wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:53 PM GMT

PDB ID	:	3UOI
Title	:	Mycobacterium tuberculosis bacterioferritin, BfrA
Authors	:	McMath, L.M.; Goulding, C.W.; TB Structural Genomics Consortium (TB-SGC)
Deposited on	:	2011-11-16
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

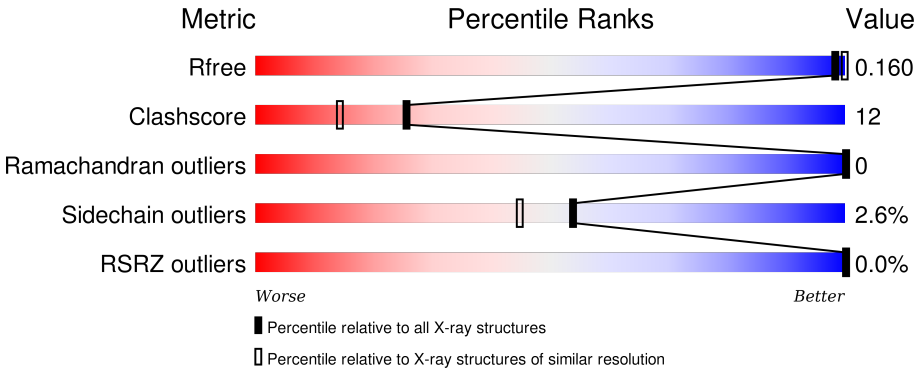
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	161	63% 32%
1	B	161	70% 27%
1	C	161	57% 39%
1	D	161	58% 39%
1	E	161	57% 37% 6%

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Mol	Chain	Length	Quality of chain
1	F	161	60% 35%
1	G	161	61% 34%
1	H	161	68% 27%
1	I	161	65% 32%
1	J	161	69% 27%
1	K	161	58% 37%
1	L	161	63% 35%
1	M	161	63% 32%
1	N	161	63% 34%
1	O	161	61% 35%
1	P	161	60% 35%
1	Q	161	52% 43%
1	R	161	58% 36% 5%
1	S	161	69% 25%
1	T	161	58% 38%
1	U	161	63% 34%
1	V	161	68% 27%
1	W	161	53% 43%
1	X	161	67% 30%
1	a	161	89% 10%
1	b	161	94% 5%
1	c	161	93% 6%
1	d	161	93% 6%
1	e	161	94%
1	f	161	% 94%

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Mol	Chain	Length	Quality of chain
1	g	161	94%
1	h	161	94%
1	i	161	93% 6%
1	j	161	91% 8%
1	k	161	90% 9%
1	l	161	95%
1	m	161	89% 9%
1	n	161	88% 11%
1	o	161	93% 6%
1	p	161	92% 7%
1	q	161	93% 5%
1	r	161	92% 7%
1	s	161	93% 6%
1	t	161	88% 11%
1	u	161	91% 7%
1	v	161	89% 9%
1	w	161	90% 9%
1	x	161	92% 7%

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	HEM	C	200	-	-	X	X
2	HEM	P	200	-	-	-	X
2	HEM	R	200	-	-	-	X
2	HEM	g	200	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 67560 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	B	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	C	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	D	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	E	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	F	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	G	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	H	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	I	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	J	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	K	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	L	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	M	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	N	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	O	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	P	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	R	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	S	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	T	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	U	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	V	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	W	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	X	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	a	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	b	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	c	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	d	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	e	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	f	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	g	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	h	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	i	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	j	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	k	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	l	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	m	159	Total	C	N	O	S	0	0	0
			1281	800	218	256	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	o	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	p	159	Total	C	N	O	S	0	0	0
			1281	800	218	256	7			
1	q	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	r	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	s	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	t	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	u	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	v	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	w	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	x	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P63697
A	0	GLY	-	EXPRESSION TAG	UNP P63697
B	-1	MET	-	EXPRESSION TAG	UNP P63697
B	0	GLY	-	EXPRESSION TAG	UNP P63697
C	-1	MET	-	EXPRESSION TAG	UNP P63697
C	0	GLY	-	EXPRESSION TAG	UNP P63697
D	-1	MET	-	EXPRESSION TAG	UNP P63697
D	0	GLY	-	EXPRESSION TAG	UNP P63697
E	-1	MET	-	EXPRESSION TAG	UNP P63697
E	0	GLY	-	EXPRESSION TAG	UNP P63697
F	-1	MET	-	EXPRESSION TAG	UNP P63697
F	0	GLY	-	EXPRESSION TAG	UNP P63697
G	-1	MET	-	EXPRESSION TAG	UNP P63697
G	0	GLY	-	EXPRESSION TAG	UNP P63697
H	-1	MET	-	EXPRESSION TAG	UNP P63697
H	0	GLY	-	EXPRESSION TAG	UNP P63697
I	-1	MET	-	EXPRESSION TAG	UNP P63697

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	GLY	-	EXPRESSION TAG	UNP P63697
J	-1	MET	-	EXPRESSION TAG	UNP P63697
J	0	GLY	-	EXPRESSION TAG	UNP P63697
K	-1	MET	-	EXPRESSION TAG	UNP P63697
K	0	GLY	-	EXPRESSION TAG	UNP P63697
L	-1	MET	-	EXPRESSION TAG	UNP P63697
L	0	GLY	-	EXPRESSION TAG	UNP P63697
M	-1	MET	-	EXPRESSION TAG	UNP P63697
M	0	GLY	-	EXPRESSION TAG	UNP P63697
N	-1	MET	-	EXPRESSION TAG	UNP P63697
N	0	GLY	-	EXPRESSION TAG	UNP P63697
O	-1	MET	-	EXPRESSION TAG	UNP P63697
O	0	GLY	-	EXPRESSION TAG	UNP P63697
P	-1	MET	-	EXPRESSION TAG	UNP P63697
P	0	GLY	-	EXPRESSION TAG	UNP P63697
Q	-1	MET	-	EXPRESSION TAG	UNP P63697
Q	0	GLY	-	EXPRESSION TAG	UNP P63697
R	-1	MET	-	EXPRESSION TAG	UNP P63697
R	0	GLY	-	EXPRESSION TAG	UNP P63697
S	-1	MET	-	EXPRESSION TAG	UNP P63697
S	0	GLY	-	EXPRESSION TAG	UNP P63697
T	-1	MET	-	EXPRESSION TAG	UNP P63697
T	0	GLY	-	EXPRESSION TAG	UNP P63697
U	-1	MET	-	EXPRESSION TAG	UNP P63697
U	0	GLY	-	EXPRESSION TAG	UNP P63697
V	-1	MET	-	EXPRESSION TAG	UNP P63697
V	0	GLY	-	EXPRESSION TAG	UNP P63697
W	-1	MET	-	EXPRESSION TAG	UNP P63697
W	0	GLY	-	EXPRESSION TAG	UNP P63697
X	-1	MET	-	EXPRESSION TAG	UNP P63697
X	0	GLY	-	EXPRESSION TAG	UNP P63697
a	-1	MET	-	EXPRESSION TAG	UNP P63697
a	0	GLY	-	EXPRESSION TAG	UNP P63697
b	-1	MET	-	EXPRESSION TAG	UNP P63697
b	0	GLY	-	EXPRESSION TAG	UNP P63697
c	-1	MET	-	EXPRESSION TAG	UNP P63697
c	0	GLY	-	EXPRESSION TAG	UNP P63697
d	-1	MET	-	EXPRESSION TAG	UNP P63697
d	0	GLY	-	EXPRESSION TAG	UNP P63697
e	-1	MET	-	EXPRESSION TAG	UNP P63697
e	0	GLY	-	EXPRESSION TAG	UNP P63697
f	-1	MET	-	EXPRESSION TAG	UNP P63697

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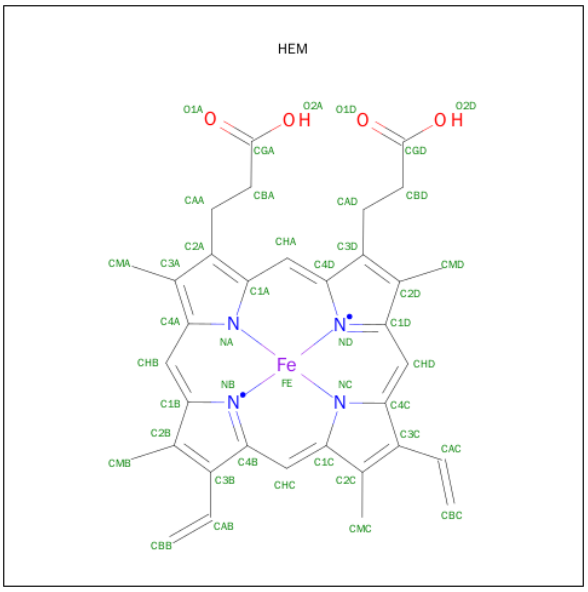
Chain	Residue	Modelled	Actual	Comment	Reference
f	0	GLY	-	EXPRESSION TAG	UNP P63697
g	-1	MET	-	EXPRESSION TAG	UNP P63697
g	0	GLY	-	EXPRESSION TAG	UNP P63697
h	-1	MET	-	EXPRESSION TAG	UNP P63697
h	0	GLY	-	EXPRESSION TAG	UNP P63697
i	-1	MET	-	EXPRESSION TAG	UNP P63697
i	0	GLY	-	EXPRESSION TAG	UNP P63697
j	-1	MET	-	EXPRESSION TAG	UNP P63697
j	0	GLY	-	EXPRESSION TAG	UNP P63697
k	-1	MET	-	EXPRESSION TAG	UNP P63697
k	0	GLY	-	EXPRESSION TAG	UNP P63697
l	-1	MET	-	EXPRESSION TAG	UNP P63697
l	0	GLY	-	EXPRESSION TAG	UNP P63697
m	-1	MET	-	EXPRESSION TAG	UNP P63697
m	0	GLY	-	EXPRESSION TAG	UNP P63697
n	-1	MET	-	EXPRESSION TAG	UNP P63697
n	0	GLY	-	EXPRESSION TAG	UNP P63697
o	-1	MET	-	EXPRESSION TAG	UNP P63697
o	0	GLY	-	EXPRESSION TAG	UNP P63697
p	-1	MET	-	EXPRESSION TAG	UNP P63697
p	0	GLY	-	EXPRESSION TAG	UNP P63697
q	-1	MET	-	EXPRESSION TAG	UNP P63697
q	0	GLY	-	EXPRESSION TAG	UNP P63697
r	-1	MET	-	EXPRESSION TAG	UNP P63697
r	0	GLY	-	EXPRESSION TAG	UNP P63697
s	-1	MET	-	EXPRESSION TAG	UNP P63697
s	0	GLY	-	EXPRESSION TAG	UNP P63697
t	-1	MET	-	EXPRESSION TAG	UNP P63697
t	0	GLY	-	EXPRESSION TAG	UNP P63697
u	-1	MET	-	EXPRESSION TAG	UNP P63697
u	0	GLY	-	EXPRESSION TAG	UNP P63697
v	-1	MET	-	EXPRESSION TAG	UNP P63697
v	0	GLY	-	EXPRESSION TAG	UNP P63697
w	-1	MET	-	EXPRESSION TAG	UNP P63697
w	0	GLY	-	EXPRESSION TAG	UNP P63697
x	-1	MET	-	EXPRESSION TAG	UNP P63697
x	0	GLY	-	EXPRESSION TAG	UNP P63697

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	a	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	c	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	g	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	j	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	k	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	n	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	o	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	t	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	x	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	120	Total	O	0	0
			120	120		
3	C	89	Total	O	0	0
			89	89		
3	D	105	Total	O	0	0
			105	105		
3	E	104	Total	O	0	0
			104	104		
3	F	102	Total	O	0	0
			102	102		
3	G	115	Total	O	0	0
			115	115		
3	H	135	Total	O	0	0
			135	135		
3	I	127	Total	O	0	0
			127	127		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	142	Total O 142 142	0	0
3	K	115	Total O 115 115	0	0
3	L	116	Total O 116 116	0	0
3	M	115	Total O 115 115	0	0
3	N	122	Total O 122 122	0	0
3	O	127	Total O 127 127	0	0
3	P	127	Total O 127 127	0	0
3	Q	108	Total O 108 108	0	0
3	R	104	Total O 104 104	0	0
3	S	73	Total O 73 73	0	0
3	T	136	Total O 136 136	0	0
3	U	151	Total O 151 151	0	0
3	V	119	Total O 119 119	0	0
3	W	91	Total O 91 91	0	0
3	X	131	Total O 131 131	0	0
3	a	65	Total O 65 65	0	0
3	b	59	Total O 59 59	0	0
3	c	94	Total O 94 94	0	0
3	d	57	Total O 57 57	0	0
3	e	103	Total O 103 103	0	0
3	f	105	Total O 105 105	0	0

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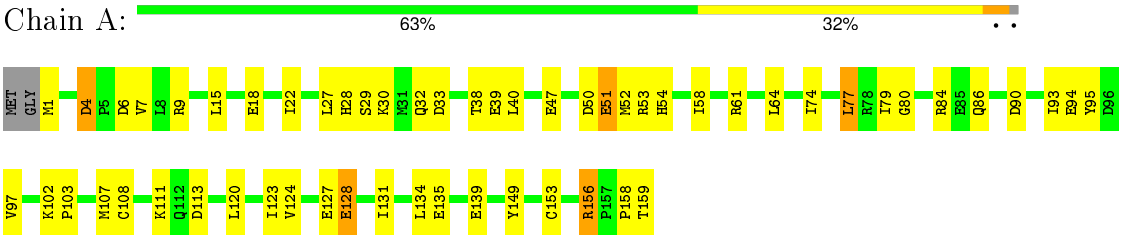
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	g	59	Total O 59 59	0	0
3	h	63	Total O 63 63	0	0
3	i	128	Total O 128 128	0	0
3	j	74	Total O 74 74	0	0
3	k	102	Total O 102 102	0	0
3	l	120	Total O 120 120	0	0
3	m	58	Total O 58 58	0	0
3	n	41	Total O 41 41	0	0
3	o	106	Total O 106 106	0	0
3	p	69	Total O 69 69	0	0
3	q	91	Total O 91 91	0	0
3	r	96	Total O 96 96	0	0
3	s	65	Total O 65 65	0	0
3	t	69	Total O 69 69	0	0
3	u	131	Total O 131 131	0	0
3	v	74	Total O 74 74	0	0
3	w	100	Total O 100 100	0	0
3	x	122	Total O 122 122	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

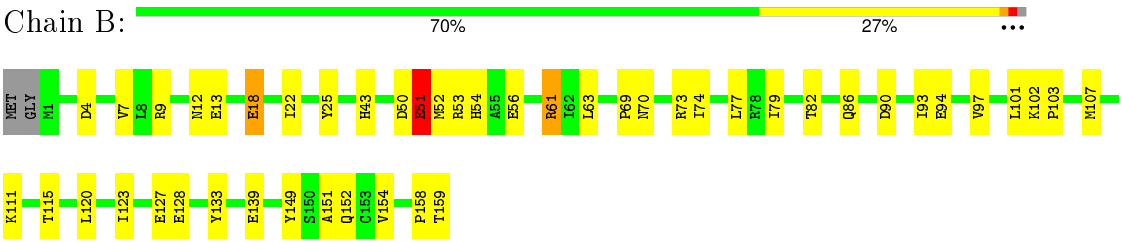
- Molecule 1: Bacterioferritin

Chain A:



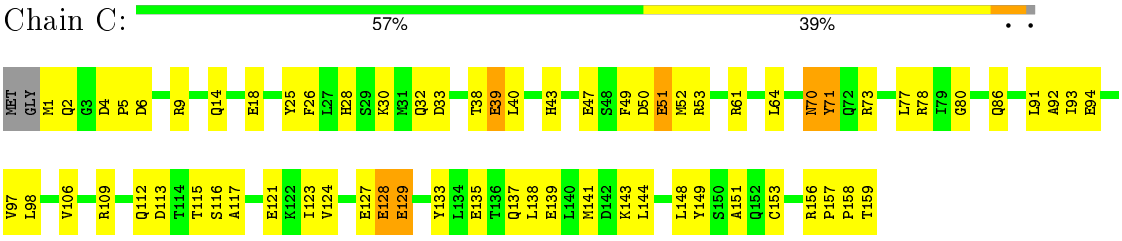
- Molecule 1: Bacterioferritin

Chain B:



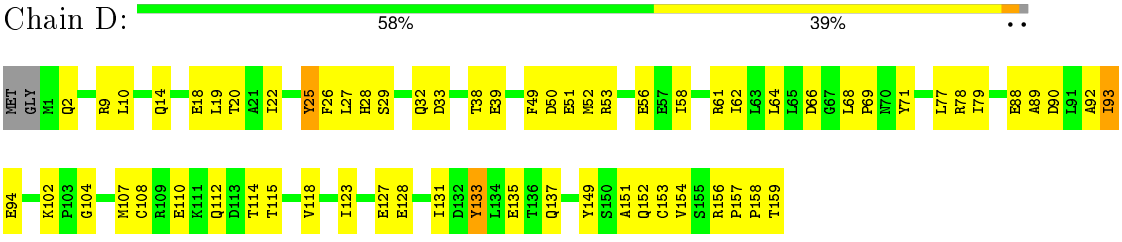
- Molecule 1: Bacterioferritin

Chain C:



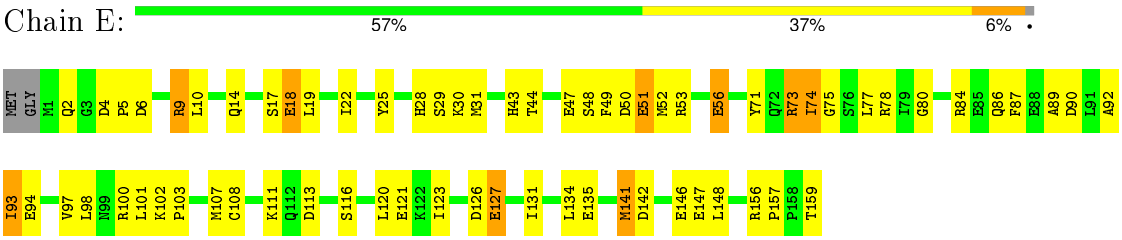
- Molecule 1: Bacterioferritin

Chain D:



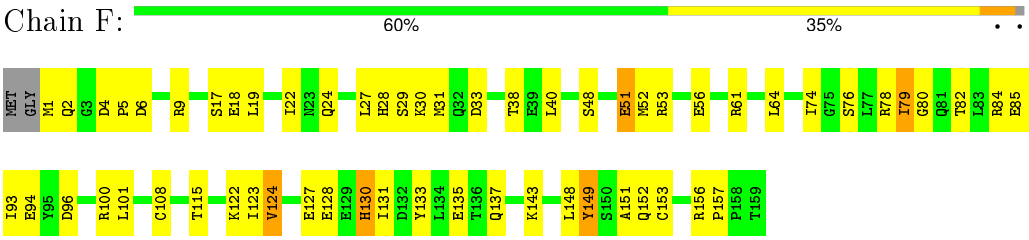
• Molecule 1: Bacterioferritin

Chain E:



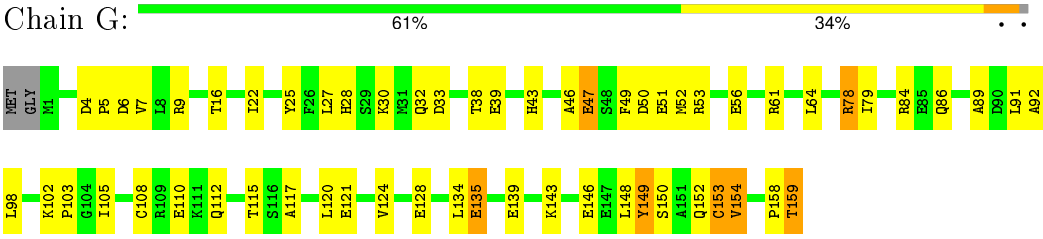
• Molecule 1: Bacterioferritin

Chain F:



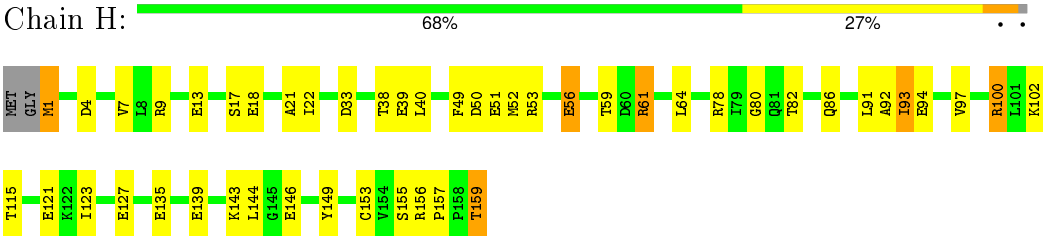
• Molecule 1: Bacterioferritin

Chain G:



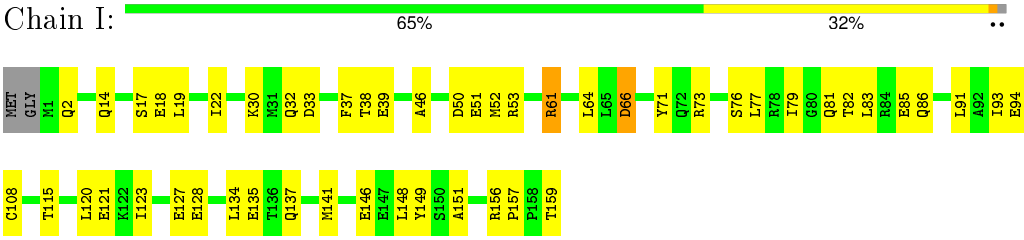
• Molecule 1: Bacterioferritin

Chain H:



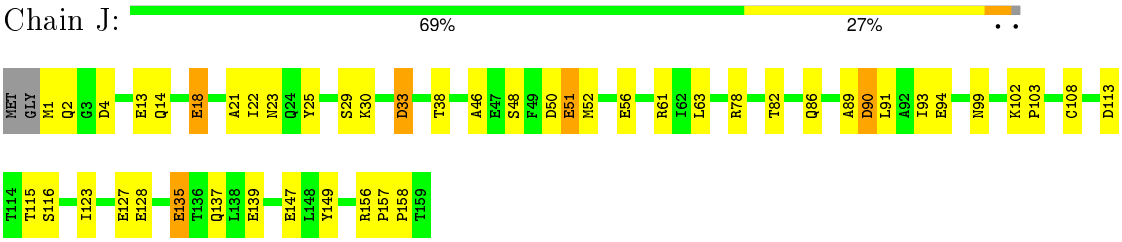
• Molecule 1: Bacterioferritin

Chain I:



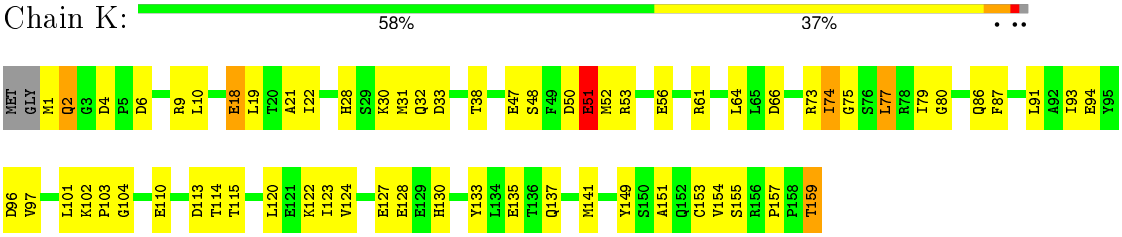
• Molecule 1: Bacterioferritin

Chain J:



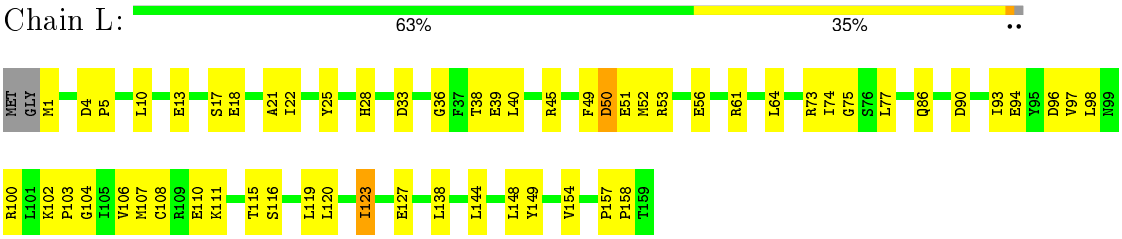
• Molecule 1: Bacterioferritin

Chain K:



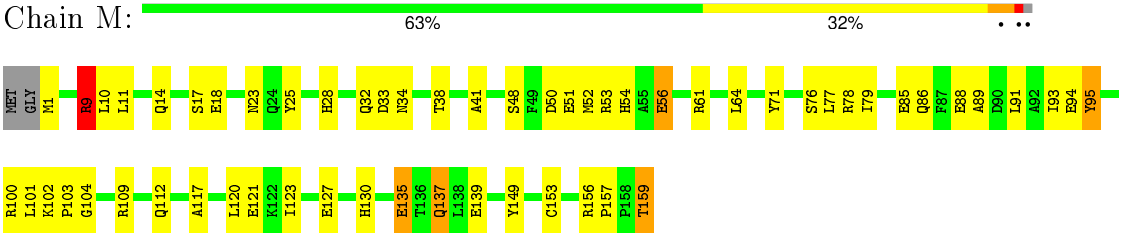
• Molecule 1: Bacterioferritin

Chain L:



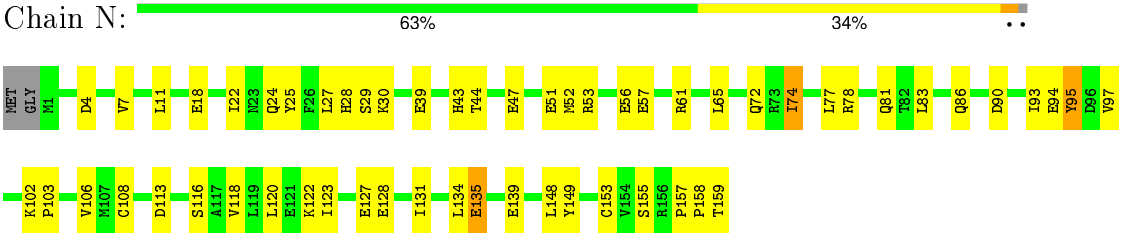
• Molecule 1: Bacterioferritin

Chain M:



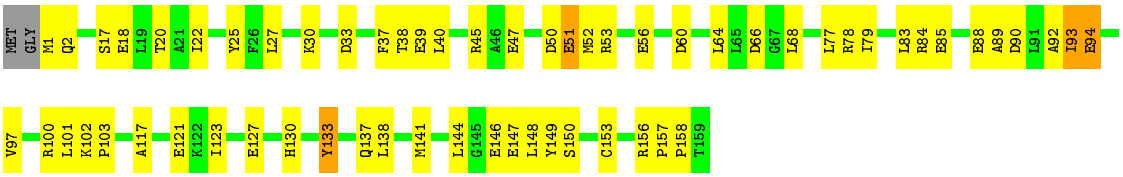
• Molecule 1: Bacterioferritin

Chain N:



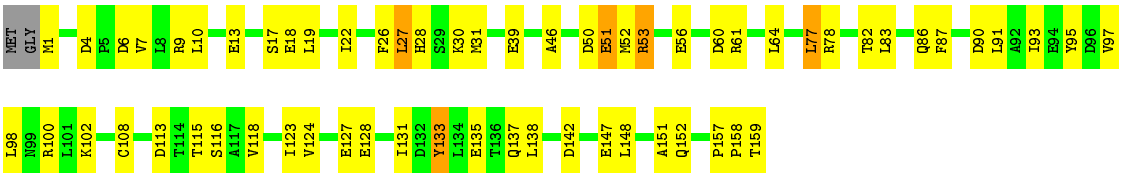
• Molecule 1: Bacterioferritin

Chain O:



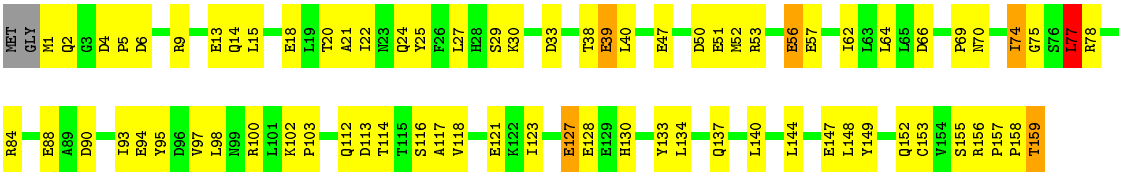
• Molecule 1: Bacterioferritin

Chain P:



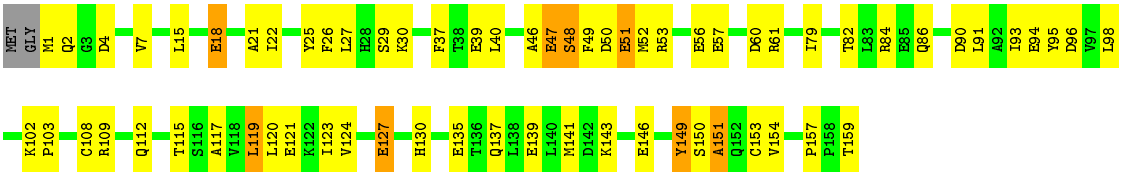
• Molecule 1: Bacterioferritin

Chain Q:



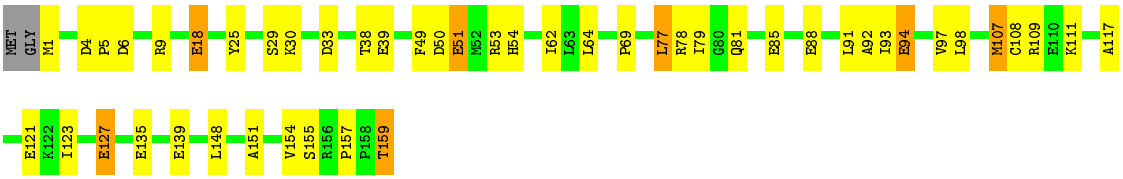
• Molecule 1: Bacterioferritin

Chain R:



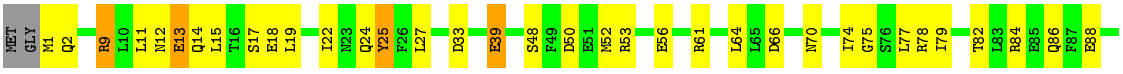
• Molecule 1: Bacterioferritin

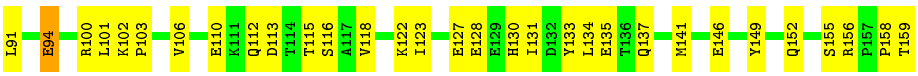
Chain S:



• Molecule 1: Bacterioferritin

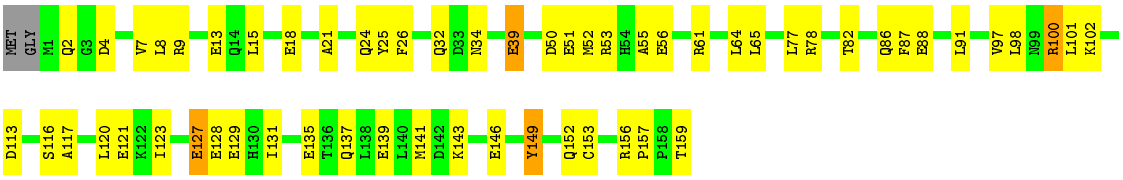
Chain T:





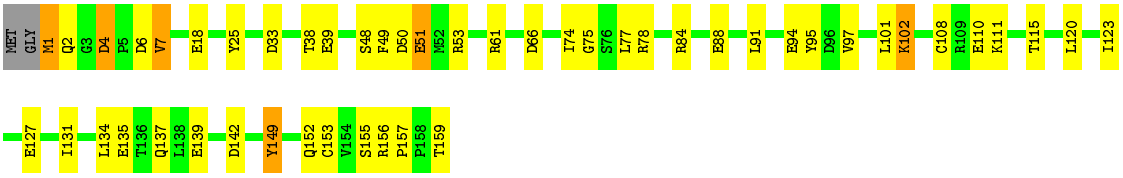
• Molecule 1: Bacterioferritin

Chain U:



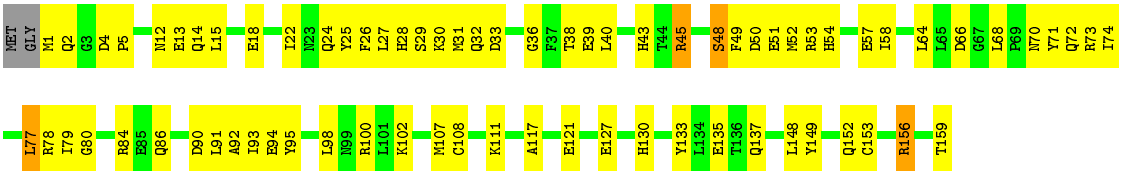
• Molecule 1: Bacterioferritin

Chain V:



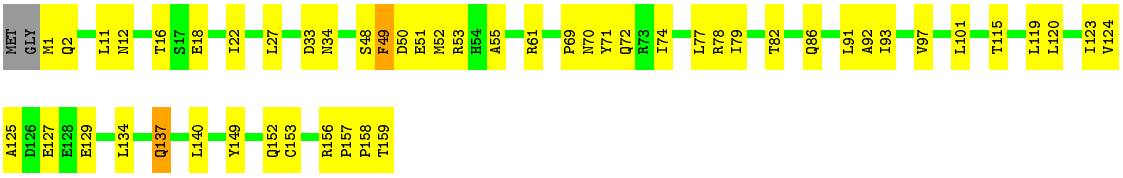
• Molecule 1: Bacterioferritin

Chain W:



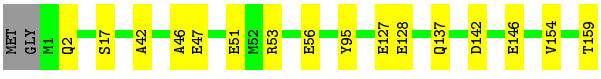
• Molecule 1: Bacterioferritin

Chain X:



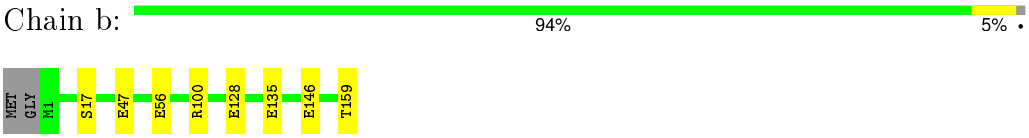
• Molecule 1: Bacterioferritin

Chain a:



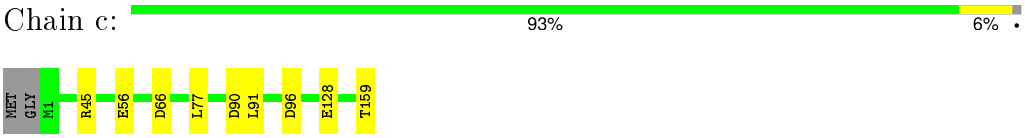
• Molecule 1: Bacterioferritin

Chain b:



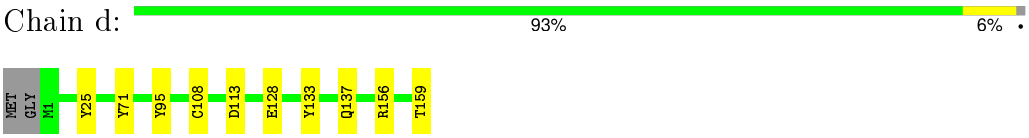
• Molecule 1: Bacterioferritin

Chain c:



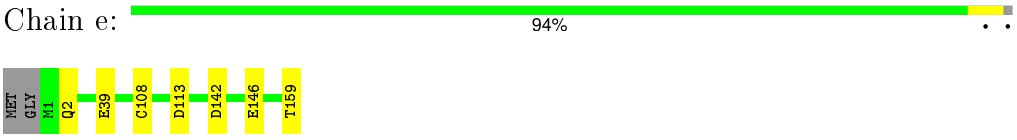
• Molecule 1: Bacterioferritin

Chain d:



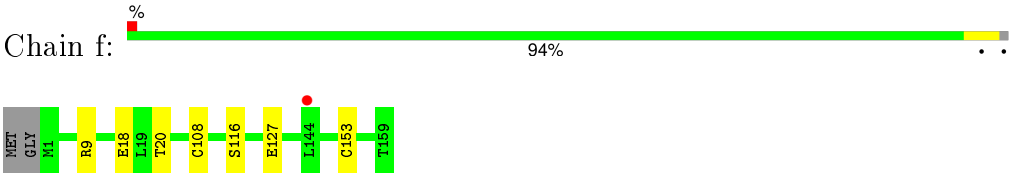
• Molecule 1: Bacterioferritin

Chain e:



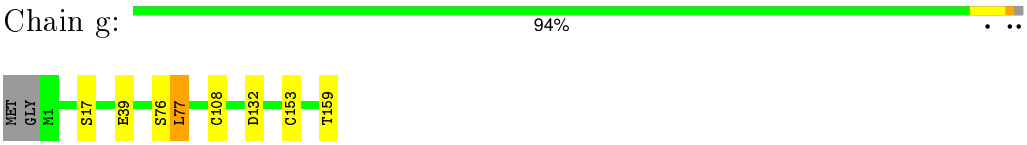
• Molecule 1: Bacterioferritin

Chain f:



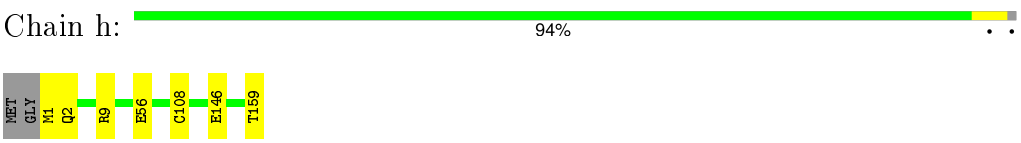
• Molecule 1: Bacterioferritin

Chain g:



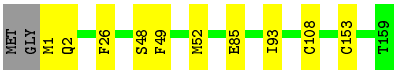
• Molecule 1: Bacterioferritin

Chain h:



• Molecule 1: Bacterioferritin

Chain i:

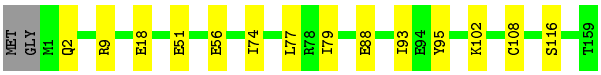


• Molecule 1: Bacterioferritin

Chain j:

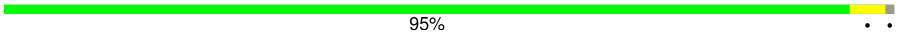
• Molecule 1: Bacterioferritin

Chain k:



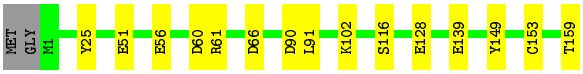
• Molecule 1: Bacterioferritin

Chain l:



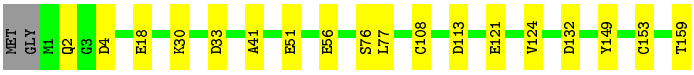
• Molecule 1: Bacterioferritin

Chain m:



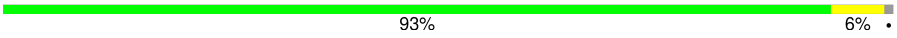
• Molecule 1: Bacterioferritin

Chain n:



• Molecule 1: Bacterioferritin

Chain o:

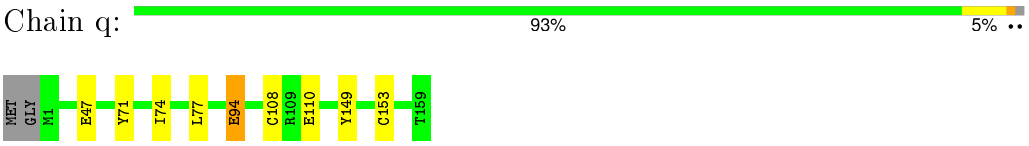


• Molecule 1: Bacterioferritin

Chain p:

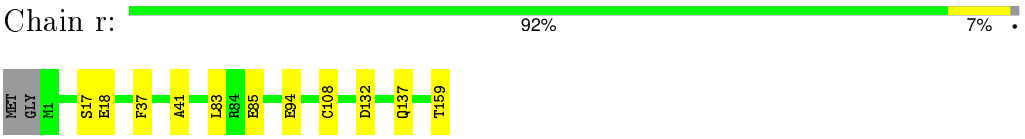
• Molecule 1: Bacterioferritin

Chain q:



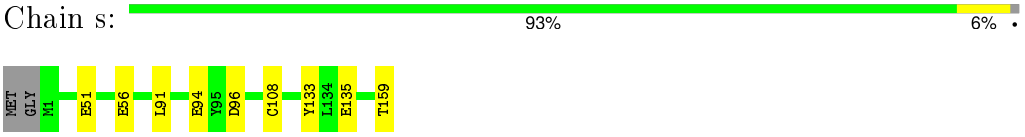
• Molecule 1: Bacterioferritin

Chain r:



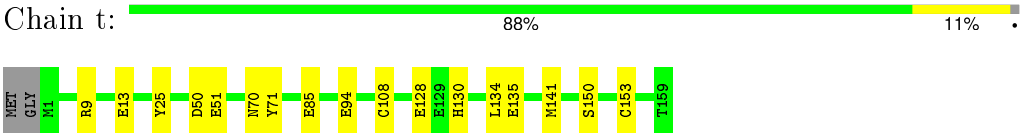
• Molecule 1: Bacterioferritin

Chain s:



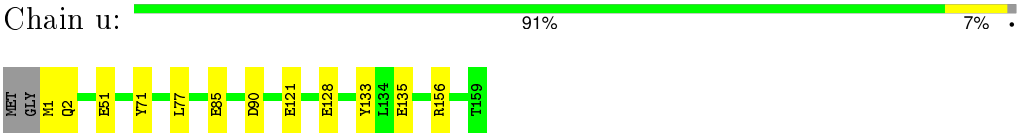
• Molecule 1: Bacterioferritin

Chain t:



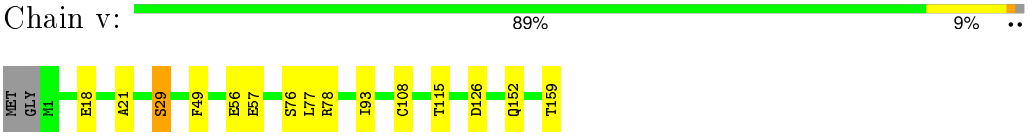
• Molecule 1: Bacterioferritin

Chain u:



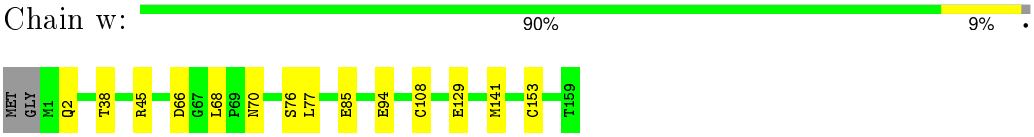
• Molecule 1: Bacterioferritin

Chain v:



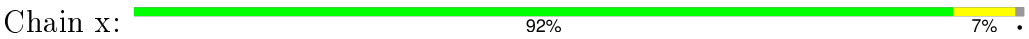
• Molecule 1: Bacterioferritin

Chain w:



• Molecule 1: Bacterioferritin

Chain x:




MET
GLY
M1
Q2
S29
Y71
L77
R78
I93
D96
L119
Y149
C153
V154
T159

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	122.96Å 123.22Å 175.45Å 89.95° 89.95° 90.00°	Depositor
Resolution (Å)	32.56 – 1.90 32.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.4 (32.56-1.90) 86.6 (32.56-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.148 , 0.194 0.162 , 0.160	Depositor DCC
R_{free} test set	34859 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.315 for 1.000H, 1.000K, L 0.208 for -1.000H, -1.000K, L 0.232 for 1.000K, -1.000H, L 0.245 for -1.000K, 1.000H, L 0.458 for k,-h,l 0.458 for -k,h,l 0.089 for h,-k,-l 0.089 for -h,k,-l 0.469 for -h,-k,l 0.089 for k,h,-l 0.089 for -k,-h,-l	Xtriage
Reported twinning fraction	0.315 for 1.000H, 1.000K, L 0.208 for -1.000H, -1.000K, L 0.232 for 1.000K, -1.000H, L 0.245 for -1.000K, 1.000H, L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 718159 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	67560	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.20 % 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 4.3600e-05.*

5 Model quality

5.1 Standard geometry

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

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	1.58	6/1304 (0.5%)	0.95	3/1763 (0.2%)
1	B	1.60	3/1304 (0.2%)	0.98	1/1763 (0.1%)
1	C	1.60	4/1304 (0.3%)	1.01	1/1763 (0.1%)
1	D	1.63	5/1304 (0.4%)	0.96	0/1763
1	E	1.56	7/1304 (0.5%)	1.05	4/1763 (0.2%)
1	F	1.62	6/1304 (0.5%)	0.98	1/1763 (0.1%)
1	G	1.67	9/1304 (0.7%)	0.99	1/1763 (0.1%)
1	H	1.64	6/1304 (0.5%)	0.96	1/1763 (0.1%)
1	I	1.57	2/1304 (0.2%)	1.00	4/1763 (0.2%)
1	J	1.66	10/1304 (0.8%)	1.02	7/1763 (0.4%)
1	K	1.57	7/1304 (0.5%)	0.94	3/1763 (0.2%)
1	L	1.60	4/1304 (0.3%)	1.00	3/1763 (0.2%)
1	M	1.64	7/1304 (0.5%)	0.96	1/1763 (0.1%)
1	N	1.71	8/1304 (0.6%)	0.98	4/1763 (0.2%)
1	O	1.62	6/1304 (0.5%)	0.98	1/1763 (0.1%)
1	P	1.69	11/1304 (0.8%)	0.95	3/1763 (0.2%)
1	Q	1.66	12/1304 (0.9%)	0.97	1/1763 (0.1%)
1	R	1.57	10/1304 (0.8%)	1.04	6/1763 (0.3%)
1	S	1.63	6/1304 (0.5%)	1.04	4/1763 (0.2%)
1	T	1.71	10/1304 (0.8%)	1.00	3/1763 (0.2%)
1	U	1.77	13/1304 (1.0%)	0.98	2/1763 (0.1%)
1	V	1.61	5/1304 (0.4%)	0.98	4/1763 (0.2%)
1	W	1.61	4/1304 (0.3%)	0.97	2/1763 (0.1%)
1	X	1.66	3/1304 (0.2%)	0.98	1/1763 (0.1%)
1	a	1.71	15/1304 (1.2%)	0.97	2/1763 (0.1%)
1	b	1.66	6/1304 (0.5%)	0.98	2/1763 (0.1%)
1	c	1.56	3/1304 (0.2%)	0.99	3/1763 (0.2%)
1	d	1.56	7/1304 (0.5%)	0.96	2/1763 (0.1%)
1	e	1.48	2/1304 (0.2%)	0.96	2/1763 (0.1%)
1	f	1.58	5/1304 (0.4%)	1.01	4/1763 (0.2%)
1	g	1.60	4/1304 (0.3%)	0.97	2/1763 (0.1%)
1	h	1.53	3/1304 (0.2%)	0.95	0/1763

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	i	1.59	8/1304 (0.6%)	0.98	3/1763 (0.2%)
1	j	1.65	7/1304 (0.5%)	1.01	3/1763 (0.2%)
1	k	1.62	7/1304 (0.5%)	0.99	2/1763 (0.1%)
1	l	1.62	5/1304 (0.4%)	0.96	0/1763
1	m	1.67	9/1300 (0.7%)	0.97	3/1758 (0.2%)
1	n	1.69	9/1304 (0.7%)	1.02	3/1763 (0.2%)
1	o	1.71	8/1304 (0.6%)	0.97	0/1763
1	p	1.59	6/1300 (0.5%)	0.95	2/1758 (0.1%)
1	q	1.56	5/1304 (0.4%)	0.96	1/1763 (0.1%)
1	r	1.60	7/1304 (0.5%)	0.99	2/1763 (0.1%)
1	s	1.60	7/1304 (0.5%)	0.96	2/1763 (0.1%)
1	t	1.77	14/1304 (1.1%)	0.99	2/1763 (0.1%)
1	u	1.72	10/1304 (0.8%)	1.01	2/1763 (0.1%)
1	v	1.67	8/1304 (0.6%)	0.99	2/1763 (0.1%)
1	w	1.61	5/1304 (0.4%)	1.05	6/1763 (0.3%)
1	x	1.68	6/1304 (0.5%)	0.94	1/1763 (0.1%)
All	All	1.63	330/62584 (0.5%)	0.98	112/84614 (0.1%)

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	q	0	1

The worst 5 of 330 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	108	CYS	CB-SG	-10.43	1.64	1.82
1	W	108	CYS	CB-SG	-9.99	1.65	1.82
1	k	108	CYS	CB-SG	-9.76	1.65	1.82
1	N	93	ILE	C-N	9.53	1.55	1.34
1	M	153	CYS	CB-SG	-9.14	1.66	1.82

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	9	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	f	9	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	q	94	GLU	O-C-N	-8.12	109.70	122.70
1	w	45	ARG	NE-CZ-NH2	8.01	124.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	w	94	GLU	O-C-N	-8.00	109.91	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	q	94	GLU	Mainchain

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	1285	0	1260	57	0
1	B	1285	0	1260	54	0
1	C	1285	0	1260	70	0
1	D	1285	0	1260	66	0
1	E	1285	0	1259	80	0
1	F	1285	0	1260	54	0
1	G	1285	0	1260	59	0
1	H	1285	0	1260	49	0
1	I	1285	0	1260	49	0
1	J	1285	0	1260	32	0
1	K	1285	0	1260	66	0
1	L	1285	0	1259	58	0
1	M	1285	0	1260	65	0
1	N	1285	0	1260	37	0
1	O	1285	0	1260	63	0
1	P	1285	0	1259	50	0
1	Q	1285	0	1260	84	0
1	R	1285	0	1260	50	0
1	S	1285	0	1260	46	0
1	T	1285	0	1260	63	0
1	U	1285	0	1260	50	0
1	V	1285	0	1260	43	0
1	W	1285	0	1260	76	0
1	X	1285	0	1260	66	0
1	a	1285	0	1260	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1285	0	1260	0	0
1	c	1285	0	1260	0	0
1	d	1285	0	1259	0	0
1	e	1285	0	1260	0	0
1	f	1285	0	1259	0	0
1	g	1285	0	1260	0	0
1	h	1285	0	1260	0	0
1	i	1285	0	1259	0	0
1	j	1285	0	1260	0	0
1	k	1285	0	1260	0	0
1	l	1285	0	1260	0	0
1	m	1281	0	1256	0	0
1	n	1285	0	1260	0	0
1	o	1285	0	1260	0	0
1	p	1281	0	1256	0	0
1	q	1285	0	1260	0	0
1	r	1285	0	1260	0	0
1	s	1285	0	1260	0	0
1	t	1285	0	1259	0	0
1	u	1285	0	1260	0	0
1	v	1285	0	1260	0	0
1	w	1285	0	1259	0	0
1	x	1285	0	1260	0	0
2	B	43	0	30	9	0
2	C	43	0	30	28	0
2	F	43	0	30	4	0
2	H	43	0	30	6	0
2	I	43	0	30	5	0
2	L	43	0	30	11	0
2	M	43	0	30	8	0
2	P	43	0	30	9	0
2	R	43	0	30	14	0
2	S	43	0	30	5	0
2	U	43	0	30	4	0
2	X	43	0	30	14	0
2	a	43	0	30	0	0
2	c	43	0	30	0	0
2	e	43	0	30	0	0
2	g	43	0	30	0	0
2	j	43	0	30	0	0
2	k	43	0	30	0	0
2	n	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	o	43	0	30	0	0
2	q	43	0	30	0	0
2	t	43	0	30	0	0
2	v	43	0	30	0	0
2	x	43	0	30	0	0
3	A	131	0	0	9	0
3	B	120	0	0	2	0
3	C	89	0	0	20	0
3	D	105	0	0	14	0
3	E	104	0	0	12	0
3	F	102	0	0	3	0
3	G	115	0	0	10	0
3	H	135	0	0	13	0
3	I	127	0	0	12	0
3	J	142	0	0	6	0
3	K	115	0	0	9	0
3	L	116	0	0	17	0
3	M	115	0	0	9	0
3	N	122	0	0	5	0
3	O	127	0	0	9	0
3	P	127	0	0	3	0
3	Q	108	0	0	12	0
3	R	104	0	0	11	0
3	S	73	0	0	3	0
3	T	136	0	0	7	0
3	U	151	0	0	9	0
3	V	119	0	0	12	0
3	W	91	0	0	19	0
3	X	131	0	0	16	0
3	a	65	0	0	0	0
3	b	59	0	0	0	0
3	c	94	0	0	0	0
3	d	57	0	0	0	0
3	e	103	0	0	0	0
3	f	105	0	0	0	0
3	g	59	0	0	0	0
3	h	63	0	0	0	0
3	i	128	0	0	0	0
3	j	74	0	0	0	0
3	k	102	0	0	0	0
3	l	120	0	0	0	0
3	m	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	n	41	0	0	0	0
3	o	106	0	0	0	0
3	p	69	0	0	0	0
3	q	91	0	0	0	0
3	r	96	0	0	0	0
3	s	65	0	0	0	0
3	t	69	0	0	0	0
3	u	131	0	0	0	0
3	v	74	0	0	0	0
3	w	100	0	0	0	0
3	x	122	0	0	0	0
All	All	67560	0	61184	1347	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 12.

The worst 5 of 1347 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LEU:HB2	3:C:356:HOH:O	22.83	1.32
1:I:76:SER:HB2	3:I:320:HOH:O	1.39	1.23
1:W:73:ARG:HD3	3:W:217:HOH:O	1.38	1.23
1:X:74:ILE:HA	3:X:403:HOH:O	1.39	1.19
1:F:78:ARG:HD3	3:F:309:HOH:O	1.40	1.16

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	157/161 (98%)	155 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	C	157/161 (98%)	157 (100%)	0	0	100	100
1	D	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	E	157/161 (98%)	157 (100%)	0	0	100	100
1	F	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	G	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	H	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	I	157/161 (98%)	157 (100%)	0	0	100	100
1	J	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	K	157/161 (98%)	157 (100%)	0	0	100	100
1	L	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	M	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	N	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	O	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	P	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	Q	157/161 (98%)	157 (100%)	0	0	100	100
1	R	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	S	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	T	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	U	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	V	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	W	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	X	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	a	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	b	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	c	157/161 (98%)	157 (100%)	0	0	100	100
1	d	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	e	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	f	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	g	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	h	157/161 (98%)	156 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	157/161 (98%)	157 (100%)	0	0	100	100
1	j	157/161 (98%)	157 (100%)	0	0	100	100
1	k	157/161 (98%)	157 (100%)	0	0	100	100
1	l	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	m	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	n	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	o	157/161 (98%)	157 (100%)	0	0	100	100
1	p	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	q	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	r	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	s	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	t	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	u	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	v	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	w	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	x	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
All	All	7536/7728 (98%)	7492 (99%)	44 (1%)	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	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	B	142/143 (99%)	140 (99%)	2 (1%)	74	71
1	C	142/143 (99%)	136 (96%)	6 (4%)	36	24
1	D	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	E	142/143 (99%)	135 (95%)	7 (5%)	31	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	G	142/143 (99%)	140 (99%)	2 (1%)	74	71
1	H	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	I	142/143 (99%)	139 (98%)	3 (2%)	61	55
1	J	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	K	142/143 (99%)	137 (96%)	5 (4%)	43	31
1	L	142/143 (99%)	142 (100%)	0	100	100
1	M	142/143 (99%)	136 (96%)	6 (4%)	36	24
1	N	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	O	142/143 (99%)	142 (100%)	0	100	100
1	P	142/143 (99%)	139 (98%)	3 (2%)	61	55
1	Q	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	R	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	S	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	T	142/143 (99%)	137 (96%)	5 (4%)	43	31
1	U	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	V	142/143 (99%)	136 (96%)	6 (4%)	36	24
1	W	142/143 (99%)	137 (96%)	5 (4%)	43	31
1	X	142/143 (99%)	140 (99%)	2 (1%)	74	71
1	a	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	b	142/143 (99%)	140 (99%)	2 (1%)	74	71
1	c	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	d	142/143 (99%)	140 (99%)	2 (1%)	74	71
1	e	142/143 (99%)	139 (98%)	3 (2%)	61	55
1	f	142/143 (99%)	141 (99%)	1 (1%)	88	88
1	g	142/143 (99%)	139 (98%)	3 (2%)	61	55
1	h	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	i	142/143 (99%)	140 (99%)	2 (1%)	74	71
1	j	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	k	142/143 (99%)	135 (95%)	7 (5%)	31	18
1	l	142/143 (99%)	141 (99%)	1 (1%)	88	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	m	141/143 (99%)	136 (96%)	5 (4%)	43	31
1	n	142/143 (99%)	135 (95%)	7 (5%)	31	18
1	o	142/143 (99%)	141 (99%)	1 (1%)	88	88
1	p	141/143 (99%)	137 (97%)	4 (3%)	51	41
1	q	142/143 (99%)	139 (98%)	3 (2%)	61	55
1	r	142/143 (99%)	139 (98%)	3 (2%)	61	55
1	s	142/143 (99%)	141 (99%)	1 (1%)	88	88
1	t	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	u	142/143 (99%)	138 (97%)	4 (3%)	51	41
1	v	142/143 (99%)	135 (95%)	7 (5%)	31	18
1	w	142/143 (99%)	136 (96%)	6 (4%)	36	24
1	x	142/143 (99%)	137 (96%)	5 (4%)	43	31
All	All	6814/6864 (99%)	6635 (97%)	179 (3%)	54	45

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	2	GLN
1	c	91	LEU
1	v	115	THR
1	V	77	LEU
1	X	2	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	112	GLN
1	f	24	GLN
1	w	70	ASN
1	b	34	ASN
1	d	137	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

24 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	HEM	B	200	1	30,50,50	2.37	8 (26%)	24,82,82	2.94	13 (54%)
2	HEM	C	200	1	30,50,50	3.55	11 (36%)	24,82,82	3.26	12 (50%)
2	HEM	F	200	1	30,50,50	2.44	8 (26%)	24,82,82	2.49	12 (50%)
2	HEM	H	200	1	30,50,50	2.34	6 (20%)	24,82,82	3.30	14 (58%)
2	HEM	I	200	1	30,50,50	2.44	11 (36%)	24,82,82	3.57	12 (50%)
2	HEM	L	200	1	30,50,50	2.68	12 (40%)	24,82,82	3.18	14 (58%)
2	HEM	M	200	1	30,50,50	2.03	9 (30%)	24,82,82	2.85	13 (54%)
2	HEM	P	200	1	30,50,50	2.87	9 (30%)	24,82,82	3.41	14 (58%)
2	HEM	R	200	1	30,50,50	2.27	7 (23%)	24,82,82	2.56	10 (41%)
2	HEM	S	200	1	30,50,50	3.59	13 (43%)	24,82,82	3.27	13 (54%)
2	HEM	U	200	1	30,50,50	2.42	8 (26%)	24,82,82	2.98	15 (62%)
2	HEM	X	200	1	30,50,50	2.65	8 (26%)	24,82,82	2.98	13 (54%)
2	HEM	a	200	1	30,50,50	2.18	9 (30%)	24,82,82	4.28	17 (70%)
2	HEM	c	200	1	30,50,50	2.33	6 (20%)	24,82,82	3.11	13 (54%)
2	HEM	e	200	1	30,50,50	2.49	8 (26%)	24,82,82	2.83	12 (50%)
2	HEM	g	200	1	30,50,50	2.57	7 (23%)	24,82,82	3.12	10 (41%)
2	HEM	j	200	1	30,50,50	2.74	7 (23%)	24,82,82	3.61	13 (54%)
2	HEM	k	200	1	30,50,50	2.09	7 (23%)	24,82,82	2.88	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	n	200	1	30,50,50	2.66	9 (30%)	24,82,82	2.46	13 (54%)
2	HEM	o	200	1	30,50,50	2.64	6 (20%)	24,82,82	2.30	6 (25%)
2	HEM	q	200	1	30,50,50	2.92	6 (20%)	24,82,82	2.56	10 (41%)
2	HEM	t	200	1	30,50,50	2.37	10 (33%)	24,82,82	2.63	10 (41%)
2	HEM	v	200	1	30,50,50	2.45	9 (30%)	24,82,82	3.00	15 (62%)
2	HEM	x	200	1	30,50,50	2.99	4 (13%)	24,82,82	3.08	14 (58%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	200	1	-	0/10/54/54	0/0/8/8
2	HEM	C	200	1	-	0/10/54/54	0/0/8/8
2	HEM	F	200	1	-	0/10/54/54	0/0/8/8
2	HEM	H	200	1	-	0/10/54/54	0/0/8/8
2	HEM	I	200	1	-	0/10/54/54	0/0/8/8
2	HEM	L	200	1	-	0/10/54/54	0/0/8/8
2	HEM	M	200	1	-	0/10/54/54	0/0/8/8
2	HEM	P	200	1	-	0/10/54/54	0/0/8/8
2	HEM	R	200	1	-	0/10/54/54	0/0/8/8
2	HEM	S	200	1	-	0/10/54/54	0/0/8/8
2	HEM	U	200	1	-	0/10/54/54	0/0/8/8
2	HEM	X	200	1	-	0/10/54/54	0/0/8/8
2	HEM	a	200	1	-	0/10/54/54	0/0/8/8
2	HEM	c	200	1	-	0/10/54/54	0/0/8/8
2	HEM	e	200	1	-	0/10/54/54	0/0/8/8
2	HEM	g	200	1	-	0/10/54/54	0/0/8/8
2	HEM	j	200	1	-	0/10/54/54	0/0/8/8
2	HEM	k	200	1	-	0/10/54/54	0/0/8/8
2	HEM	n	200	1	-	0/10/54/54	0/0/8/8
2	HEM	o	200	1	-	0/10/54/54	0/0/8/8
2	HEM	q	200	1	-	0/10/54/54	0/0/8/8
2	HEM	t	200	1	-	0/10/54/54	0/0/8/8
2	HEM	v	200	1	-	0/10/54/54	0/0/8/8
2	HEM	x	200	1	-	0/10/54/54	0/0/8/8

The worst 5 of 198 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	200	HEM	C3B-C4B	-14.09	1.39	1.51
2	x	200	HEM	C3B-C4B	-11.81	1.41	1.51
2	q	200	HEM	C3B-C4B	-10.83	1.42	1.51
2	P	200	HEM	C3B-C4B	-10.75	1.42	1.51
2	n	200	HEM	C3B-C4B	-9.66	1.43	1.51

The worst 5 of 296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	200	HEM	C3C-CAC-CBC	-11.48	106.86	124.46
2	I	200	HEM	CBA-CAA-C2A	-8.29	97.67	112.53
2	j	200	HEM	C3C-CAC-CBC	-7.68	112.68	124.46
2	k	200	HEM	C3B-CAB-CBB	-7.59	112.82	124.46
2	X	200	HEM	C3C-CAC-CBC	-7.42	113.08	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 117 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	200	HEM	9	0
2	C	200	HEM	28	0
2	F	200	HEM	4	0
2	H	200	HEM	6	0
2	I	200	HEM	5	0
2	L	200	HEM	11	0
2	M	200	HEM	8	0
2	P	200	HEM	9	0
2	R	200	HEM	14	0
2	S	200	HEM	5	0
2	U	200	HEM	4	0
2	X	200	HEM	14	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	159/161 (98%)	-0.29	0	100	100	16, 24, 32, 39	0
1	B	159/161 (98%)	-0.29	0	100	100	15, 25, 33, 41	0
1	C	159/161 (98%)	-0.20	0	100	100	16, 25, 33, 39	0
1	D	159/161 (98%)	-0.25	0	100	100	16, 24, 33, 43	0
1	E	159/161 (98%)	-0.10	0	100	100	16, 25, 34, 42	0
1	F	159/161 (98%)	-0.19	0	100	100	16, 24, 32, 39	0
1	G	159/161 (98%)	-0.23	0	100	100	16, 23, 32, 36	0
1	H	159/161 (98%)	-0.24	0	100	100	12, 22, 30, 41	0
1	I	159/161 (98%)	-0.33	0	100	100	14, 22, 31, 36	0
1	J	159/161 (98%)	-0.32	0	100	100	14, 22, 30, 41	0
1	K	159/161 (98%)	-0.28	0	100	100	15, 25, 33, 37	0
1	L	159/161 (98%)	-0.29	0	100	100	14, 24, 33, 42	0
1	M	159/161 (98%)	-0.25	0	100	100	17, 26, 34, 45	0
1	N	159/161 (98%)	-0.28	0	100	100	17, 24, 34, 39	0
1	O	159/161 (98%)	-0.23	0	100	100	16, 22, 31, 40	0
1	P	159/161 (98%)	-0.27	0	100	100	13, 23, 31, 38	0
1	Q	159/161 (98%)	-0.10	0	100	100	16, 26, 36, 44	0
1	R	159/161 (98%)	-0.13	0	100	100	16, 24, 32, 46	0
1	S	159/161 (98%)	-0.24	0	100	100	13, 20, 29, 35	0
1	T	159/161 (98%)	-0.26	0	100	100	12, 20, 28, 42	0
1	U	159/161 (98%)	-0.25	0	100	100	13, 21, 30, 39	0
1	V	159/161 (98%)	-0.33	0	100	100	15, 22, 30, 36	0
1	W	159/161 (98%)	-0.18	0	100	100	17, 26, 35, 42	0
1	X	159/161 (98%)	-0.30	0	100	100	14, 23, 31, 44	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	a	159/161 (98%)	-0.26	0 100 100	13, 22, 31, 38	0
1	b	159/161 (98%)	-0.21	0 100 100	14, 23, 32, 40	0
1	c	159/161 (98%)	-0.28	0 100 100	17, 25, 34, 40	0
1	d	159/161 (98%)	-0.24	0 100 100	17, 25, 34, 43	0
1	e	159/161 (98%)	-0.25	0 100 100	20, 28, 36, 46	0
1	f	159/161 (98%)	-0.25	1 (0%) 90 91	17, 25, 34, 42	0
1	g	159/161 (98%)	-0.20	0 100 100	15, 24, 32, 39	0
1	h	159/161 (98%)	-0.32	0 100 100	16, 23, 32, 42	0
1	i	159/161 (98%)	-0.33	0 100 100	15, 22, 34, 38	0
1	j	159/161 (98%)	-0.31	0 100 100	14, 22, 30, 39	0
1	k	159/161 (98%)	-0.18	0 100 100	14, 23, 33, 38	0
1	l	159/161 (98%)	-0.29	0 100 100	14, 23, 32, 39	0
1	m	159/161 (98%)	-0.23	0 100 100	15, 22, 33, 38	0
1	n	159/161 (98%)	-0.22	0 100 100	15, 23, 32, 42	0
1	o	159/161 (98%)	-0.26	0 100 100	16, 24, 30, 36	0
1	p	159/161 (98%)	-0.29	0 100 100	18, 24, 31, 41	0
1	q	159/161 (98%)	-0.18	0 100 100	20, 28, 36, 43	0
1	r	159/161 (98%)	-0.19	0 100 100	18, 27, 36, 43	0
1	s	159/161 (98%)	-0.30	0 100 100	14, 23, 31, 37	0
1	t	159/161 (98%)	-0.30	0 100 100	14, 21, 30, 34	0
1	u	159/161 (98%)	-0.25	0 100 100	13, 21, 29, 37	0
1	v	159/161 (98%)	-0.34	0 100 100	14, 22, 32, 39	0
1	w	159/161 (98%)	-0.25	0 100 100	16, 25, 34, 44	0
1	x	159/161 (98%)	-0.22	0 100 100	14, 21, 29, 38	0
All	All	7632/7728 (98%)	-0.25	1 (0%) 100 100	12, 24, 33, 46	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	f	144	LEU	2.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	C	200	43/43	0.96	0.15	3.93	18,31,44,47	0
2	HEM	g	200	43/43	0.97	0.14	2.94	17,29,40,42	0
2	HEM	P	200	43/43	0.96	0.14	2.44	12,25,37,39	0
2	HEM	R	200	43/43	0.96	0.15	2.07	21,28,38,40	0
2	HEM	e	200	43/43	0.97	0.14	1.88	19,31,38,40	0
2	HEM	v	200	43/43	0.96	0.12	1.83	14,24,33,35	0
2	HEM	c	200	43/43	0.97	0.12	1.71	17,27,40,43	0
2	HEM	t	200	43/43	0.97	0.12	1.49	10,21,34,37	0
2	HEM	k	200	43/43	0.97	0.12	1.48	10,21,34,37	0
2	HEM	n	200	43/43	0.96	0.13	1.46	10,21,34,37	0
2	HEM	M	200	43/43	0.98	0.11	1.26	14,24,43,53	0
2	HEM	L	200	43/43	0.97	0.11	1.24	14,21,42,48	0
2	HEM	o	200	43/43	0.97	0.11	1.24	12,22,37,44	0
2	HEM	I	200	43/43	0.98	0.11	1.04	10,21,34,37	0
2	HEM	j	200	43/43	0.98	0.11	1.01	6,18,36,37	0
2	HEM	S	200	43/43	0.98	0.12	0.77	8,16,30,33	0
2	HEM	F	200	43/43	0.97	0.12	0.74	16,28,46,52	0
2	HEM	B	200	43/43	0.97	0.11	0.67	18,27,38,45	0
2	HEM	x	200	43/43	0.96	0.12	0.54	10,22,34,38	0
2	HEM	a	200	43/43	0.97	0.11	0.44	13,22,29,33	0
2	HEM	U	200	43/43	0.98	0.10	0.27	10,20,26,33	0
2	HEM	q	200	43/43	0.96	0.10	-0.08	25,32,42,45	0
2	HEM	H	200	43/43	0.97	0.10	-0.23	14,24,32,35	0
2	HEM	X	200	43/43	0.97	0.10	-0.25	13,24,37,41	0

6.5 Other polymers (i)

There are no such residues in this entry.