



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 12:56 am BST

PDB ID : 6IPC  
Title : Non-native human ferritin 8-mer  
Authors : Zang, J.C.; Chen, H.; Zhao, G.  
Deposited on : 2018-11-03  
Resolution : 4.44 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

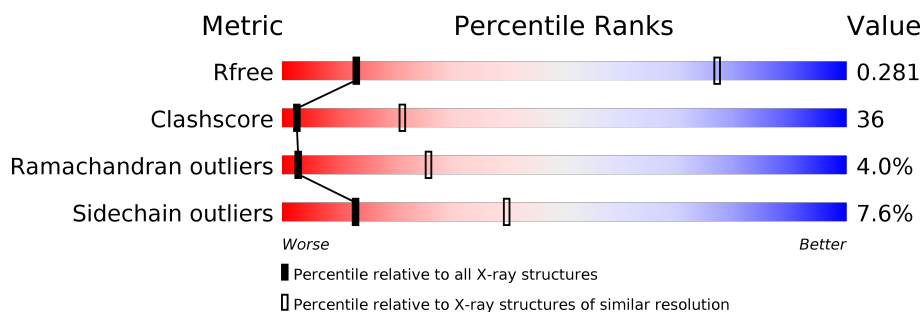
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.44 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.




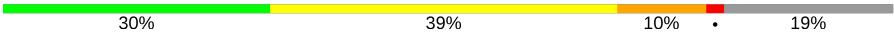
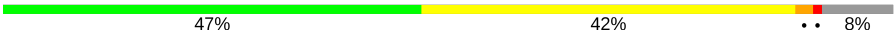

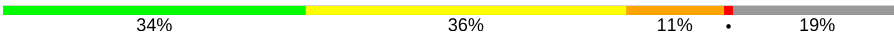

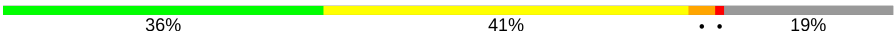
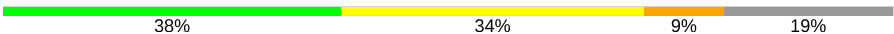
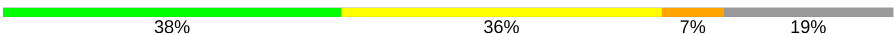
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1048 (5.08-3.80)
Clashscore	141614	1116 (5.08-3.80)
Ramachandran outliers	138981	1063 (5.08-3.80)
Sidechain outliers	138945	1045 (5.08-3.80)

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 on 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	176	
1	B	176	
1	C	176	
1	E	176	
1	F	176	
1	G	176	
1	H	176	

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Mol	Chain	Length	Quality of chain
1	I	176	
1	J	176	
1	K	176	
1	M	176	
1	N	176	
1	O	176	
1	P	176	
2	D	176	
2	L	176	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20183 atoms, of which 28 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	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	B	143	Total	C	N	O	S	0	0	0
			1184	744	208	229	3			
1	C	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	E	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	F	143	Total	C	N	O	S	0	0	0
			1184	744	208	229	3			
1	G	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	H	143	Total	C	N	O	S	0	0	0
			1184	744	208	229	3			
1	I	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	J	143	Total	C	N	O	S	0	0	0
			1184	744	208	229	3			
1	K	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	M	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	N	143	Total	C	N	O	S	0	0	0
			1184	744	208	229	3			
1	O	162	Total	C	N	O	S	0	0	0
			1331	839	231	257	4			
1	P	143	Total	C	N	O	S	0	0	0
			1184	744	208	229	3			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	ALA	CYS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	LYS	deletion	UNP P02794
F	?	-	ALA	deletion	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
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
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
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
K	90	ALA	CYS	engineered mutation	UNP P02794
K	102	ALA	CYS	engineered mutation	UNP P02794
K	130	ALA	CYS	engineered mutation	UNP P02794
K	?	-	ASN	deletion	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	GLU	deletion	UNP P02794
K	?	-	GLN	deletion	UNP P02794
K	?	-	VAL	deletion	UNP P02794
K	?	-	LYS	deletion	UNP P02794
K	?	-	ALA	deletion	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
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
N	?	-	LYS	deletion	UNP P02794
N	?	-	ALA	deletion	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
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

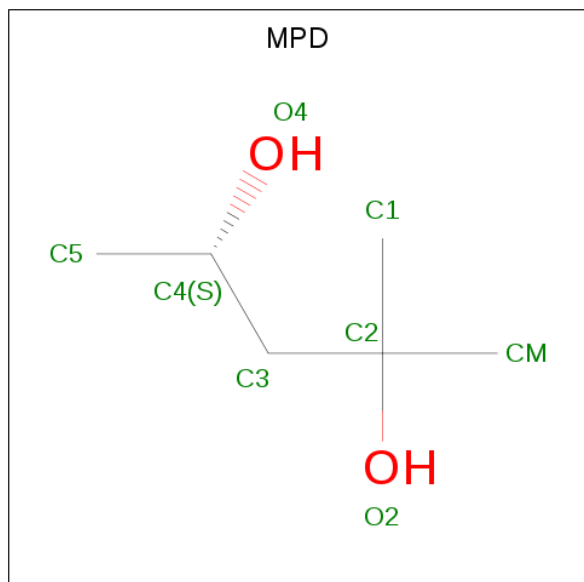
- Molecule 2 is a protein called Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1185	744	208	229	4			
2	L	143	Total	C	N	O	S	0	0	0
			1185	744	208	229	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ALA	CYS	engineered mutation	UNP P02794
D	102	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
L	90	ALA	CYS	engineered mutation	UNP P02794
L	102	ALA	CYS	engineered mutation	UNP P02794
L	?	-	ASN	deletion	UNP P02794
L	?	-	GLU	deletion	UNP P02794
L	?	-	GLN	deletion	UNP P02794
L	?	-	VAL	deletion	UNP P02794
L	?	-	LYS	deletion	UNP P02794
L	?	-	ALA	deletion	UNP P02794

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	K	1	Total	C	H	O	0	0
			22	6	14	2		

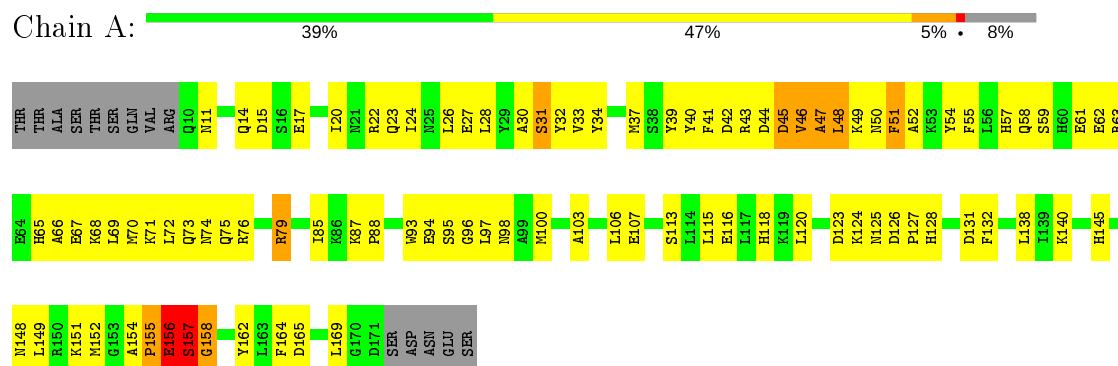
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	O	0	0
			3	3		
4	D	2	Total	O	0	0
			2	2		
4	E	2	Total	O	0	0
			2	2		
4	G	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		
4	I	1	Total	O	0	0
			1	1		
4	J	1	Total	O	0	0
			1	1		
4	K	2	Total	O	0	0
			2	2		
4	L	1	Total	O	0	0
			1	1		
4	M	2	Total	O	0	0
			2	2		
4	O	1	Total	O	0	0
			1	1		

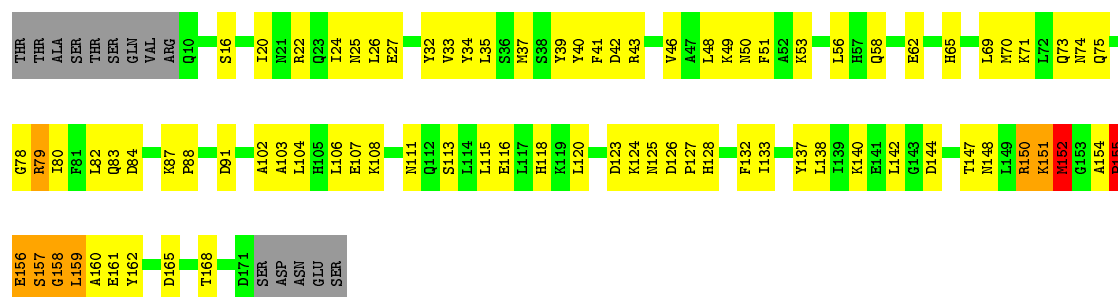
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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

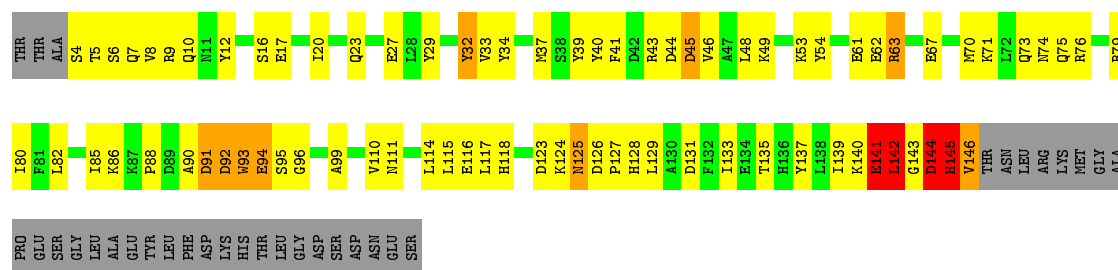


Chain E: 



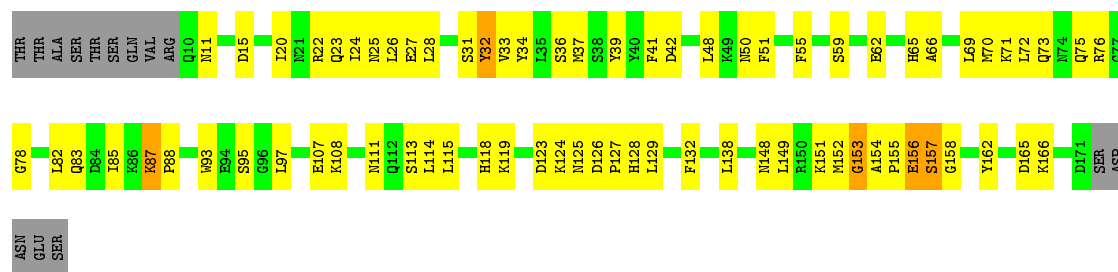
• Molecule 1: Ferritin heavy chain

Chain F: 



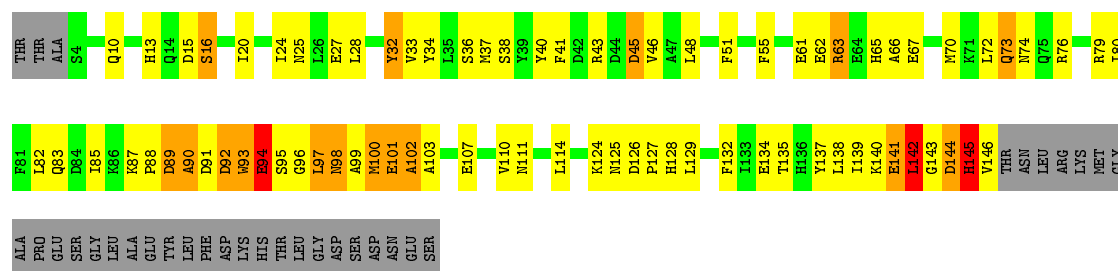
• Molecule 1: Ferritin heavy chain

Chain G: 



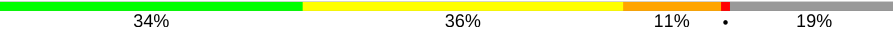
• Molecule 1: Ferritin heavy chain

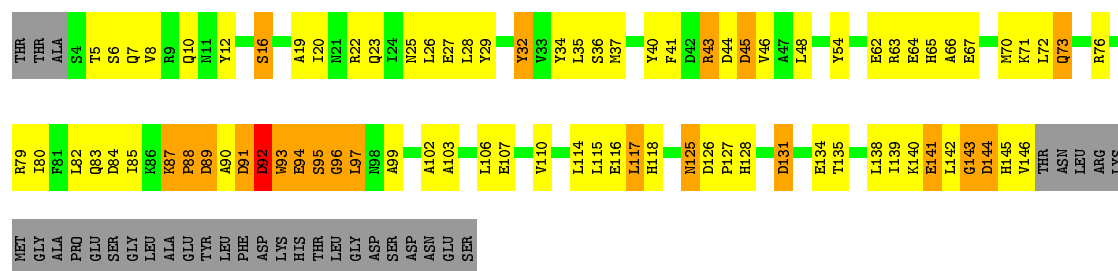
Chain H: 



• Molecule 1: Ferritin heavy chain

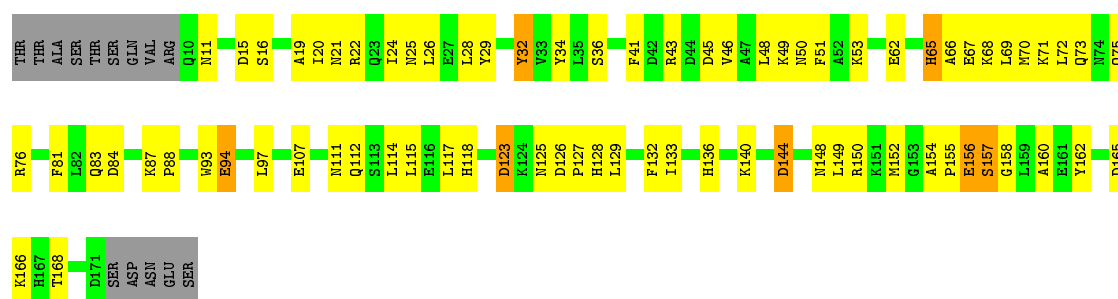


Chain N: 



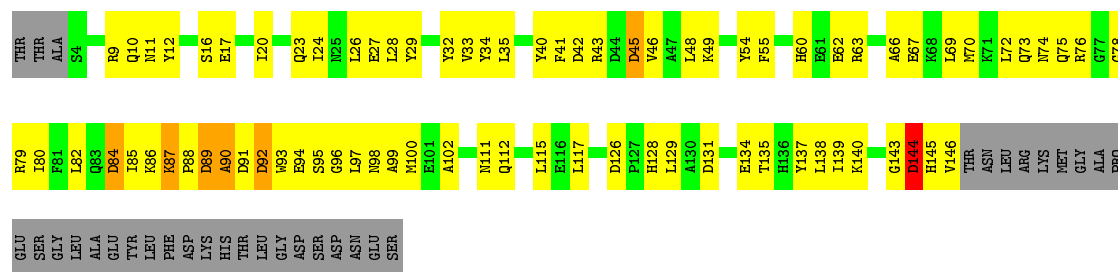
- Molecule 1: Ferritin heavy chain

Chain O: 



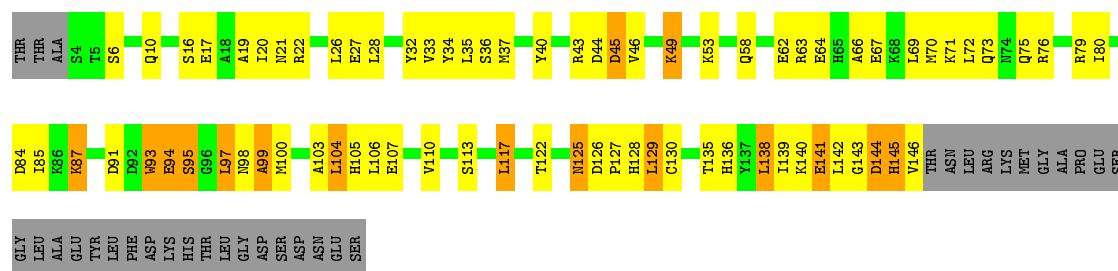
- Molecule 1: Ferritin heavy chain

Chain P: 

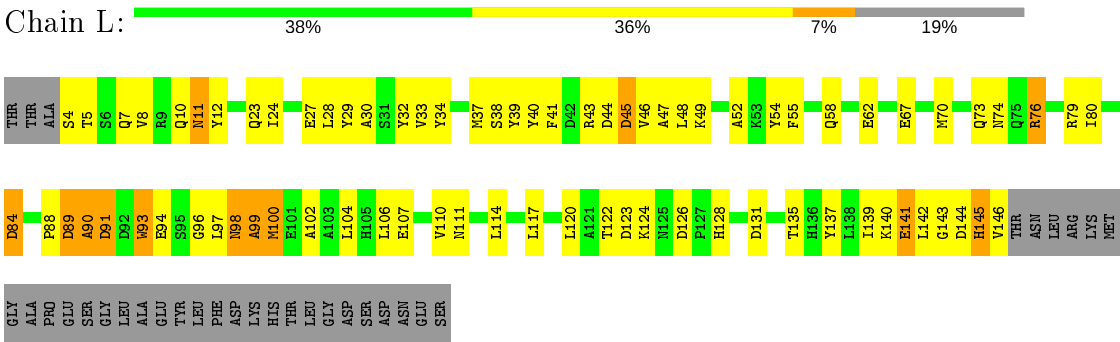


- Molecule 2: Ferritin heavy chain

Chain D: 



- Molecule 2: Ferritin heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.30Å 139.22Å 139.11Å 90.10° 90.28° 90.18°	Depositor
Resolution (Å)	49.25 – 4.44 49.25 – 4.44	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.25-4.44) 87.3 (49.25-4.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.207 , 0.277 0.215 , 0.281	Depositor DCC
$R_{free}$ test set	883 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	127.5	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 21.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.299 for h,-l,k 0.299 for h,l,-k 0.309 for h,-k,-l 0.287 for -h,-k,l 0.318 for -h,k,-l 0.297 for -h,l,k 0.347 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	20183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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

### 5.1 Standard geometry

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

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	0.32	0/1360	0.48	0/1833
1	B	0.51	2/1209 (0.2%)	0.62	3/1630 (0.2%)
1	C	0.32	0/1360	0.45	0/1833
1	E	0.31	0/1360	0.50	2/1833 (0.1%)
1	F	0.29	0/1209	0.45	0/1630
1	G	0.32	0/1360	0.46	0/1833
1	H	0.33	0/1209	0.50	0/1630
1	I	0.33	0/1360	0.46	0/1833
1	J	0.43	1/1209 (0.1%)	0.59	1/1630 (0.1%)
1	K	0.31	0/1360	0.48	1/1833 (0.1%)
1	M	0.32	0/1360	0.46	0/1833
1	N	0.32	0/1209	0.60	1/1630 (0.1%)
1	O	0.32	0/1360	0.47	0/1833
1	P	0.30	0/1209	0.45	0/1630
2	D	0.30	0/1210	0.52	1/1631 (0.1%)
2	L	0.29	0/1210	0.44	0/1631
All	All	0.34	3/20554 (0.0%)	0.50	9/27706 (0.0%)

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	J	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	TRP	CB-CG	8.51	1.65	1.50
1	J	93	TRP	CB-CG	-5.46	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	GLY	CA-C	5.04	1.59	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	87	LYS	C-N-CD	-11.86	94.51	120.60
1	B	96	GLY	C-N-CA	8.18	142.15	121.70
2	D	97	LEU	CA-CB-CG	7.84	133.33	115.30
1	B	93	TRP	CA-CB-CG	6.34	125.76	113.70
1	B	96	GLY	N-CA-C	5.51	126.86	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	87	LYS	Peptide
1	J	92	ASP	Peptide
1	J	93	TRP	Peptide
1	J	94	GLU	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1331	0	1271	123	0
1	B	1184	0	1131	112	1
1	C	1331	0	1272	68	0
1	E	1331	0	1270	104	0
1	F	1184	0	1131	91	0
1	G	1331	0	1272	88	0
1	H	1184	0	1131	112	0
1	I	1331	0	1272	90	0
1	J	1184	0	1131	156	1
1	K	1331	0	1272	91	0
1	M	1331	0	1272	94	0
1	N	1184	0	1131	110	0
1	O	1331	0	1272	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1184	0	1131	71	0
2	D	1185	0	1131	103	0
2	L	1185	0	1131	80	0
3	A	8	14	14	0	0
3	K	8	14	14	0	0
4	C	3	0	0	1	0
4	D	2	0	0	5	0
4	E	2	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	3	0
4	I	1	0	0	1	0
4	J	1	0	0	4	0
4	K	2	0	0	1	0
4	L	1	0	0	0	0
4	M	2	0	0	1	0
4	O	1	0	0	0	0
All	All	20155	28	19249	1436	1

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 36.

The worst 5 of 1436 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:A:152:MET:HA	1:E:159:LEU:CD1	1.12	1.53
1:A:152:MET:CA	1:E:159:LEU:HD11	1.06	1.50
1:N:87:LYS:CG	1:N:88:PRO:HD2	1.37	1.50
1:N:87:LYS:HG2	1:N:88:PRO:CD	1.54	1.36
1:E:147:THR:O	1:E:151:LYS:HB2	1.28	1.33

All (1) 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:B:98:ASN:N	1:J:96:GLY:O[1_665]	2.04	0.16

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	160/176 (91%)	139 (87%)	15 (9%)	6 (4%)	3	27
1	B	141/176 (80%)	114 (81%)	15 (11%)	12 (8%)	1	13
1	C	160/176 (91%)	147 (92%)	10 (6%)	3 (2%)	8	41
1	E	160/176 (91%)	144 (90%)	11 (7%)	5 (3%)	4	31
1	F	141/176 (80%)	120 (85%)	13 (9%)	8 (6%)	1	20
1	G	160/176 (91%)	142 (89%)	15 (9%)	3 (2%)	8	41
1	H	141/176 (80%)	114 (81%)	16 (11%)	11 (8%)	1	15
1	I	160/176 (91%)	142 (89%)	15 (9%)	3 (2%)	8	41
1	J	141/176 (80%)	114 (81%)	18 (13%)	9 (6%)	1	19
1	K	160/176 (91%)	136 (85%)	21 (13%)	3 (2%)	8	41
1	M	160/176 (91%)	145 (91%)	14 (9%)	1 (1%)	25	65
1	N	141/176 (80%)	116 (82%)	15 (11%)	10 (7%)	1	16
1	O	160/176 (91%)	141 (88%)	17 (11%)	2 (1%)	12	48
1	P	141/176 (80%)	124 (88%)	11 (8%)	6 (4%)	2	25
2	D	141/176 (80%)	111 (79%)	24 (17%)	6 (4%)	2	25
2	L	141/176 (80%)	114 (81%)	18 (13%)	9 (6%)	1	19
All	All	2408/2816 (86%)	2063 (86%)	248 (10%)	97 (4%)	3	26

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	PRO
1	A	156	GLU
1	A	157	SER
1	A	158	GLY
1	B	93	TRP

### 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	141/154 (92%)	131 (93%)	10 (7%)	14	41
1	B	127/154 (82%)	117 (92%)	10 (8%)	12	38
1	C	141/154 (92%)	134 (95%)	7 (5%)	24	51
1	E	141/154 (92%)	133 (94%)	8 (6%)	20	48
1	F	127/154 (82%)	113 (89%)	14 (11%)	6	25
1	G	141/154 (92%)	136 (96%)	5 (4%)	36	60
1	H	127/154 (82%)	112 (88%)	15 (12%)	5	23
1	I	141/154 (92%)	135 (96%)	6 (4%)	29	55
1	J	127/154 (82%)	112 (88%)	15 (12%)	5	23
1	K	141/154 (92%)	135 (96%)	6 (4%)	29	55
1	M	141/154 (92%)	136 (96%)	5 (4%)	36	60
1	N	127/154 (82%)	112 (88%)	15 (12%)	5	23
1	O	141/154 (92%)	134 (95%)	7 (5%)	24	51
1	P	127/154 (82%)	118 (93%)	9 (7%)	14	41
2	D	128/155 (83%)	110 (86%)	18 (14%)	3	19
2	L	128/155 (83%)	115 (90%)	13 (10%)	7	27
All	All	2146/2466 (87%)	1983 (92%)	163 (8%)	13	40

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	32	TYR
1	I	156	GLU
1	O	68	LYS
1	H	61	GLU
1	H	97	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	57	HIS
1	I	65	HIS
1	M	118	HIS
1	I	23	GLN
1	N	73	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	MPD	K	201	-	7,7,7	0.55	0	9,10,10	0.56	0
3	MPD	A	201	-	7,7,7	0.49	0	9,10,10	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	K	201	-	-	1/5/5/5	-
3	MPD	A	201	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	MPD	C2-C3-C4-O4
3	A	201	MPD	C2-C3-C4-C5
3	K	201	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.