



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:58 PM UTC

PDB ID : 3ERZ / pdb_00003erz
Title : Directing Noble Metal Ion Chemistry within a Designed Ferritin Protein. Mercury Ions on the Three-Fold Channel
Authors : Di Costanzo, L.; Christianson, D.W.
Deposited on : 2008-10-03
Resolution : 3.06 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

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

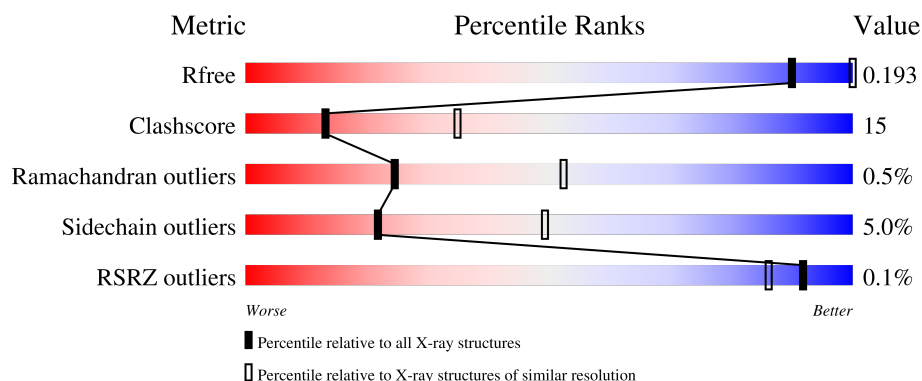
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	183	
1	B	183	
1	C	183	
1	D	183	
1	E	183	

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Mol	Chain	Length	Quality of chain
1	F	183	
1	G	183	
1	H	183	
1	I	183	
1	J	183	
1	K	183	
1	L	183	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	533	X	-	-	-
2	MPD	B	540	X	-	-	X
2	MPD	B	630	X	-	-	-
2	MPD	C	535	X	-	-	-
2	MPD	E	631	X	-	-	-
2	MPD	F	543	X	-	-	X
2	MPD	G	537	X	-	-	-
2	MPD	H	538	X	-	-	-
2	MPD	H	542	X	-	-	X
2	MPD	I	539	X	-	-	-
2	MPD	K	541	X	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17139 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	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	B	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	C	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	D	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	E	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	F	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	G	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	H	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	I	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	J	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	K	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			
1	L	172	Total	C	N	O	S	0	0	0
			1402	877	247	269	9			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	HIS	engineered mutation	UNP P02794
A	64	CYS	GLU	engineered mutation	UNP P02794
A	90	ARG	CYS	engineered mutation	UNP P02794
A	102	ALA	CYS	engineered mutation	UNP P02794
A	105	GLN	HIS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
A	140	CYS	GLU	engineered mutation	UNP P02794
A	143	CYS	LYS	engineered mutation	UNP P02794
A	147	CYS	GLU	engineered mutation	UNP P02794
B	13	ASP	HIS	engineered mutation	UNP P02794
B	64	CYS	GLU	engineered mutation	UNP P02794
B	90	ARG	CYS	engineered mutation	UNP P02794
B	102	ALA	CYS	engineered mutation	UNP P02794
B	105	GLN	HIS	engineered mutation	UNP P02794
B	140	CYS	GLU	engineered mutation	UNP P02794
B	143	CYS	LYS	engineered mutation	UNP P02794
B	147	CYS	GLU	engineered mutation	UNP P02794
C	13	ASP	HIS	engineered mutation	UNP P02794
C	64	CYS	GLU	engineered mutation	UNP P02794
C	90	ARG	CYS	engineered mutation	UNP P02794
C	102	ALA	CYS	engineered mutation	UNP P02794
C	105	GLN	HIS	engineered mutation	UNP P02794
C	140	CYS	GLU	engineered mutation	UNP P02794
C	143	CYS	LYS	engineered mutation	UNP P02794
C	147	CYS	GLU	engineered mutation	UNP P02794
D	13	ASP	HIS	engineered mutation	UNP P02794
D	64	CYS	GLU	engineered mutation	UNP P02794
D	90	ARG	CYS	engineered mutation	UNP P02794
D	102	ALA	CYS	engineered mutation	UNP P02794
D	105	GLN	HIS	engineered mutation	UNP P02794
D	140	CYS	GLU	engineered mutation	UNP P02794
D	143	CYS	LYS	engineered mutation	UNP P02794
D	147	CYS	GLU	engineered mutation	UNP P02794
E	13	ASP	HIS	engineered mutation	UNP P02794
E	64	CYS	GLU	engineered mutation	UNP P02794
E	90	ARG	CYS	engineered mutation	UNP P02794
E	102	ALA	CYS	engineered mutation	UNP P02794
E	105	GLN	HIS	engineered mutation	UNP P02794
E	140	CYS	GLU	engineered mutation	UNP P02794
E	143	CYS	LYS	engineered mutation	UNP P02794
E	147	CYS	GLU	engineered mutation	UNP P02794
F	13	ASP	HIS	engineered mutation	UNP P02794
F	64	CYS	GLU	engineered mutation	UNP P02794
F	90	ARG	CYS	engineered mutation	UNP P02794
F	102	ALA	CYS	engineered mutation	UNP P02794
F	105	GLN	HIS	engineered mutation	UNP P02794
F	140	CYS	GLU	engineered mutation	UNP P02794
F	143	CYS	LYS	engineered mutation	UNP P02794

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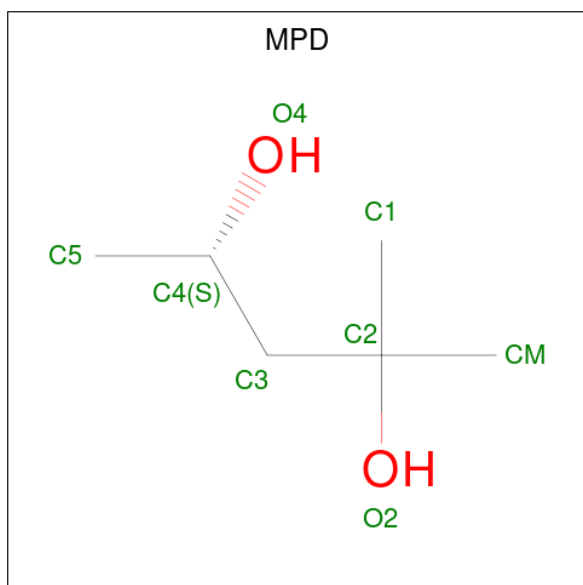
Chain	Residue	Modelled	Actual	Comment	Reference
F	147	CYS	GLU	engineered mutation	UNP P02794
G	13	ASP	HIS	engineered mutation	UNP P02794
G	64	CYS	GLU	engineered mutation	UNP P02794
G	90	ARG	CYS	engineered mutation	UNP P02794
G	102	ALA	CYS	engineered mutation	UNP P02794
G	105	GLN	HIS	engineered mutation	UNP P02794
G	140	CYS	GLU	engineered mutation	UNP P02794
G	143	CYS	LYS	engineered mutation	UNP P02794
G	147	CYS	GLU	engineered mutation	UNP P02794
H	13	ASP	HIS	engineered mutation	UNP P02794
H	64	CYS	GLU	engineered mutation	UNP P02794
H	90	ARG	CYS	engineered mutation	UNP P02794
H	102	ALA	CYS	engineered mutation	UNP P02794
H	105	GLN	HIS	engineered mutation	UNP P02794
H	140	CYS	GLU	engineered mutation	UNP P02794
H	143	CYS	LYS	engineered mutation	UNP P02794
H	147	CYS	GLU	engineered mutation	UNP P02794
I	13	ASP	HIS	engineered mutation	UNP P02794
I	64	CYS	GLU	engineered mutation	UNP P02794
I	90	ARG	CYS	engineered mutation	UNP P02794
I	102	ALA	CYS	engineered mutation	UNP P02794
I	105	GLN	HIS	engineered mutation	UNP P02794
I	140	CYS	GLU	engineered mutation	UNP P02794
I	143	CYS	LYS	engineered mutation	UNP P02794
I	147	CYS	GLU	engineered mutation	UNP P02794
J	13	ASP	HIS	engineered mutation	UNP P02794
J	64	CYS	GLU	engineered mutation	UNP P02794
J	90	ARG	CYS	engineered mutation	UNP P02794
J	102	ALA	CYS	engineered mutation	UNP P02794
J	105	GLN	HIS	engineered mutation	UNP P02794
J	140	CYS	GLU	engineered mutation	UNP P02794
J	143	CYS	LYS	engineered mutation	UNP P02794
J	147	CYS	GLU	engineered mutation	UNP P02794
K	13	ASP	HIS	engineered mutation	UNP P02794
K	64	CYS	GLU	engineered mutation	UNP P02794
K	90	ARG	CYS	engineered mutation	UNP P02794
K	102	ALA	CYS	engineered mutation	UNP P02794
K	105	GLN	HIS	engineered mutation	UNP P02794
K	140	CYS	GLU	engineered mutation	UNP P02794
K	143	CYS	LYS	engineered mutation	UNP P02794
K	147	CYS	GLU	engineered mutation	UNP P02794
L	13	ASP	HIS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
L	64	CYS	GLU	engineered mutation	UNP P02794
L	90	ARG	CYS	engineered mutation	UNP P02794
L	102	ALA	CYS	engineered mutation	UNP P02794
L	105	GLN	HIS	engineered mutation	UNP P02794
L	140	CYS	GLU	engineered mutation	UNP P02794
L	143	CYS	LYS	engineered mutation	UNP P02794
L	147	CYS	GLU	engineered mutation	UNP P02794

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	H	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			8	6	2		
2	I	1	Total	C	O	0	0
			8	6	2		
2	K	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Hg	0	0
			1	1		
3	B	1	Total	Hg	0	0
			1	1		
3	C	1	Total	Hg	0	0
			1	1		
3	D	1	Total	Hg	0	0
			1	1		
3	E	1	Total	Hg	0	0
			1	1		
3	F	1	Total	Hg	0	0
			1	1		
3	G	1	Total	Hg	0	0
			1	1		
3	H	1	Total	Hg	0	0
			1	1		
3	I	1	Total	Hg	0	0
			1	1		
3	J	1	Total	Hg	0	0
			1	1		
3	K	1	Total	Hg	0	0
			1	1		
3	L	1	Total	Hg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	G	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		
5	I	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		
6	B	16	Total	O	0	0
			16	16		
6	C	19	Total	O	0	0
			19	19		
6	D	21	Total	O	0	0
			21	21		
6	E	17	Total	O	0	0
			17	17		
6	F	26	Total	O	0	0
			26	26		
6	G	15	Total	O	0	0
			15	15		
6	H	14	Total	O	0	0
			14	14		
6	I	13	Total	O	0	0
			13	13		
6	J	13	Total	O	0	0
			13	13		
6	K	16	Total	O	0	0
			16	16		

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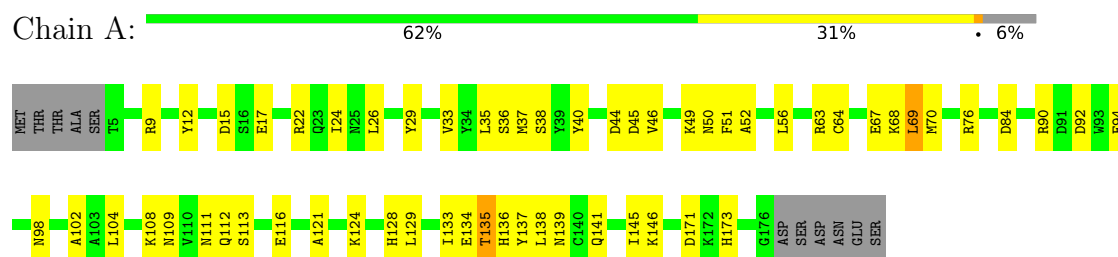
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	16	Total	O	0	0
			16	16		

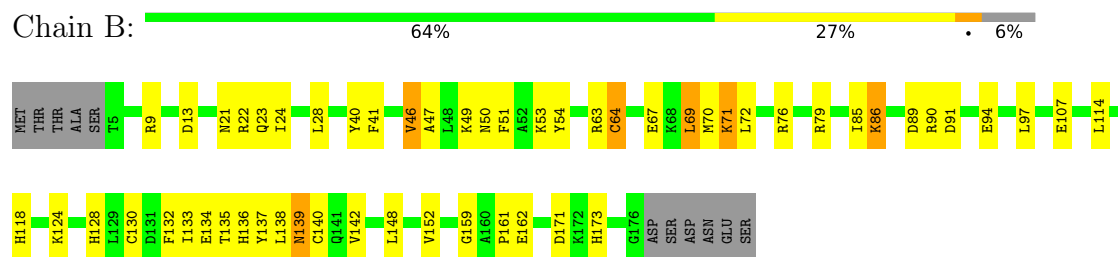
3 Residue-property plots [i](#)

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.

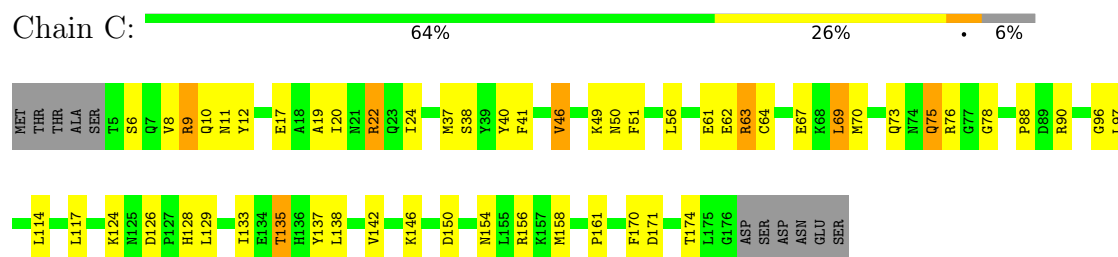
- Molecule 1: Ferritin heavy chain



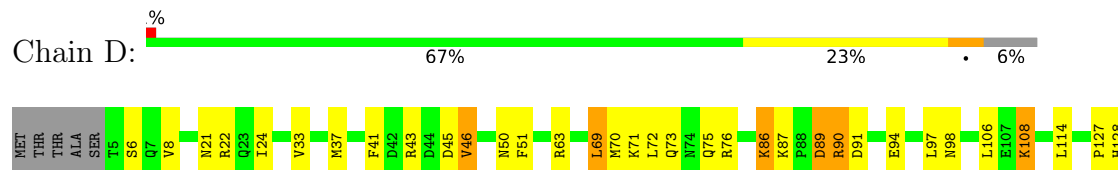
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

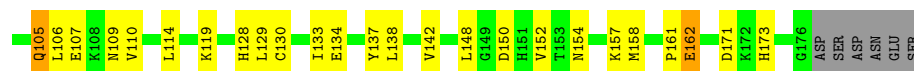


- Molecule 1: Ferritin heavy chain

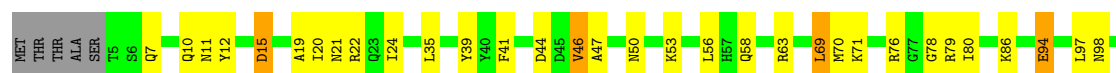




• Molecule 1: Ferritin heavy chain



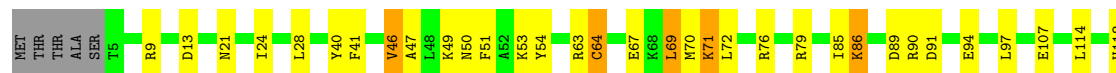
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain

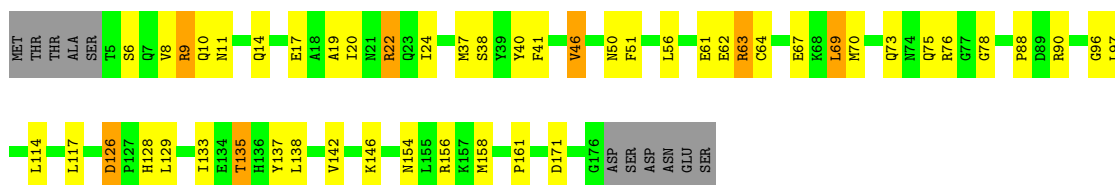


• Molecule 1: Ferritin heavy chain



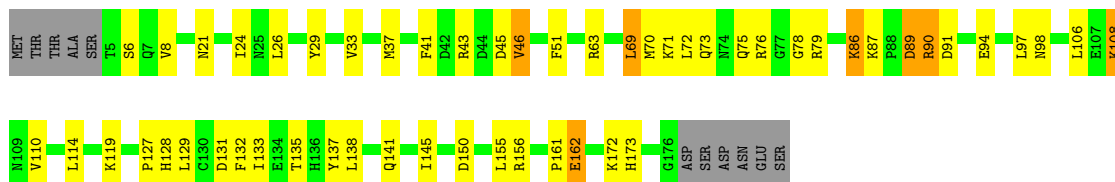
• Molecule 1: Ferritin heavy chain





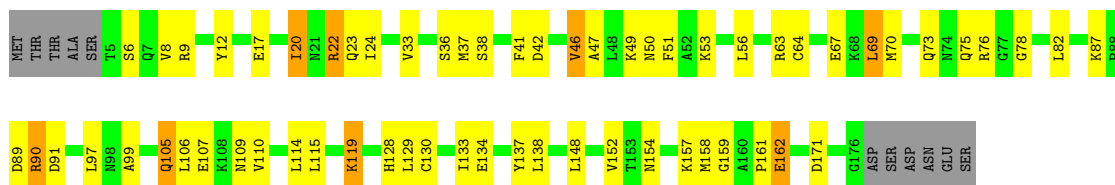
• Molecule 1: Ferritin heavy chain

Chain J: 64% 26% 6%



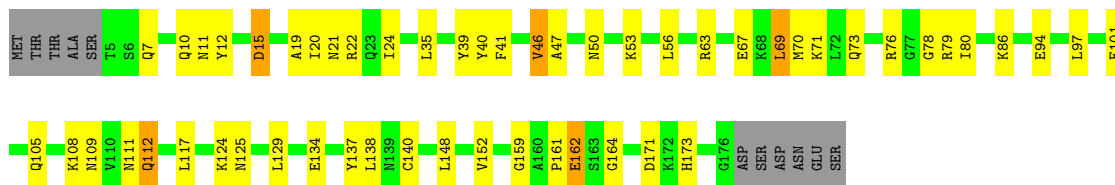
• Molecule 1: Ferritin heavy chain

Chain K: 60% 30% 6%



• Molecule 1: Ferritin heavy chain

Chain L: 64% 27% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.94Å 170.94Å 190.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 3.06 28.80 – 3.06	Depositor EDS
% Data completeness (in resolution range)	85.8 (28.80-3.06) 87.8 (28.80-3.06)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.199 , 0.256 0.196 , 0.193	Depositor DCC
R_{free} test set	2381 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17139	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

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

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	0.47	0/1429	0.88	5/1925 (0.3%)
1	B	0.48	0/1429	0.92	7/1925 (0.4%)
1	C	0.44	0/1429	0.94	3/1925 (0.2%)
1	D	0.47	0/1429	0.91	5/1925 (0.3%)
1	E	0.46	0/1429	0.88	4/1925 (0.2%)
1	F	0.49	0/1429	0.88	4/1925 (0.2%)
1	G	0.46	0/1429	0.89	5/1925 (0.3%)
1	H	0.47	0/1429	0.92	6/1925 (0.3%)
1	I	0.47	0/1429	0.94	5/1925 (0.3%)
1	J	0.45	0/1429	0.91	4/1925 (0.2%)
1	K	0.47	0/1429	0.89	3/1925 (0.2%)
1	L	0.46	0/1429	0.88	5/1925 (0.3%)
All	All	0.47	0/17148	0.91	56/23100 (0.2%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	46	VAL	N-CA-C	-11.43	102.59	111.62
1	C	46	VAL	N-CA-C	-10.39	103.41	111.62
1	H	46	VAL	N-CA-C	-8.91	103.90	111.56
1	B	46	VAL	N-CA-C	-8.61	104.16	111.56
1	B	91	ASP	N-CA-C	-8.15	104.48	114.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1402	0	1351	47	0
1	B	1402	0	1351	46	0
1	C	1402	0	1351	44	0
1	D	1402	0	1351	42	0
1	E	1402	0	1351	46	0
1	F	1402	0	1351	49	0
1	G	1402	0	1351	44	0
1	H	1402	0	1351	55	0
1	I	1402	0	1351	38	0
1	J	1402	0	1351	44	0
1	K	1402	0	1351	50	0
1	L	1402	0	1351	40	0
2	A	8	0	13	0	0
2	B	16	0	27	0	0
2	C	8	0	13	0	0
2	E	8	0	13	0	0
2	F	8	0	13	2	0
2	G	8	0	13	0	0
2	H	16	0	26	3	0
2	I	8	0	13	0	0
2	K	8	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
6	A	21	0	0	2	0
6	B	16	0	0	2	0
6	C	19	0	0	5	0
6	D	21	0	0	2	0
6	E	17	0	0	0	0
6	F	26	0	0	3	0
6	G	15	0	0	2	0
6	H	14	0	0	2	0
6	I	13	0	0	0	0
6	J	13	0	0	2	0
6	K	16	0	0	3	0
6	L	16	0	0	2	0
All	All	17139	0	16356	497	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 497 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:C:63:ARG:HB3	1:C:63:ARG:HH11	1.15	1.08
1:I:63:ARG:HH11	1:I:63:ARG:HB3	1.15	1.06
1:H:86:LYS:HA	1:H:86:LYS:HZ3	1.31	0.96
1:C:63:ARG:HB3	1:C:63:ARG:NH1	1.84	0.92
1:I:63:ARG:HB3	1:I:63:ARG:NH1	1.85	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/183 (93%)	162 (95%)	8 (5%)	0	100	100
1	B	170/183 (93%)	159 (94%)	10 (6%)	1 (1%)	21	48
1	C	170/183 (93%)	159 (94%)	11 (6%)	0	100	100
1	D	170/183 (93%)	162 (95%)	7 (4%)	1 (1%)	21	48
1	E	170/183 (93%)	160 (94%)	9 (5%)	1 (1%)	21	48
1	F	170/183 (93%)	159 (94%)	9 (5%)	2 (1%)	10	32
1	G	170/183 (93%)	162 (95%)	8 (5%)	0	100	100
1	H	170/183 (93%)	160 (94%)	9 (5%)	1 (1%)	21	48
1	I	170/183 (93%)	159 (94%)	11 (6%)	0	100	100
1	J	170/183 (93%)	162 (95%)	7 (4%)	1 (1%)	21	48
1	K	170/183 (93%)	160 (94%)	9 (5%)	1 (1%)	21	48
1	L	170/183 (93%)	159 (94%)	9 (5%)	2 (1%)	10	32
All	All	2040/2196 (93%)	1923 (94%)	107 (5%)	10 (0%)	24	52

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	94	GLU
1	J	94	GLU
1	E	47	ALA
1	K	47	ALA
1	L	47	ALA

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	152/162 (94%)	147 (97%)	5 (3%)	33	60
1	B	152/162 (94%)	145 (95%)	7 (5%)	24	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	152/162 (94%)	142 (93%)	10 (7%)	15	40
1	D	152/162 (94%)	145 (95%)	7 (5%)	24	52
1	E	152/162 (94%)	143 (94%)	9 (6%)	18	44
1	F	152/162 (94%)	144 (95%)	8 (5%)	20	47
1	G	152/162 (94%)	147 (97%)	5 (3%)	33	60
1	H	152/162 (94%)	145 (95%)	7 (5%)	24	52
1	I	152/162 (94%)	142 (93%)	10 (7%)	15	40
1	J	152/162 (94%)	145 (95%)	7 (5%)	24	52
1	K	152/162 (94%)	143 (94%)	9 (6%)	18	44
1	L	152/162 (94%)	144 (95%)	8 (5%)	20	47
All	All	1824/1944 (94%)	1732 (95%)	92 (5%)	22	49

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	139	ASN
1	J	90	ARG
1	I	22	ARG
1	I	75	GLN
1	K	8	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	141	GLN
1	I	98	ASN
1	L	10	GLN
1	H	7	GLN
1	H	139	ASN

5.3.3 RNA ⓘ

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](#)

Of 31 ligands modelled in this entry, 20 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	MPD	E	631	-	7,7,7	2.16	2 (28%)	9,10,10	1.59	2 (22%)
2	MPD	B	630	-	7,7,7	1.58	2 (28%)	9,10,10	1.42	2 (22%)
2	MPD	H	542	-	7,7,7	1.11	1 (14%)	9,10,10	1.53	1 (11%)
2	MPD	A	533	-	7,7,7	1.24	1 (14%)	9,10,10	1.49	1 (11%)
2	MPD	I	539	-	7,7,7	1.14	1 (14%)	9,10,10	1.48	1 (11%)
2	MPD	B	540	-	7,7,7	1.11	1 (14%)	9,10,10	1.50	1 (11%)
2	MPD	K	541	-	7,7,7	1.06	1 (14%)	9,10,10	1.52	1 (11%)
2	MPD	F	543	-	7,7,7	0.95	1 (14%)	9,10,10	1.63	2 (22%)
2	MPD	G	537	-	7,7,7	1.15	1 (14%)	9,10,10	1.45	1 (11%)
2	MPD	C	535	-	7,7,7	1.25	1 (14%)	9,10,10	1.41	1 (11%)
2	MPD	H	538	-	7,7,7	1.14	1 (14%)	9,10,10	1.53	2 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	E	631	-	1/1/2/2	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	B	630	-	1/1/2/2	3/5/5/5	-
2	MPD	H	542	-	1/1/2/2	0/5/5/5	-
2	MPD	A	533	-	1/1/2/2	0/5/5/5	-
2	MPD	I	539	-	1/1/2/2	1/5/5/5	-
2	MPD	B	540	-	1/1/2/2	1/5/5/5	-
2	MPD	K	541	-	1/1/2/2	1/5/5/5	-
2	MPD	F	543	-	1/1/2/2	0/5/5/5	-
2	MPD	G	537	-	1/1/2/2	0/5/5/5	-
2	MPD	C	535	-	1/1/2/2	2/5/5/5	-
2	MPD	H	538	-	1/1/2/2	2/5/5/5	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	631	MPD	C3-C2	-5.22	1.38	1.54
2	B	630	MPD	C3-C2	-3.47	1.44	1.54
2	C	535	MPD	O2-C2	-2.50	1.38	1.44
2	H	542	MPD	O2-C2	-2.30	1.39	1.44
2	E	631	MPD	O2-C2	-2.25	1.39	1.44

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	543	MPD	O4-C4-C3	3.90	126.88	111.35
2	E	631	MPD	O4-C4-C3	3.79	126.43	111.35
2	H	542	MPD	O4-C4-C3	3.71	126.13	111.35
2	H	538	MPD	O4-C4-C3	3.66	125.92	111.35
2	K	541	MPD	O4-C4-C3	3.64	125.84	111.35

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	533	MPD	C4
2	B	540	MPD	C4
2	B	630	MPD	C4
2	C	535	MPD	C4
2	E	631	MPD	C4

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	538	MPD	CM-C2-C3-C4
2	B	630	MPD	C1-C2-C3-C4
2	B	630	MPD	CM-C2-C3-C4
2	C	535	MPD	CM-C2-C3-C4
2	E	631	MPD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	542	MPD	1	0
2	F	543	MPD	2	0
2	H	538	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	172/183 (93%)	-0.29	0 100 100	22, 35, 54, 64	0
1	B	172/183 (93%)	-0.39	0 100 100	21, 33, 49, 55	0
1	C	172/183 (93%)	-0.37	0 100 100	22, 34, 51, 59	0
1	D	172/183 (93%)	-0.30	1 (0%) 85 69	23, 34, 52, 61	0
1	E	172/183 (93%)	-0.26	0 100 100	24, 35, 52, 59	0
1	F	172/183 (93%)	-0.33	0 100 100	22, 34, 50, 58	0
1	G	172/183 (93%)	-0.30	0 100 100	24, 37, 56, 63	0
1	H	172/183 (93%)	-0.27	1 (0%) 85 69	24, 35, 51, 58	0
1	I	172/183 (93%)	-0.37	0 100 100	20, 33, 51, 59	0
1	J	172/183 (93%)	-0.34	0 100 100	24, 36, 52, 61	0
1	K	172/183 (93%)	-0.37	0 100 100	23, 34, 52, 62	0
1	L	172/183 (93%)	-0.39	0 100 100	24, 36, 52, 59	0
All	All	2064/2196 (93%)	-0.33	2 (0%) 92 86	20, 35, 52, 64	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	ASN	2.3
1	H	123	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ZN	H	709	1/1	0.45	0.16	30,30,30,30	1
2	MPD	H	542	8/8	0.68	0.57	39,43,44,45	8
2	MPD	F	543	8/8	0.68	0.52	48,49,49,51	8
2	MPD	K	541	8/8	0.70	0.55	47,49,52,53	8
5	ZN	B	708	1/1	0.71	0.23	23,23,23,23	1
2	MPD	B	540	8/8	0.73	0.55	41,43,44,46	8
2	MPD	B	630	8/8	0.85	0.19	45,53,58,63	8
4	CA	G	813	1/1	0.87	0.12	50,50,50,50	1
4	CA	J	811	1/1	0.87	0.09	47,47,47,47	1
4	CA	A	812	1/1	0.91	0.12	52,52,52,52	1
2	MPD	H	538	8/8	0.92	0.16	49,50,52,53	0
2	MPD	A	533	8/8	0.92	0.15	33,37,42,43	0
2	MPD	G	537	8/8	0.93	0.12	38,42,48,48	0
2	MPD	C	535	8/8	0.94	0.14	46,51,54,57	0
2	MPD	E	631	8/8	0.94	0.15	48,56,58,64	8
2	MPD	I	539	8/8	0.95	0.10	37,41,42,44	0
3	HG	L	534	1/1	0.97	0.11	73,73,73,73	1
3	HG	H	533	1/1	0.97	0.10	59,59,59,59	1
5	ZN	I	710	1/1	0.97	0.10	28,28,28,28	1
3	HG	J	532	1/1	0.98	0.10	63,63,63,63	1
3	HG	K	530	1/1	0.98	0.08	63,63,63,63	1
3	HG	B	526	1/1	0.98	0.08	53,53,53,53	1
3	HG	C	525	1/1	0.98	0.07	65,65,65,65	1
3	HG	D	527	1/1	0.98	0.08	63,63,63,63	1
3	HG	E	523	1/1	0.98	0.07	66,66,66,66	1
3	HG	F	528	1/1	0.98	0.08	61,61,61,61	1
5	ZN	G	707	1/1	0.98	0.29	20,20,20,20	1
3	HG	A	524	1/1	0.98	0.08	65,65,65,65	1
3	HG	I	531	1/1	0.98	0.09	65,65,65,65	1
3	HG	G	529	1/1	0.99	0.09	70,70,70,70	1
5	ZN	A	706	1/1	0.99	0.14	15,15,15,15	1

6.5 Other polymers [i](#)

There are no such residues in this entry.