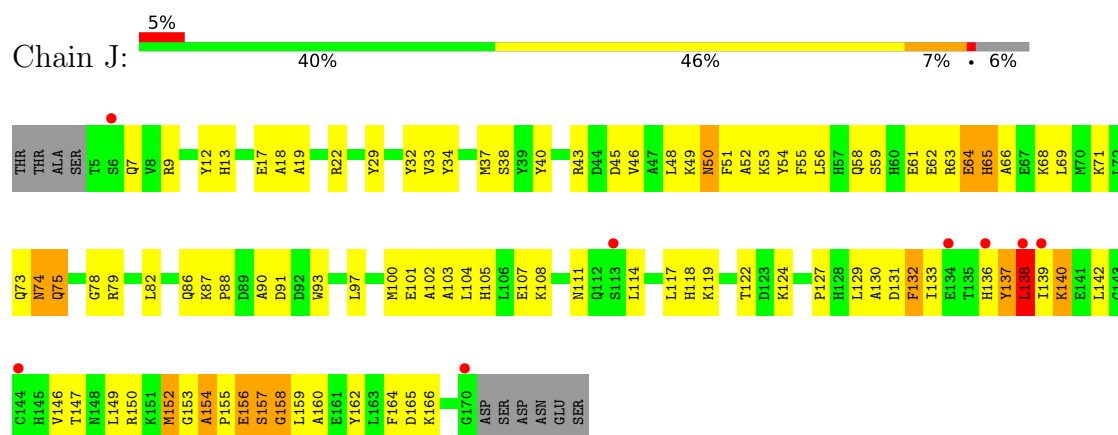
● Molecule 1: Ferritin heavy chain



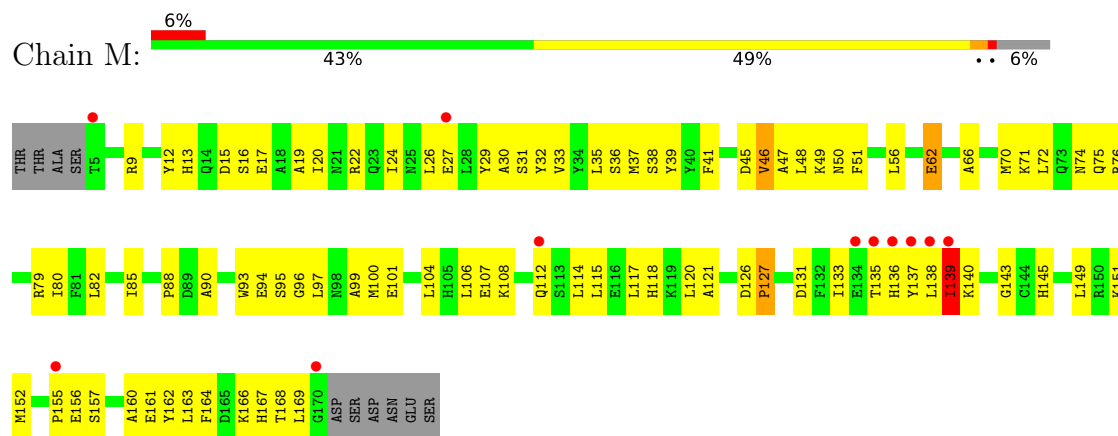
- Molecule 1: Ferritin heavy chain



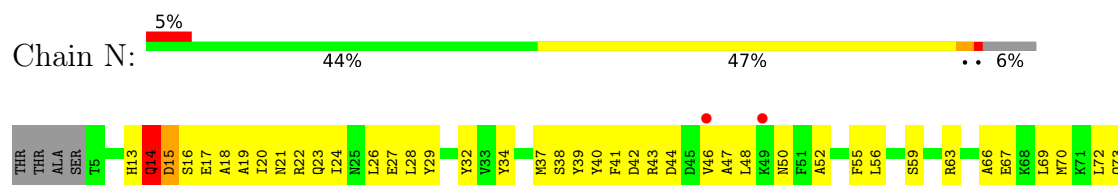
- Molecule 1: Ferritin heavy chain

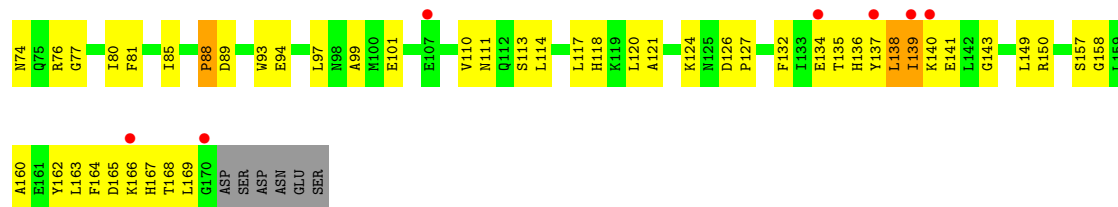


- Molecule 1: Ferritin heavy chain

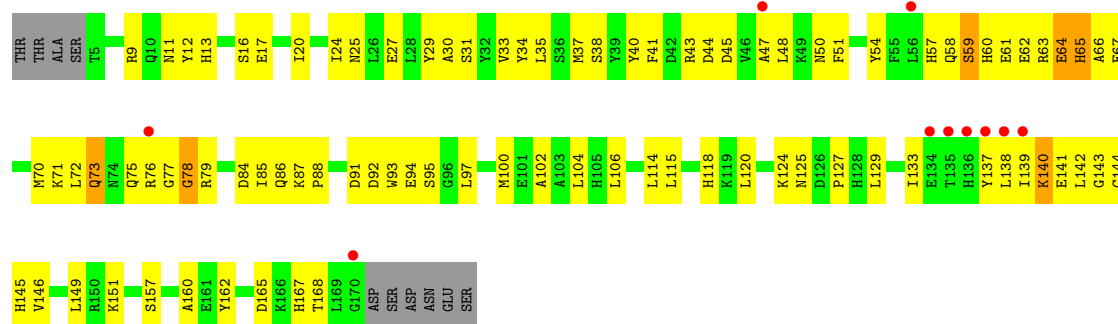
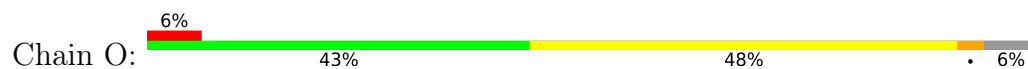


- Molecule 1: Ferritin heavy chain

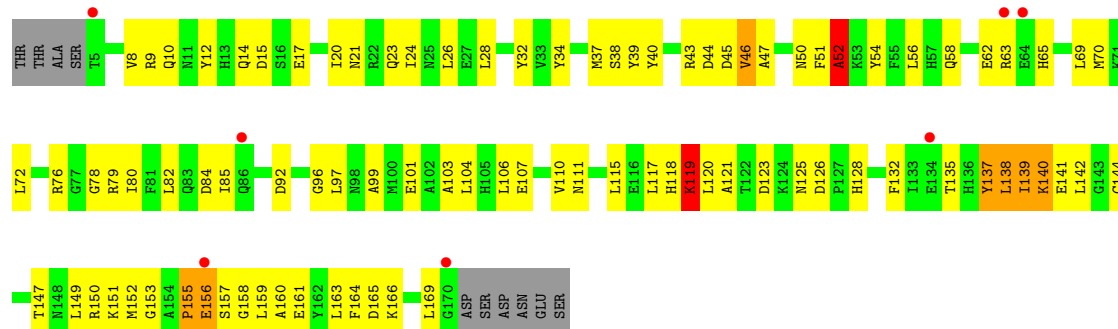




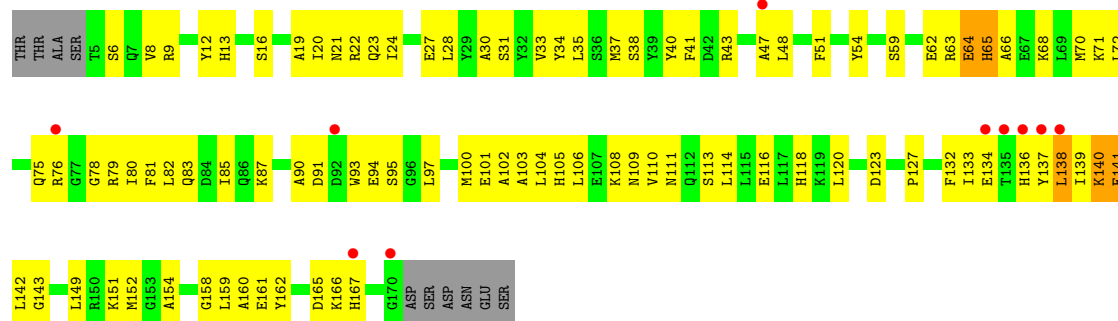
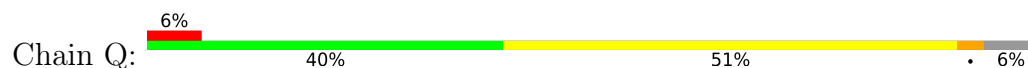
● Molecule 1: Ferritin heavy chain



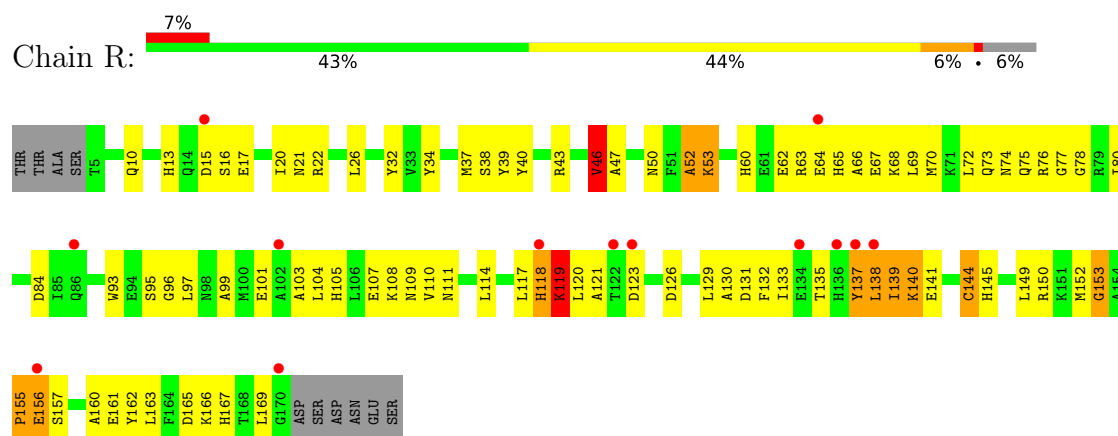
● Molecule 1: Ferritin heavy chain



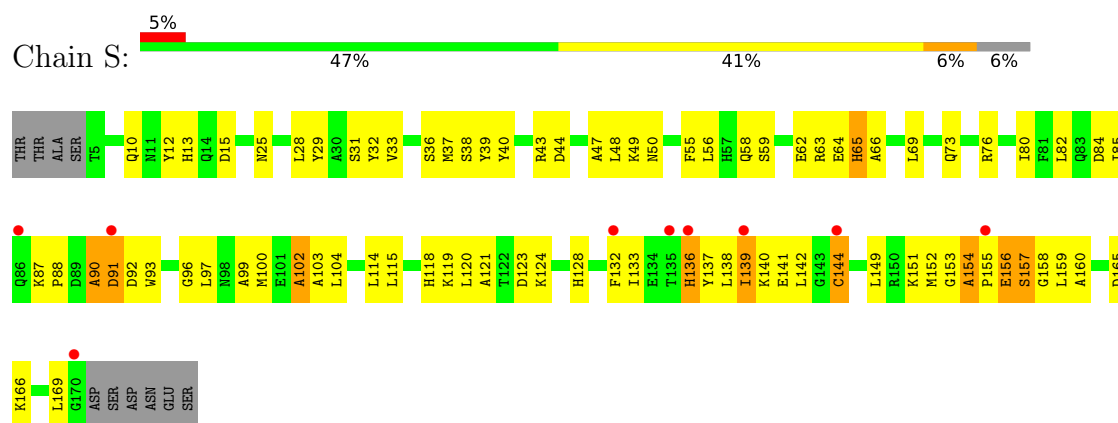
● Molecule 1: Ferritin heavy chain



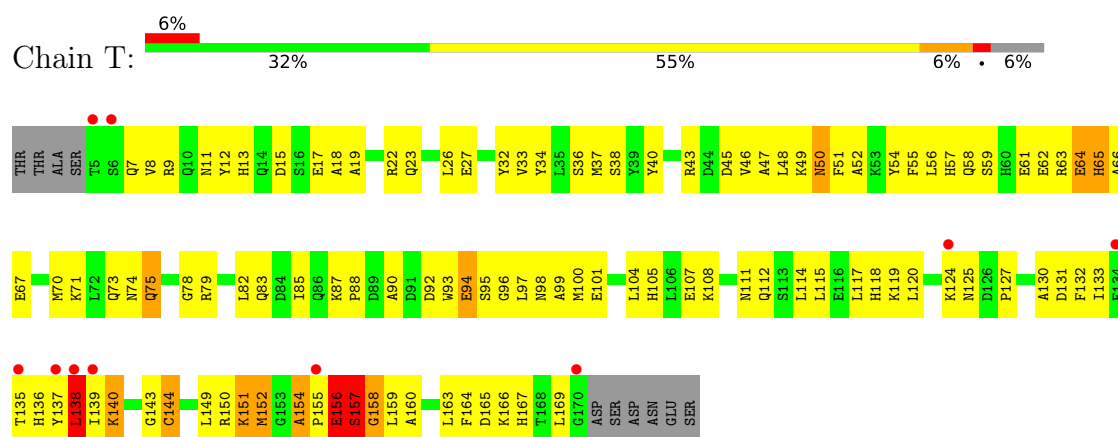
- Molecule 1: Ferritin heavy chain



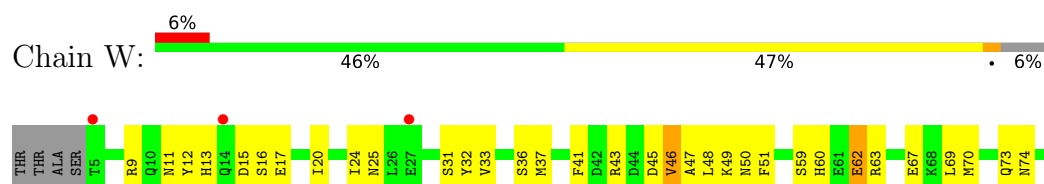
- Molecule 1: Ferritin heavy chain

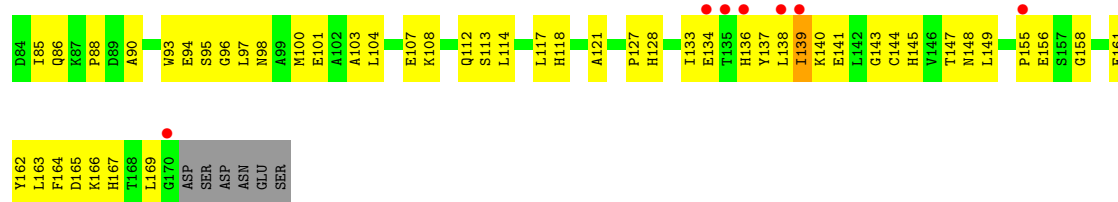


- Molecule 1: Ferritin heavy chain

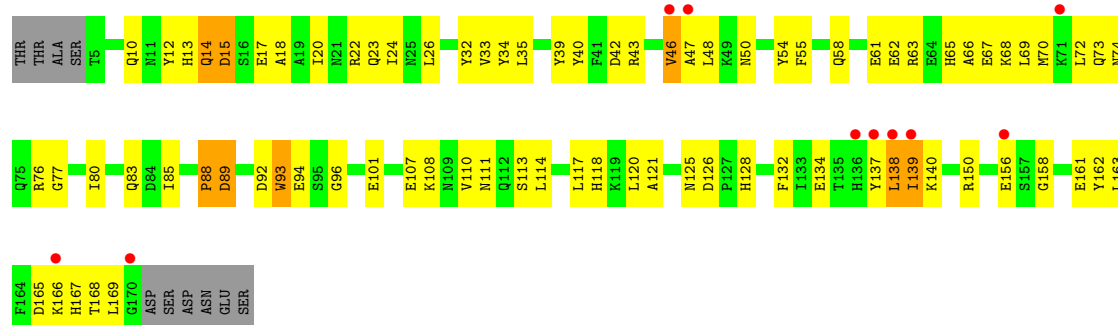


- Molecule 1: Ferritin heavy chain

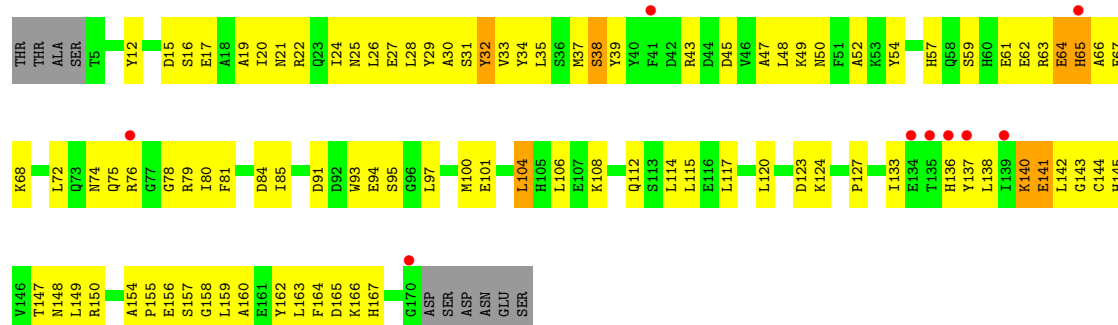




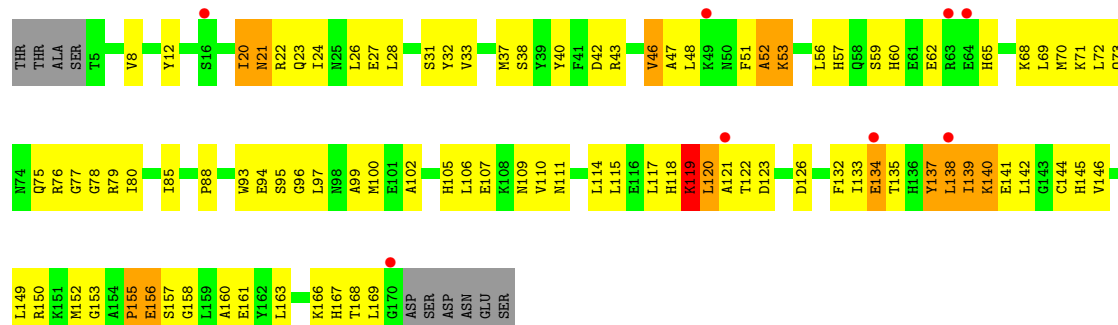
● Molecule 1: Ferritin heavy chain



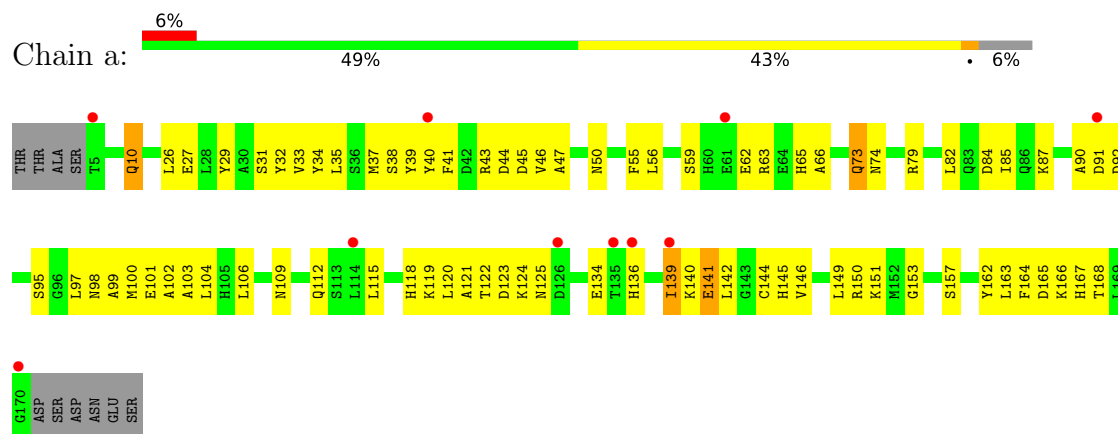
● Molecule 1: Ferritin heavy chain



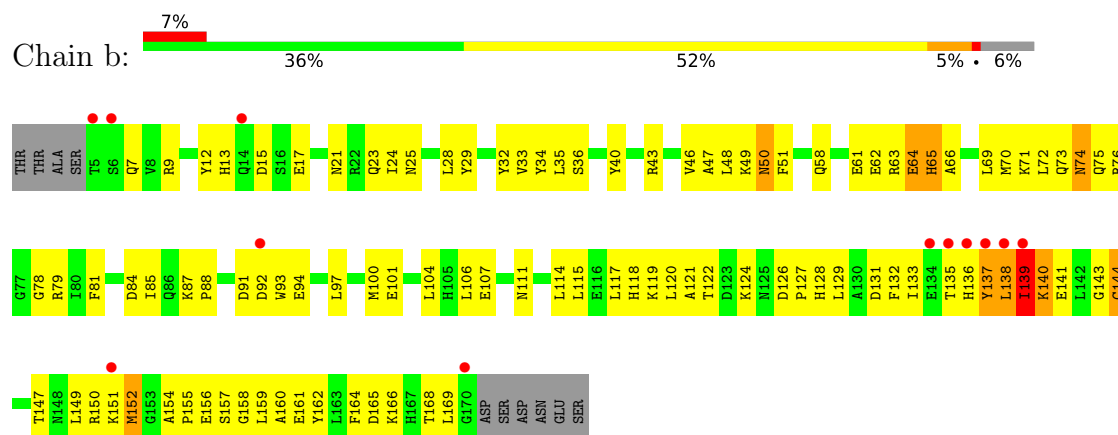
● Molecule 1: Ferritin heavy chain



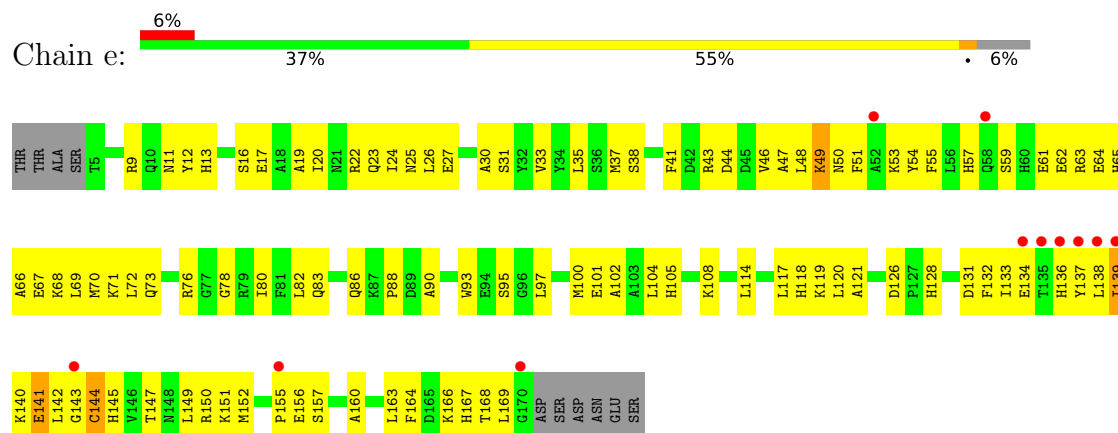
- Molecule 1: Ferritin heavy chain



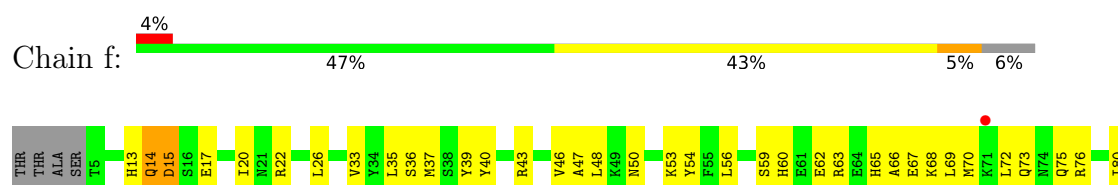
- Molecule 1: Ferritin heavy chain

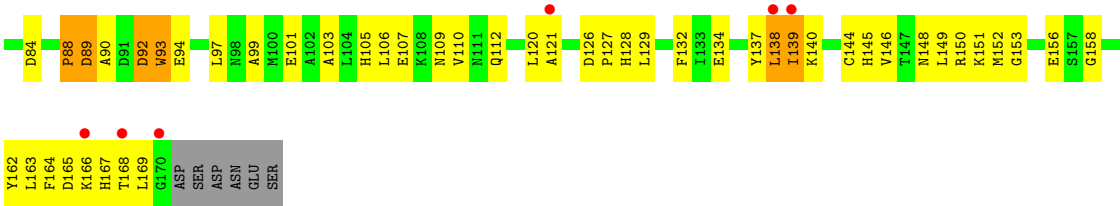


- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain





4 Data and refinement statistics

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 40.87 – 3.87	Depositor EDS
% Data completeness (in resolution range)	92.4 (40.87-3.87) 92.3 (40.87-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.88Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.243 , 0.328 0.248 , 0.332	Depositor DCC
R_{free} test set	2731 reflections (4.64%)	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)	0.36 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	0.81	4/1385 (0.3%)	0.82	2/1867 (0.1%)
1	B	0.93	6/1385 (0.4%)	1.13	14/1867 (0.7%)
1	C	0.76	0/1385	1.03	4/1867 (0.2%)
1	D	0.75	0/1385	1.06	5/1867 (0.3%)
1	G	0.66	0/1380	0.79	0/1859
1	H	0.64	0/1385	0.91	5/1867 (0.3%)
1	I	0.66	0/1381	0.91	5/1862 (0.3%)
1	J	0.70	0/1385	1.00	4/1867 (0.2%)
1	M	0.65	0/1380	0.80	1/1859 (0.1%)
1	N	0.65	0/1385	0.93	2/1867 (0.1%)
1	O	0.62	0/1385	0.77	0/1867
1	P	0.63	0/1385	0.88	4/1867 (0.2%)
1	Q	0.67	0/1385	0.81	0/1867
1	R	0.67	0/1385	0.92	6/1867 (0.3%)
1	S	0.73	1/1381 (0.1%)	0.92	5/1862 (0.3%)
1	T	0.66	1/1385 (0.1%)	0.92	3/1867 (0.2%)
1	W	0.63	0/1380	0.78	0/1859
1	X	0.65	0/1385	0.96	8/1867 (0.4%)
1	Y	0.64	0/1385	0.81	0/1867
1	Z	0.66	0/1385	0.91	5/1867 (0.3%)
1	a	0.67	0/1380	0.85	0/1859
1	b	0.70	1/1384 (0.1%)	0.96	5/1864 (0.3%)
1	e	0.66	0/1380	0.88	1/1859 (0.1%)
1	f	0.65	0/1385	0.94	7/1867 (0.4%)
All	All	0.69	13/33206 (0.0%)	0.91	86/44755 (0.2%)

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

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	CYS	CB-SG	12.01	2.20	1.81
1	B	140	LYS	C-N	-11.87	1.17	1.33
1	A	65	HIS	CE1-NE2	-11.83	1.20	1.32
1	A	65	HIS	CG-ND1	-10.83	1.26	1.38
1	A	65	HIS	CG-CD2	-7.53	1.27	1.35

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	154	ALA	N-CA-C	-13.59	90.00	110.39
1	B	140	LYS	CA-C-O	12.76	138.76	120.51
1	D	157	SER	CA-C-N	-10.17	101.48	121.41
1	D	157	SER	C-N-CA	-10.17	101.48	121.41
1	C	154	ALA	N-CA-C	-9.73	95.80	110.39

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	119	LYS	Peptide
1	B	141	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	G	139	ILE	Peptide
1	G	45	ASP	Peptide
1	H	88	PRO	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	1356	0	1300	103	0
1	B	1356	0	1300	101	0
1	C	1356	0	1300	93	0
1	D	1356	0	1298	142	0
1	G	1352	0	1295	81	0
1	H	1356	0	1300	100	0
1	I	1352	0	1294	104	0
1	J	1356	0	1300	96	0
1	M	1352	0	1295	86	0
1	N	1356	0	1300	84	0
1	O	1356	0	1300	97	0
1	P	1356	0	1300	89	0
1	Q	1356	0	1300	88	0
1	R	1356	0	1300	88	0
1	S	1352	0	1294	83	1
1	T	1356	0	1300	101	2
1	W	1352	0	1295	81	0
1	X	1356	0	1300	74	2
1	Y	1356	0	1300	104	0
1	Z	1356	0	1300	100	0
1	a	1352	0	1293	67	1
1	b	1356	0	1299	98	0
1	e	1352	0	1295	92	0
1	f	1356	0	1300	88	0
2	D	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	2	0
2	N	1	0	0	0	0
2	T	1	0	0	1	0
2	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1	0	0	0	0
All	All	32524	0	31158	1993	3

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 31.

The worst 5 of 1993 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:S:97:LEU:CD2	1:S:155:PRO:HG3	1.54	1.35
1:B:144:CYS:SG	1:B:144:CYS:CB	2.20	1.30
1:S:97:LEU:HD23	1:S:155:PRO:CG	1.67	1.24
1:D:156:GLU:O	1:D:158:GLY:N	1.69	1.23
1:D:152:MET:HE1	1:D:160:ALA:O	1.38	1.20

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:156:GLU:OE1	1:X:150:ARG:CD[2_545]	1.83	0.37
1:T:157:SER:OG	1:X:156:GLU:OE2[2_545]	1.85	0.35
1:S:156:GLU:OE2	1:a:150:ARG:CD[2_555]	2.14	0.06

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%)	2	22
1	B	164/176 (93%)	128 (78%)	22 (13%)	14 (8%)	0	10
1	C	164/176 (93%)	122 (74%)	27 (16%)	15 (9%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	164/176 (93%)	121 (74%)	27 (16%)	16 (10%)	0	8
1	G	162/176 (92%)	129 (80%)	27 (17%)	6 (4%)	2	22
1	H	164/176 (93%)	137 (84%)	23 (14%)	4 (2%)	4	30
1	I	164/176 (93%)	136 (83%)	22 (13%)	6 (4%)	2	22
1	J	164/176 (93%)	128 (78%)	22 (13%)	14 (8%)	0	10
1	M	162/176 (92%)	130 (80%)	26 (16%)	6 (4%)	2	22
1	N	164/176 (93%)	134 (82%)	26 (16%)	4 (2%)	4	30
1	O	164/176 (93%)	132 (80%)	25 (15%)	7 (4%)	2	20
1	P	164/176 (93%)	138 (84%)	16 (10%)	10 (6%)	1	15
1	Q	164/176 (93%)	134 (82%)	23 (14%)	7 (4%)	2	20
1	R	164/176 (93%)	132 (80%)	20 (12%)	12 (7%)	1	13
1	S	164/176 (93%)	131 (80%)	25 (15%)	8 (5%)	1	18
1	T	164/176 (93%)	126 (77%)	23 (14%)	15 (9%)	0	10
1	W	162/176 (92%)	135 (83%)	21 (13%)	6 (4%)	2	22
1	X	164/176 (93%)	142 (87%)	16 (10%)	6 (4%)	2	22
1	Y	164/176 (93%)	133 (81%)	22 (13%)	9 (6%)	1	17
1	Z	164/176 (93%)	129 (79%)	21 (13%)	14 (8%)	0	10
1	a	162/176 (92%)	137 (85%)	19 (12%)	6 (4%)	2	22
1	b	162/176 (92%)	130 (80%)	21 (13%)	11 (7%)	1	14
1	e	162/176 (92%)	129 (80%)	27 (17%)	6 (4%)	2	22
1	f	164/176 (93%)	142 (87%)	17 (10%)	5 (3%)	3	26
All	All	3924/4224 (93%)	3168 (81%)	543 (14%)	213 (5%)	1	17

5 of 213 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	94	GLU
1	A	139	ILE
1	A	140	LYS
1	B	16	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/154 (94%)	144 (100%)	0	100	100
1	B	144/154 (94%)	144 (100%)	0	100	100
1	C	144/154 (94%)	143 (99%)	1 (1%)	76	78
1	D	144/154 (94%)	141 (98%)	3 (2%)	47	65
1	G	143/154 (93%)	143 (100%)	0	100	100
1	H	144/154 (94%)	144 (100%)	0	100	100
1	I	143/154 (93%)	143 (100%)	0	100	100
1	J	144/154 (94%)	143 (99%)	1 (1%)	76	78
1	M	143/154 (93%)	143 (100%)	0	100	100
1	N	144/154 (94%)	144 (100%)	0	100	100
1	O	144/154 (94%)	143 (99%)	1 (1%)	76	78
1	P	144/154 (94%)	143 (99%)	1 (1%)	76	78
1	Q	144/154 (94%)	144 (100%)	0	100	100
1	R	144/154 (94%)	144 (100%)	0	100	100
1	S	143/154 (93%)	141 (99%)	2 (1%)	59	70
1	T	144/154 (94%)	141 (98%)	3 (2%)	47	65
1	W	143/154 (93%)	143 (100%)	0	100	100
1	X	144/154 (94%)	143 (99%)	1 (1%)	76	78
1	Y	144/154 (94%)	143 (99%)	1 (1%)	76	78
1	Z	144/154 (94%)	144 (100%)	0	100	100
1	a	143/154 (93%)	143 (100%)	0	100	100
1	b	144/154 (94%)	143 (99%)	1 (1%)	76	78
1	e	143/154 (93%)	143 (100%)	0	100	100
1	f	144/154 (94%)	143 (99%)	1 (1%)	76	78
All	All	3449/3696 (93%)	3433 (100%)	16 (0%)	81	82

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	111	ASN
1	Y	32	TYR
1	S	156	GLU
1	X	61	GLU
1	S	136	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	112	GLN
1	X	13	HIS
1	T	23	GLN
1	W	11	ASN
1	X	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 oligosaccharides 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

The worst 5 of 7 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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	166/176 (94%)	0.67	12 (7%)	21 19	33, 55, 77, 102	0
1	B	166/176 (94%)	0.56	5 (3%)	52 36	36, 53, 79, 145	0
1	C	166/176 (94%)	0.67	12 (7%)	21 19	33, 50, 81, 109	0
1	D	166/176 (94%)	0.62	10 (6%)	27 23	29, 47, 87, 119	0
1	G	166/176 (94%)	0.70	12 (7%)	21 19	24, 50, 69, 106	0
1	H	166/176 (94%)	0.59	8 (4%)	35 27	32, 47, 77, 98	0
1	I	166/176 (94%)	0.53	9 (5%)	31 25	34, 51, 69, 108	0
1	J	166/176 (94%)	0.55	8 (4%)	35 27	30, 50, 80, 111	0
1	M	166/176 (94%)	0.69	11 (6%)	24 21	26, 52, 74, 104	0
1	N	166/176 (94%)	0.63	9 (5%)	31 25	34, 53, 76, 86	0
1	O	166/176 (94%)	0.59	10 (6%)	27 23	32, 52, 75, 101	0
1	P	166/176 (94%)	0.52	7 (4%)	40 30	37, 49, 72, 114	0
1	Q	166/176 (94%)	0.58	10 (6%)	27 23	30, 50, 70, 106	0
1	R	166/176 (94%)	0.59	13 (7%)	19 18	29, 49, 77, 125	0
1	S	166/176 (94%)	0.53	9 (5%)	31 25	34, 50, 76, 105	0
1	T	166/176 (94%)	0.61	10 (6%)	27 23	32, 52, 81, 115	0
1	W	166/176 (94%)	0.58	10 (6%)	27 23	36, 53, 75, 114	0
1	X	166/176 (94%)	0.67	10 (6%)	27 23	36, 52, 75, 100	0
1	Y	166/176 (94%)	0.62	9 (5%)	31 25	29, 53, 72, 113	0
1	Z	166/176 (94%)	0.54	8 (4%)	35 27	31, 50, 76, 119	0
1	a	166/176 (94%)	0.66	10 (6%)	27 23	35, 53, 73, 120	0
1	b	166/176 (94%)	0.64	12 (7%)	21 19	27, 52, 79, 119	0
1	e	166/176 (94%)	0.65	11 (6%)	24 21	28, 50, 75, 112	0
1	f	166/176 (94%)	0.57	7 (4%)	40 30	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%)	0.61	232 (5%)	29	23	24, 51, 78, 145	0

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	134	GLU	8.6
1	J	134	GLU	5.7
1	f	170	GLY	5.4
1	Q	134	GLU	4.8
1	a	135	THR	4.6

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 oligosaccharides 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.