



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 PM UTC

PDB ID : 5GOU / pdb_00005gou
Title : Structure of a 16-mer protein nanocage fabricated from its 24-mer analogue
by subunit interface redesign
Authors : Zhang, S.; Zang, J.; Wang, W.; Wang, H.; Zhao, G.
Deposited on : 2016-07-29
Resolution : 2.91 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
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

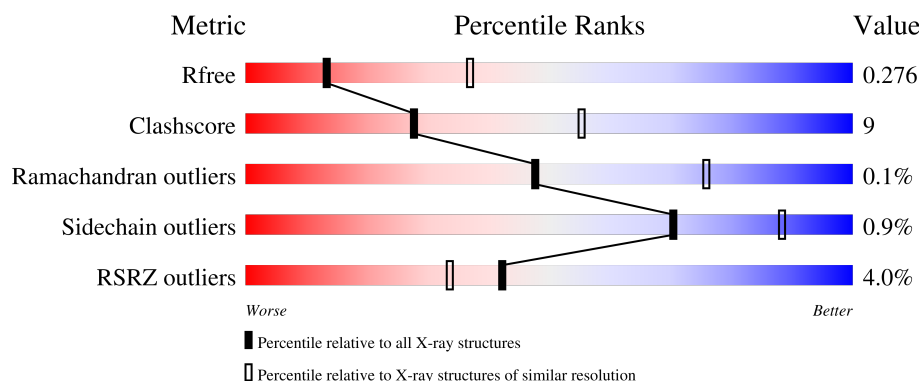
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	190	3% 55% 19% 26%
1	B	190	3% 55% 14% 31%
1	C	190	2% 65% 13% 22%
1	D	190	5% 51% 18% 31%
1	E	190	6% 48% 21% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	190	
1	G	190	
1	H	190	
1	I	190	
1	J	190	
1	K	190	
1	L	190	
1	M	190	
1	N	190	
1	O	190	
1	P	190	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18625 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	141	Total	C	N	O	S	0	0	0
			1153	725	201	221	6			
1	B	131	Total	C	N	O	S	0	0	0
			1088	680	191	211	6			
1	C	148	Total	C	N	O	S	0	0	0
			1207	758	211	232	6			
1	D	131	Total	C	N	O	S	0	0	0
			1088	680	191	211	6			
1	F	152	Total	C	N	O	S	0	0	0
			1246	783	219	238	6			
1	E	132	Total	C	N	O	S	0	0	0
			1103	691	194	212	6			
1	H	145	Total	C	N	O	S	0	0	0
			1183	744	206	227	6			
1	G	134	Total	C	N	O	S	0	0	0
			1109	692	196	215	6			
1	J	146	Total	C	N	O	S	0	0	0
			1188	747	207	228	6			
1	I	133	Total	C	N	O	S	0	0	0
			1104	689	195	214	6			
1	L	146	Total	C	N	O	S	0	0	0
			1192	749	208	229	6			
1	K	133	Total	C	N	O	S	0	0	0
			1104	689	195	214	6			
1	N	144	Total	C	N	O	S	0	0	0
			1176	741	205	224	6			
1	M	133	Total	C	N	O	S	0	0	0
			1110	695	195	214	6			
1	P	143	Total	C	N	O	S	0	0	0
			1168	735	204	223	6			
1	O	133	Total	C	N	O	S	0	0	0
			1110	695	195	214	6			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	LEU	-	insertion	UNP P02794
A	140	ASN	-	insertion	UNP P02794
A	141	GLU	-	insertion	UNP P02794
A	142	GLN	-	insertion	UNP P02794
A	143	VAL	-	insertion	UNP P02794
A	144	LYS	-	insertion	UNP P02794
A	145	ALA	-	insertion	UNP P02794
B	139	LEU	-	insertion	UNP P02794
B	140	ASN	-	insertion	UNP P02794
B	141	GLU	-	insertion	UNP P02794
B	142	GLN	-	insertion	UNP P02794
B	143	VAL	-	insertion	UNP P02794
B	144	LYS	-	insertion	UNP P02794
B	145	ALA	-	insertion	UNP P02794
C	139	LEU	-	insertion	UNP P02794
C	140	ASN	-	insertion	UNP P02794
C	141	GLU	-	insertion	UNP P02794
C	142	GLN	-	insertion	UNP P02794
C	143	VAL	-	insertion	UNP P02794
C	144	LYS	-	insertion	UNP P02794
C	145	ALA	-	insertion	UNP P02794
D	139	LEU	-	insertion	UNP P02794
D	140	ASN	-	insertion	UNP P02794
D	141	GLU	-	insertion	UNP P02794
D	142	GLN	-	insertion	UNP P02794
D	143	VAL	-	insertion	UNP P02794
D	144	LYS	-	insertion	UNP P02794
D	145	ALA	-	insertion	UNP P02794
F	139	LEU	-	insertion	UNP P02794
F	140	ASN	-	insertion	UNP P02794
F	141	GLU	-	insertion	UNP P02794
F	142	GLN	-	insertion	UNP P02794
F	143	VAL	-	insertion	UNP P02794
F	144	LYS	-	insertion	UNP P02794
F	145	ALA	-	insertion	UNP P02794
E	139	LEU	-	insertion	UNP P02794
E	140	ASN	-	insertion	UNP P02794
E	141	GLU	-	insertion	UNP P02794
E	142	GLN	-	insertion	UNP P02794
E	143	VAL	-	insertion	UNP P02794
E	144	LYS	-	insertion	UNP P02794
E	145	ALA	-	insertion	UNP P02794

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	139	LEU	-	insertion	UNP P02794
H	140	ASN	-	insertion	UNP P02794
H	141	GLU	-	insertion	UNP P02794
H	142	GLN	-	insertion	UNP P02794
H	143	VAL	-	insertion	UNP P02794
H	144	LYS	-	insertion	UNP P02794
H	145	ALA	-	insertion	UNP P02794
G	139	LEU	-	insertion	UNP P02794
G	140	ASN	-	insertion	UNP P02794
G	141	GLU	-	insertion	UNP P02794
G	142	GLN	-	insertion	UNP P02794
G	143	VAL	-	insertion	UNP P02794
G	144	LYS	-	insertion	UNP P02794
G	145	ALA	-	insertion	UNP P02794
J	139	LEU	-	insertion	UNP P02794
J	140	ASN	-	insertion	UNP P02794
J	141	GLU	-	insertion	UNP P02794
J	142	GLN	-	insertion	UNP P02794
J	143	VAL	-	insertion	UNP P02794
J	144	LYS	-	insertion	UNP P02794
J	145	ALA	-	insertion	UNP P02794
I	139	LEU	-	insertion	UNP P02794
I	140	ASN	-	insertion	UNP P02794
I	141	GLU	-	insertion	UNP P02794
I	142	GLN	-	insertion	UNP P02794
I	143	VAL	-	insertion	UNP P02794
I	144	LYS	-	insertion	UNP P02794
I	145	ALA	-	insertion	UNP P02794
L	139	LEU	-	insertion	UNP P02794
L	140	ASN	-	insertion	UNP P02794
L	141	GLU	-	insertion	UNP P02794
L	142	GLN	-	insertion	UNP P02794
L	143	VAL	-	insertion	UNP P02794
L	144	LYS	-	insertion	UNP P02794
L	145	ALA	-	insertion	UNP P02794
K	139	LEU	-	insertion	UNP P02794
K	140	ASN	-	insertion	UNP P02794
K	141	GLU	-	insertion	UNP P02794
K	142	GLN	-	insertion	UNP P02794
K	143	VAL	-	insertion	UNP P02794
K	144	LYS	-	insertion	UNP P02794
K	145	ALA	-	insertion	UNP P02794

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	139	LEU	-	insertion	UNP P02794
N	140	ASN	-	insertion	UNP P02794
N	141	GLU	-	insertion	UNP P02794
N	142	GLN	-	insertion	UNP P02794
N	143	VAL	-	insertion	UNP P02794
N	144	LYS	-	insertion	UNP P02794
N	145	ALA	-	insertion	UNP P02794
M	139	LEU	-	insertion	UNP P02794
M	140	ASN	-	insertion	UNP P02794
M	141	GLU	-	insertion	UNP P02794
M	142	GLN	-	insertion	UNP P02794
M	143	VAL	-	insertion	UNP P02794
M	144	LYS	-	insertion	UNP P02794
M	145	ALA	-	insertion	UNP P02794
P	139	LEU	-	insertion	UNP P02794
P	140	ASN	-	insertion	UNP P02794
P	141	GLU	-	insertion	UNP P02794
P	142	GLN	-	insertion	UNP P02794
P	143	VAL	-	insertion	UNP P02794
P	144	LYS	-	insertion	UNP P02794
P	145	ALA	-	insertion	UNP P02794
O	139	LEU	-	insertion	UNP P02794
O	140	ASN	-	insertion	UNP P02794
O	141	GLU	-	insertion	UNP P02794
O	142	GLN	-	insertion	UNP P02794
O	143	VAL	-	insertion	UNP P02794
O	144	LYS	-	insertion	UNP P02794
O	145	ALA	-	insertion	UNP P02794

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	22	Total O 22 22	0	0
2	B	13	Total O 13 13	0	0
2	C	29	Total O 29 29	0	0
2	D	13	Total O 13 13	0	0
2	F	24	Total O 24 24	0	0

Continued on next page...

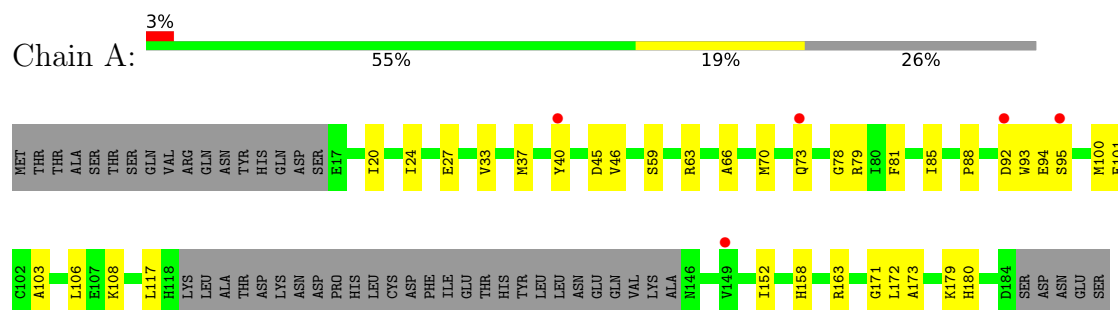
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	14	Total 14	O 14	0	0
2	H	20	Total 20	O 20	0	0
2	G	12	Total 12	O 12	0	0
2	J	22	Total 22	O 22	0	0
2	I	11	Total 11	O 11	0	0
2	L	15	Total 15	O 15	0	0
2	K	8	Total 8	O 8	0	0
2	N	26	Total 26	O 26	0	0
2	M	20	Total 20	O 20	0	0
2	P	30	Total 30	O 30	0	0
2	O	17	Total 17	O 17	0	0

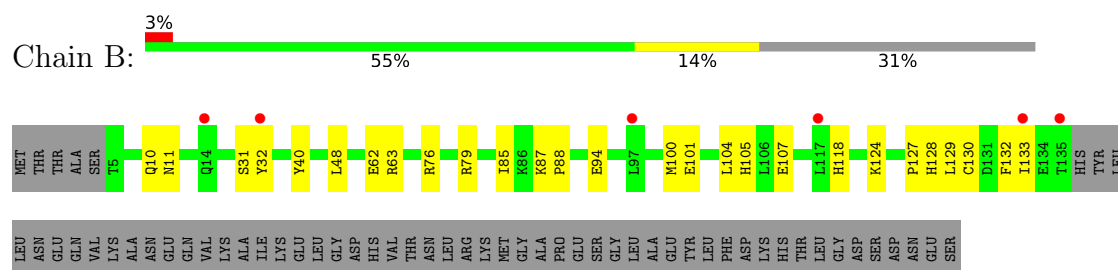
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

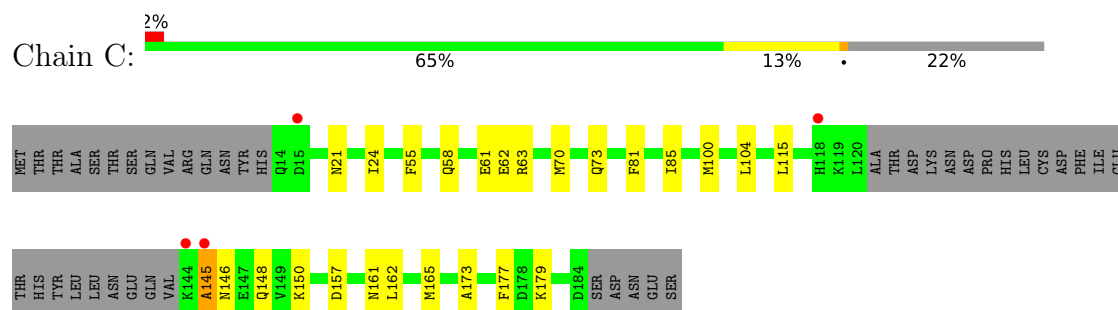
• Molecule 1: Ferritin heavy chain



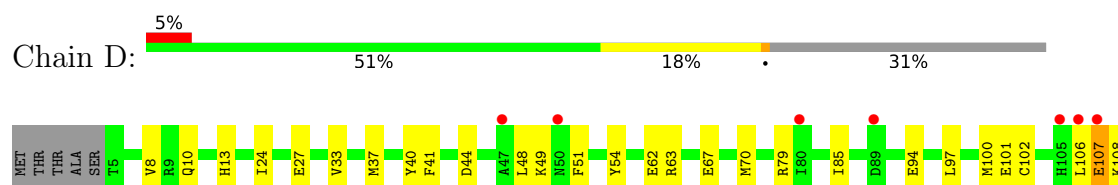
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



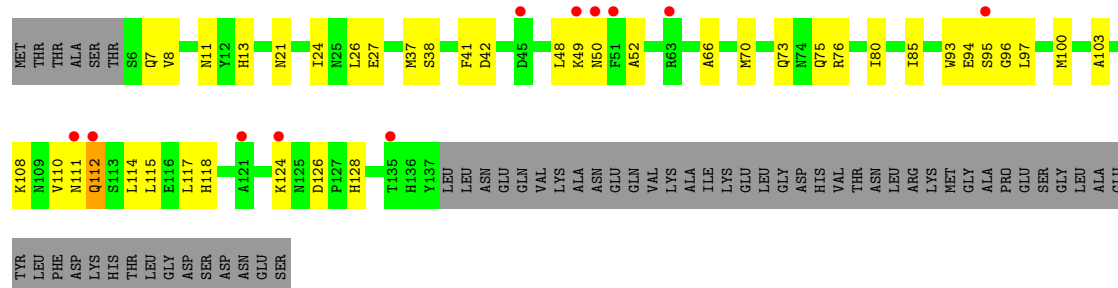
• Molecule 1: Ferritin heavy chain



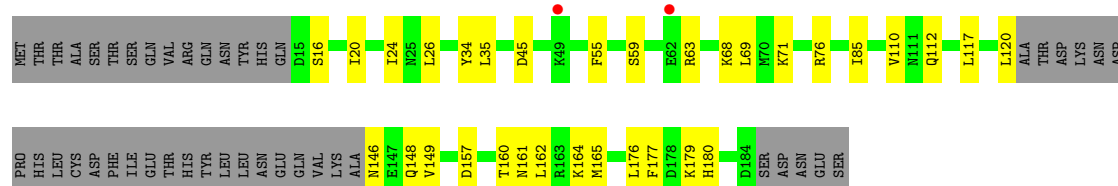
- Molecule 1: Ferritin heavy chain



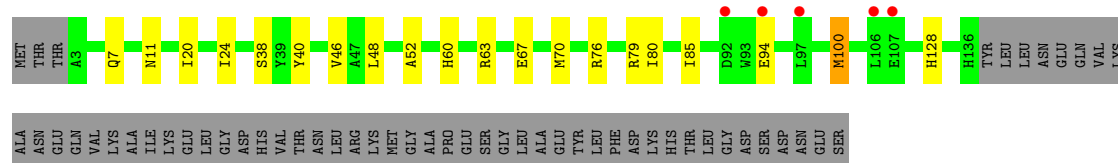
- Molecule 1: Ferritin heavy chain



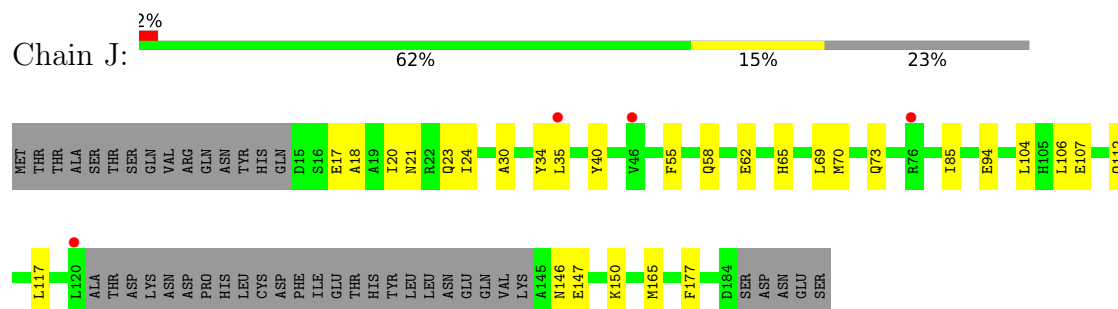
- Molecule 1: Ferritin heavy chain



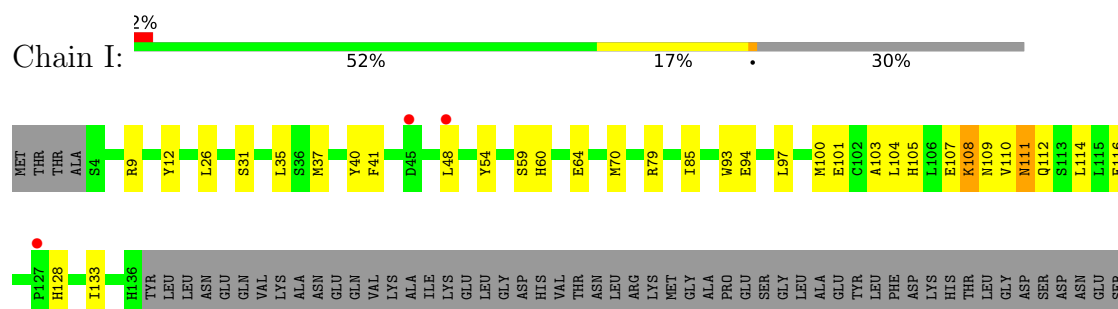
- Molecule 1: Ferritin heavy chain



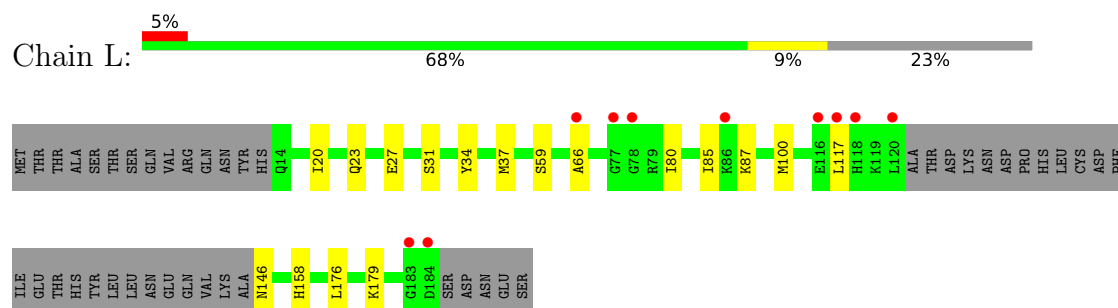
- Molecule 1: Ferritin heavy chain



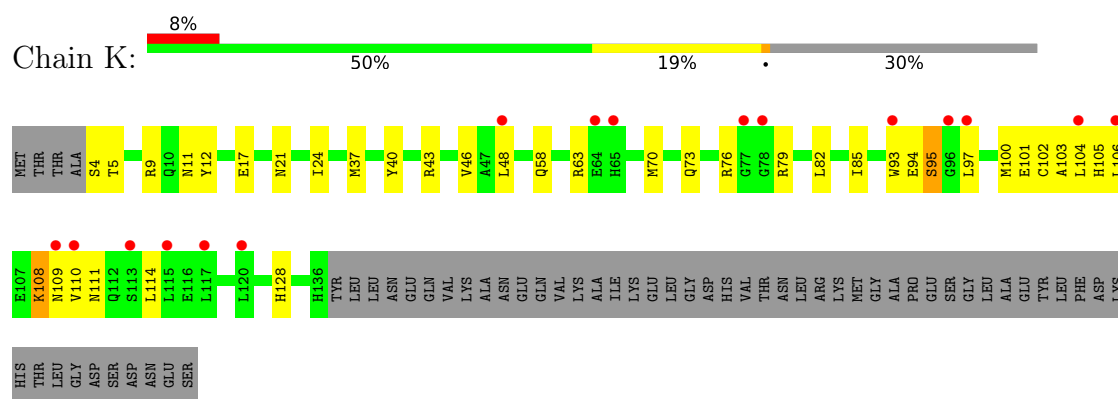
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.59Å 95.46Å 111.97Å 67.08° 68.29° 70.06°	Depositor
Resolution (Å)	49.55 – 2.91 49.55 – 2.91	Depositor EDS
% Data completeness (in resolution range)	85.1 (49.55-2.91) 81.4 (49.55-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.228 , 0.275 0.230 , 0.276	Depositor DCC
R_{free} test set	3165 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18625	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.00% 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

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	0.10	0/1174	0.32	0/1576
1	B	0.19	0/1110	0.32	0/1495
1	C	0.09	0/1228	0.29	0/1647
1	D	0.14	0/1110	0.36	0/1495
1	E	0.11	0/1127	0.36	0/1518
1	F	0.10	0/1268	0.29	0/1702
1	G	0.15	0/1132	0.33	0/1525
1	H	0.10	0/1204	0.28	0/1615
1	I	0.11	0/1127	0.32	0/1518
1	J	0.10	0/1209	0.27	0/1622
1	K	0.11	0/1127	0.36	0/1518
1	L	0.10	0/1213	0.28	0/1627
1	M	0.09	0/1134	0.26	0/1528
1	N	0.11	0/1197	0.30	0/1606
1	O	0.10	0/1134	0.30	0/1528
1	P	0.10	0/1189	0.29	0/1595
All	All	0.11	0/18683	0.31	0/25115

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	C	0	1
1	D	0	1
1	E	0	1
1	I	0	2
1	P	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	145	ALA	Peptide
1	D	107	GLU	Peptide
1	E	112	GLN	Peptide
1	I	108	LYS	Peptide
1	I	111	ASN	Peptide
1	P	14	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1153	0	1114	37	0
1	B	1088	0	1035	41	0
1	C	1207	0	1173	20	0
1	D	1088	0	1035	34	0
1	E	1103	0	1044	34	0
1	F	1246	0	1213	15	0
1	G	1109	0	1052	19	0
1	H	1183	0	1147	28	0
1	I	1104	0	1047	32	0
1	J	1188	0	1152	19	0
1	K	1104	0	1047	28	0
1	L	1192	0	1155	11	0
1	M	1110	0	1051	12	0
1	N	1176	0	1145	15	0
1	O	1110	0	1051	29	0
1	P	1168	0	1134	20	0
2	A	22	0	0	0	0
2	B	13	0	0	0	0
2	C	29	0	0	1	0
2	D	13	0	0	0	0
2	E	14	0	0	0	0
2	F	24	0	0	2	0
2	G	12	0	0	0	0
2	H	20	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	11	0	0	0	0
2	J	22	0	0	0	0
2	K	8	0	0	0	0
2	L	15	0	0	0	0
2	M	20	0	0	0	0
2	N	26	0	0	0	0
2	O	17	0	0	0	0
2	P	30	0	0	0	0
All	All	18625	0	17595	324	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 9.

All (324) 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:B:118:HIS:CD2	1:B:133:ILE:CD1	1.97	1.46
1:B:118:HIS:CD2	1:B:133:ILE:HD11	1.50	1.45
1:B:118:HIS:HD2	1:B:133:ILE:CD1	1.39	1.22
1:A:73:GLN:HE21	1:A:79:ARG:N	1.41	1.18
1:B:118:HIS:CD2	1:B:133:ILE:HD12	1.76	1.10
1:B:118:HIS:CG	1:B:133:ILE:CD1	2.38	1.05
1:A:73:GLN:NE2	1:A:79:ARG:C	2.16	1.04
1:D:51:PHE:CZ	1:I:104:LEU:CD2	2.42	1.03
1:D:51:PHE:CZ	1:I:104:LEU:HD21	1.92	1.03
1:A:73:GLN:NE2	1:A:79:ARG:N	2.08	1.01
1:H:63:ARG:HH12	1:G:60:HIS:CE1	1.78	1.00
1:A:73:GLN:NE2	1:A:79:ARG:H	1.60	0.99
1:B:118:HIS:CG	1:B:133:ILE:HD11	1.97	0.99
1:D:51:PHE:CE2	1:I:104:LEU:CD2	2.45	0.99
1:D:51:PHE:CE2	1:I:104:LEU:HD21	1.97	0.98
1:A:73:GLN:NE2	1:A:79:ARG:O	1.99	0.93
1:D:107:GLU:HB3	1:D:110:VAL:HB	1.52	0.90
1:E:108:LYS:HA	1:E:111:ASN:HB2	1.52	0.90
1:G:100:MET:HE1	1:M:51:PHE:CZ	2.08	0.88
1:B:118:HIS:CB	1:B:133:ILE:CD1	2.51	0.88
1:B:118:HIS:HB2	1:B:133:ILE:CD1	2.05	0.87
1:A:73:GLN:HE22	1:A:79:ARG:C	1.81	0.85
1:H:165:MET:HE1	1:H:177:PHE:HB2	1.59	0.85
1:D:51:PHE:CZ	1:I:104:LEU:HD23	2.12	0.84
1:G:40:TYR:OH	1:G:94:GLU:O	1.95	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:GLN:HE21	1:E:115:LEU:HG	1.42	0.83
1:B:118:HIS:CG	1:B:133:ILE:HD12	2.13	0.78
1:A:73:GLN:HE21	1:A:79:ARG:H	0.79	0.78
1:D:106:LEU:HG	1:D:107:GLU:HG2	1.66	0.77
1:B:100:MET:HE2	1:O:100:MET:HE2	1.67	0.75
1:D:110:VAL:O	1:D:114:LEU:N	2.19	0.74
1:G:24:ILE:HD12	1:G:70:MET:HG3	1.70	0.73
1:F:160:THR:HG21	1:H:45:ASP:HA	1.69	0.72
1:A:152:ILE:HG22	1:D:8:VAL:HG13	1.72	0.72
1:B:40:TYR:OH	1:B:94:GLU:O	2.05	0.72
1:D:51:PHE:HZ	1:I:104:LEU:HD23	1.55	0.72
1:N:100:MET:HE2	1:N:158:HIS:HB2	1.72	0.71
1:A:59:SER:OG	1:B:63:ARG:NH2	2.21	0.71
1:I:111:ASN:HA	1:I:114:LEU:HB2	1.73	0.70
1:L:59:SER:OG	1:K:63:ARG:NH2	2.24	0.70
1:B:118:HIS:HB2	1:B:133:ILE:HD13	1.73	0.69
1:E:42:ASP:OD1	1:E:49:LYS:NZ	2.26	0.69
1:H:20:ILE:HD13	1:H:117:LEU:HD21	1.75	0.68
1:B:118:HIS:HD2	1:B:133:ILE:HD12	1.25	0.68
1:K:37:MET:HE1	1:K:103:ALA:HB2	1.75	0.68
1:L:179:LYS:HG2	1:N:180:HIS:HB3	1.73	0.68
1:N:85:ILE:HB	1:M:85:ILE:HB	1.77	0.67
1:K:9:ARG:NH1	1:K:12:TYR:O	2.28	0.67
1:B:118:HIS:HB2	1:B:133:ILE:HD12	1.76	0.67
1:F:44:ASP:OD2	1:E:8:VAL:HG13	1.94	0.67
1:J:35:LEU:HD21	1:I:70:MET:HE1	1.77	0.66
1:H:63:ARG:NH1	1:G:60:HIS:CE1	2.59	0.66
1:D:33:VAL:HG12	1:D:37:MET:HE2	1.77	0.66
1:D:110:VAL:HA	1:D:113:SER:HB3	1.78	0.66
1:D:41:PHE:HB3	1:D:48:LEU:HB2	1.78	0.65
1:C:148:GLN:NE2	2:C:202:HOH:O	2.29	0.65
1:H:85:ILE:HB	1:G:85:ILE:HB	1.78	0.64
1:D:48:LEU:HB3	1:D:51:PHE:HD2	1.62	0.64
1:E:13:HIS:H	1:E:124:LYS:HE2	1.63	0.64
1:J:165:MET:HE1	1:J:177:PHE:HB2	1.79	0.64
1:A:73:GLN:NE2	1:A:79:ARG:CA	2.61	0.63
1:A:73:GLN:CG	1:A:78:GLY:HA3	2.28	0.63
1:A:108:LYS:O	1:D:10:GLN:NE2	2.30	0.63
1:O:40:TYR:OH	1:O:94:GLU:O	2.10	0.63
1:E:38:SER:OG	1:E:52:ALA:O	2.16	0.62
1:K:105:HIS:HA	1:K:108:LYS:HB3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASN:OD1	1:C:73:GLN:NE2	2.33	0.61
1:J:20:ILE:HG12	1:J:117:LEU:HD11	1.81	0.61
1:B:118:HIS:HD2	1:B:133:ILE:CG1	2.09	0.61
1:A:172:LEU:HD11	1:H:176:LEU:HD12	1.83	0.60
1:D:100:MET:HG3	1:I:100:MET:HG2	1.84	0.60
1:F:13:HIS:N	2:F:206:HOH:O	2.35	0.60
1:E:114:LEU:HA	1:E:117:LEU:HB2	1.83	0.60
1:B:101:GLU:OE1	1:B:105:HIS:NE2	2.35	0.60
1:H:146:ASN:OD1	1:H:148:GLN:NE2	2.34	0.60
1:E:97:LEU:HD11	1:K:97:LEU:HB2	1.84	0.59
1:O:67:GLU:HA	1:O:70:MET:HE3	1.84	0.59
1:C:85:ILE:HB	1:D:85:ILE:HB	1.85	0.59
1:L:100:MET:HE2	1:L:158:HIS:HB2	1.83	0.59
1:K:9:ARG:NH2	1:K:17:GLU:OE1	2.35	0.59
1:M:38:SER:OG	1:M:52:ALA:O	2.14	0.59
1:D:40:TYR:OH	1:D:94:GLU:O	2.12	0.59
1:A:73:GLN:HG3	1:A:78:GLY:HA3	1.85	0.59
1:A:85:ILE:HB	1:B:85:ILE:HB	1.85	0.59
1:O:43:ARG:NE	1:O:45:ASP:OD1	2.34	0.58
1:B:118:HIS:CB	1:B:133:ILE:HD13	2.30	0.58
1:K:108:LYS:HG2	1:K:109:ASN:N	2.18	0.58
1:N:165:MET:HE1	1:N:177:PHE:HB2	1.85	0.58
1:O:107:GLU:O	1:O:111:ASN:ND2	2.33	0.58
1:A:63:ARG:HH21	1:B:63:ARG:HD3	1.69	0.58
1:G:67:GLU:HA	1:G:70:MET:HE3	1.85	0.57
1:D:107:GLU:O	1:D:111:ASN:ND2	2.37	0.57
1:A:92:ASP:OD1	1:A:94:GLU:HG3	2.05	0.57
1:I:128:HIS:NE2	1:L:146:ASN:OD1	2.37	0.57
1:K:21:ASN:OD1	1:K:73:GLN:NE2	2.38	0.57
1:E:97:LEU:HD11	1:K:97:LEU:HD13	1.85	0.57
1:N:23:GLN:HB3	1:N:69:LEU:HD13	1.86	0.57
1:C:115:LEU:HD13	1:E:11:ASN:HD22	1.69	0.56
1:B:32:TYR:CE2	1:B:87:LYS:HA	2.40	0.56
1:B:127:PRO:O	1:B:129:LEU:N	2.39	0.56
1:H:26:LEU:HG	1:H:110:VAL:HG22	1.87	0.56
1:A:45:ASP:HA	1:H:160:THR:HG21	1.88	0.56
1:H:35:LEU:HD21	1:G:70:MET:HE1	1.88	0.56
1:F:85:ILE:HB	1:E:85:ILE:HB	1.87	0.56
1:B:32:TYR:HE2	1:B:87:LYS:HA	1.71	0.56
1:B:48:LEU:HD11	1:O:104:LEU:HD22	1.88	0.56
1:F:180:HIS:HB3	1:H:179:LYS:HD3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:ILE:O	1:G:24:ILE:HG12	2.06	0.56
1:G:40:TYR:CZ	1:G:46:VAL:HG21	2.41	0.56
1:J:23:GLN:HG3	1:J:117:LEU:HD22	1.88	0.56
1:I:40:TYR:OH	1:I:94:GLU:O	2.20	0.56
1:A:27:GLU:HB2	1:A:66:ALA:HB2	1.88	0.55
1:A:20:ILE:HG12	1:A:117:LEU:HD11	1.89	0.55
1:N:108:LYS:HG2	1:N:152:ILE:HD12	1.87	0.55
1:P:85:ILE:HB	1:O:85:ILE:HB	1.88	0.55
1:P:35:LEU:HD21	1:O:70:MET:HE1	1.87	0.55
1:F:160:THR:HG23	1:G:7:GLN:HE22	1.72	0.55
1:J:104:LEU:HD21	1:O:7:GLN:HB3	1.89	0.55
1:H:16:SER:OG	1:H:76:ARG:NH2	2.39	0.54
1:L:34:TYR:HD1	1:L:37:MET:HE2	1.72	0.54
1:C:165:MET:HE1	1:C:177:PHE:HB2	1.88	0.54
1:K:46:VAL:HG12	1:K:48:LEU:HD13	1.88	0.54
1:B:104:LEU:HD11	1:O:48:LEU:HD13	1.90	0.54
1:E:50:ASN:ND2	1:K:58:GLN:OE1	2.41	0.54
1:E:100:MET:HE2	1:K:100:MET:HE2	1.89	0.54
1:H:59:SER:OG	1:G:63:ARG:NH2	2.41	0.54
1:J:65:HIS:NE2	1:J:147:GLU:OE1	2.40	0.54
1:A:33:VAL:HG21	1:A:106:LEU:HD13	1.90	0.53
1:K:102:CYS:O	1:K:106:LEU:N	2.41	0.53
1:M:114:LEU:HD12	1:M:133:ILE:HG23	1.91	0.53
1:E:93:TRP:O	1:E:95:SER:N	2.42	0.53
1:J:23:GLN:HB3	1:J:69:LEU:HD13	1.90	0.53
1:G:11:ASN:O	1:G:76:ARG:NH2	2.42	0.53
1:D:97:LEU:HD21	1:I:101:GLU:HG2	1.90	0.53
1:N:37:MET:HE3	1:N:99:ALA:HB1	1.90	0.52
1:A:40:TYR:OH	1:A:94:GLU:HA	2.09	0.52
1:K:40:TYR:OH	1:K:94:GLU:HA	2.09	0.52
1:E:124:LYS:HD3	1:E:126:ASP:HB2	1.91	0.52
1:C:63:ARG:HH21	1:D:63:ARG:HG2	1.74	0.52
1:E:21:ASN:OD1	1:E:73:GLN:NE2	2.36	0.52
1:K:93:TRP:O	1:K:95:SER:N	2.43	0.52
1:H:24:ILE:HG22	1:H:69:LEU:HB2	1.91	0.52
1:B:32:TYR:CE2	1:B:88:PRO:HD3	2.45	0.52
1:I:9:ARG:NH1	1:I:12:TYR:O	2.43	0.52
1:I:103:ALA:O	1:I:107:GLU:N	2.38	0.52
1:F:40:TYR:OH	1:F:94:GLU:O	2.20	0.51
1:J:40:TYR:OH	1:J:94:GLU:O	2.20	0.51
1:E:96:GLY:O	1:E:100:MET:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:CYS:O	1:B:133:ILE:HG13	2.11	0.51
1:B:128:HIS:O	1:B:132:PHE:N	2.44	0.50
1:C:55:PHE:HZ	1:C:100:MET:HG2	1.76	0.50
1:E:11:ASN:OD1	1:E:124:LYS:NZ	2.45	0.50
1:C:146:ASN:HD21	1:E:75:GLN:HE22	1.58	0.50
1:P:27:GLU:HB2	1:P:66:ALA:HB2	1.92	0.50
1:D:102:CYS:O	1:D:106:LEU:N	2.45	0.49
1:B:118:HIS:CB	1:B:133:ILE:HD12	2.31	0.49
1:I:41:PHE:HD1	1:I:48:LEU:HB2	1.77	0.49
1:B:31:SER:OG	1:B:62:GLU:HB3	2.12	0.49
1:N:73:GLN:HG2	1:N:78:GLY:HA3	1.95	0.49
1:A:40:TYR:CZ	1:A:94:GLU:HA	2.47	0.49
1:D:63:ARG:NE	1:D:67:GLU:OE1	2.44	0.49
1:A:73:GLN:HG2	1:A:78:GLY:HA3	1.93	0.49
1:C:21:ASN:HD22	1:C:81:PHE:HB2	1.78	0.49
1:I:111:ASN:O	1:I:111:ASN:ND2	2.45	0.49
1:A:33:VAL:HG12	1:A:88:PRO:HG3	1.94	0.49
1:J:58:GLN:O	1:J:62:GLU:HG2	2.12	0.49
1:O:76:ARG:HD3	1:O:128:HIS:CE1	2.48	0.49
1:O:14:GLN:HA	1:O:17:GLU:HB3	1.95	0.48
1:A:37:MET:HE1	1:A:103:ALA:HB2	1.95	0.48
1:J:112:GLN:HG2	1:O:10:GLN:NE2	2.28	0.48
1:K:76:ARG:HD2	1:K:128:HIS:ND1	2.28	0.48
1:O:37:MET:HG2	1:O:93:TRP:CE2	2.48	0.48
1:J:70:MET:HE1	1:I:35:LEU:HD21	1.94	0.48
1:P:72:LEU:O	1:P:76:ARG:HG3	2.14	0.48
1:O:38:SER:OG	1:O:52:ALA:O	2.26	0.48
1:K:106:LEU:HA	1:K:109:ASN:HD21	1.79	0.48
1:B:10:GLN:NE2	1:H:112:GLN:HB2	2.29	0.48
1:D:108:LYS:HD2	1:I:48:LEU:HD21	1.96	0.48
1:H:148:GLN:NE2	1:H:148:GLN:H	2.11	0.48
1:F:27:GLU:HB2	1:F:66:ALA:HB2	1.96	0.48
1:I:108:LYS:HG2	1:I:111:ASN:HB3	1.95	0.47
1:A:40:TYR:CE1	1:A:46:VAL:HG21	2.50	0.47
1:P:32:TYR:CD2	1:P:88:PRO:HD3	2.49	0.47
1:O:96:GLY:O	1:O:100:MET:HG2	2.15	0.47
1:F:17:GLU:HG2	1:F:21:ASN:HD21	1.80	0.47
1:J:24:ILE:HD13	1:J:70:MET:HG2	1.97	0.47
1:K:40:TYR:CE1	1:K:43:ARG:HD3	2.49	0.47
1:A:171:GLY:C	1:A:173:ALA:H	2.23	0.47
1:A:180:HIS:O	1:C:179:LYS:NZ	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ALA:HB3	1:C:148:GLN:HG2	1.96	0.47
1:H:63:ARG:HH22	1:G:60:HIS:CD2	2.33	0.47
1:O:121:ALA:HB2	1:O:129:LEU:HD23	1.96	0.47
1:E:37:MET:HE1	1:E:103:ALA:HB2	1.97	0.47
1:P:17:GLU:HG3	1:P:73:GLN:NE2	2.30	0.47
1:P:39:TYR:HE1	1:O:71:LYS:HG3	1.80	0.47
1:D:49:LYS:H	1:D:49:LYS:HD2	1.79	0.46
1:D:79:ARG:HA	1:D:79:ARG:HD3	1.76	0.46
1:O:41:PHE:HE2	1:O:55:PHE:HE2	1.62	0.46
1:C:104:LEU:HD21	1:E:7:GLN:HG2	1.97	0.46
1:O:124:LYS:HE3	1:O:126:ASP:HB2	1.97	0.46
1:E:114:LEU:O	1:E:118:HIS:N	2.35	0.46
1:K:4:SER:OG	1:K:5:THR:N	2.46	0.46
1:P:84:ASP:OD1	1:O:87:LYS:N	2.47	0.46
1:E:26:LEU:HD21	1:E:110:VAL:HA	1.97	0.46
1:A:40:TYR:CE1	1:A:94:GLU:HG2	2.51	0.46
1:I:112:GLN:O	1:I:116:GLU:HG3	2.15	0.46
1:C:162:LEU:HA	1:C:165:MET:HE3	1.98	0.46
1:I:114:LEU:HD22	1:I:133:ILE:HG23	1.97	0.46
1:K:110:VAL:O	1:K:114:LEU:N	2.41	0.46
1:N:50:ASN:ND2	1:N:178:ASP:O	2.40	0.46
1:A:101:GLU:OE2	1:A:163:ARG:NH1	2.49	0.45
1:F:163:ARG:NH2	2:F:208:HOH:O	2.48	0.45
1:L:27:GLU:HB2	1:L:66:ALA:HB2	1.98	0.45
1:H:162:LEU:HA	1:H:165:MET:HE2	1.99	0.45
1:I:26:LEU:HD21	1:I:110:VAL:HA	1.98	0.45
1:I:37:MET:HG2	1:I:93:TRP:CE2	2.51	0.45
1:H:68:LYS:HA	1:H:71:LYS:HG2	1.98	0.45
1:N:71:LYS:O	1:N:75:GLN:HG2	2.17	0.45
1:P:80:ILE:HG22	1:P:82:LEU:HD21	1.99	0.45
1:D:107:GLU:OE1	1:D:110:VAL:HG23	2.16	0.45
1:E:114:LEU:HD23	1:E:117:LEU:HD12	1.98	0.45
1:H:16:SER:HB3	1:H:120:LEU:HB3	1.98	0.45
1:K:79:ARG:HA	1:K:79:ARG:HD3	1.80	0.45
1:D:97:LEU:CD1	1:I:104:LEU:HD12	2.47	0.44
1:O:133:ILE:O	1:O:137:TYR:HB2	2.18	0.44
1:E:26:LEU:HG	1:E:110:VAL:HG22	1.98	0.44
1:L:176:LEU:HD21	1:N:176:LEU:HD13	2.00	0.44
1:K:101:GLU:HA	1:K:104:LEU:HD12	1.99	0.44
1:F:181:THR:OG1	1:H:179:LYS:HE3	2.18	0.44
1:A:79:ARG:HE	1:A:81:PHE:HE2	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:82:LEU:HD22	1:O:32:TYR:OH	2.18	0.44
1:B:76:ARG:HD3	1:B:128:HIS:CE1	2.52	0.44
1:B:124:LYS:HD2	1:B:124:LYS:HA	1.67	0.44
1:L:20:ILE:HA	1:L:117:LEU:HD11	1.98	0.44
1:N:26:LEU:HG	1:N:110:VAL:HG22	2.00	0.44
1:A:179:LYS:HG2	1:H:180:HIS:HB3	1.99	0.44
1:B:101:GLU:OE2	1:O:97:LEU:HD11	2.18	0.44
1:D:54:TYR:CE1	1:I:54:TYR:HB2	2.52	0.44
1:F:17:GLU:HG2	1:F:21:ASN:ND2	2.33	0.44
1:P:58:GLN:O	1:P:62:GLU:HG2	2.17	0.44
1:P:26:LEU:HG	1:P:110:VAL:HG22	2.00	0.44
1:P:96:GLY:H	1:P:174:GLU:CD	2.26	0.44
1:P:15:ASP:O	1:P:19:ALA:N	2.50	0.43
1:P:32:TYR:HE1	1:O:28:LEU:HD13	1.83	0.43
1:E:124:LYS:O	1:E:124:LYS:HG2	2.18	0.43
1:J:18:ALA:HA	1:J:21:ASN:HD22	1.83	0.43
1:M:101:GLU:OE1	1:M:105:HIS:NE2	2.51	0.43
1:G:70:MET:HG2	1:G:80:ILE:HD13	2.00	0.43
1:K:70:MET:HE3	1:K:82:LEU:HD21	1.99	0.43
1:C:157:ASP:O	1:C:161:ASN:ND2	2.50	0.43
1:D:129:LEU:O	1:D:133:ILE:HG13	2.19	0.43
1:E:27:GLU:HB2	1:E:66:ALA:HB2	2.00	0.43
1:O:11:ASN:O	1:O:124:LYS:NZ	2.50	0.43
1:B:10:GLN:HE21	1:H:112:GLN:HB2	1.83	0.43
1:F:70:MET:HB3	1:F:80:ILE:HD13	2.00	0.43
1:F:72:LEU:HD22	1:F:142:GLN:HB2	2.00	0.43
1:E:41:PHE:HB3	1:E:48:LEU:O	2.19	0.43
1:J:34:TYR:OH	1:J:107:GLU:HG2	2.18	0.43
1:J:30:ALA:HA	1:J:106:LEU:HD21	2.01	0.43
1:K:40:TYR:O	1:K:43:ARG:HG2	2.19	0.43
1:C:24:ILE:HD13	1:C:70:MET:HG2	2.00	0.43
1:I:105:HIS:O	1:I:109:ASN:HB2	2.18	0.43
1:O:41:PHE:HD1	1:O:46:VAL:HG11	1.84	0.43
1:D:13:HIS:CG	1:D:124:LYS:HE2	2.54	0.42
1:H:157:ASP:O	1:H:161:ASN:ND2	2.51	0.42
1:I:31:SER:O	1:I:59:SER:OG	2.30	0.42
1:I:41:PHE:HB3	1:I:48:LEU:O	2.19	0.42
1:C:55:PHE:CZ	1:C:100:MET:HG2	2.54	0.42
1:D:101:GLU:HB2	1:I:97:LEU:HD21	2.01	0.42
1:E:76:ARG:HD3	1:E:128:HIS:CE1	2.54	0.42
1:P:14:GLN:O	1:P:17:GLU:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:TYR:CZ	1:B:88:PRO:HD3	2.54	0.42
1:P:82:LEU:HD13	1:O:32:TYR:CZ	2.55	0.42
1:B:128:HIS:CE1	1:H:149:VAL:HG11	2.54	0.42
1:J:34:TYR:HB3	1:J:55:PHE:O	2.20	0.42
1:L:85:ILE:HB	1:K:85:ILE:HB	2.00	0.42
1:A:100:MET:HE2	1:A:158:HIS:HB2	2.00	0.42
1:G:46:VAL:HG12	1:G:48:LEU:HG	2.02	0.42
1:N:24:ILE:HD13	1:N:82:LEU:HD23	2.02	0.42
1:A:93:TRP:O	1:A:95:SER:N	2.47	0.42
1:C:100:MET:HE2	1:C:100:MET:HB3	1.65	0.42
1:K:11:ASN:O	1:K:76:ARG:NH1	2.53	0.42
1:N:17:GLU:OE2	1:N:79:ARG:N	2.46	0.42
1:P:32:TYR:CE2	1:P:88:PRO:HD3	2.54	0.42
1:B:11:ASN:O	1:B:76:ARG:NH2	2.52	0.42
1:C:58:GLN:O	1:C:62:GLU:HG2	2.20	0.42
1:C:150:LYS:HA	1:C:150:LYS:HD2	1.76	0.41
1:G:38:SER:OG	1:G:52:ALA:O	2.28	0.41
1:B:107:GLU:CD	1:O:50:ASN:HB2	2.45	0.41
1:E:24:ILE:HD13	1:E:70:MET:HG2	2.01	0.41
1:I:60:HIS:O	1:I:64:GLU:HG2	2.20	0.41
1:D:24:ILE:HD13	1:D:70:MET:HG2	2.02	0.41
1:E:70:MET:HE3	1:E:80:ILE:HG21	2.01	0.41
1:C:165:MET:HB3	1:C:173:ALA:HB1	2.02	0.41
1:D:27:GLU:OE1	1:D:62:GLU:OE1	2.37	0.41
1:F:24:ILE:HD13	1:F:70:MET:HG2	2.02	0.41
1:H:161:ASN:HA	1:H:164:LYS:HE3	2.01	0.41
1:J:85:ILE:HB	1:I:85:ILE:HB	2.02	0.41
1:K:111:ASN:HA	1:K:114:LEU:HB2	2.02	0.41
1:M:48:LEU:HD12	1:M:48:LEU:HA	1.91	0.41
1:M:56:LEU:O	1:M:60:HIS:ND1	2.54	0.41
1:I:79:ARG:HD3	1:I:79:ARG:HA	1.92	0.41
1:A:24:ILE:HD13	1:A:70:MET:HG2	2.03	0.41
1:E:13:HIS:N	1:E:124:LYS:HE2	2.32	0.41
1:M:76:ARG:HD3	1:M:128:HIS:ND1	2.35	0.41
1:A:33:VAL:O	1:A:37:MET:HG3	2.21	0.41
1:J:146:ASN:O	1:J:150:LYS:HG2	2.20	0.41
1:G:79:ARG:HA	1:G:79:ARG:HD3	1.78	0.41
1:K:97:LEU:HA	1:K:100:MET:HG2	2.03	0.41
1:N:150:LYS:HE3	1:N:150:LYS:HB2	1.84	0.41
1:P:30:ALA:HA	1:P:106:LEU:HD21	2.03	0.41
1:E:76:ARG:HH11	1:E:128:HIS:HD1	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:TYR:HB3	1:H:55:PHE:O	2.21	0.40
1:J:17:GLU:HG3	1:J:73:GLN:HE22	1.85	0.40
1:E:49:LYS:HD2	1:E:49:LYS:HA	1.75	0.40
1:G:76:ARG:HD3	1:G:128:HIS:ND1	2.36	0.40
1:L:23:GLN:HG3	1:L:117:LEU:HD13	2.04	0.40
1:B:31:SER:OG	1:B:63:ARG:N	2.54	0.40
1:B:79:ARG:HA	1:B:79:ARG:HD3	1.85	0.40
1:M:27:GLU:HB2	1:M:66:ALA:HB2	2.02	0.40
1:M:53:LYS:HB3	1:M:53:LYS:HE3	1.84	0.40
1:L:31:SER:O	1:L:59:SER:OG	2.37	0.40
1:M:10:GLN:NE2	1:P:112:GLN:HB2	2.37	0.40
1:M:93:TRP:O	1:M:95:SER:N	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	137/190 (72%)	128 (93%)	9 (7%)	0	100	100
1	B	129/190 (68%)	120 (93%)	9 (7%)	0	100	100
1	C	144/190 (76%)	140 (97%)	4 (3%)	0	100	100
1	D	129/190 (68%)	124 (96%)	5 (4%)	0	100	100
1	E	130/190 (68%)	123 (95%)	6 (5%)	1 (1%)	16	43
1	F	148/190 (78%)	145 (98%)	3 (2%)	0	100	100
1	G	132/190 (70%)	127 (96%)	5 (4%)	0	100	100
1	H	141/190 (74%)	139 (99%)	2 (1%)	0	100	100
1	I	131/190 (69%)	128 (98%)	3 (2%)	0	100	100
1	J	142/190 (75%)	135 (95%)	7 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	131/190 (69%)	125 (95%)	5 (4%)	1 (1%)	16	43
1	L	142/190 (75%)	138 (97%)	4 (3%)	0	100	100
1	M	131/190 (69%)	128 (98%)	3 (2%)	0	100	100
1	N	140/190 (74%)	136 (97%)	4 (3%)	0	100	100
1	O	131/190 (69%)	125 (95%)	6 (5%)	0	100	100
1	P	139/190 (73%)	136 (98%)	2 (1%)	1 (1%)	18	46
All	All	2177/3040 (72%)	2097 (96%)	77 (4%)	3 (0%)	48	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	94	GLU
1	K	95	SER
1	P	94	GLU

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	123/169 (73%)	123 (100%)	0	100	100
1	B	119/169 (70%)	119 (100%)	0	100	100
1	C	129/169 (76%)	128 (99%)	1 (1%)	73	89
1	D	119/169 (70%)	118 (99%)	1 (1%)	73	89
1	E	120/169 (71%)	120 (100%)	0	100	100
1	F	134/169 (79%)	134 (100%)	0	100	100
1	G	121/169 (72%)	120 (99%)	1 (1%)	73	89
1	H	127/169 (75%)	127 (100%)	0	100	100
1	I	121/169 (72%)	121 (100%)	0	100	100
1	J	127/169 (75%)	127 (100%)	0	100	100
1	K	121/169 (72%)	119 (98%)	2 (2%)	53	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	128/169 (76%)	126 (98%)	2 (2%)	55	81
1	M	121/169 (72%)	118 (98%)	3 (2%)	42	73
1	N	126/169 (75%)	126 (100%)	0	100	100
1	O	121/169 (72%)	117 (97%)	4 (3%)	33	65
1	P	125/169 (74%)	122 (98%)	3 (2%)	43	73
All	All	1982/2704 (73%)	1965 (99%)	17 (1%)	70	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	61	GLU
1	D	44	ASP
1	G	100	MET
1	L	80	ILE
1	L	87	LYS
1	K	24	ILE
1	K	108	LYS
1	M	43	ARG
1	M	101	GLU
1	M	106	LEU
1	P	17	GLU
1	P	91	ASP
1	P	148	GLN
1	O	23	GLN
1	O	50	ASN
1	O	58	GLN
1	O	133	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	73	GLN
1	A	148	GLN
1	A	158	HIS
1	B	7	GLN
1	B	10	GLN
1	B	25	ASN
1	B	118	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	21	ASN
1	C	57	HIS
1	C	73	GLN
1	C	146	ASN
1	D	23	GLN
1	D	98	ASN
1	F	57	HIS
1	F	98	ASN
1	E	50	ASN
1	H	105	HIS
1	H	111	ASN
1	H	148	GLN
1	G	7	GLN
1	G	23	GLN
1	G	60	HIS
1	G	125	ASN
1	J	23	GLN
1	J	73	GLN
1	J	112	GLN
1	I	65	HIS
1	L	158	HIS
1	L	161	ASN
1	K	7	GLN
1	K	10	GLN
1	K	23	GLN
1	K	105	HIS
1	K	109	ASN
1	N	73	GLN
1	N	111	ASN
1	N	161	ASN
1	M	11	ASN
1	M	50	ASN
1	M	98	ASN
1	M	118	HIS
1	P	57	HIS
1	P	75	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	141/190 (74%)	0.37	5 (3%) 47 38	36, 50, 78, 97	0
1	B	131/190 (68%)	0.39	6 (4%) 37 29	36, 58, 79, 87	0
1	C	148/190 (77%)	0.17	4 (2%) 56 46	35, 48, 72, 111	0
1	D	131/190 (68%)	0.52	9 (6%) 23 18	45, 66, 83, 98	0
1	E	132/190 (69%)	0.52	11 (8%) 17 14	37, 60, 90, 107	0
1	F	152/190 (80%)	0.13	4 (2%) 57 47	30, 47, 82, 102	0
1	G	134/190 (70%)	0.46	5 (3%) 45 36	34, 55, 75, 87	0
1	H	145/190 (76%)	0.17	2 (1%) 73 65	31, 45, 64, 90	0
1	I	133/190 (70%)	0.40	3 (2%) 61 51	43, 62, 81, 90	0
1	J	146/190 (76%)	0.23	4 (2%) 56 46	32, 46, 69, 81	0
1	K	133/190 (70%)	0.74	16 (12%) 9 7	45, 69, 92, 98	0
1	L	146/190 (76%)	0.54	10 (6%) 23 19	38, 55, 87, 101	0
1	M	133/190 (70%)	0.21	2 (1%) 72 64	34, 52, 73, 83	0
1	N	144/190 (75%)	0.25	5 (3%) 47 38	33, 50, 83, 99	0
1	O	133/190 (70%)	0.26	2 (1%) 72 64	31, 52, 74, 84	0
1	P	143/190 (75%)	0.01	1 (0%) 84 79	28, 40, 66, 97	0
All	All	2225/3040 (73%)	0.33	89 (4%) 42 33	28, 53, 82, 111	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	32	TYR	6.3
1	B	32	TYR	5.0
1	K	77	GLY	4.0
1	K	48	LEU	3.9
1	D	105	HIS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	117	LEU	3.7
1	D	107	GLU	3.5
1	L	183	GLY	3.4
1	E	121	ALA	3.4
1	L	77	GLY	3.2
1	E	45	ASP	3.2
1	B	117	LEU	3.2
1	K	93	TRP	3.1
1	D	50	ASN	3.0
1	D	134	GLU	2.9
1	E	49	LYS	2.9
1	F	145	ALA	2.9
1	E	111	ASN	2.8
1	D	135	THR	2.8
1	L	118	HIS	2.8
1	K	117	LEU	2.8
1	L	184	ASP	2.8
1	E	51	PHE	2.8
1	N	32	TYR	2.8
1	N	118	HIS	2.7
1	P	183	GLY	2.7
1	A	149	VAL	2.7
1	C	15	ASP	2.7
1	K	64	GLU	2.6
1	K	96	GLY	2.6
1	D	106	LEU	2.6
1	I	45	ASP	2.6
1	E	50	ASN	2.5
1	E	135	THR	2.5
1	K	65	HIS	2.5
1	B	97	LEU	2.5
1	I	127	PRO	2.5
1	K	106	LEU	2.5
1	L	86	LYS	2.5
1	J	120	LEU	2.5
1	A	73	GLN	2.5
1	B	14	GLN	2.5
1	E	124	LYS	2.5
1	C	118	HIS	2.5
1	L	120	LEU	2.4
1	G	97	LEU	2.4
1	N	36	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	145	ALA	2.4
1	A	95	SER	2.4
1	A	40	TYR	2.4
1	H	49	LYS	2.3
1	M	46	VAL	2.3
1	F	32	TYR	2.3
1	L	78	GLY	2.3
1	A	92	ASP	2.3
1	N	16	SER	2.3
1	C	144	LYS	2.3
1	J	76	ARG	2.3
1	M	105	HIS	2.3
1	G	94	GLU	2.2
1	G	107	GLU	2.2
1	F	120	LEU	2.2
1	I	48	LEU	2.2
1	O	97	LEU	2.2
1	B	135	THR	2.2
1	K	78	GLY	2.2
1	K	120	LEU	2.2
1	K	109	ASN	2.2
1	E	112	GLN	2.2
1	E	95	SER	2.2
1	K	115	LEU	2.2
1	D	47	ALA	2.2
1	H	62	GLU	2.2
1	B	133	ILE	2.1
1	J	35	LEU	2.1
1	K	97	LEU	2.1
1	K	104	LEU	2.1
1	E	63	ARG	2.1
1	L	116	GLU	2.1
1	D	80	ILE	2.1
1	D	89	ASP	2.1
1	G	106	LEU	2.1
1	J	46	VAL	2.1
1	G	92	ASP	2.1
1	L	66	ALA	2.1
1	K	113	SER	2.0
1	F	146	ASN	2.0
1	K	110	VAL	2.0
1	N	179	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.