



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:55 am BST

PDB ID : 3WNW
Title : Structure of Mouse H-chain modified ferritin
Authors : Zarivach, R.; Lewin, L.
Deposited on : 2013-12-17
Resolution : 2.24 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 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

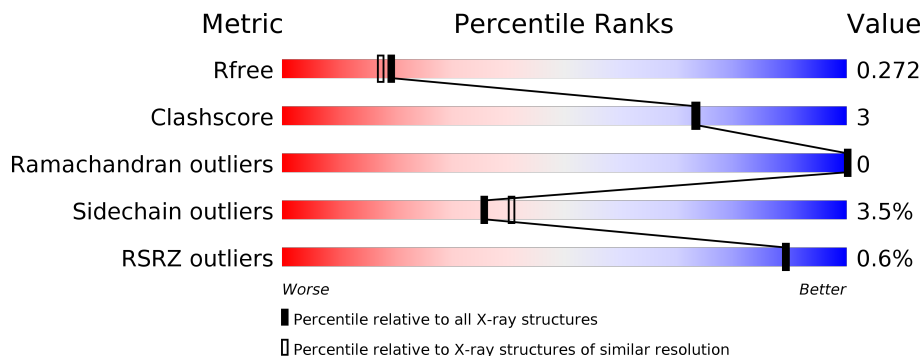
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 ≥ 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	212	
1	B	212	
1	C	212	
1	D	212	
1	E	212	
1	F	212	

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Mol	Chain	Length	Quality of chain
1	G	212	 70% 10% 18%
1	H	212	 68% 13% 18%
1	I	212	 70% 10% 18%
1	J	212	 74% 8% 18%
1	K	212	 74% 7% 18%
1	L	212	 74% 8% 18%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18648 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	173	1423	892	251	272	8	0	1	0
1	B	173	1435	901	250	276	8	0	3	0
1	C	173	1426	894	249	275	8	0	2	0
1	D	173	1415	887	248	272	8	0	0	0
1	E	173	1432	898	253	273	8	0	2	0
1	F	174	1433	898	254	273	8	0	1	0
1	G	174	1437	902	253	274	8	0	2	0
1	H	173	1431	897	254	272	8	0	2	0
1	I	173	1440	903	252	277	8	0	4	0
1	J	174	1425	893	251	273	8	0	0	0
1	K	173	1430	897	251	274	8	0	2	0
1	L	174	1449	909	254	278	8	0	3	0

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	EXPRESSION TAG	UNP P09528
A	-16	SER	-	EXPRESSION TAG	UNP P09528
A	-15	HIS	-	EXPRESSION TAG	UNP P09528
A	-14	MET	-	EXPRESSION TAG	UNP P09528
A	-13	ALA	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	SER	-	EXPRESSION TAG	UNP P09528
A	-11	MET	-	EXPRESSION TAG	UNP P09528
A	-10	THR	-	EXPRESSION TAG	UNP P09528
A	-9	GLY	-	EXPRESSION TAG	UNP P09528
A	-8	GLY	-	EXPRESSION TAG	UNP P09528
A	-7	GLN	-	EXPRESSION TAG	UNP P09528
A	-6	GLN	-	EXPRESSION TAG	UNP P09528
A	-5	MET	-	EXPRESSION TAG	UNP P09528
A	-4	GLY	-	EXPRESSION TAG	UNP P09528
A	-3	ARG	-	EXPRESSION TAG	UNP P09528
A	-2	GLY	-	EXPRESSION TAG	UNP P09528
A	-1	SER	-	EXPRESSION TAG	UNP P09528
A	182	GLY	-	EXPRESSION TAG	UNP P09528
A	183	ASP	-	EXPRESSION TAG	UNP P09528
A	184	ILE	-	EXPRESSION TAG	UNP P09528
A	185	GLU	-	EXPRESSION TAG	UNP P09528
A	186	SER	-	EXPRESSION TAG	UNP P09528
A	187	ALA	-	EXPRESSION TAG	UNP P09528
A	188	GLN	-	EXPRESSION TAG	UNP P09528
A	189	SER	-	EXPRESSION TAG	UNP P09528
A	190	ASP	-	EXPRESSION TAG	UNP P09528
A	191	GLU	-	EXPRESSION TAG	UNP P09528
A	192	GLU	-	EXPRESSION TAG	UNP P09528
A	193	VAL	-	EXPRESSION TAG	UNP P09528
A	194	GLU	-	EXPRESSION TAG	UNP P09528
B	-17	GLY	-	EXPRESSION TAG	UNP P09528
B	-16	SER	-	EXPRESSION TAG	UNP P09528
B	-15	HIS	-	EXPRESSION TAG	UNP P09528
B	-14	MET	-	EXPRESSION TAG	UNP P09528
B	-13	ALA	-	EXPRESSION TAG	UNP P09528
B	-12	SER	-	EXPRESSION TAG	UNP P09528
B	-11	MET	-	EXPRESSION TAG	UNP P09528
B	-10	THR	-	EXPRESSION TAG	UNP P09528
B	-9	GLY	-	EXPRESSION TAG	UNP P09528
B	-8	GLY	-	EXPRESSION TAG	UNP P09528
B	-7	GLN	-	EXPRESSION TAG	UNP P09528
B	-6	GLN	-	EXPRESSION TAG	UNP P09528
B	-5	MET	-	EXPRESSION TAG	UNP P09528
B	-4	GLY	-	EXPRESSION TAG	UNP P09528
B	-3	ARG	-	EXPRESSION TAG	UNP P09528
B	-2	GLY	-	EXPRESSION TAG	UNP P09528
B	-1	SER	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	GLY	-	EXPRESSION TAG	UNP P09528
B	183	ASP	-	EXPRESSION TAG	UNP P09528
B	184	ILE	-	EXPRESSION TAG	UNP P09528
B	185	GLU	-	EXPRESSION TAG	UNP P09528
B	186	SER	-	EXPRESSION TAG	UNP P09528
B	187	ALA	-	EXPRESSION TAG	UNP P09528
B	188	GLN	-	EXPRESSION TAG	UNP P09528
B	189	SER	-	EXPRESSION TAG	UNP P09528
B	190	ASP	-	EXPRESSION TAG	UNP P09528
B	191	GLU	-	EXPRESSION TAG	UNP P09528
B	192	GLU	-	EXPRESSION TAG	UNP P09528
B	193	VAL	-	EXPRESSION TAG	UNP P09528
B	194	GLU	-	EXPRESSION TAG	UNP P09528
C	-17	GLY	-	EXPRESSION TAG	UNP P09528
C	-16	SER	-	EXPRESSION TAG	UNP P09528
C	-15	HIS	-	EXPRESSION TAG	UNP P09528
C	-14	MET	-	EXPRESSION TAG	UNP P09528
C	-13	ALA	-	EXPRESSION TAG	UNP P09528
C	-12	SER	-	EXPRESSION TAG	UNP P09528
C	-11	MET	-	EXPRESSION TAG	UNP P09528
C	-10	THR	-	EXPRESSION TAG	UNP P09528
C	-9	GLY	-	EXPRESSION TAG	UNP P09528
C	-8	GLY	-	EXPRESSION TAG	UNP P09528
C	-7	GLN	-	EXPRESSION TAG	UNP P09528
C	-6	GLN	-	EXPRESSION TAG	UNP P09528
C	-5	MET	-	EXPRESSION TAG	UNP P09528
C	-4	GLY	-	EXPRESSION TAG	UNP P09528
C	-3	ARG	-	EXPRESSION TAG	UNP P09528
C	-2	GLY	-	EXPRESSION TAG	UNP P09528
C	-1	SER	-	EXPRESSION TAG	UNP P09528
C	182	GLY	-	EXPRESSION TAG	UNP P09528
C	183	ASP	-	EXPRESSION TAG	UNP P09528
C	184	ILE	-	EXPRESSION TAG	UNP P09528
C	185	GLU	-	EXPRESSION TAG	UNP P09528
C	186	SER	-	EXPRESSION TAG	UNP P09528
C	187	ALA	-	EXPRESSION TAG	UNP P09528
C	188	GLN	-	EXPRESSION TAG	UNP P09528
C	189	SER	-	EXPRESSION TAG	UNP P09528
C	190	ASP	-	EXPRESSION TAG	UNP P09528
C	191	GLU	-	EXPRESSION TAG	UNP P09528
C	192	GLU	-	EXPRESSION TAG	UNP P09528
C	193	VAL	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
C	194	GLU	-	EXPRESSION TAG	UNP P09528
D	-17	GLY	-	EXPRESSION TAG	UNP P09528
D	-16	SER	-	EXPRESSION TAG	UNP P09528
D	-15	HIS	-	EXPRESSION TAG	UNP P09528
D	-14	MET	-	EXPRESSION TAG	UNP P09528
D	-13	ALA	-	EXPRESSION TAG	UNP P09528
D	-12	SER	-	EXPRESSION TAG	UNP P09528
D	-11	MET	-	EXPRESSION TAG	UNP P09528
D	-10	THR	-	EXPRESSION TAG	UNP P09528
D	-9	GLY	-	EXPRESSION TAG	UNP P09528
D	-8	GLY	-	EXPRESSION TAG	UNP P09528
D	-7	GLN	-	EXPRESSION TAG	UNP P09528
D	-6	GLN	-	EXPRESSION TAG	UNP P09528
D	-5	MET	-	EXPRESSION TAG	UNP P09528
D	-4	GLY	-	EXPRESSION TAG	UNP P09528
D	-3	ARG	-	EXPRESSION TAG	UNP P09528
D	-2	GLY	-	EXPRESSION TAG	UNP P09528
D	-1	SER	-	EXPRESSION TAG	UNP P09528
D	182	GLY	-	EXPRESSION TAG	UNP P09528
D	183	ASP	-	EXPRESSION TAG	UNP P09528
D	184	ILE	-	EXPRESSION TAG	UNP P09528
D	185	GLU	-	EXPRESSION TAG	UNP P09528
D	186	SER	-	EXPRESSION TAG	UNP P09528
D	187	ALA	-	EXPRESSION TAG	UNP P09528
D	188	GLN	-	EXPRESSION TAG	UNP P09528
D	189	SER	-	EXPRESSION TAG	UNP P09528
D	190	ASP	-	EXPRESSION TAG	UNP P09528
D	191	GLU	-	EXPRESSION TAG	UNP P09528
D	192	GLU	-	EXPRESSION TAG	UNP P09528
D	193	VAL	-	EXPRESSION TAG	UNP P09528
D	194	GLU	-	EXPRESSION TAG	UNP P09528
E	-17	GLY	-	EXPRESSION TAG	UNP P09528
E	-16	SER	-	EXPRESSION TAG	UNP P09528
E	-15	HIS	-	EXPRESSION TAG	UNP P09528
E	-14	MET	-	EXPRESSION TAG	UNP P09528
E	-13	ALA	-	EXPRESSION TAG	UNP P09528
E	-12	SER	-	EXPRESSION TAG	UNP P09528
E	-11	MET	-	EXPRESSION TAG	UNP P09528
E	-10	THR	-	EXPRESSION TAG	UNP P09528
E	-9	GLY	-	EXPRESSION TAG	UNP P09528
E	-8	GLY	-	EXPRESSION TAG	UNP P09528
E	-7	GLN	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLN	-	EXPRESSION TAG	UNP P09528
E	-5	MET	-	EXPRESSION TAG	UNP P09528
E	-4	GLY	-	EXPRESSION TAG	UNP P09528
E	-3	ARG	-	EXPRESSION TAG	UNP P09528
E	-2	GLY	-	EXPRESSION TAG	UNP P09528
E	-1	SER	-	EXPRESSION TAG	UNP P09528
E	182	GLY	-	EXPRESSION TAG	UNP P09528
E	183	ASP	-	EXPRESSION TAG	UNP P09528
E	184	ILE	-	EXPRESSION TAG	UNP P09528
E	185	GLU	-	EXPRESSION TAG	UNP P09528
E	186	SER	-	EXPRESSION TAG	UNP P09528
E	187	ALA	-	EXPRESSION TAG	UNP P09528
E	188	GLN	-	EXPRESSION TAG	UNP P09528
E	189	SER	-	EXPRESSION TAG	UNP P09528
E	190	ASP	-	EXPRESSION TAG	UNP P09528
E	191	GLU	-	EXPRESSION TAG	UNP P09528
E	192	GLU	-	EXPRESSION TAG	UNP P09528
E	193	VAL	-	EXPRESSION TAG	UNP P09528
E	194	GLU	-	EXPRESSION TAG	UNP P09528
F	-17	GLY	-	EXPRESSION TAG	UNP P09528
F	-16	SER	-	EXPRESSION TAG	UNP P09528
F	-15	HIS	-	EXPRESSION TAG	UNP P09528
F	-14	MET	-	EXPRESSION TAG	UNP P09528
F	-13	ALA	-	EXPRESSION TAG	UNP P09528
F	-12	SER	-	EXPRESSION TAG	UNP P09528
F	-11	MET	-	EXPRESSION TAG	UNP P09528
F	-10	THR	-	EXPRESSION TAG	UNP P09528
F	-9	GLY	-	EXPRESSION TAG	UNP P09528
F	-8	GLY	-	EXPRESSION TAG	UNP P09528
F	-7	GLN	-	EXPRESSION TAG	UNP P09528
F	-6	GLN	-	EXPRESSION TAG	UNP P09528
F	-5	MET	-	EXPRESSION TAG	UNP P09528
F	-4	GLY	-	EXPRESSION TAG	UNP P09528
F	-3	ARG	-	EXPRESSION TAG	UNP P09528
F	-2	GLY	-	EXPRESSION TAG	UNP P09528
F	-1	SER	-	EXPRESSION TAG	UNP P09528
F	182	GLY	-	EXPRESSION TAG	UNP P09528
F	183	ASP	-	EXPRESSION TAG	UNP P09528
F	184	ILE	-	EXPRESSION TAG	UNP P09528
F	185	GLU	-	EXPRESSION TAG	UNP P09528
F	186	SER	-	EXPRESSION TAG	UNP P09528
F	187	ALA	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
F	188	GLN	-	EXPRESSION TAG	UNP P09528
F	189	SER	-	EXPRESSION TAG	UNP P09528
F	190	ASP	-	EXPRESSION TAG	UNP P09528
F	191	GLU	-	EXPRESSION TAG	UNP P09528
F	192	GLU	-	EXPRESSION TAG	UNP P09528
F	193	VAL	-	EXPRESSION TAG	UNP P09528
F	194	GLU	-	EXPRESSION TAG	UNP P09528
G	-17	GLY	-	EXPRESSION TAG	UNP P09528
G	-16	SER	-	EXPRESSION TAG	UNP P09528
G	-15	HIS	-	EXPRESSION TAG	UNP P09528
G	-14	MET	-	EXPRESSION TAG	UNP P09528
G	-13	ALA	-	EXPRESSION TAG	UNP P09528
G	-12	SER	-	EXPRESSION TAG	UNP P09528
G	-11	MET	-	EXPRESSION TAG	UNP P09528
G	-10	THR	-	EXPRESSION TAG	UNP P09528
G	-9	GLY	-	EXPRESSION TAG	UNP P09528
G	-8	GLY	-	EXPRESSION TAG	UNP P09528
G	-7	GLN	-	EXPRESSION TAG	UNP P09528
G	-6	GLN	-	EXPRESSION TAG	UNP P09528
G	-5	MET	-	EXPRESSION TAG	UNP P09528
G	-4	GLY	-	EXPRESSION TAG	UNP P09528
G	-3	ARG	-	EXPRESSION TAG	UNP P09528
G	-2	GLY	-	EXPRESSION TAG	UNP P09528
G	-1	SER	-	EXPRESSION TAG	UNP P09528
G	182	GLY	-	EXPRESSION TAG	UNP P09528
G	183	ASP	-	EXPRESSION TAG	UNP P09528
G	184	ILE	-	EXPRESSION TAG	UNP P09528
G	185	GLU	-	EXPRESSION TAG	UNP P09528
G	186	SER	-	EXPRESSION TAG	UNP P09528
G	187	ALA	-	EXPRESSION TAG	UNP P09528
G	188	GLN	-	EXPRESSION TAG	UNP P09528
G	189	SER	-	EXPRESSION TAG	UNP P09528
G	190	ASP	-	EXPRESSION TAG	UNP P09528
G	191	GLU	-	EXPRESSION TAG	UNP P09528
G	192	GLU	-	EXPRESSION TAG	UNP P09528
G	193	VAL	-	EXPRESSION TAG	UNP P09528
G	194	GLU	-	EXPRESSION TAG	UNP P09528
H	-17	GLY	-	EXPRESSION TAG	UNP P09528
H	-16	SER	-	EXPRESSION TAG	UNP P09528
H	-15	HIS	-	EXPRESSION TAG	UNP P09528
H	-14	MET	-	EXPRESSION TAG	UNP P09528
H	-13	ALA	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-12	SER	-	EXPRESSION TAG	UNP P09528
H	-11	MET	-	EXPRESSION TAG	UNP P09528
H	-10	THR	-	EXPRESSION TAG	UNP P09528
H	-9	GLY	-	EXPRESSION TAG	UNP P09528
H	-8	GLY	-	EXPRESSION TAG	UNP P09528
H	-7	GLN	-	EXPRESSION TAG	UNP P09528
H	-6	GLN	-	EXPRESSION TAG	UNP P09528
H	-5	MET	-	EXPRESSION TAG	UNP P09528
H	-4	GLY	-	EXPRESSION TAG	UNP P09528
H	-3	ARG	-	EXPRESSION TAG	UNP P09528
H	-2	GLY	-	EXPRESSION TAG	UNP P09528
H	-1	SER	-	EXPRESSION TAG	UNP P09528
H	182	GLY	-	EXPRESSION TAG	UNP P09528
H	183	ASP	-	EXPRESSION TAG	UNP P09528
H	184	ILE	-	EXPRESSION TAG	UNP P09528
H	185	GLU	-	EXPRESSION TAG	UNP P09528
H	186	SER	-	EXPRESSION TAG	UNP P09528
H	187	ALA	-	EXPRESSION TAG	UNP P09528
H	188	GLN	-	EXPRESSION TAG	UNP P09528
H	189	SER	-	EXPRESSION TAG	UNP P09528
H	190	ASP	-	EXPRESSION TAG	UNP P09528
H	191	GLU	-	EXPRESSION TAG	UNP P09528
H	192	GLU	-	EXPRESSION TAG	UNP P09528
H	193	VAL	-	EXPRESSION TAG	UNP P09528
H	194	GLU	-	EXPRESSION TAG	UNP P09528
I	-17	GLY	-	EXPRESSION TAG	UNP P09528
I	-16	SER	-	EXPRESSION TAG	UNP P09528
I	-15	HIS	-	EXPRESSION TAG	UNP P09528
I	-14	MET	-	EXPRESSION TAG	UNP P09528
I	-13	ALA	-	EXPRESSION TAG	UNP P09528
I	-12	SER	-	EXPRESSION TAG	UNP P09528
I	-11	MET	-	EXPRESSION TAG	UNP P09528
I	-10	THR	-	EXPRESSION TAG	UNP P09528
I	-9	GLY	-	EXPRESSION TAG	UNP P09528
I	-8	GLY	-	EXPRESSION TAG	UNP P09528
I	-7	GLN	-	EXPRESSION TAG	UNP P09528
I	-6	GLN	-	EXPRESSION TAG	UNP P09528
I	-5	MET	-	EXPRESSION TAG	UNP P09528
I	-4	GLY	-	EXPRESSION TAG	UNP P09528
I	-3	ARG	-	EXPRESSION TAG	UNP P09528
I	-2	GLY	-	EXPRESSION TAG	UNP P09528
I	-1	SER	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
I	182	GLY	-	EXPRESSION TAG	UNP P09528
I	183	ASP	-	EXPRESSION TAG	UNP P09528
I	184	ILE	-	EXPRESSION TAG	UNP P09528
I	185	GLU	-	EXPRESSION TAG	UNP P09528
I	186	SER	-	EXPRESSION TAG	UNP P09528
I	187	ALA	-	EXPRESSION TAG	UNP P09528
I	188	GLN	-	EXPRESSION TAG	UNP P09528
I	189	SER	-	EXPRESSION TAG	UNP P09528
I	190	ASP	-	EXPRESSION TAG	UNP P09528
I	191	GLU	-	EXPRESSION TAG	UNP P09528
I	192	GLU	-	EXPRESSION TAG	UNP P09528
I	193	VAL	-	EXPRESSION TAG	UNP P09528
I	194	GLU	-	EXPRESSION TAG	UNP P09528
J	-17	GLY	-	EXPRESSION TAG	UNP P09528
J	-16	SER	-	EXPRESSION TAG	UNP P09528
J	-15	HIS	-	EXPRESSION TAG	UNP P09528
J	-14	MET	-	EXPRESSION TAG	UNP P09528
J	-13	ALA	-	EXPRESSION TAG	UNP P09528
J	-12	SER	-	EXPRESSION TAG	UNP P09528
J	-11	MET	-	EXPRESSION TAG	UNP P09528
J	-10	THR	-	EXPRESSION TAG	UNP P09528
J	-9	GLY	-	EXPRESSION TAG	UNP P09528
J	-8	GLY	-	EXPRESSION TAG	UNP P09528
J	-7	GLN	-	EXPRESSION TAG	UNP P09528
J	-6	GLN	-	EXPRESSION TAG	UNP P09528
J	-5	MET	-	EXPRESSION TAG	UNP P09528
J	-4	GLY	-	EXPRESSION TAG	UNP P09528
J	-3	ARG	-	EXPRESSION TAG	UNP P09528
J	-2	GLY	-	EXPRESSION TAG	UNP P09528
J	-1	SER	-	EXPRESSION TAG	UNP P09528
J	182	GLY	-	EXPRESSION TAG	UNP P09528
J	183	ASP	-	EXPRESSION TAG	UNP P09528
J	184	ILE	-	EXPRESSION TAG	UNP P09528
J	185	GLU	-	EXPRESSION TAG	UNP P09528
J	186	SER	-	EXPRESSION TAG	UNP P09528
J	187	ALA	-	EXPRESSION TAG	UNP P09528
J	188	GLN	-	EXPRESSION TAG	UNP P09528
J	189	SER	-	EXPRESSION TAG	UNP P09528
J	190	ASP	-	EXPRESSION TAG	UNP P09528
J	191	GLU	-	EXPRESSION TAG	UNP P09528
J	192	GLU	-	EXPRESSION TAG	UNP P09528
J	193	VAL	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
J	194	GLU	-	EXPRESSION TAG	UNP P09528
K	-17	GLY	-	EXPRESSION TAG	UNP P09528
K	-16	SER	-	EXPRESSION TAG	UNP P09528
K	-15	HIS	-	EXPRESSION TAG	UNP P09528
K	-14	MET	-	EXPRESSION TAG	UNP P09528
K	-13	ALA	-	EXPRESSION TAG	UNP P09528
K	-12	SER	-	EXPRESSION TAG	UNP P09528
K	-11	MET	-	EXPRESSION TAG	UNP P09528
K	-10	THR	-	EXPRESSION TAG	UNP P09528
K	-9	GLY	-	EXPRESSION TAG	UNP P09528
K	-8	GLY	-	EXPRESSION TAG	UNP P09528
K	-7	GLN	-	EXPRESSION TAG	UNP P09528
K	-6	GLN	-	EXPRESSION TAG	UNP P09528
K	-5	MET	-	EXPRESSION TAG	UNP P09528
K	-4	GLY	-	EXPRESSION TAG	UNP P09528
K	-3	ARG	-	EXPRESSION TAG	UNP P09528
K	-2	GLY	-	EXPRESSION TAG	UNP P09528
K	-1	SER	-	EXPRESSION TAG	UNP P09528
K	182	GLY	-	EXPRESSION TAG	UNP P09528
K	183	ASP	-	EXPRESSION TAG	UNP P09528
K	184	ILE	-	EXPRESSION TAG	UNP P09528
K	185	GLU	-	EXPRESSION TAG	UNP P09528
K	186	SER	-	EXPRESSION TAG	UNP P09528
K	187	ALA	-	EXPRESSION TAG	UNP P09528
K	188	GLN	-	EXPRESSION TAG	UNP P09528
K	189	SER	-	EXPRESSION TAG	UNP P09528
K	190	ASP	-	EXPRESSION TAG	UNP P09528
K	191	GLU	-	EXPRESSION TAG	UNP P09528
K	192	GLU	-	EXPRESSION TAG	UNP P09528
K	193	VAL	-	EXPRESSION TAG	UNP P09528
K	194	GLU	-	EXPRESSION TAG	UNP P09528
L	-17	GLY	-	EXPRESSION TAG	UNP P09528
L	-16	SER	-	EXPRESSION TAG	UNP P09528
L	-15	HIS	-	EXPRESSION TAG	UNP P09528
L	-14	MET	-	EXPRESSION TAG	UNP P09528
L	-13	ALA	-	EXPRESSION TAG	UNP P09528
L	-12	SER	-	EXPRESSION TAG	UNP P09528
L	-11	MET	-	EXPRESSION TAG	UNP P09528
L	-10	THR	-	EXPRESSION TAG	UNP P09528
L	-9	GLY	-	EXPRESSION TAG	UNP P09528
L	-8	GLY	-	EXPRESSION TAG	UNP P09528
L	-7	GLN	-	EXPRESSION TAG	UNP P09528

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	GLN	-	EXPRESSION TAG	UNP P09528
L	-5	MET	-	EXPRESSION TAG	UNP P09528
L	-4	GLY	-	EXPRESSION TAG	UNP P09528
L	-3	ARG	-	EXPRESSION TAG	UNP P09528
L	-2	GLY	-	EXPRESSION TAG	UNP P09528
L	-1	SER	-	EXPRESSION TAG	UNP P09528
L	182	GLY	-	EXPRESSION TAG	UNP P09528
L	183	ASP	-	EXPRESSION TAG	UNP P09528
L	184	ILE	-	EXPRESSION TAG	UNP P09528
L	185	GLU	-	EXPRESSION TAG	UNP P09528
L	186	SER	-	EXPRESSION TAG	UNP P09528
L	187	ALA	-	EXPRESSION TAG	UNP P09528
L	188	GLN	-	EXPRESSION TAG	UNP P09528
L	189	SER	-	EXPRESSION TAG	UNP P09528
L	190	ASP	-	EXPRESSION TAG	UNP P09528
L	191	GLU	-	EXPRESSION TAG	UNP P09528
L	192	GLU	-	EXPRESSION TAG	UNP P09528
L	193	VAL	-	EXPRESSION TAG	UNP P09528
L	194	GLU	-	EXPRESSION TAG	UNP P09528

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	K	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

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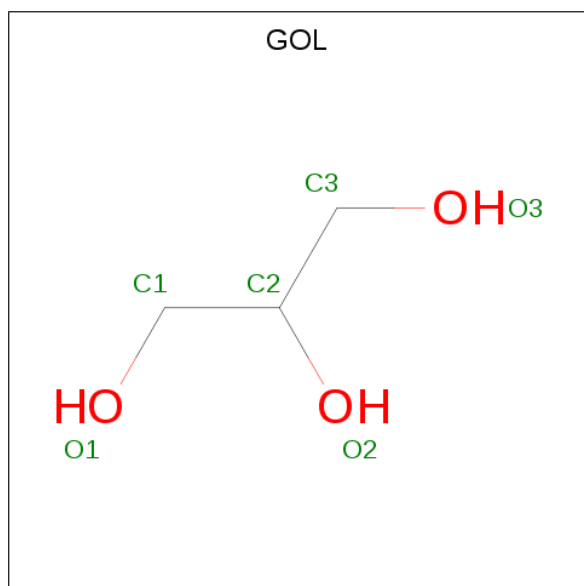
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	124	Total O 124 124	0	0
6	B	117	Total O 117 117	0	0
6	C	103	Total O 103 103	0	0
6	D	130	Total O 130 130	0	0
6	E	114	Total O 114 114	0	0
6	F	105	Total O 105 105	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	147	Total 147	O 147	0	0
6	H	114	Total 114	O 114	0	0
6	I	102	Total 102	O 102	0	0
6	J	96	Total 96	O 96	0	0
6	K	110	Total 110	O 110	0	0
6	L	112	Total 112	O 112	0	0

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

• Molecule 1: Ferritin heavy chain



GLY
SER
HIS
MET
ALA
SER
MET
THR
GLY
GLY
GLN
GLN
MET
GLY
ARG
GLY
SER
MET
THR
THR
ALA
S4
Y32
D44
K49
K53
Y54
Q88
R63
E64
H65
K71
L72
Q73
R79
I80
D84
K87
H118
P127
D131
Q141
K142
K143
S144
I145

D150
G176
HIS
GLY
ASP
GLU
SER
GLY
GLY
ASP
ILE
GLU
SER
ALA
GLN
SER
ASP
SER
MET
THR
THR
GLU
VAL
GLU

• Molecule 1: Ferritin heavy chain



GLY
SER
HIS
MET
ALA
SER
MET
THR
GLY
GLY
GLN
GLN
MET
GLY
ARG
GLY
SER
MET
THR
THR
ALA
S4
I20
Y32
R43
K49
K53
R63
E67
L72
R79
D81
D82
Q112
L117
H118
Q141
D150
K157
H177
GLY
ASP
GLU
SER

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

• Molecule 1: Ferritin heavy chain



GLY
SER
HIS
MET
ALA
SER
MET
THR
GLY
GLY
GLN
GLN
MET
GLY
GLY
ARG
GLY
SER
MET
THR
THR
ALA
S4
R9
Q14
D15
A19
Y32
R43
K49
K53
R63
E67
K71
D84
I85
R86
D81
E101
L104
E107
K108
L117
H118

D126
E140
L148
R156
K157
H177
GLY
ASP
GLU
SER
SER
GLY
GLY
ASP
ILE
GLU
SER
ALA
GLN
SER
ASP
GLU
GLU
VAL
GLU

• Molecule 1: Ferritin heavy chain

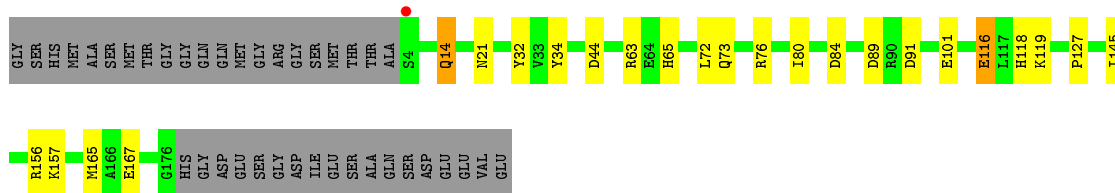


GLY
SER
HIS
MET
ALA
SER
MET
THR
GLY
GLY
GLN
GLN
MET
GLY
GLY
ARG
GLY
SER
MET
THR
THR
ALA
S4
V8
R22
Q23
Y32
D44
D45
V46
K49
S59
R63
E64
K71
L72
Q73
N74
G78
R79
I80
F81
L82
Q83
D84
D91
D92
E107
L114

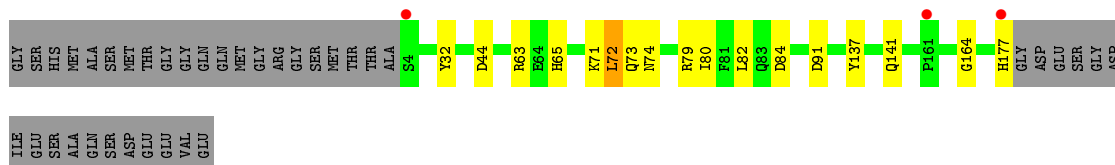
P127
L148
K157
P161
E162
A163
G164
G176
HIS
GLY
ASP
GLU
SER
GLY
ILE
GLU
SER
SER
ALA
GLN
SER
ASP
GLU
GLU
VAL
GLU

• Molecule 1: Ferritin heavy chain





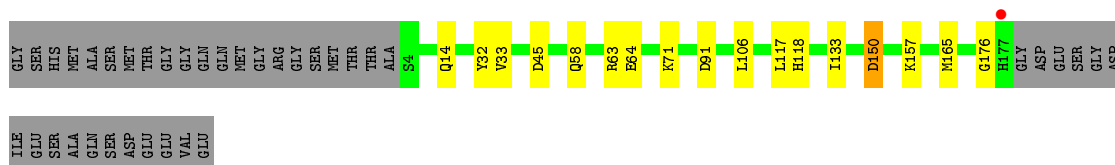
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	218.15Å 218.15Å 147.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 2.24 49.81 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.86-2.24) 94.5 (49.81-2.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.25Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.220 , 0.265 0.228 , 0.272	Depositor DCC
R_{free} test set	8052 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18648	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1694e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, K, FE

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	0.99	0/1455	0.98	2/1957 (0.1%)
1	B	1.03	2/1470 (0.1%)	1.04	8/1978 (0.4%)
1	C	0.98	0/1461	1.04	6/1966 (0.3%)
1	D	1.00	1/1444 (0.1%)	1.00	4/1943 (0.2%)
1	E	1.02	0/1464	1.00	5/1968 (0.3%)
1	F	0.96	0/1466	1.00	5/1972 (0.3%)
1	G	0.97	1/1473 (0.1%)	0.99	9/1981 (0.5%)
1	H	1.00	0/1466	1.00	7/1971 (0.4%)
1	I	1.05	1/1481 (0.1%)	1.02	5/1992 (0.3%)
1	J	0.97	0/1455	0.98	5/1958 (0.3%)
1	K	1.05	1/1462 (0.1%)	1.02	5/1966 (0.3%)
1	L	0.97	0/1491	0.99	5/2006 (0.2%)
All	All	1.00	6/17588 (0.0%)	1.00	66/23658 (0.3%)

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	H	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLU	CG-CD	6.76	1.62	1.51
1	B	64	GLU	CD-OE1	6.12	1.32	1.25
1	I	34	TYR	CE1-CZ	-5.82	1.30	1.38
1	G	140	GLU	CD-OE2	5.33	1.31	1.25
1	D	123	ASP	CB-CG	5.26	1.62	1.51

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	79	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	E	79	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	J	84	ASP	CB-CG-OD1	9.18	126.56	118.30
1	H	84	ASP	CB-CG-OD1	8.88	126.30	118.30
1	D	63	ARG	NE-CZ-NH1	8.31	124.45	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	46	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1423	0	1377	13	0
1	B	1435	0	1388	9	0
1	C	1426	0	1375	14	0
1	D	1415	0	1364	12	0
1	E	1432	0	1389	14	0
1	F	1433	0	1384	7	0
1	G	1437	0	1392	11	0
1	H	1431	0	1390	20	0
1	I	1440	0	1395	16	0
1	J	1425	0	1371	8	0
1	K	1430	0	1384	14	0
1	L	1449	0	1401	7	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	16	0	0
4	C	12	0	16	0	0
4	D	12	0	16	0	0
4	E	12	0	16	1	0
4	K	12	0	16	0	0
4	L	12	0	16	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	124	0	0	1	0
6	B	117	0	0	1	0
6	C	103	0	0	5	0
6	D	130	0	0	3	0
6	E	114	0	0	2	0
6	F	105	0	0	1	0
6	G	147	0	0	3	0
6	H	114	0	0	2	0
6	I	102	0	0	2	0
6	J	96	0	0	0	0
6	K	110	0	0	4	0
6	L	112	0	0	2	0
All	All	18648	0	16706	113	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 3.

The worst 5 of 113 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:H:22[B]:ARG:NH2	6:H:406:HOH:O	2.01	0.93
1:K:91:ASP:OD2	6:K:394:HOH:O	1.94	0.84
1:H:63[B]:ARG:NH1	1:K:63:ARG:HG2	1.94	0.83
1:E:71[B]:LYS:HE3	4:E:203:GOL:O1	1.80	0.81
1:K:119[B]:LYS:HD2	6:K:327:HOH:O	1.85	0.77

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	172/212 (81%)	170 (99%)	2 (1%)	0	100	100
1	B	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
1	C	173/212 (82%)	170 (98%)	3 (2%)	0	100	100
1	D	171/212 (81%)	168 (98%)	3 (2%)	0	100	100
1	E	173/212 (82%)	171 (99%)	2 (1%)	0	100	100
1	F	173/212 (82%)	169 (98%)	4 (2%)	0	100	100
1	G	174/212 (82%)	173 (99%)	1 (1%)	0	100	100
1	H	173/212 (82%)	170 (98%)	3 (2%)	0	100	100
1	I	175/212 (82%)	173 (99%)	2 (1%)	0	100	100
1	J	172/212 (81%)	169 (98%)	3 (2%)	0	100	100
1	K	173/212 (82%)	171 (99%)	2 (1%)	0	100	100
1	L	176/212 (83%)	171 (97%)	5 (3%)	0	100	100
All	All	2079/2544 (82%)	2045 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	154/182 (85%)	148 (96%)	6 (4%)	32	35
1	B	156/182 (86%)	152 (97%)	4 (3%)	46	52
1	C	155/182 (85%)	151 (97%)	4 (3%)	46	52
1	D	153/182 (84%)	149 (97%)	4 (3%)	46	52
1	E	155/182 (85%)	144 (93%)	11 (7%)	14	11
1	F	155/182 (85%)	148 (96%)	7 (4%)	27	29
1	G	156/182 (86%)	148 (95%)	8 (5%)	24	23
1	H	155/182 (85%)	148 (96%)	7 (4%)	27	29
1	I	157/182 (86%)	150 (96%)	7 (4%)	27	29
1	J	154/182 (85%)	149 (97%)	5 (3%)	39	44
1	K	155/182 (85%)	152 (98%)	3 (2%)	57	64
1	L	158/182 (87%)	153 (97%)	5 (3%)	39	44
All	All	1863/2184 (85%)	1792 (96%)	71 (4%)	36	36

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	53	LYS
1	G	63	ARG
1	K	165	MET
1	F	91	ASP
1	G	32	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	21	ASN
1	L	177	HIS
1	L	14	GLN
1	H	10	GLN
1	I	23	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](#)

Of 38 ligands modelled in this entry, 26 are monoatomic - leaving 12 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
4	GOL	K	203	-	5,5,5	0.80	0	5,5,5	1.38	1 (20%)
4	GOL	E	204	-	5,5,5	0.65	0	5,5,5	1.10	0
4	GOL	C	204	-	5,5,5	0.75	0	5,5,5	1.07	0
4	GOL	A	204	-	5,5,5	0.34	0	5,5,5	1.20	0
4	GOL	L	202	-	5,5,5	0.15	0	5,5,5	0.64	0
4	GOL	K	204	-	5,5,5	0.47	0	5,5,5	1.19	1 (20%)
4	GOL	D	203	-	5,5,5	0.55	0	5,5,5	1.69	1 (20%)
4	GOL	D	204	-	5,5,5	0.39	0	5,5,5	0.85	0
4	GOL	L	203	-	5,5,5	0.49	0	5,5,5	1.60	1 (20%)
4	GOL	C	205	-	5,5,5	0.83	0	5,5,5	2.68	2 (40%)
4	GOL	A	205	-	5,5,5	0.57	0	5,5,5	1.02	0
4	GOL	E	203	-	5,5,5	0.65	0	5,5,5	1.23	1 (20%)

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
4	GOL	K	203	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	204	-	-	0/4/4/4	-
4	GOL	C	204	-	-	0/4/4/4	-
4	GOL	A	204	-	-	4/4/4/4	-
4	GOL	L	202	-	-	0/4/4/4	-
4	GOL	K	204	-	-	2/4/4/4	-
4	GOL	D	203	-	-	2/4/4/4	-
4	GOL	D	204	-	-	0/4/4/4	-
4	GOL	L	203	-	-	2/4/4/4	-
4	GOL	C	205	-	-	0/4/4/4	-
4	GOL	A	205	-	-	2/4/4/4	-
4	GOL	E	203	-	-	2/4/4/4	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	205	GOL	O2-C2-C3	4.12	127.27	109.12
4	C	205	GOL	C3-C2-C1	-3.65	97.51	111.70
4	L	203	GOL	C3-C2-C1	-3.00	100.02	111.70
4	K	203	GOL	O2-C2-C1	2.62	120.66	109.12
4	D	203	GOL	O3-C3-C2	2.42	121.81	110.20

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	204	GOL	C1-C2-C3-O3
4	K	204	GOL	O2-C2-C3-O3
4	A	204	GOL	O2-C2-C3-O3
4	K	203	GOL	C1-C2-C3-O3
4	A	205	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	203	GOL	1	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 [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, 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	173/212 (81%)	-0.47	1 (0%) 89 89	8, 13, 25, 42	0
1	B	173/212 (81%)	-0.47	1 (0%) 89 89	9, 13, 27, 48	0
1	C	173/212 (81%)	-0.42	1 (0%) 89 89	9, 13, 26, 48	0
1	D	173/212 (81%)	-0.51	1 (0%) 89 89	8, 13, 25, 46	0
1	E	173/212 (81%)	-0.39	1 (0%) 89 89	9, 14, 28, 51	0
1	F	174/212 (82%)	-0.46	1 (0%) 89 89	9, 13, 27, 61	0
1	G	174/212 (82%)	-0.48	1 (0%) 89 89	8, 12, 27, 70	0
1	H	173/212 (81%)	-0.49	1 (0%) 89 89	9, 13, 26, 51	0
1	I	173/212 (81%)	-0.48	1 (0%) 89 89	9, 13, 26, 46	0
1	J	174/212 (82%)	-0.45	3 (1%) 70 71	8, 13, 28, 71	0
1	K	173/212 (81%)	-0.44	0 100 100	9, 13, 27, 48	0
1	L	174/212 (82%)	-0.48	1 (0%) 89 89	9, 13, 27, 71	0
All	All	2080/2544 (81%)	-0.46	13 (0%) 89 89	8, 13, 27, 71	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	177	HIS	4.7
1	J	177	HIS	4.6
1	J	4	SER	3.7
1	A	4	SER	3.5
1	L	177	HIS	3.5

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 carbohydrates 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(Å ²)	Q<0.9
4	GOL	C	205	6/6	0.82	0.19	21,23,26,31	0
4	GOL	D	203	6/6	0.82	0.22	22,26,30,32	0
4	GOL	E	203	6/6	0.84	0.21	21,26,30,35	0
2	MG	E	201	1/1	0.88	0.20	38,38,38,38	0
4	GOL	A	205	6/6	0.89	0.13	22,26,27,27	0
2	MG	J	201	1/1	0.89	0.06	28,28,28,28	0
4	GOL	A	204	6/6	0.89	0.17	25,29,33,35	0
4	GOL	L	203	6/6	0.89	0.19	20,24,25,28	0
4	GOL	E	204	6/6	0.90	0.17	18,25,27,27	0
4	GOL	D	204	6/6	0.90	0.15	20,24,27,28	0
4	GOL	K	204	6/6	0.91	0.23	20,21,26,35	0
4	GOL	K	203	6/6	0.91	0.17	19,22,26,29	0
2	MG	B	201	1/1	0.92	0.06	25,25,25,25	0
2	MG	K	201	1/1	0.92	0.12	42,42,42,42	0
2	MG	I	201	1/1	0.93	0.07	38,38,38,38	0
2	MG	D	201	1/1	0.93	0.07	24,24,24,24	0
2	MG	E	202	1/1	0.93	0.10	28,28,28,28	0
5	K	C	206	1/1	0.94	0.22	53,53,53,53	0
2	MG	C	201	1/1	0.94	0.09	26,26,26,26	0
2	MG	H	201	1/1	0.94	0.07	23,23,23,23	0
4	GOL	L	202	6/6	0.94	0.12	21,22,23,23	0
4	GOL	C	204	6/6	0.94	0.10	21,23,24,25	0
2	MG	A	202	1/1	0.95	0.08	23,23,23,23	0
2	MG	K	202	1/1	0.96	0.06	19,19,19,19	0
2	MG	J	202	1/1	0.96	0.10	21,21,21,21	0
2	MG	I	202	1/1	0.96	0.08	19,19,19,19	0
2	MG	C	202	1/1	0.97	0.09	23,23,23,23	0
5	K	B	203	1/1	0.97	0.19	40,40,40,40	0
2	MG	A	201	1/1	0.97	0.06	28,28,28,28	0
2	MG	G	202	1/1	0.97	0.05	18,18,18,18	0
2	MG	F	201	1/1	0.98	0.07	24,24,24,24	0
2	MG	L	201	1/1	0.98	0.05	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	G	201	1/1	0.98	0.05	25,25,25,25	0
2	MG	D	202	1/1	0.98	0.05	20,20,20,20	0
3	FE	H	202	1/1	0.99	0.06	34,34,34,34	1
3	FE	A	203	1/1	0.99	0.06	31,31,31,31	0
3	FE	B	202	1/1	0.99	0.05	32,32,32,32	1
3	FE	C	203	1/1	1.00	0.04	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.