



# wwPDB X-ray Structure Validation Summary Report ⓘ

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

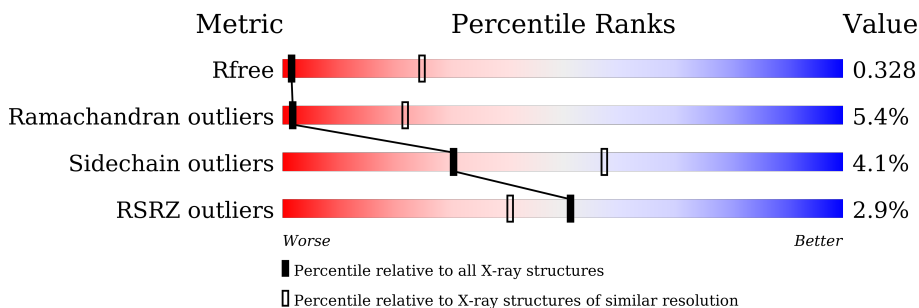
# 1 Overall quality at a glance

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  $\geq 3$ , 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	
1	B	176	
1	C	176	
1	D	176	
1	G	176	
1	H	176	
1	I	176	

Continued on next page...

Continued from previous page...

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

*Continued on next page...*

Continued from previous page...

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

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

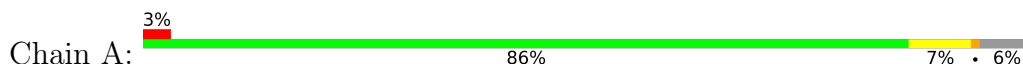
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
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

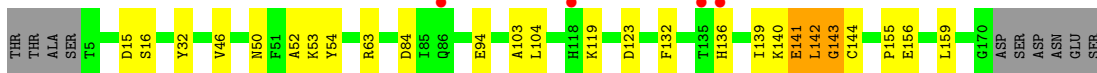
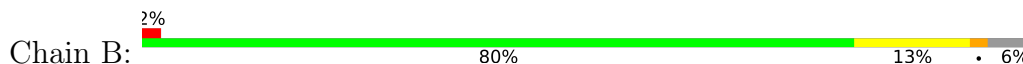
### 3 Residue-property plots [i](#)

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.

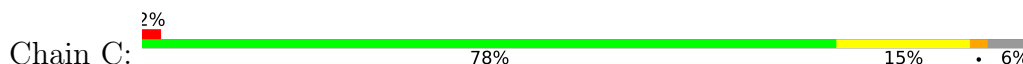
- Molecule 1: Ferritin heavy chain



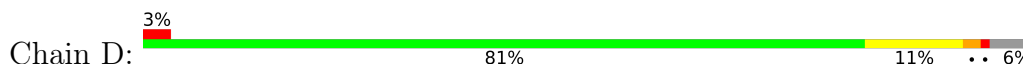
- Molecule 1: Ferritin heavy chain



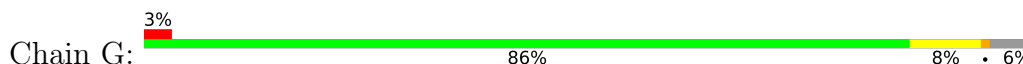
- Molecule 1: Ferritin heavy chain



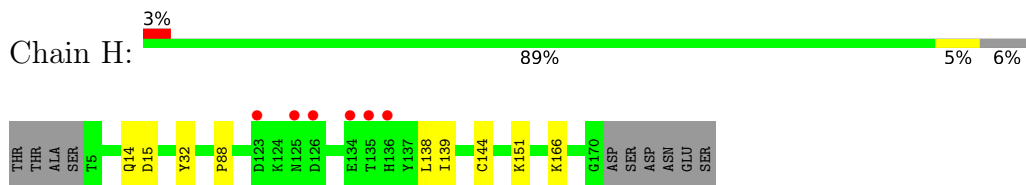
- Molecule 1: Ferritin heavy chain



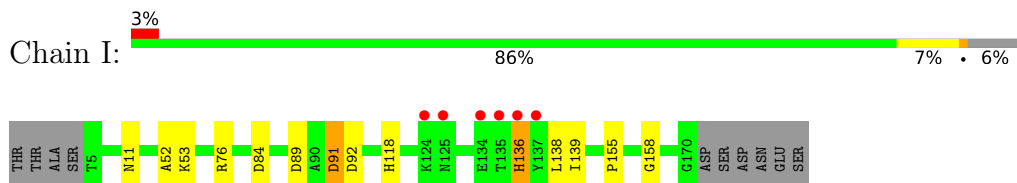
- Molecule 1: Ferritin heavy chain



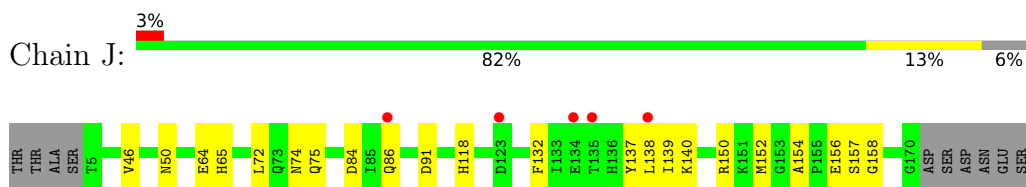
- Molecule 1: Ferritin heavy chain



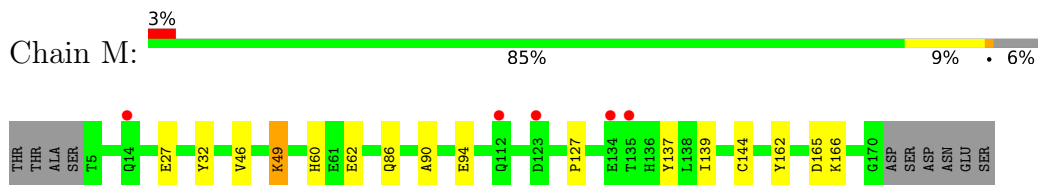
- Molecule 1: Ferritin heavy chain



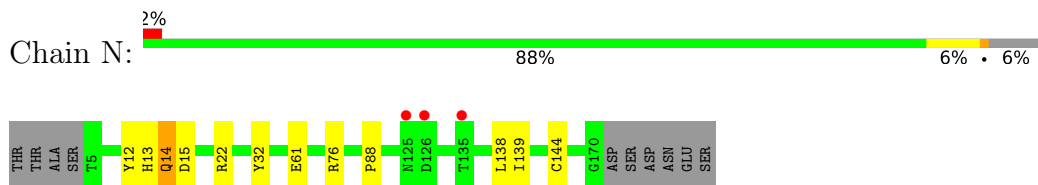
- Molecule 1: Ferritin heavy chain



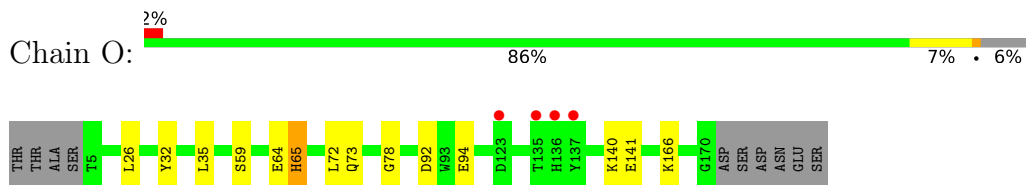
- Molecule 1: Ferritin heavy chain



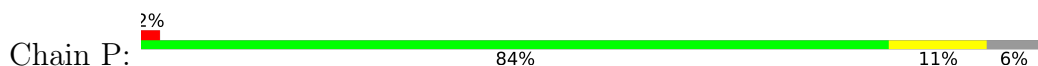
- Molecule 1: Ferritin heavy chain

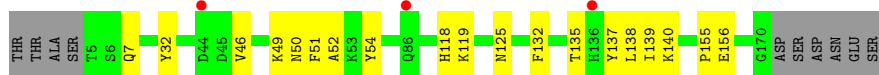


- Molecule 1: Ferritin heavy chain

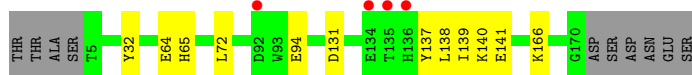
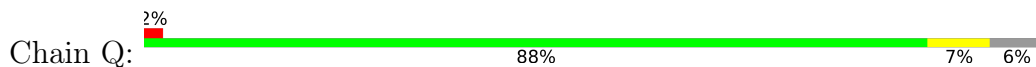


- Molecule 1: Ferritin heavy chain

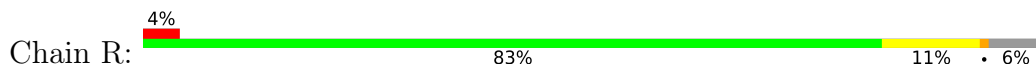




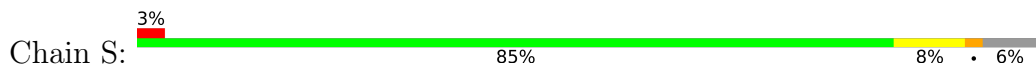
- Molecule 1: Ferritin heavy chain



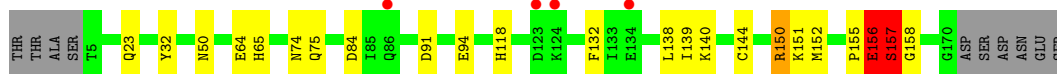
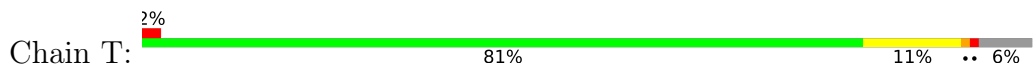
- Molecule 1: Ferritin heavy chain



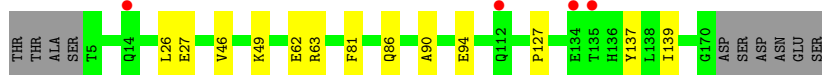
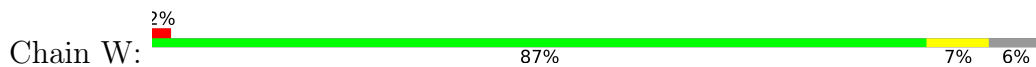
- Molecule 1: Ferritin heavy chain



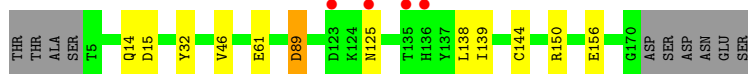
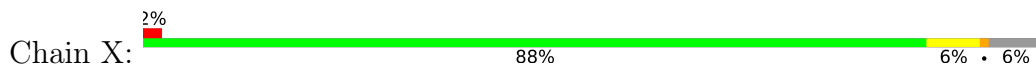
- Molecule 1: Ferritin heavy chain



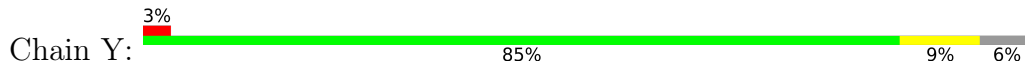
- Molecule 1: Ferritin heavy chain



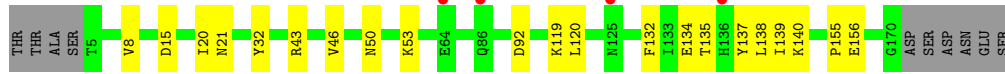
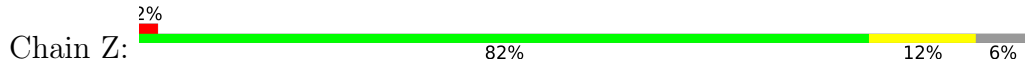
- Molecule 1: Ferritin heavy chain



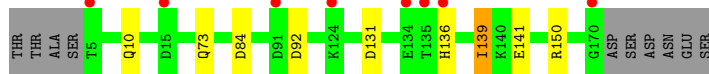
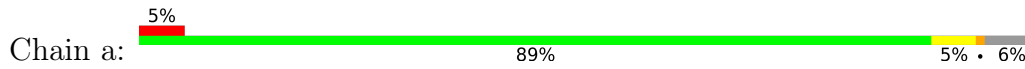
- Molecule 1: Ferritin heavy chain



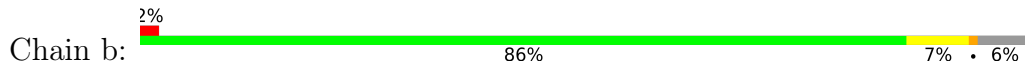
• Molecule 1: Ferritin heavy chain



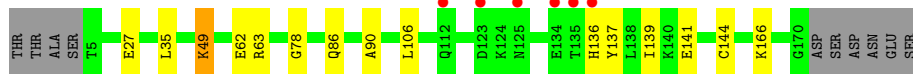
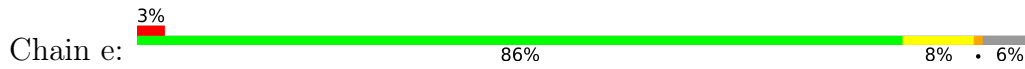
• Molecule 1: Ferritin heavy chain



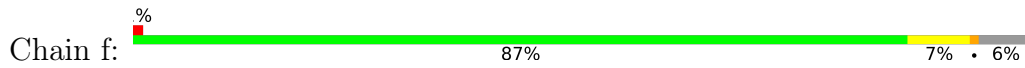
• Molecule 1: Ferritin heavy chain



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 3.88Å)	Xtrriage
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 <sup>2</sup> )	66.4	Xtrriage
Anisotropy	0.853	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 77.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	32524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.76	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

*Continued on next page...*

*Continued from previous page...*

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 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

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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

*Continued on next page...*

*Continued from previous page...*

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](#)

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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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 [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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	17	GLU
1	Y	131	ASP
1	b	150	ARG
1	J	72	LEU
1	I	136	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	125	ASN
1	Y	148	ASN
1	b	50	ASN
1	N	73	GLN
1	M	167	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](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	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

*Continued on next page...*



*Continued from previous page...*

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

The worst 5 of 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

## 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.