



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:40 AM UTC

PDB ID : 6Z3D / pdb_00006z3d
Title : L-FerritinMSA
Authors : Davidov, G.; Zarivach, R.
Deposited on : 2020-05-20
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

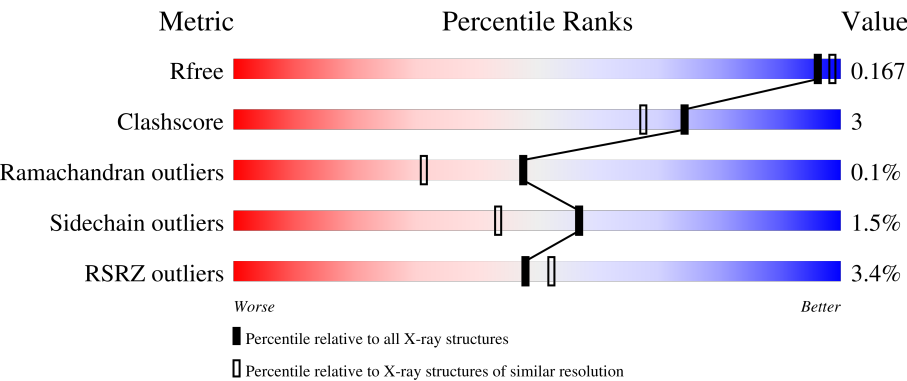
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	2% 73% 5% 22%
1	B	216	2% 73% 5% 21%
1	C	216	2% 75% • 21%
1	D	216	3% 73% 5% 21%
1	E	216	3% 74% • 21%

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Mol	Chain	Length	Quality of chain
1	F	216	

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	ACT	A	201	-	-	X	-
2	ACT	A	202	-	-	X	-
2	ACT	C	201	-	-	X	-
2	ACT	D	201	-	-	X	-
2	ACT	E	201	-	-	X	-
2	ACT	E	202	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9643 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	6	0
			1409	889	255	259	6			
1	B	170	Total	C	N	O	S	0	5	0
			1412	888	254	264	6			
1	C	170	Total	C	N	O	S	0	5	0
			1411	889	254	262	6			
1	D	170	Total	C	N	O	S	0	5	0
			1416	891	258	261	6			
1	E	170	Total	C	N	O	S	0	7	0
			1427	898	259	264	6			
1	F	170	Total	C	N	O	S	0	4	0
			1407	883	258	261	5			

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9CPX4
A	-18	GLY	-	expression tag	UNP Q9CPX4
A	-17	SER	-	expression tag	UNP Q9CPX4
A	-16	SER	-	expression tag	UNP Q9CPX4
A	-15	HIS	-	expression tag	UNP Q9CPX4
A	-14	HIS	-	expression tag	UNP Q9CPX4
A	-13	HIS	-	expression tag	UNP Q9CPX4
A	-12	HIS	-	expression tag	UNP Q9CPX4
A	-11	HIS	-	expression tag	UNP Q9CPX4
A	-10	HIS	-	expression tag	UNP Q9CPX4
A	-9	SER	-	expression tag	UNP Q9CPX4
A	-8	SER	-	expression tag	UNP Q9CPX4
A	-7	GLY	-	expression tag	UNP Q9CPX4
A	-6	LEU	-	expression tag	UNP Q9CPX4
A	-5	VAL	-	expression tag	UNP Q9CPX4
A	-4	PRO	-	expression tag	UNP Q9CPX4
A	-3	ARG	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9CPX4
A	-1	SER	-	expression tag	UNP Q9CPX4
A	0	HIS	-	expression tag	UNP Q9CPX4
A	184	GLY	-	expression tag	UNP Q9CPX4
A	185	ASP	-	expression tag	UNP Q9CPX4
A	186	ILE	-	expression tag	UNP Q9CPX4
A	187	GLU	-	expression tag	UNP Q9CPX4
A	188	SER	-	expression tag	UNP Q9CPX4
A	189	ALA	-	expression tag	UNP Q9CPX4
A	190	GLN	-	expression tag	UNP Q9CPX4
A	191	SER	-	expression tag	UNP Q9CPX4
A	192	ASP	-	expression tag	UNP Q9CPX4
A	193	GLU	-	expression tag	UNP Q9CPX4
A	194	GLU	-	expression tag	UNP Q9CPX4
A	195	VAL	-	expression tag	UNP Q9CPX4
A	196	GLU	-	expression tag	UNP Q9CPX4
B	-19	MET	-	initiating methionine	UNP Q9CPX4
B	-18	GLY	-	expression tag	UNP Q9CPX4
B	-17	SER	-	expression tag	UNP Q9CPX4
B	-16	SER	-	expression tag	UNP Q9CPX4
B	-15	HIS	-	expression tag	UNP Q9CPX4
B	-14	HIS	-	expression tag	UNP Q9CPX4
B	-13	HIS	-	expression tag	UNP Q9CPX4
B	-12	HIS	-	expression tag	UNP Q9CPX4
B	-11	HIS	-	expression tag	UNP Q9CPX4
B	-10	HIS	-	expression tag	UNP Q9CPX4
B	-9	SER	-	expression tag	UNP Q9CPX4
B	-8	SER	-	expression tag	UNP Q9CPX4
B	-7	GLY	-	expression tag	UNP Q9CPX4
B	-6	LEU	-	expression tag	UNP Q9CPX4
B	-5	VAL	-	expression tag	UNP Q9CPX4
B	-4	PRO	-	expression tag	UNP Q9CPX4
B	-3	ARG	-	expression tag	UNP Q9CPX4
B	-2	GLY	-	expression tag	UNP Q9CPX4
B	-1	SER	-	expression tag	UNP Q9CPX4
B	0	HIS	-	expression tag	UNP Q9CPX4
B	184	GLY	-	expression tag	UNP Q9CPX4
B	185	ASP	-	expression tag	UNP Q9CPX4
B	186	ILE	-	expression tag	UNP Q9CPX4
B	187	GLU	-	expression tag	UNP Q9CPX4
B	188	SER	-	expression tag	UNP Q9CPX4
B	189	ALA	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	190	GLN	-	expression tag	UNP Q9CPX4
B	191	SER	-	expression tag	UNP Q9CPX4
B	192	ASP	-	expression tag	UNP Q9CPX4
B	193	GLU	-	expression tag	UNP Q9CPX4
B	194	GLU	-	expression tag	UNP Q9CPX4
B	195	VAL	-	expression tag	UNP Q9CPX4
B	196	GLU	-	expression tag	UNP Q9CPX4
C	-19	MET	-	initiating methionine	UNP Q9CPX4
C	-18	GLY	-	expression tag	UNP Q9CPX4
C	-17	SER	-	expression tag	UNP Q9CPX4
C	-16	SER	-	expression tag	UNP Q9CPX4
C	-15	HIS	-	expression tag	UNP Q9CPX4
C	-14	HIS	-	expression tag	UNP Q9CPX4
C	-13	HIS	-	expression tag	UNP Q9CPX4
C	-12	HIS	-	expression tag	UNP Q9CPX4
C	-11	HIS	-	expression tag	UNP Q9CPX4
C	-10	HIS	-	expression tag	UNP Q9CPX4
C	-9	SER	-	expression tag	UNP Q9CPX4
C	-8	SER	-	expression tag	UNP Q9CPX4
C	-7	GLY	-	expression tag	UNP Q9CPX4
C	-6	LEU	-	expression tag	UNP Q9CPX4
C	-5	VAL	-	expression tag	UNP Q9CPX4
C	-4	PRO	-	expression tag	UNP Q9CPX4
C	-3	ARG	-	expression tag	UNP Q9CPX4
C	-2	GLY	-	expression tag	UNP Q9CPX4
C	-1	SER	-	expression tag	UNP Q9CPX4
C	0	HIS	-	expression tag	UNP Q9CPX4
C	184	GLY	-	expression tag	UNP Q9CPX4
C	185	ASP	-	expression tag	UNP Q9CPX4
C	186	ILE	-	expression tag	UNP Q9CPX4
C	187	GLU	-	expression tag	UNP Q9CPX4
C	188	SER	-	expression tag	UNP Q9CPX4
C	189	ALA	-	expression tag	UNP Q9CPX4
C	190	GLN	-	expression tag	UNP Q9CPX4
C	191	SER	-	expression tag	UNP Q9CPX4
C	192	ASP	-	expression tag	UNP Q9CPX4
C	193	GLU	-	expression tag	UNP Q9CPX4
C	194	GLU	-	expression tag	UNP Q9CPX4
C	195	VAL	-	expression tag	UNP Q9CPX4
C	196	GLU	-	expression tag	UNP Q9CPX4
D	-19	MET	-	initiating methionine	UNP Q9CPX4
D	-18	GLY	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP Q9CPX4
D	-16	SER	-	expression tag	UNP Q9CPX4
D	-15	HIS	-	expression tag	UNP Q9CPX4
D	-14	HIS	-	expression tag	UNP Q9CPX4
D	-13	HIS	-	expression tag	UNP Q9CPX4
D	-12	HIS	-	expression tag	UNP Q9CPX4
D	-11	HIS	-	expression tag	UNP Q9CPX4
D	-10	HIS	-	expression tag	UNP Q9CPX4
D	-9	SER	-	expression tag	UNP Q9CPX4
D	-8	SER	-	expression tag	UNP Q9CPX4
D	-7	GLY	-	expression tag	UNP Q9CPX4
D	-6	LEU	-	expression tag	UNP Q9CPX4
D	-5	VAL	-	expression tag	UNP Q9CPX4
D	-4	PRO	-	expression tag	UNP Q9CPX4
D	-3	ARG	-	expression tag	UNP Q9CPX4
D	-2	GLY	-	expression tag	UNP Q9CPX4
D	-1	SER	-	expression tag	UNP Q9CPX4
D	0	HIS	-	expression tag	UNP Q9CPX4
D	184	GLY	-	expression tag	UNP Q9CPX4
D	185	ASP	-	expression tag	UNP Q9CPX4
D	186	ILE	-	expression tag	UNP Q9CPX4
D	187	GLU	-	expression tag	UNP Q9CPX4
D	188	SER	-	expression tag	UNP Q9CPX4
D	189	ALA	-	expression tag	UNP Q9CPX4
D	190	GLN	-	expression tag	UNP Q9CPX4
D	191	SER	-	expression tag	UNP Q9CPX4
D	192	ASP	-	expression tag	UNP Q9CPX4
D	193	GLU	-	expression tag	UNP Q9CPX4
D	194	GLU	-	expression tag	UNP Q9CPX4
D	195	VAL	-	expression tag	UNP Q9CPX4
D	196	GLU	-	expression tag	UNP Q9CPX4
E	-19	MET	-	initiating methionine	UNP Q9CPX4
E	-18	GLY	-	expression tag	UNP Q9CPX4
E	-17	SER	-	expression tag	UNP Q9CPX4
E	-16	SER	-	expression tag	UNP Q9CPX4
E	-15	HIS	-	expression tag	UNP Q9CPX4
E	-14	HIS	-	expression tag	UNP Q9CPX4
E	-13	HIS	-	expression tag	UNP Q9CPX4
E	-12	HIS	-	expression tag	UNP Q9CPX4
E	-11	HIS	-	expression tag	UNP Q9CPX4
E	-10	HIS	-	expression tag	UNP Q9CPX4
E	-9	SER	-	expression tag	UNP Q9CPX4

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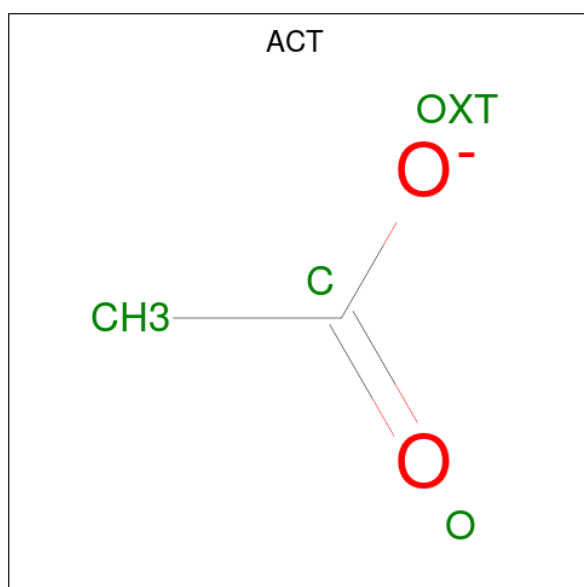
Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	SER	-	expression tag	UNP Q9CPX4
E	-7	GLY	-	expression tag	UNP Q9CPX4
E	-6	LEU	-	expression tag	UNP Q9CPX4
E	-5	VAL	-	expression tag	UNP Q9CPX4
E	-4	PRO	-	expression tag	UNP Q9CPX4
E	-3	ARG	-	expression tag	UNP Q9CPX4
E	-2	GLY	-	expression tag	UNP Q9CPX4
E	-1	SER	-	expression tag	UNP Q9CPX4
E	0	HIS	-	expression tag	UNP Q9CPX4
E	184	GLY	-	expression tag	UNP Q9CPX4
E	185	ASP	-	expression tag	UNP Q9CPX4
E	186	ILE	-	expression tag	UNP Q9CPX4
E	187	GLU	-	expression tag	UNP Q9CPX4
E	188	SER	-	expression tag	UNP Q9CPX4
E	189	ALA	-	expression tag	UNP Q9CPX4
E	190	GLN	-	expression tag	UNP Q9CPX4
E	191	SER	-	expression tag	UNP Q9CPX4
E	192	ASP	-	expression tag	UNP Q9CPX4
E	193	GLU	-	expression tag	UNP Q9CPX4
E	194	GLU	-	expression tag	UNP Q9CPX4
E	195	VAL	-	expression tag	UNP Q9CPX4
E	196	GLU	-	expression tag	UNP Q9CPX4
F	-19	MET	-	initiating methionine	UNP Q9CPX4
F	-18	GLY	-	expression tag	UNP Q9CPX4
F	-17	SER	-	expression tag	UNP Q9CPX4
F	-16	SER	-	expression tag	UNP Q9CPX4
F	-15	HIS	-	expression tag	UNP Q9CPX4
F	-14	HIS	-	expression tag	UNP Q9CPX4
F	-13	HIS	-	expression tag	UNP Q9CPX4
F	-12	HIS	-	expression tag	UNP Q9CPX4
F	-11	HIS	-	expression tag	UNP Q9CPX4
F	-10	HIS	-	expression tag	UNP Q9CPX4
F	-9	SER	-	expression tag	UNP Q9CPX4
F	-8	SER	-	expression tag	UNP Q9CPX4
F	-7	GLY	-	expression tag	UNP Q9CPX4
F	-6	LEU	-	expression tag	UNP Q9CPX4
F	-5	VAL	-	expression tag	UNP Q9CPX4
F	-4	PRO	-	expression tag	UNP Q9CPX4
F	-3	ARG	-	expression tag	UNP Q9CPX4
F	-2	GLY	-	expression tag	UNP Q9CPX4
F	-1	SER	-	expression tag	UNP Q9CPX4
F	0	HIS	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	184	GLY	-	expression tag	UNP Q9CPX4
F	185	ASP	-	expression tag	UNP Q9CPX4
F	186	ILE	-	expression tag	UNP Q9CPX4
F	187	GLU	-	expression tag	UNP Q9CPX4
F	188	SER	-	expression tag	UNP Q9CPX4
F	189	ALA	-	expression tag	UNP Q9CPX4
F	190	GLN	-	expression tag	UNP Q9CPX4
F	191	SER	-	expression tag	UNP Q9CPX4
F	192	ASP	-	expression tag	UNP Q9CPX4
F	193	GLU	-	expression tag	UNP Q9CPX4
F	194	GLU	-	expression tag	UNP Q9CPX4
F	195	VAL	-	expression tag	UNP Q9CPX4
F	196	GLU	-	expression tag	UNP Q9CPX4

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			4	2	2		

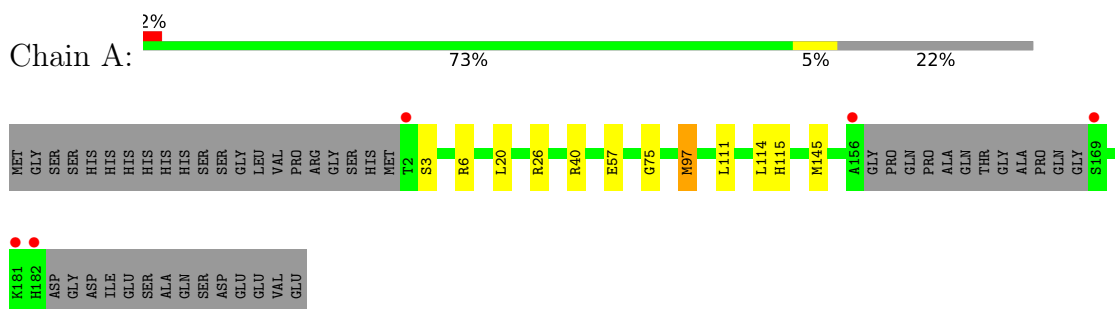
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	221	Total	O	0	0
			221	221		
3	C	173	Total	O	0	0
			173	173		
3	D	198	Total	O	0	0
			198	198		
3	E	163	Total	O	0	0
			163	163		
3	F	168	Total	O	0	0
			168	168		

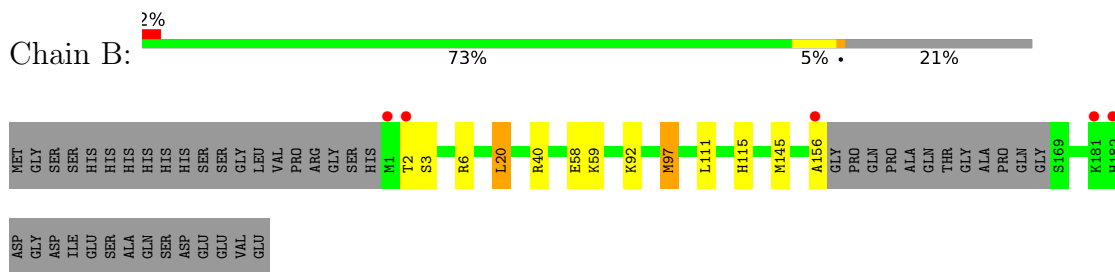
3 Residue-property plots [i](#)

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.

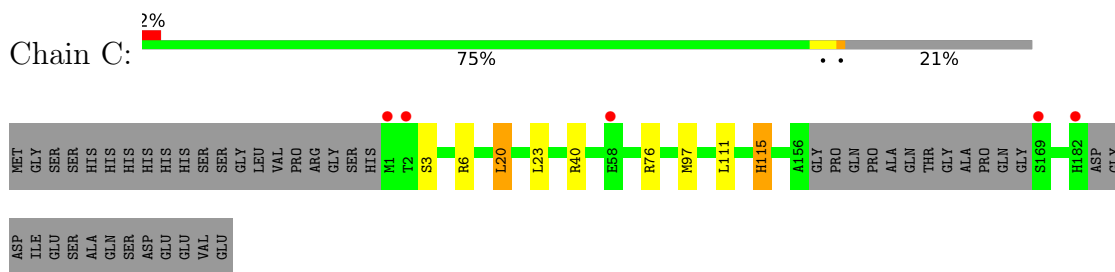
- Molecule 1: Ferritin



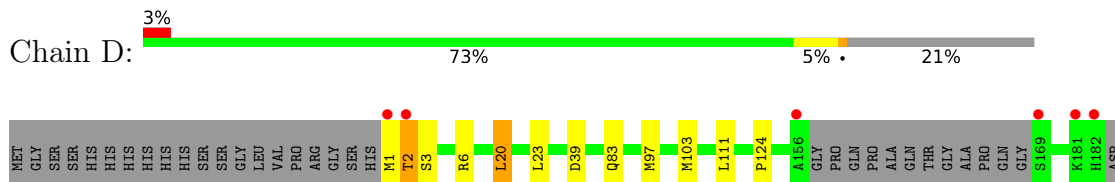
- Molecule 1: Ferritin



- Molecule 1: Ferritin

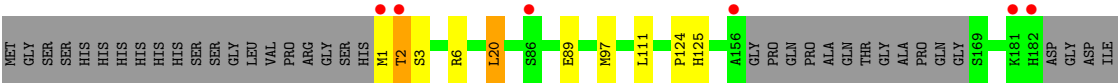


- Molecule 1: Ferritin



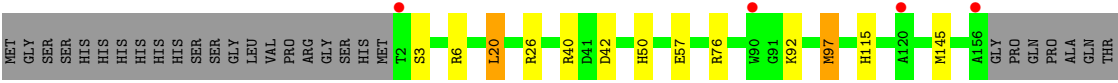
GLY
ASP
ILE
GLU
SER
ALA
GLN
SER
ASP
GLU
VAL
GLU

● Molecule 1: Ferritin



GLU
SER
ALA
GLN
SER
ASP
GLU
GLU
VAL
GLU

● Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.30Å 134.30Å 166.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	166.85 – 1.70 166.85 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (166.85-1.70) 100.0 (166.85-1.70)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.155 , 0.176 0.168 , 0.167	Depositor DCC
R_{free} test set	8447 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9643	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: ACT

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	1.01	1/1447 (0.1%)	1.14	1/1941 (0.1%)
1	B	1.08	3/1447 (0.2%)	1.18	1/1940 (0.1%)
1	C	1.00	1/1446 (0.1%)	1.17	1/1939 (0.1%)
1	D	1.02	0/1448	1.16	0/1941
1	E	0.98	1/1468 (0.1%)	1.12	1/1968 (0.1%)
1	F	1.00	1/1442 (0.1%)	1.14	0/1934
All	All	1.02	7/8698 (0.1%)	1.15	4/11663 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	125	HIS	CE1-NE2	7.47	1.40	1.32
1	B	115	HIS	CE1-NE2	7.17	1.39	1.32
1	C	115	HIS	CE1-NE2	6.81	1.39	1.32
1	B	40	ARG	NE-CZ	5.54	1.39	1.33
1	F	115	HIS	CE1-NE2	5.34	1.37	1.32
1	A	75	GLY	C-O	5.32	1.29	1.23
1	B	2	THR	C-O	-5.17	1.17	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ALA	CA-C-O	-7.11	108.71	120.80
1	A	57	GLU	CB-CG-CD	6.01	122.82	112.60
1	E	2	THR	N-CA-CB	5.53	118.70	110.29
1	C	76	ARG	CB-CA-C	5.21	118.80	110.16

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	1409	0	1403	11	0
1	B	1412	0	1397	7	0
1	C	1411	0	1400	7	0
1	D	1416	0	1409	9	0
1	E	1427	0	1421	5	0
1	F	1407	0	1391	7	0
2	A	8	0	6	3	0
2	C	4	0	3	2	0
2	D	4	0	3	2	0
2	E	8	0	6	4	0
3	A	214	0	0	4	1
3	B	221	0	0	1	1
3	C	173	0	0	3	0
3	D	198	0	0	4	0
3	E	163	0	0	0	0
3	F	168	0	0	2	0
All	All	9643	0	8439	52	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 3.

All (52) 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:F:57:GLU:OE1	3:F:201:HOH:O	1.81	0.99
1:B:58[B]:GLU:OE2	1:B:59:LYS:HE2	1.69	0.91
2:A:201:ACT:H3	2:A:202:ACT:H1	1.58	0.83
1:E:89:GLU:OE1	1:F:76[B]:ARG:NH1	2.12	0.83
2:E:201:ACT:H1	2:E:202:ACT:H3	1.66	0.77
1:B:58[B]:GLU:CD	1:B:59:LYS:HE2	2.12	0.74
1:E:20:LEU:HD11	1:E:111:LEU:HD23	1.70	0.73
1:A:20[B]:LEU:HD12	1:A:114:LEU:HD22	1.70	0.72
1:B:20:LEU:HD11	1:B:111:LEU:HD23	1.72	0.72
1:B:58[A]:GLU:OE1	3:B:202:HOH:O	2.09	0.70
1:C:20:LEU:HD11	1:C:111:LEU:HD23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LEU:HD11	1:D:111:LEU:HD23	1.73	0.69
1:D:103:MET:SD	3:D:461:HOH:O	2.50	0.69
1:F:50:HIS:CE1	1:F:183:ASP:C	2.77	0.63
1:F:40[B]:ARG:NH2	1:F:42:ASP:OD2	2.34	0.61
1:A:3:SER:OG	3:A:301:HOH:O	2.08	0.60
1:F:20:LEU:HD22	3:F:289:HOH:O	2.03	0.58
1:C:40[A]:ARG:NH2	3:C:301:HOH:O	2.37	0.57
2:C:201:ACT:H3	2:D:201:ACT:H1	1.87	0.57
1:A:3:SER:CB	3:A:301:HOH:O	2.54	0.56
1:F:3:SER:HB3	1:F:6:ARG:HB2	1.88	0.55
2:A:201:ACT:H3	2:A:202:ACT:CH3	2.32	0.54
1:A:26:ARG:HG3	3:A:396:HOH:O	2.08	0.54
1:A:20[A]:LEU:HD21	1:A:111:LEU:HD23	1.89	0.54
1:C:23[B]:LEU:HG	3:C:412:HOH:O	2.08	0.54
1:A:3:SER:HB3	1:A:6:ARG:HB2	1.89	0.53
1:C:3:SER:HB3	1:C:6:ARG:HB2	1.90	0.53
2:E:201:ACT:H1	2:E:202:ACT:CH3	2.38	0.52
1:C:115:HIS:CE1	1:E:124:PRO:HB3	2.46	0.51
1:B:3:SER:HB3	1:B:6:ARG:HB2	1.92	0.51
1:E:3:SER:HB3	1:E:6:ARG:HB2	1.92	0.51
1:F:97[A]:MET:HE1	1:F:145:MET:HA	1.93	0.51
1:D:3:SER:HB3	1:D:6:ARG:HB2	1.91	0.51
1:D:23[B]:LEU:HD23	3:D:330:HOH:O	2.11	0.50
2:A:201:ACT:CH3	2:A:202:ACT:H1	2.36	0.49
2:E:201:ACT:CH3	2:E:202:ACT:H3	2.41	0.49
1:B:97[A]:MET:HE1	1:B:145:MET:HA	1.94	0.49
1:D:97[A]:MET:HB3	1:D:97[A]:MET:HE2	1.64	0.48
1:A:40[A]:ARG:NH1	3:A:309:HOH:O	2.46	0.47
1:C:97:MET:HB3	1:C:97:MET:HE2	1.71	0.46
1:A:97[A]:MET:HE1	1:A:145:MET:HA	1.97	0.46
1:D:39:ASP:OD2	3:D:301:HOH:O	2.21	0.46
2:E:201:ACT:OXT	2:E:202:ACT:H3	2.18	0.44
1:C:23[B]:LEU:HD23	3:C:334:HOH:O	2.18	0.43
1:A:20[A]:LEU:HD21	1:A:111:LEU:CD2	2.49	0.43
1:D:83:GLN:NE2	3:D:308:HOH:O	2.50	0.43
2:C:201:ACT:CH3	2:D:201:ACT:H1	2.49	0.42
1:D:1:MET:O	1:D:2:THR:O	2.37	0.42
1:A:115:HIS:CE1	1:D:124:PRO:HB3	2.55	0.42
1:E:97[A]:MET:HE2	1:E:97[A]:MET:HB3	1.67	0.41
1:A:20[B]:LEU:HD12	1:A:114:LEU:CD2	2.46	0.41
1:B:59:LYS:HA	1:B:59:LYS:HD3	1.94	0.40

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)
3:A:302:HOH:O	3:B:214:HOH:O[3_445]	2.18	0.02

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	171/216 (79%)	170 (99%)	1 (1%)	0	100	100
1	B	171/216 (79%)	170 (99%)	1 (1%)	0	100	100
1	C	171/216 (79%)	169 (99%)	2 (1%)	0	100	100
1	D	171/216 (79%)	168 (98%)	2 (1%)	1 (1%)	21	9
1	E	173/216 (80%)	171 (99%)	2 (1%)	0	100	100
1	F	170/216 (79%)	167 (98%)	3 (2%)	0	100	100
All	All	1027/1296 (79%)	1015 (99%)	11 (1%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	THR

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	149/180 (83%)	147 (99%)	2 (1%)	61	48
1	B	149/180 (83%)	145 (97%)	4 (3%)	39	23
1	C	149/180 (83%)	148 (99%)	1 (1%)	76	69
1	D	149/180 (83%)	148 (99%)	1 (1%)	76	69
1	E	151/180 (84%)	148 (98%)	3 (2%)	48	32
1	F	148/180 (82%)	143 (97%)	5 (3%)	32	16
All	All	895/1080 (83%)	879 (98%)	16 (2%)	57	36

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97[A]	MET
1	A	97[B]	MET
1	B	20	LEU
1	B	92	LYS
1	B	97[A]	MET
1	B	97[B]	MET
1	C	20	LEU
1	D	20	LEU
1	E	1	MET
1	E	2	THR
1	E	20	LEU
1	F	20	LEU
1	F	26	ARG
1	F	92	LYS
1	F	97[A]	MET
1	F	97[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	83	GLN
1	A	182	HIS
1	B	50	HIS
1	B	182	HIS
1	C	50	HIS
1	D	50	HIS
1	D	182	HIS
1	E	50	HIS

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Mol	Chain	Res	Type
1	E	182	HIS
1	F	50	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
2	ACT	E	202	-	3,3,3	1.13	0	3,3,3	0.80	0
2	ACT	D	201	-	3,3,3	1.02	0	3,3,3	0.92	0
2	ACT	E	201	-	3,3,3	1.10	0	3,3,3	0.91	0
2	ACT	C	201	-	3,3,3	1.04	0	3,3,3	0.82	0
2	ACT	A	201	-	3,3,3	1.23	0	3,3,3	0.80	0
2	ACT	A	202	-	3,3,3	1.14	0	3,3,3	1.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	202	ACT	4	0
2	D	201	ACT	2	0
2	E	201	ACT	4	0
2	C	201	ACT	2	0
2	A	201	ACT	3	0
2	A	202	ACT	3	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	169/216 (78%)	-0.22	5 (2%)	52	56	10, 21, 35, 54	6 (3%)
1	B	170/216 (78%)	-0.28	5 (2%)	53	58	11, 19, 31, 83	5 (2%)
1	C	170/216 (78%)	-0.00	5 (2%)	53	58	12, 25, 38, 89	5 (2%)
1	D	170/216 (78%)	-0.11	6 (3%)	47	52	12, 23, 38, 89	5 (2%)
1	E	170/216 (78%)	0.10	6 (3%)	47	52	16, 28, 41, 86	7 (4%)
1	F	170/216 (78%)	0.10	8 (4%)	36	40	16, 27, 39, 78	4 (2%)
All	All	1019/1296 (78%)	-0.07	35 (3%)	48	52	10, 24, 39, 89	32 (3%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.8
1	E	1	MET	4.7
1	B	1	MET	4.6
1	C	1	MET	4.4
1	D	182	HIS	4.2
1	F	2	THR	4.2
1	A	2	THR	4.1
1	B	2	THR	3.4
1	C	2	THR	3.2
1	E	2	THR	3.1
1	F	183	ASP	2.9
1	F	156	ALA	2.9
1	E	156	ALA	2.8
1	E	182	HIS	2.8
1	F	181	LYS	2.7
1	F	182	HIS	2.7
1	C	182	HIS	2.6
1	B	181	LYS	2.6
1	A	169	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	169	SER	2.4
1	D	156	ALA	2.4
1	A	182	HIS	2.4
1	E	86	SER	2.3
1	E	181	LYS	2.3
1	B	156	ALA	2.3
1	B	182	HIS	2.3
1	D	169	SER	2.3
1	F	90	TRP	2.2
1	D	2	THR	2.2
1	F	169	SER	2.2
1	F	120	ALA	2.1
1	D	181	LYS	2.1
1	A	156	ALA	2.1
1	A	181	LYS	2.1
1	C	58	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	ACT	E	202	4/4	0.72	0.27	55,57,58,62	0
2	ACT	A	202	4/4	0.74	0.21	39,41,44,49	0
2	ACT	A	201	4/4	0.74	0.24	45,47,49,53	0
2	ACT	D	201	4/4	0.78	0.25	52,52,56,59	0
2	ACT	E	201	4/4	0.79	0.24	61,61,63,66	0
2	ACT	C	201	4/4	0.82	0.18	51,51,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.