Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:37 PM GMT

PDB ID	:	4TOE
Title	:	2.20A resolution structure of Iron Bound BfrB (D34F) from Pseudomonas aeruginosa
Authors	:	Lovell, S.; Battaile, K.P.; Yao, H.; Kumar, R.; Eshelman, K.; Rivera, M.
Deposited on	:	2014-06-05
Resolution	:	2.20 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
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:

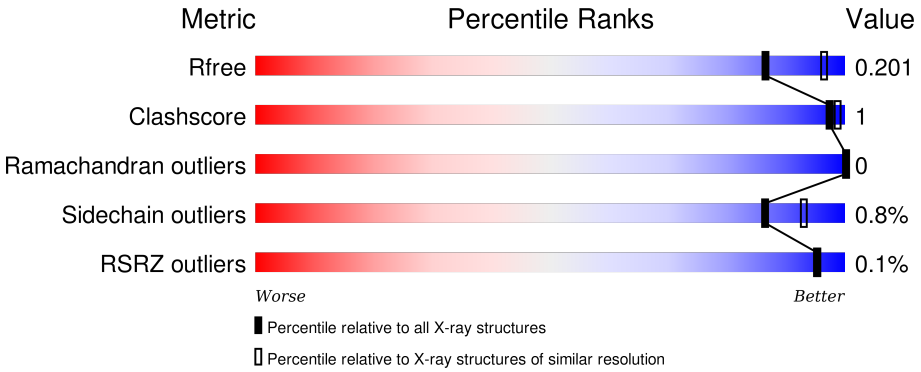
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	158	96%
1	B	158	94%
1	C	158	96%
1	D	158	94%
1	E	158	92% 5%

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Mol	Chain	Length	Quality of chain
1	F	158	94%
1	G	158	96%
1	H	158	97%
1	I	158	95%
1	J	158	95%
1	K	158	94%
1	L	158	97%
1	M	158	91% 7%
1	N	158	95%
1	O	158	93%
1	P	158	96%
1	Q	158	92% 5%
1	R	158	94%
1	S	158	93%
1	T	158	95%
1	U	158	95%
1	V	158	% 96%
1	W	158	96%
1	X	158	% 96%

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	FE2	A	205	-	-	-	X
2	FE2	B	204	-	-	-	X
2	FE2	C	204	-	-	-	X
2	FE2	F	203	-	-	-	X
2	FE2	H	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FE2	J	202	-	-	-	X
2	FE2	J	204	-	-	-	X
2	FE2	L	203	-	-	-	X
2	FE2	M	203	-	-	-	X
2	FE2	N	204	-	-	-	X
2	FE2	O	203	-	-	-	X
2	FE2	P	203	-	-	-	X
2	FE2	Q	203	-	-	-	X
2	FE2	Q	204	-	-	-	X
2	FE2	R	204	-	-	-	X
2	FE2	S	202	-	-	-	X
2	FE2	S	203	-	-	-	X
2	FE2	T	202	-	-	-	X
2	FE2	U	203	-	-	-	X
2	FE2	V	203	-	-	-	X
2	FE2	W	203	-	-	-	X
2	FE2	X	202	-	-	-	X
3	HEM	R	208	-	-	-	X
4	K	E	208	-	-	-	X
4	K	G	209	-	-	-	X
5	SO4	A	209	-	-	-	X
5	SO4	B	209	-	-	-	X
5	SO4	D	208	-	-	-	X
5	SO4	I	208	-	-	X	-
5	SO4	K	207	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33246 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	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	B	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	C	155	Total	C	N	O	S	0	0	0
			1265	802	216	241	6			
1	D	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	E	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	F	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	G	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	H	155	Total	C	N	O	S	0	0	0
			1267	804	216	241	6			
1	I	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	J	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	K	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	L	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	M	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	N	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	O	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	P	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	R	155	Total	C	N	O	S	0	0	0
			1265	802	216	241	6			
1	S	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	T	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	U	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	V	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			
1	W	155	Total	C	N	O	S	0	0	0
			1265	802	216	241	6			
1	X	154	Total	C	N	O	S	0	0	0
			1260	799	215	240	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	PHE	ASP	engineered mutation	UNP Q9HY79
B	34	PHE	ASP	engineered mutation	UNP Q9HY79
C	34	PHE	ASP	engineered mutation	UNP Q9HY79
D	34	PHE	ASP	engineered mutation	UNP Q9HY79
E	34	PHE	ASP	engineered mutation	UNP Q9HY79
F	34	PHE	ASP	engineered mutation	UNP Q9HY79
G	34	PHE	ASP	engineered mutation	UNP Q9HY79
H	34	PHE	ASP	engineered mutation	UNP Q9HY79
I	34	PHE	ASP	engineered mutation	UNP Q9HY79
J	34	PHE	ASP	engineered mutation	UNP Q9HY79
K	34	PHE	ASP	engineered mutation	UNP Q9HY79
L	34	PHE	ASP	engineered mutation	UNP Q9HY79
M	34	PHE	ASP	engineered mutation	UNP Q9HY79
N	34	PHE	ASP	engineered mutation	UNP Q9HY79
O	34	PHE	ASP	engineered mutation	UNP Q9HY79
P	34	PHE	ASP	engineered mutation	UNP Q9HY79
Q	34	PHE	ASP	engineered mutation	UNP Q9HY79
R	34	PHE	ASP	engineered mutation	UNP Q9HY79
S	34	PHE	ASP	engineered mutation	UNP Q9HY79
T	34	PHE	ASP	engineered mutation	UNP Q9HY79
U	34	PHE	ASP	engineered mutation	UNP Q9HY79
V	34	PHE	ASP	engineered mutation	UNP Q9HY79
W	34	PHE	ASP	engineered mutation	UNP Q9HY79

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Chain	Residue	Modelled	Actual	Comment	Reference
X	34	PHE	ASP	engineered mutation	UNP Q9HY79

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	6	Total Fe 6 6	0	0
2	K	6	Total Fe 6 6	0	0
2	B	7	Total Fe 7 7	0	0
2	W	6	Total Fe 6 6	0	0
2	N	8	Total Fe 8 8	0	0
2	X	4	Total Fe 4 4	0	0
2	S	5	Total Fe 5 5	0	0
2	J	6	Total Fe 6 6	0	0
2	E	6	Total Fe 6 6	0	0
2	V	5	Total Fe 5 5	0	0
2	A	6	Total Fe 6 6	0	0
2	R	7	Total Fe 7 7	0	0
2	M	6	Total Fe 6 6	0	0
2	D	6	Total Fe 6 6	0	0
2	I	6	Total Fe 6 6	0	0
2	U	6	Total Fe 6 6	0	0
2	L	6	Total Fe 6 6	0	0
2	G	7	Total Fe 7 7	0	0
2	Q	6	Total Fe 6 6	0	0

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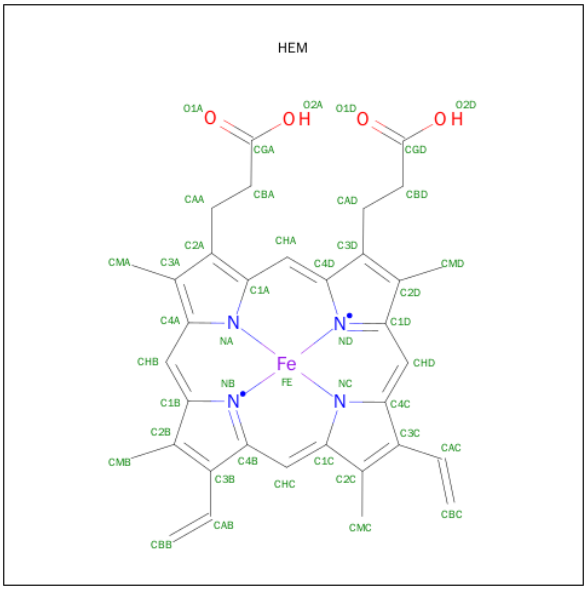
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	5	Total Fe 5 5	0	0
2	C	7	Total Fe 7 7	0	0
2	T	5	Total Fe 5 5	0	0
2	O	6	Total Fe 6 6	0	0
2	F	6	Total Fe 6 6	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	E	1	Total C Fe N O 43 34 1 4 4	0	0
3	G	1	Total C Fe N O 43 34 1 4 4	0	0
3	I	1	Total C Fe N O 43 34 1 4 4	0	0
3	L	1	Total C Fe N O 43 34 1 4 4	0	0

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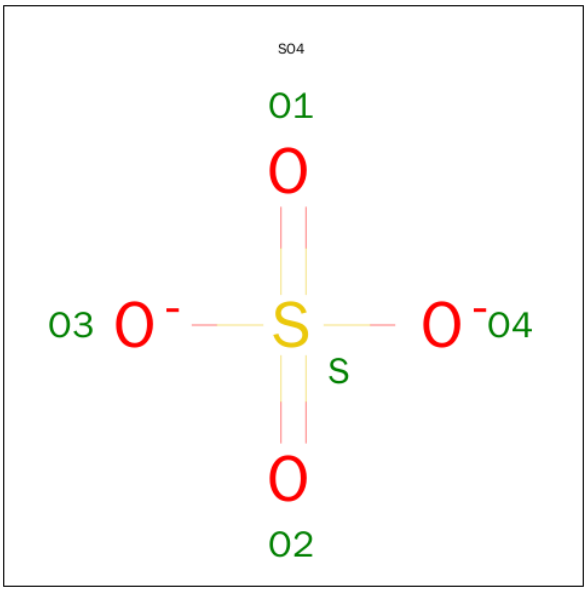
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	N	1	Total	K	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0
5	X	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	80	Total O 80 80	0	0
6	B	96	Total O 96 96	0	0
6	C	82	Total O 82 82	0	0
6	D	91	Total O 91 91	0	0

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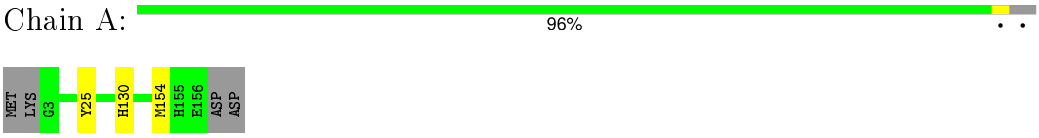
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	96	Total O 96 96	0	0
6	F	106	Total O 106 106	0	0
6	G	85	Total O 85 85	0	0
6	H	80	Total O 80 80	0	0
6	I	96	Total O 96 96	0	0
6	J	102	Total O 102 102	0	0
6	K	104	Total O 104 104	0	0
6	L	95	Total O 95 95	0	0
6	M	94	Total O 94 94	0	0
6	N	106	Total O 106 106	0	0
6	O	104	Total O 104 104	0	0
6	P	88	Total O 88 88	0	0
6	Q	99	Total O 99 99	0	0
6	R	113	Total O 113 113	0	0
6	S	102	Total O 102 102	0	0
6	T	102	Total O 102 102	0	0
6	U	97	Total O 97 97	0	0
6	V	89	Total O 89 89	0	0
6	W	82	Total O 82 82	0	0
6	X	89	Total O 89 89	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.

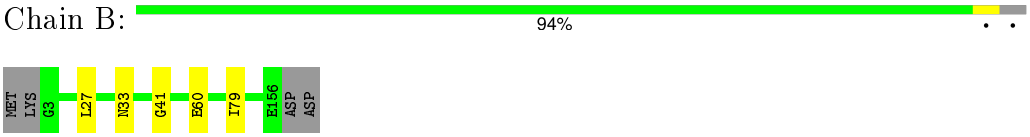
- Molecule 1: Bacterioferritin

Chain A:



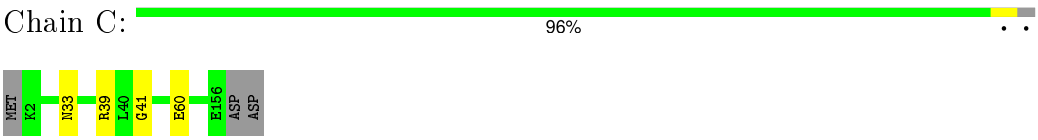
- Molecule 1: Bacterioferritin

Chain B:



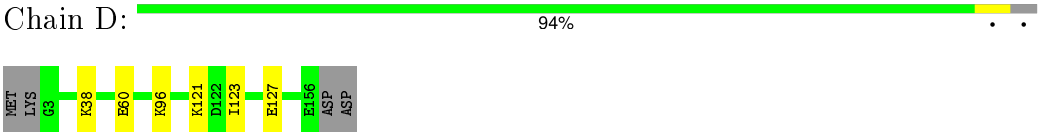
- Molecule 1: Bacterioferritin

Chain C:



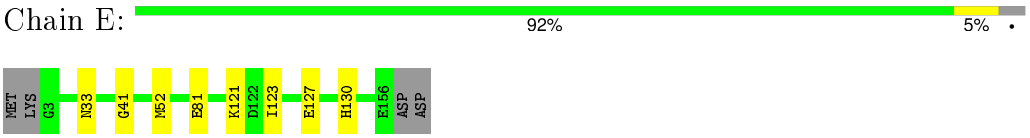
- Molecule 1: Bacterioferritin

Chain D:



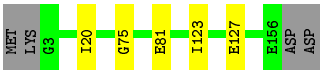
- Molecule 1: Bacterioferritin

Chain E:



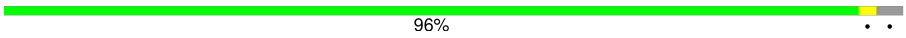
- Molecule 1: Bacterioferritin

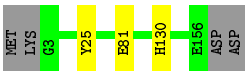
Chain F:



• Molecule 1: Bacterioferritin

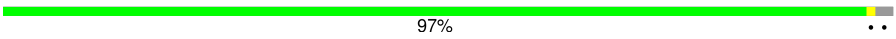
Chain G:

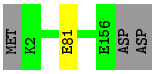




• Molecule 1: Bacterioferritin

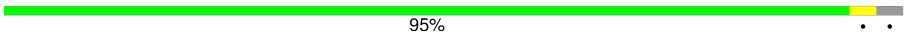
Chain H:

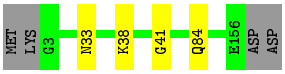




• Molecule 1: Bacterioferritin

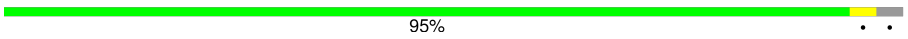
Chain I:

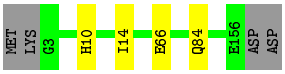




• Molecule 1: Bacterioferritin

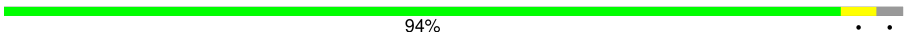
Chain J:





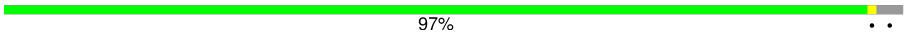
• Molecule 1: Bacterioferritin

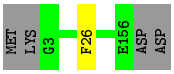
Chain K:



• Molecule 1: Bacterioferritin

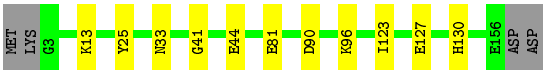
Chain L:





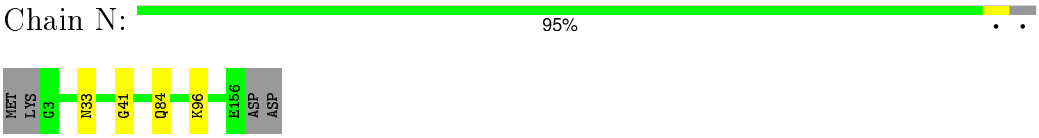
• Molecule 1: Bacterioferritin

Chain M:



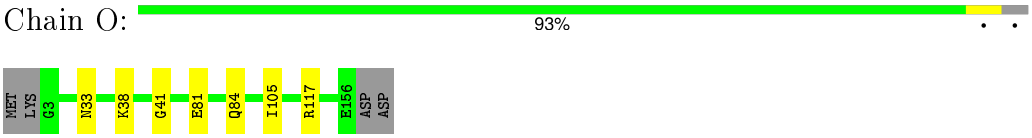
• Molecule 1: Bacterioferritin

Chain N:



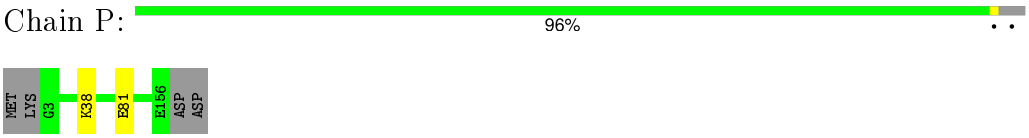
- Molecule 1: Bacterioferritin

Chain O:



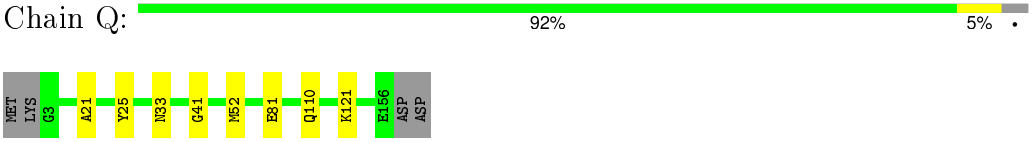
- Molecule 1: Bacterioferritin

Chain P:



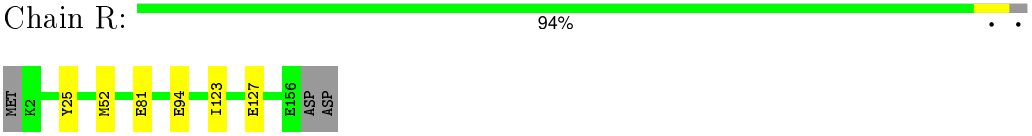
- Molecule 1: Bacterioferritin

Chain Q:



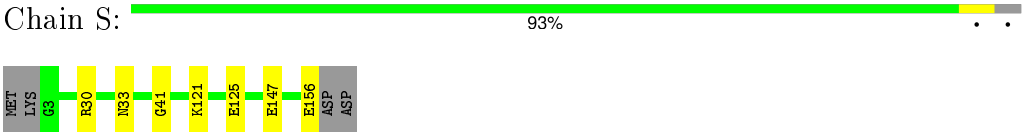
- Molecule 1: Bacterioferritin

Chain R:



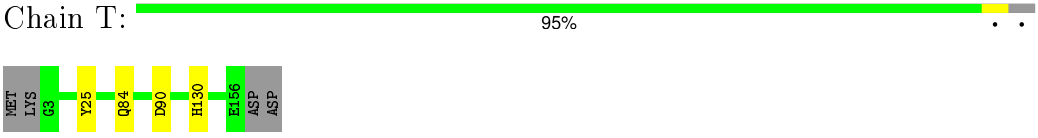
- Molecule 1: Bacterioferritin

Chain S:



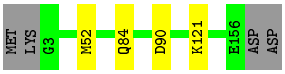
- Molecule 1: Bacterioferritin

Chain T:



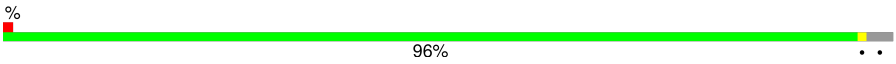
- Molecule 1: Bacterioferritin

Chain U:



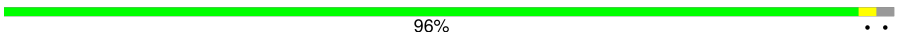
• Molecule 1: Bacterioferritin

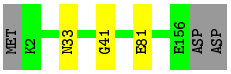
Chain V:



• Molecule 1: Bacterioferritin

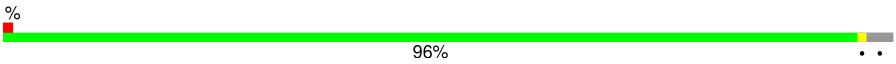
Chain W:

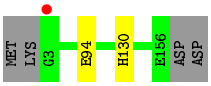




• Molecule 1: Bacterioferritin

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.49Å 203.40Å 207.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.20 48.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (48.39-2.20) 96.3 (48.39-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1450)	Depositor
R, R_{free}	0.149 , 0.187 0.167 , 0.201	Depositor DCC
R_{free} test set	12949 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.5	EDS
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 257583 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33246	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, K, FE2, SO4

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	0.49	0/1282	0.55	0/1729
1	B	0.49	0/1282	0.56	0/1729
1	C	0.53	0/1287	0.59	1/1736 (0.1%)
1	D	0.53	0/1282	0.57	0/1729
1	E	0.56	0/1282	0.59	0/1729
1	F	0.50	0/1282	0.55	0/1729
1	G	0.51	0/1282	0.58	0/1729
1	H	0.49	0/1289	0.55	0/1738
1	I	0.53	0/1282	0.58	0/1729
1	J	0.55	0/1282	0.59	0/1729
1	K	0.55	0/1282	0.58	0/1729
1	L	0.51	0/1282	0.56	0/1729
1	M	0.55	0/1282	0.61	0/1729
1	N	0.54	0/1282	0.58	0/1729
1	O	0.55	0/1282	0.60	0/1729
1	P	0.54	0/1282	0.58	0/1729
1	Q	0.53	0/1282	0.58	0/1729
1	R	0.53	0/1287	0.57	0/1736
1	S	0.56	0/1282	0.61	1/1729 (0.1%)
1	T	0.53	0/1282	0.62	1/1729 (0.1%)
1	U	0.52	0/1282	0.58	2/1729 (0.1%)
1	V	0.49	0/1282	0.58	0/1729
1	W	0.51	0/1287	0.57	0/1736
1	X	0.50	0/1282	0.61	0/1729
All	All	0.52	0/30790	0.58	5/41526 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	90	ASP	CB-CG-OD1	5.98	123.68	118.30
1	T	90	ASP	CB-CG-OD1	5.28	123.05	118.30
1	U	90	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	S	30	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	39	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1260	0	1226	2	0
1	B	1260	0	1226	3	0
1	C	1265	0	1228	2	0
1	D	1260	0	1226	3	0
1	E	1260	0	1226	4	0
1	F	1260	0	1226	2	0
1	G	1260	0	1226	1	0
1	H	1267	0	1232	0	0
1	I	1260	0	1226	3	0
1	J	1260	0	1226	2	0
1	K	1260	0	1226	3	0
1	L	1260	0	1226	3	0
1	M	1260	0	1226	5	0
1	N	1260	0	1226	2	0
1	O	1260	0	1226	3	0
1	P	1260	0	1226	1	0
1	Q	1260	0	1226	3	0
1	R	1265	0	1228	3	0
1	S	1260	0	1226	2	0
1	T	1260	0	1226	2	0
1	U	1260	0	1226	2	0
1	V	1260	0	1226	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1265	0	1228	1	0
1	X	1260	0	1226	1	0
2	A	6	0	0	0	0
2	B	7	0	0	0	0
2	C	7	0	0	0	0
2	D	6	0	0	0	0
2	E	6	0	0	0	0
2	F	6	0	0	0	0
2	G	7	0	0	0	0
2	H	5	0	0	0	0
2	I	6	0	0	0	0
2	J	6	0	0	0	0
2	K	6	0	0	0	0
2	L	6	0	0	0	0
2	M	6	0	0	0	0
2	N	8	0	0	0	0
2	O	6	0	0	0	0
2	P	6	0	0	0	0
2	Q	6	0	0	0	0
2	R	7	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
2	U	6	0	0	0	0
2	V	5	0	0	0	0
2	W	6	0	0	0	0
2	X	4	0	0	0	0
3	A	43	0	30	1	0
3	D	43	0	30	1	0
3	E	43	0	30	1	0
3	G	43	0	30	1	0
3	I	43	0	30	2	0
3	L	43	0	30	5	0
3	M	43	0	30	1	0
3	O	43	0	30	2	0
3	R	43	0	30	4	0
3	T	43	0	30	1	0
3	V	43	0	30	2	0
3	W	43	0	30	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1	0	0	0	0
4	N	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	1	0
5	F	5	0	0	1	0
5	I	5	0	0	2	0
5	K	5	0	0	0	0
5	R	5	0	0	0	0
5	X	5	0	0	0	0
6	A	80	0	0	0	0
6	B	96	0	0	1	0
6	C	82	0	0	1	0
6	D	91	0	0	3	0
6	E	96	0	0	1	0
6	F	106	0	0	1	0
6	G	85	0	0	0	0
6	H	80	0	0	0	0
6	I	96	0	0	4	0
6	J	102	0	0	1	0
6	K	104	0	0	1	0
6	L	95	0	0	1	0
6	M	94	0	0	1	0
6	N	106	0	0	1	0
6	O	104	0	0	1	0
6	P	88	0	0	1	0
6	Q	99	0	0	0	0
6	R	113	0	0	0	0
6	S	102	0	0	1	0
6	T	102	0	0	1	0
6	U	97	0	0	1	0
6	V	89	0	0	1	0
6	W	82	0	0	0	0
6	X	89	0	0	0	0
All	All	33246	0	29796	73	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 1.

All (73) 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:60:GLU:OE1	6:B:350:HOH:O	2.10	0.70
3:L:207:HEM:HHD	3:L:207:HEM:HBC2	1.73	0.69
5:I:208:SO4:O4	6:I:334:HOH:O	2.10	0.69
3:R:208:HEM:HBB2	3:R:208:HEM:HHC	1.75	0.68
1:T:84:GLN:OE1	6:T:366:HOH:O	2.11	0.67
1:V:118:ASP:OD2	6:V:388:HOH:O	2.13	0.66
3:O:207:HEM:HBC2	3:O:207:HEM:HHD	1.76	0.66
1:U:84:GLN:NE2	6:U:341:HOH:O	2.32	0.62
5:F:207:SO4:O2	6:F:403:HOH:O	2.15	0.61
5:D:208:SO4:O3	6:D:304:HOH:O	2.16	0.57
1:C:60:GLU:OE1	6:C:340:HOH:O	2.19	0.53
3:V:206:HEM:HBC2	3:V:206:HEM:HHD	1.90	0.53
3:R:208:HEM:HBC2	3:R:208:HEM:HHD	1.90	0.53
3:I:207:HEM:HBC2	3:I:207:HEM:HHD	1.92	0.51
3:T:206:HEM:HBC2	3:T:206:HEM:HHD	1.90	0.51
1:J:84:GLN:NE2	6:J:339:HOH:O	2.44	0.50
1:N:33:ASN:ND2	1:N:41:GLY:HA3	2.27	0.50
1:M:13:LYS:NZ	6:M:381:HOH:O	2.32	0.49
5:I:208:SO4:O1	6:I:391:HOH:O	2.18	0.49
1:S:33:ASN:ND2	1:S:41:GLY:HA3	2.28	0.49
3:W:207:HEM:HMC1	3:W:207:HEM:HBC2	1.96	0.48
1:S:147:GLU:OE2	6:S:301:HOH:O	2.20	0.48
1:O:84:GLN:NE2	6:O:331:HOH:O	2.46	0.47
3:D:207:HEM:HBC2	3:D:207:HEM:HMC2	1.96	0.47
1:L:26:PHE:CE1	3:L:207:HEM:CBC	2.98	0.47
1:M:123:ILE:O	1:M:127:GLU:HG2	2.15	0.46
1:D:123:ILE:O	1:D:127:GLU:HG2	2.15	0.46
1:W:33:ASN:ND2	1:W:41:GLY:HA3	2.30	0.46
1:E:33:ASN:ND2	1:E:41:GLY:HA3	2.31	0.45
1:B:33:ASN:ND2	1:B:41:GLY:HA3	2.30	0.45
1:A:25:TYR:CE2	1:A:130:HIS:HE1	2.35	0.45
1:N:84:GLN:NE2	6:N:314:HOH:O	2.50	0.45
1:M:25:TYR:CE2	1:M:130:HIS:HE1	2.35	0.45
1:B:27:LEU:HD23	1:B:79:ILE:HD12	1.99	0.45
1:L:26:PHE:CZ	3:L:207:HEM:CBC	3.01	0.44
1:F:20:ILE:HD11	1:F:75:GLY:HA3	2.00	0.44
1:M:33:ASN:ND2	1:M:41:GLY:HA3	2.33	0.43
3:M:207:HEM:HBC2	3:M:207:HEM:HMC1	2.00	0.43
3:G:208:HEM:HMC2	3:G:208:HEM:HBC2	2.00	0.43
1:X:94:GLU:OE2	1:X:130:HIS:ND1	2.50	0.43
1:D:60:GLU:OE1	6:D:337:HOH:O	2.21	0.43
1:F:123:ILE:O	1:F:127:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:21:ALA:HB1	1:Q:25:TYR:CE2	2.54	0.43
1:A:154:MET:HB3	1:A:154:MET:HE2	1.77	0.43
3:O:207:HEM:HBC2	3:O:207:HEM:CHD	2.48	0.42
1:K:33:ASN:ND2	1:K:41:GLY:HA3	2.34	0.42
1:E:130:HIS:HB2	6:E:367:HOH:O	2.19	0.42
1:R:25:TYR:OH	1:R:94:GLU:OE2	2.30	0.42
3:L:207:HEM:O1D	6:L:383:HOH:O	2.22	0.42
1:G:25:TYR:CE2	1:G:130:HIS:HE1	2.37	0.42
1:I:38:LYS:CE	6:I:337:HOH:O	2.67	0.42
1:R:52:MET:HB3	3:R:208:HEM:CHB	2.50	0.42
1:O:105:ILE:HG23	1:O:117:ARG:HG3	2.00	0.42
1:U:52:MET:HB3	3:V:206:HEM:CHD	2.50	0.41
1:C:33:ASN:ND2	1:C:41:GLY:HA3	2.35	0.41
1:J:10:HIS:O	1:J:14:ILE:HG12	2.20	0.41
1:T:25:TYR:CE2	1:T:130:HIS:HE1	2.38	0.41
1:M:44:GLU:OE2	1:M:90:ASP:OD2	2.38	0.41
1:Q:33:ASN:ND2	1:Q:41:GLY:HA3	2.35	0.41
1:I:84:GLN:NE2	6:I:310:HOH:O	2.54	0.41
3:I:207:HEM:HBB2	3:I:207:HEM:CMB	2.51	0.41
1:E:123:ILE:O	1:E:127:GLU:HG2	2.20	0.41
1:Q:52:MET:HB3	3:R:208:HEM:CHD	2.51	0.41
1:I:33:ASN:ND2	1:I:41:GLY:HA3	2.36	0.41
1:E:52:MET:HB3	3:E:207:HEM:CHD	2.51	0.41
1:K:130:HIS:NE2	6:K:312:HOH:O	2.37	0.41
1:O:33:ASN:ND2	1:O:41:GLY:HA3	2.36	0.41
1:P:38:LYS:HE2	6:P:335:HOH:O	2.21	0.41
1:K:123:ILE:O	1:K:127:GLU:HG2	2.21	0.41
1:L:26:PHE:CE1	3:L:207:HEM:HBC1	2.57	0.40
1:D:38:LYS:CE	6:D:329:HOH:O	2.70	0.40
1:R:123:ILE:O	1:R:127:GLU:HG2	2.22	0.40
3:A:207:HEM:HMC2	3:A:207:HEM:HBC2	2.04	0.40

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	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	B	152/158 (96%)	152 (100%)	0	0	100	100
1	C	153/158 (97%)	152 (99%)	1 (1%)	0	100	100
1	D	152/158 (96%)	152 (100%)	0	0	100	100
1	E	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	F	152/158 (96%)	152 (100%)	0	0	100	100
1	G	152/158 (96%)	152 (100%)	0	0	100	100
1	H	153/158 (97%)	153 (100%)	0	0	100	100
1	I	152/158 (96%)	152 (100%)	0	0	100	100
1	J	152/158 (96%)	152 (100%)	0	0	100	100
1	K	152/158 (96%)	152 (100%)	0	0	100	100
1	L	152/158 (96%)	152 (100%)	0	0	100	100
1	M	152/158 (96%)	152 (100%)	0	0	100	100
1	N	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	O	152/158 (96%)	152 (100%)	0	0	100	100
1	P	152/158 (96%)	152 (100%)	0	0	100	100
1	Q	152/158 (96%)	152 (100%)	0	0	100	100
1	R	153/158 (97%)	153 (100%)	0	0	100	100
1	S	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	T	152/158 (96%)	152 (100%)	0	0	100	100
1	U	152/158 (96%)	152 (100%)	0	0	100	100
1	V	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	W	153/158 (97%)	153 (100%)	0	0	100	100
1	X	152/158 (96%)	152 (100%)	0	0	100	100
All	All	3652/3792 (96%)	3645 (100%)	7 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	136/144 (94%)	136 (100%)	0	100	100
1	B	136/144 (94%)	136 (100%)	0	100	100
1	C	136/144 (94%)	136 (100%)	0	100	100
1	D	136/144 (94%)	134 (98%)	2 (2%)	72	84
1	E	136/144 (94%)	134 (98%)	2 (2%)	72	84
1	F	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	G	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	H	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	I	136/144 (94%)	136 (100%)	0	100	100
1	J	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	K	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	L	136/144 (94%)	136 (100%)	0	100	100
1	M	136/144 (94%)	134 (98%)	2 (2%)	72	84
1	N	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	O	136/144 (94%)	134 (98%)	2 (2%)	72	84
1	P	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	Q	136/144 (94%)	133 (98%)	3 (2%)	60	72
1	R	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	S	136/144 (94%)	133 (98%)	3 (2%)	60	72
1	T	136/144 (94%)	136 (100%)	0	100	100
1	U	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	V	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	W	136/144 (94%)	135 (99%)	1 (1%)	88	94
1	X	136/144 (94%)	136 (100%)	0	100	100
All	All	3264/3456 (94%)	3239 (99%)	25 (1%)	86	93

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	96	LYS

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Mol	Chain	Res	Type
1	D	121	LYS
1	E	81	GLU
1	E	121	LYS
1	F	81	GLU
1	G	81	GLU
1	H	81	GLU
1	J	66	GLU
1	K	81	GLU
1	M	81	GLU
1	M	96	LYS
1	N	96	LYS
1	O	38	LYS
1	O	81	GLU
1	P	81	GLU
1	Q	81	GLU
1	Q	110	GLN
1	Q	121	LYS
1	R	81	GLU
1	S	121	LYS
1	S	125	GLU
1	S	156	GLU
1	U	121	LYS
1	V	81	GLU
1	W	81	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	130	HIS
1	B	33	ASN
1	C	33	ASN
1	D	33	ASN
1	D	54	HIS
1	D	137	GLN
1	E	33	ASN
1	E	137	GLN
1	F	33	ASN
1	F	112	HIS
1	F	130	HIS
1	G	33	ASN
1	G	110	GLN

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Mol	Chain	Res	Type
1	H	33	ASN
1	H	84	GLN
1	H	112	HIS
1	H	130	HIS
1	H	137	GLN
1	I	9	GLN
1	I	33	ASN
1	I	84	GLN
1	I	112	HIS
1	I	137	GLN
1	J	9	GLN
1	J	33	ASN
1	J	84	GLN
1	K	33	ASN
1	K	54	HIS
1	L	33	ASN
1	L	43	HIS
1	L	54	HIS
1	M	9	GLN
1	M	33	ASN
1	M	112	HIS
1	M	130	HIS
1	N	33	ASN
1	N	43	HIS
1	N	84	GLN
1	N	137	GLN
1	O	33	ASN
1	O	43	HIS
1	O	84	GLN
1	O	130	HIS
1	P	9	GLN
1	P	33	ASN
1	P	112	HIS
1	Q	33	ASN
1	Q	43	HIS
1	Q	84	GLN
1	Q	137	GLN
1	R	9	GLN
1	R	33	ASN
1	R	84	GLN
1	S	33	ASN
1	S	112	HIS

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Mol	Chain	Res	Type
1	T	9	GLN
1	T	33	ASN
1	T	84	GLN
1	T	112	HIS
1	T	130	HIS
1	U	9	GLN
1	U	33	ASN
1	U	43	HIS
1	U	137	GLN
1	V	9	GLN
1	V	33	ASN
1	V	84	GLN
1	V	130	HIS
1	W	9	GLN
1	W	33	ASN
1	W	130	HIS
1	X	9	GLN
1	X	33	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 170 ligands modelled in this entry, 150 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	A	207	1	30,50,50	2.18	5 (16%)	24,82,82	2.62	9 (37%)
5	SO4	A	209	-	4,4,4	0.23	0	6,6,6	0.18	0
5	SO4	B	209	-	4,4,4	0.26	0	6,6,6	0.20	0
3	HEM	D	207	1	30,50,50	2.34	7 (23%)	24,82,82	2.56	10 (41%)
5	SO4	D	208	-	4,4,4	0.39	0	6,6,6	0.32	0
3	HEM	E	207	1	30,50,50	2.48	7 (23%)	24,82,82	2.41	9 (37%)
5	SO4	F	207	-	4,4,4	0.22	0	6,6,6	0.34	0
3	HEM	G	208	1	30,50,50	2.13	5 (16%)	24,82,82	2.51	9 (37%)
3	HEM	I	207	1	30,50,50	2.47	8 (26%)	24,82,82	2.70	12 (50%)
5	SO4	I	208	-	4,4,4	0.30	0	6,6,6	0.24	0
5	SO4	K	207	-	4,4,4	0.24	0	6,6,6	0.37	0
3	HEM	L	207	1	30,50,50	2.38	6 (20%)	24,82,82	2.51	11 (45%)
3	HEM	M	207	1	30,50,50	2.30	8 (26%)	24,82,82	2.62	9 (37%)
3	HEM	O	207	1	30,50,50	2.22	7 (23%)	24,82,82	2.62	14 (58%)
3	HEM	R	208	1	30,50,50	2.15	5 (16%)	24,82,82	2.60	11 (45%)
5	SO4	R	209	-	4,4,4	0.28	0	6,6,6	0.58	0
3	HEM	T	206	1	30,50,50	2.22	4 (13%)	24,82,82	2.46	9 (37%)
3	HEM	V	206	1	30,50,50	2.50	8 (26%)	24,82,82	2.56	10 (41%)
3	HEM	W	207	1	30,50,50	2.23	8 (26%)	24,82,82	2.50	8 (33%)
5	SO4	X	205	-	4,4,4	0.27	0	6,6,6	0.16	0

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
3	HEM	A	207	1	-	0/10/54/54	0/0/8/8
5	SO4	A	209	-	-	0/0/0/0	0/0/0/0
5	SO4	B	209	-	-	0/0/0/0	0/0/0/0
3	HEM	D	207	1	-	0/10/54/54	0/0/8/8
5	SO4	D	208	-	-	0/0/0/0	0/0/0/0
3	HEM	E	207	1	-	0/10/54/54	0/0/8/8
5	SO4	F	207	-	-	0/0/0/0	0/0/0/0
3	HEM	G	208	1	-	0/10/54/54	0/0/8/8
3	HEM	I	207	1	-	0/10/54/54	0/0/8/8
5	SO4	I	208	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	K	207	-	-	0/0/0/0	0/0/0/0
3	HEM	L	207	1	-	0/10/54/54	0/0/8/8
3	HEM	M	207	1	-	0/10/54/54	0/0/8/8
3	HEM	O	207	1	-	0/10/54/54	0/0/8/8
3	HEM	R	208	1	-	0/10/54/54	0/0/8/8
5	SO4	R	209	-	-	0/0/0/0	0/0/0/0
3	HEM	T	206	1	-	0/10/54/54	0/0/8/8
3	HEM	V	206	1	-	0/10/54/54	0/0/8/8
3	HEM	W	207	1	-	0/10/54/54	0/0/8/8
5	SO4	X	205	-	-	0/0/0/0	0/0/0/0

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	206	HEM	C3B-C4B	-9.91	1.43	1.51
3	E	207	HEM	C3B-C4B	-9.37	1.43	1.51
3	L	207	HEM	C3B-C4B	-9.03	1.43	1.51
3	I	207	HEM	C3B-C4B	-8.99	1.43	1.51
3	D	207	HEM	C3B-C4B	-8.81	1.44	1.51
3	A	207	HEM	C3B-C4B	-7.91	1.44	1.51
3	M	207	HEM	C3B-C4B	-7.84	1.44	1.51
3	G	208	HEM	C3B-C4B	-7.61	1.45	1.51
3	T	206	HEM	C3B-C4B	-7.48	1.45	1.51
3	W	207	HEM	C3B-C4B	-7.19	1.45	1.51
3	O	207	HEM	C3B-C4B	-7.18	1.45	1.51
3	R	208	HEM	C3B-C4B	-7.17	1.45	1.51
3	L	207	HEM	C3D-C4D	-6.06	1.43	1.51
3	W	207	HEM	C3D-C4D	-6.01	1.43	1.51
3	R	208	HEM	C3D-C4D	-5.98	1.43	1.51
3	O	207	HEM	C3D-C4D	-5.97	1.43	1.51
3	T	206	HEM	C3D-C4D	-5.84	1.44	1.51
3	I	207	HEM	C3D-C4D	-5.75	1.44	1.51
3	E	207	HEM	C3D-C4D	-5.68	1.44	1.51
3	D	207	HEM	C3D-C4D	-5.64	1.44	1.51
3	G	208	HEM	C3D-C4D	-5.40	1.44	1.51
3	M	207	HEM	C3D-C4D	-5.29	1.44	1.51
3	A	207	HEM	C3D-C4D	-5.13	1.45	1.51
3	V	206	HEM	C3D-C4D	-5.08	1.45	1.51
3	T	206	HEM	C2C-C1C	-4.68	1.43	1.52
3	M	207	HEM	C2C-C1C	-4.67	1.43	1.52
3	I	207	HEM	C2C-C1C	-4.47	1.44	1.52
3	V	206	HEM	C2C-C1C	-4.46	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	207	HEM	C2C-C1C	-4.31	1.44	1.52
3	E	207	HEM	C2C-C1C	-4.01	1.45	1.52
3	A	207	HEM	C2C-C1C	-4.00	1.45	1.52
3	D	207	HEM	C2C-C1C	-3.98	1.45	1.52
3	L	207	HEM	C2C-C1C	-3.78	1.45	1.52
3	R	208	HEM	C2C-C1C	-3.65	1.45	1.52
3	W	207	HEM	C2C-C1C	-3.53	1.45	1.52
3	G	208	HEM	C2C-C1C	-3.31	1.46	1.52
3	M	207	HEM	C2D-C1D	-2.86	1.42	1.51
3	W	207	HEM	C2D-C1D	-2.55	1.43	1.51
3	T	206	HEM	C2D-C1D	-2.49	1.43	1.51
3	W	207	HEM	C2B-C1B	-2.47	1.43	1.51
3	O	207	HEM	C2D-C1D	-2.43	1.43	1.51
3	R	208	HEM	C2D-C1D	-2.39	1.44	1.51
3	G	208	HEM	C2D-C1D	-2.39	1.44	1.51
3	V	206	HEM	C2B-C1B	-2.35	1.44	1.51
3	I	207	HEM	C2D-C1D	-2.31	1.44	1.51
3	L	207	HEM	C2D-C1D	-2.26	1.44	1.51
3	D	207	HEM	C2B-C1B	-2.14	1.44	1.51
3	M	207	HEM	C2B-C1B	-2.14	1.44	1.51
3	V	206	HEM	C2D-C1D	-2.11	1.45	1.51
3	A	207	HEM	C2D-C1D	-2.10	1.45	1.51
3	D	207	HEM	C2D-C1D	-2.06	1.45	1.51
3	O	207	HEM	C2B-C1B	-2.05	1.45	1.51
3	I	207	HEM	C2B-C1B	-2.03	1.45	1.51
3	E	207	HEM	C2D-C1D	-2.00	1.45	1.51
3	L	207	HEM	FE-NC	2.01	2.03	1.95
3	D	207	HEM	FE-ND	2.01	2.08	1.97
3	W	207	HEM	C1C-NC	2.01	1.38	1.36
3	V	206	HEM	C1C-NC	2.07	1.38	1.36
3	R	208	HEM	C1C-NC	2.10	1.38	1.36
3	I	207	HEM	FE-NC	2.11	2.04	1.95
3	D	207	HEM	C3B-CAB	2.11	1.55	1.51
3	W	207	HEM	FE-ND	2.14	2.08	1.97
3	M	207	HEM	FE-NB	2.14	2.08	1.97
3	E	207	HEM	FE-ND	2.16	2.08	1.97
3	W	207	HEM	FE-NC	2.22	2.04	1.95
3	M	207	HEM	FE-ND	2.26	2.09	1.97
3	A	207	HEM	FE-NC	2.26	2.04	1.95
3	E	207	HEM	C1C-NC	2.26	1.38	1.36
3	M	207	HEM	C1C-NC	2.34	1.38	1.36
3	G	208	HEM	FE-NC	2.36	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	206	HEM	FE-NC	2.44	2.05	1.95
3	V	206	HEM	FE-ND	2.51	2.10	1.97
3	O	207	HEM	FE-ND	2.57	2.11	1.97
3	L	207	HEM	FE-ND	2.60	2.11	1.97
3	O	207	HEM	FE-NC	2.69	2.06	1.95
3	I	207	HEM	FE-NB	2.83	2.12	1.97
3	I	207	HEM	C1C-NC	2.85	1.39	1.36
3	E	207	HEM	FE-NC	3.12	2.08	1.95

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	207	HEM	C3C-CAC-CBC	-5.04	116.72	124.46
3	R	208	HEM	CBA-CAA-C2A	-4.96	103.64	112.53
3	M	207	HEM	CBA-CAA-C2A	-4.66	104.18	112.53
3	V	206	HEM	CBA-CAA-C2A	-4.12	105.14	112.53
3	A	207	HEM	C3B-CAB-CBB	-3.93	118.43	124.46
3	I	207	HEM	CBA-CAA-C2A	-3.84	105.65	112.53
3	T	206	HEM	CBA-CAA-C2A	-3.84	105.65	112.53
3	L	207	HEM	CBA-CAA-C2A	-3.76	105.80	112.53
3	I	207	HEM	C3B-CAB-CBB	-3.69	118.80	124.46
3	R	208	HEM	CBD-CAD-C3D	-3.67	102.87	113.55
3	T	206	HEM	C3C-CAC-CBC	-3.65	118.86	124.46
3	I	207	HEM	CBD-CAD-C3D	-3.63	103.00	113.55
3	R	208	HEM	CAA-C2A-C1A	-3.56	123.15	127.01
3	E	207	HEM	C3C-CAC-CBC	-3.53	119.04	124.46
3	A	207	HEM	CBA-CAA-C2A	-3.52	106.22	112.53
3	W	207	HEM	CBD-CAD-C3D	-3.47	103.44	113.55
3	V	206	HEM	CBD-CAD-C3D	-3.42	103.61	113.55
3	D	207	HEM	CBD-CAD-C3D	-3.34	103.84	113.55
3	G	208	HEM	CBA-CAA-C2A	-3.33	106.56	112.53
3	O	207	HEM	CBD-CAD-C3D	-3.31	103.91	113.55
3	E	207	HEM	CBD-CAD-C3D	-3.24	104.14	113.55
3	D	207	HEM	CBA-CAA-C2A	-3.18	106.83	112.53
3	R	208	HEM	C3C-CAC-CBC	-3.10	119.70	124.46
3	G	208	HEM	CBD-CAD-C3D	-3.07	104.61	113.55
3	L	207	HEM	C3B-CAB-CBB	-3.02	119.83	124.46
3	O	207	HEM	CBA-CAA-C2A	-3.00	107.15	112.53
3	E	207	HEM	CBA-CAA-C2A	-3.00	107.16	112.53
3	D	207	HEM	C3B-CAB-CBB	-2.99	119.86	124.46
3	T	206	HEM	CBD-CAD-C3D	-2.99	104.85	113.55
3	M	207	HEM	CBD-CAD-C3D	-2.90	105.11	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	207	HEM	CAA-CBA-CGA	-2.75	107.71	112.75
3	L	207	HEM	CBD-CAD-C3D	-2.70	105.71	113.55
3	V	206	HEM	C3B-CAB-CBB	-2.68	120.34	124.46
3	I	207	HEM	CAA-C2A-C1A	-2.66	124.12	127.01
3	L	207	HEM	CAA-C2A-C1A	-2.60	124.18	127.01
3	A	207	HEM	CBD-CAD-C3D	-2.57	106.07	113.55
3	V	206	HEM	CAA-C2A-C1A	-2.54	124.25	127.01
3	O	207	HEM	C3B-CAB-CBB	-2.53	120.58	124.46
3	O	207	HEM	CAA-C2A-C1A	-2.36	124.45	127.01
3	O	207	HEM	CMA-C3A-C4A	-2.35	124.47	128.36
3	I	207	HEM	CAA-CBA-CGA	-2.30	108.53	112.75
3	O	207	HEM	C3C-CAC-CBC	-2.24	121.02	124.46
3	O	207	HEM	C3B-C4B-NB	-2.18	107.47	111.63
3	G	208	HEM	C3B-CAB-CBB	-2.12	121.21	124.46
3	M	207	HEM	C3B-CAB-CBB	-2.04	121.32	124.46
3	W	207	HEM	CAA-C2A-C1A	-2.02	124.82	127.01
3	D	207	HEM	CMA-C3A-C4A	-2.01	125.04	128.36
3	O	207	HEM	C3B-C4B-CHC	2.06	126.06	123.16
3	G	208	HEM	C2D-C3D-C4D	2.29	105.38	101.50
3	W	207	HEM	C2D-C3D-C4D	2.42	105.61	101.50
3	G	208	HEM	CMD-C2D-C3D	2.63	126.00	114.35
3	L	207	HEM	CMD-C2D-C3D	2.71	126.33	114.35
3	R	208	HEM	C2D-C3D-C4D	2.73	106.13	101.50
3	L	207	HEM	C2D-C3D-C4D	2.77	106.20	101.50
3	D	207	HEM	CMD-C2D-C3D	2.78	126.63	114.35
3	T	206	HEM	C2D-C3D-C4D	2.78	106.21	101.50
3	V	206	HEM	C2D-C3D-C4D	2.79	106.23	101.50
3	V	206	HEM	CMD-C2D-C3D	2.79	126.69	114.35
3	E	207	HEM	C2D-C3D-C4D	2.80	106.24	101.50
3	E	207	HEM	CMD-C2D-C3D	2.81	126.77	114.35
3	W	207	HEM	CMD-C2D-C3D	2.84	126.91	114.35
3	A	207	HEM	C2D-C3D-C4D	2.85	106.33	101.50
3	M	207	HEM	CMD-C2D-C3D	2.87	127.02	114.35
3	R	208	HEM	CMD-C2D-C3D	2.95	127.41	114.35
3	A	207	HEM	CMD-C2D-C3D	2.96	127.43	114.35
3	D	207	HEM	C2D-C3D-C4D	2.96	106.52	101.50
3	O	207	HEM	C2D-C3D-C4D	2.96	106.52	101.50
3	I	207	HEM	CMC-C2C-C3C	3.02	124.07	116.53
3	I	207	HEM	CMD-C2D-C3D	3.04	127.80	114.35
3	T	206	HEM	CMD-C2D-C3D	3.08	127.99	114.35
3	I	207	HEM	C2D-C3D-C4D	3.09	106.74	101.50
3	R	208	HEM	CMC-C2C-C3C	3.16	124.42	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	207	HEM	CMD-C2D-C3D	3.31	129.00	114.35
3	R	208	HEM	C3B-C4B-CHC	3.36	127.90	123.16
3	M	207	HEM	C2D-C3D-C4D	3.37	107.21	101.50
3	T	206	HEM	CMC-C2C-C3C	3.60	125.53	116.53
3	O	207	HEM	CMC-C2C-C3C	3.62	125.56	116.53
3	O	207	HEM	CAD-C3D-C4D	3.64	125.31	112.47
3	E	207	HEM	CMC-C2C-C3C	3.74	125.87	116.53
3	R	208	HEM	CMB-C2B-C3B	3.80	126.03	116.53
3	V	206	HEM	CMC-C2C-C3C	3.82	126.06	116.53
3	L	207	HEM	CMC-C2C-C3C	3.87	126.20	116.53
3	I	207	HEM	CAD-C3D-C4D	3.93	126.34	112.47
3	A	207	HEM	CAD-C3D-C4D	3.96	126.43	112.47
3	E	207	HEM	CAD-C3D-C4D	4.08	126.84	112.47
3	M	207	HEM	CAD-C3D-C2D	4.09	124.98	113.22
3	R	208	HEM	CAD-C3D-C4D	4.12	127.02	112.47
3	G	208	HEM	CAD-C3D-C2D	4.16	125.16	113.22
3	D	207	HEM	CAD-C3D-C4D	4.23	127.40	112.47
3	T	206	HEM	CAD-C3D-C2D	4.26	125.46	113.22
3	W	207	HEM	CAD-C3D-C4D	4.30	127.63	112.47
3	V	206	HEM	CAD-C3D-C4D	4.34	127.77	112.47
3	M	207	HEM	CAD-C3D-C4D	4.34	127.78	112.47
3	L	207	HEM	CAD-C3D-C4D	4.38	127.93	112.47
3	L	207	HEM	CAD-C3D-C2D	4.40	125.86	113.22
3	V	206	HEM	CAD-C3D-C2D	4.40	125.88	113.22
3	D	207	HEM	CAD-C3D-C2D	4.47	126.06	113.22
3	T	206	HEM	CAD-C3D-C4D	4.48	128.29	112.47
3	A	207	HEM	CMB-C2B-C3B	4.70	128.26	116.53
3	W	207	HEM	CAD-C3D-C2D	4.70	126.72	113.22
3	I	207	HEM	CAD-C3D-C2D	4.72	126.80	113.22
3	R	208	HEM	CAD-C3D-C2D	4.73	126.82	113.22
3	T	206	HEM	CMB-C2B-C3B	4.73	128.35	116.53
3	E	207	HEM	CAD-C3D-C2D	4.75	126.88	113.22
3	L	207	HEM	CMB-C2B-C3B	4.78	128.47	116.53
3	I	207	HEM	CMB-C2B-C3B	4.78	128.47	116.53
3	G	208	HEM	CAD-C3D-C4D	4.80	129.40	112.47
3	A	207	HEM	CAD-C3D-C2D	4.87	127.23	113.22
3	D	207	HEM	CMB-C2B-C3B	4.90	128.76	116.53
3	W	207	HEM	CMC-C2C-C3C	4.97	128.95	116.53
3	E	207	HEM	CMB-C2B-C3B	5.00	129.02	116.53
3	O	207	HEM	CAD-C3D-C2D	5.19	128.14	113.22
3	M	207	HEM	CMB-C2B-C3B	5.21	129.54	116.53
3	O	207	HEM	CMB-C2B-C3B	5.29	129.75	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	206	HEM	CMB-C2B-C3B	5.33	129.83	116.53
3	G	208	HEM	CMB-C2B-C3B	5.34	129.85	116.53
3	G	208	HEM	CMC-C2C-C3C	5.39	129.99	116.53
3	W	207	HEM	CMB-C2B-C3B	5.54	130.36	116.53
3	D	207	HEM	CMC-C2C-C3C	5.63	130.58	116.53
3	M	207	HEM	CMC-C2C-C3C	5.71	130.79	116.53
3	A	207	HEM	CMC-C2C-C3C	5.91	131.29	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	207	HEM	1	0
3	D	207	HEM	1	0
5	D	208	SO4	1	0
3	E	207	HEM	1	0
5	F	207	SO4	1	0
3	G	208	HEM	1	0
3	I	207	HEM	2	0
5	I	208	SO4	2	0
3	L	207	HEM	5	0
3	M	207	HEM	1	0
3	O	207	HEM	2	0
3	R	208	HEM	4	0
3	T	206	HEM	1	0
3	V	206	HEM	2	0
3	W	207	HEM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	154/158 (97%)	-0.68	0 100 100	20, 25, 36, 45	0
1	B	154/158 (97%)	-0.64	0 100 100	20, 25, 36, 45	0
1	C	155/158 (98%)	-0.67	0 100 100	19, 23, 34, 45	0
1	D	154/158 (97%)	-0.71	0 100 100	18, 23, 35, 42	0
1	E	154/158 (97%)	-0.69	0 100 100	17, 22, 34, 40	0
1	F	154/158 (97%)	-0.71	0 100 100	17, 23, 34, 42	0
1	G	154/158 (97%)	-0.70	0 100 100	19, 23, 35, 43	0
1	H	155/158 (98%)	-0.66	0 100 100	19, 25, 37, 47	0
1	I	154/158 (97%)	-0.68	0 100 100	17, 22, 32, 43	0
1	J	154/158 (97%)	-0.68	0 100 100	17, 22, 33, 46	0
1	K	154/158 (97%)	-0.69	0 100 100	17, 22, 31, 43	0
1	L	154/158 (97%)	-0.66	0 100 100	18, 23, 35, 42	0
1	M	154/158 (97%)	-0.72	0 100 100	17, 22, 32, 41	0
1	N	154/158 (97%)	-0.68	0 100 100	17, 22, 34, 41	0
1	O	154/158 (97%)	-0.68	0 100 100	17, 23, 33, 41	0
1	P	154/158 (97%)	-0.65	0 100 100	17, 21, 32, 40	0
1	Q	154/158 (97%)	-0.70	0 100 100	16, 21, 33, 41	0
1	R	155/158 (98%)	-0.67	0 100 100	17, 22, 34, 55	0
1	S	154/158 (97%)	-0.65	0 100 100	16, 21, 32, 41	0
1	T	154/158 (97%)	-0.69	0 100 100	16, 21, 33, 39	0
1	U	154/158 (97%)	-0.68	0 100 100	17, 22, 33, 40	0
1	V	154/158 (97%)	-0.60	1 (0%) 90 90	17, 22, 35, 44	0
1	W	155/158 (98%)	-0.68	0 100 100	19, 25, 35, 45	0
1	X	154/158 (97%)	-0.66	1 (0%) 90 90	18, 23, 35, 49	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3700/3792 (97%)	-0.68	2 (0%)	95	95	16, 23, 34, 55	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	3	GLY	3.2
1	X	3	GLY	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE2	H	202	1/1	0.87	0.33	13.76	59,59,59,59	0
2	FE2	V	203	1/1	0.96	0.25	12.08	54,54,54,54	0
2	FE2	O	203	1/1	0.92	0.24	8.74	56,56,56,56	0
2	FE2	S	202	1/1	0.98	0.21	8.46	27,27,27,27	0
5	SO4	K	207	5/5	0.95	0.14	8.11	48,54,54,64	0
2	FE2	M	203	1/1	0.88	0.22	8.06	49,49,49,49	0
2	FE2	Q	204	1/1	0.89	0.26	7.47	52,52,52,52	0
2	FE2	R	204	1/1	0.95	0.32	7.35	52,52,52,52	0
2	FE2	P	203	1/1	0.94	0.32	6.32	58,58,58,58	0
2	FE2	L	203	1/1	0.90	0.20	6.24	48,48,48,48	0
2	FE2	J	204	1/1	0.93	0.23	5.58	48,48,48,48	0
5	SO4	D	208	5/5	0.94	0.13	5.22	47,49,51,64	0
2	FE2	B	204	1/1	0.93	0.26	5.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE2	U	203	1/1	0.92	0.26	5.01	53,53,53,53	0
5	SO4	A	209	5/5	0.96	0.13	4.63	45,52,56,64	0
2	FE2	N	204	1/1	0.96	0.20	4.60	48,48,48,48	0
2	FE2	X	202	1/1	0.96	0.24	4.29	49,49,49,49	0
2	FE2	S	203	1/1	0.92	0.19	4.09	52,52,52,52	0
2	FE2	W	203	1/1	0.92	0.20	4.02	54,54,54,54	0
2	FE2	T	202	1/1	0.92	0.20	3.96	47,47,47,47	0
2	FE2	C	204	1/1	0.86	0.22	3.82	50,50,50,50	0
2	FE2	F	203	1/1	0.90	0.19	3.77	48,48,48,48	0
2	FE2	J	202	1/1	0.98	0.16	3.29	27,27,27,27	0
4	K	E	208	1/1	0.99	0.12	2.75	41,41,41,41	0
2	FE2	Q	203	1/1	0.98	0.13	2.63	28,28,28,28	0
2	FE2	A	205	1/1	0.94	0.19	2.50	54,54,54,54	0
4	K	G	209	1/1	0.99	0.11	2.37	41,41,41,41	0
5	SO4	B	209	5/5	0.94	0.11	2.35	44,48,54,62	0
3	HEM	R	208	43/43	0.93	0.13	2.33	17,22,33,37	0
3	HEM	O	207	43/43	0.93	0.12	1.79	17,22,32,37	0
3	HEM	A	207	43/43	0.94	0.12	1.69	19,26,35,39	0
2	FE2	B	203	1/1	0.99	0.15	1.56	32,32,32,32	0
3	HEM	T	206	43/43	0.94	0.11	1.39	15,19,32,35	0
2	FE2	D	204	1/1	0.94	0.17	1.36	50,50,50,50	0
3	HEM	W	207	43/43	0.94	0.12	1.34	18,23,33,39	0
3	HEM	D	207	43/43	0.94	0.12	1.27	19,23,36,37	0
3	HEM	V	206	43/43	0.93	0.12	1.11	16,21,32,35	0
5	SO4	I	208	5/5	0.91	0.12	0.63	46,49,51,67	0
3	HEM	L	207	43/43	0.93	0.11	0.57	17,21,33,35	0
3	HEM	M	207	43/43	0.93	0.12	0.56	15,22,32,40	0
3	HEM	G	208	43/43	0.94	0.11	0.56	18,23,37,45	0
5	SO4	F	207	5/5	0.95	0.10	0.43	42,44,58,63	0
3	HEM	E	207	43/43	0.95	0.11	0.25	17,23,32,39	0
3	HEM	I	207	43/43	0.94	0.10	0.25	18,22,33,38	0
2	FE2	P	202	1/1	0.97	0.12	0.15	27,27,27,27	0
5	SO4	X	205	5/5	0.94	0.10	-0.11	45,48,58,64	0
4	K	B	208	1/1	0.99	0.08	-1.66	42,42,42,42	0
5	SO4	R	209	5/5	0.97	0.08	-1.68	44,47,54,63	0
4	K	N	209	1/1	0.99	0.07	-2.75	38,38,38,38	0
4	K	A	208	1/1	0.98	0.06	-3.17	40,40,40,40	0
4	K	C	208	1/1	1.00	0.05	-3.61	35,35,35,35	0
2	FE2	C	207	1/1	0.76	0.24	-	58,58,58,58	0
2	FE2	M	202	1/1	0.99	0.11	-	25,25,25,25	0
2	FE2	C	202	1/1	0.99	0.12	-	26,26,26,26	0
2	FE2	D	206	1/1	0.83	0.22	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE2	I	201	1/1	0.98	0.12	-	27,27,27,27	0
2	FE2	D	203	1/1	0.99	0.11	-	32,32,32,32	0
2	FE2	G	205	1/1	0.99	0.13	-	35,35,35,35	0
2	FE2	V	204	1/1	0.81	0.49	-	75,75,75,75	0
2	FE2	V	201	1/1	0.97	0.12	-	27,27,27,27	0
2	FE2	A	206	1/1	0.86	0.22	-	59,59,59,59	0
2	FE2	O	202	1/1	0.97	0.14	-	31,31,31,31	0
2	FE2	L	201	1/1	0.99	0.09	-	25,25,25,25	0
2	FE2	P	201	1/1	0.99	0.12	-	25,25,25,25	0
2	FE2	D	202	1/1	0.99	0.12	-	25,25,25,25	0
2	FE2	A	202	1/1	0.99	0.09	-	26,26,26,26	0
2	FE2	A	203	1/1	0.99	0.12	-	33,33,33,33	0
2	FE2	B	206	1/1	0.81	0.33	-	68,68,68,68	0
2	FE2	N	208	1/1	0.94	0.17	-	59,59,59,59	0
2	FE2	M	204	1/1	1.00	0.11	-	28,28,28,28	0
2	FE2	I	202	1/1	0.99	0.10	-	24,24,24,24	0
2	FE2	I	204	1/1	0.92	0.23	-	44,44,44,44	0
2	FE2	B	205	1/1	0.99	0.15	-	36,36,36,36	0
2	FE2	N	201	1/1	0.99	0.13	-	28,28,28,28	0
2	FE2	B	201	1/1	0.99	0.11	-	26,26,26,26	0
2	FE2	K	206	1/1	0.90	0.28	-	63,63,63,63	0
2	FE2	W	205	1/1	0.77	0.34	-	73,73,73,73	0
2	FE2	D	201	1/1	0.99	0.12	-	27,27,27,27	0
2	FE2	M	201	1/1	0.98	0.14	-	29,29,29,29	0
2	FE2	Q	205	1/1	0.57	0.28	-	69,69,69,69	0
2	FE2	E	201	1/1	0.99	0.12	-	26,26,26,26	0
2	FE2	B	202	1/1	0.98	0.09	-	29,29,29,29	0
2	FE2	E	204	1/1	0.95	0.24	-	50,50,50,50	0
2	FE2	Q	202	1/1	1.00	0.12	-	27,27,27,27	0
2	FE2	E	202	1/1	0.95	0.15	-	29,29,29,29	0
2	FE2	R	203	1/1	0.98	0.11	-	34,34,34,34	0
2	FE2	N	206	1/1	0.74	0.35	-	71,71,71,71	0
2	FE2	C	205	1/1	0.99	0.10	-	30,30,30,30	0
2	FE2	K	201	1/1	0.98	0.09	-	23,23,23,23	0
2	FE2	N	207	1/1	0.74	0.28	-	66,66,66,66	0
2	FE2	X	204	1/1	0.96	0.20	-	60,60,60,60	0
2	FE2	T	204	1/1	0.64	0.24	-	68,68,68,68	0
2	FE2	G	202	1/1	0.98	0.14	-	29,29,29,29	0
2	FE2	A	201	1/1	0.99	0.08	-	29,29,29,29	0
2	FE2	R	201	1/1	0.99	0.08	-	24,24,24,24	0
2	FE2	C	201	1/1	0.99	0.06	-	24,24,24,24	0
2	FE2	R	205	1/1	0.93	0.23	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE2	H	201	1/1	0.99	0.15	-	27,27,27,27	0
2	FE2	V	202	1/1	0.98	0.14	-	32,32,32,32	0
2	FE2	H	204	1/1	0.90	0.38	-	71,71,71,71	0
2	FE2	L	206	1/1	0.78	0.29	-	65,65,65,65	0
2	FE2	I	205	1/1	0.84	0.40	-	76,76,76,76	0
2	FE2	E	205	1/1	0.98	0.12	-	31,31,31,31	0
2	FE2	T	201	1/1	0.99	0.13	-	24,24,24,24	0
2	FE2	U	201	1/1	0.98	0.13	-	27,27,27,27	0
2	FE2	N	205	1/1	0.99	0.08	-	23,23,23,23	0
2	FE2	J	206	1/1	0.89	0.31	-	62,62,62,62	0
2	FE2	K	202	1/1	0.96	0.15	-	28,28,28,28	0
2	FE2	G	207	1/1	0.89	0.27	-	62,62,62,62	0
2	FE2	G	206	1/1	0.76	0.28	-	68,68,68,68	0
2	FE2	S	201	1/1	1.00	0.07	-	21,21,21,21	0
2	FE2	T	203	1/1	0.98	0.12	-	30,30,30,30	0
2	FE2	H	205	1/1	0.85	0.21	-	61,61,61,61	0
2	FE2	K	204	1/1	0.88	0.19	-	49,49,49,49	0
2	FE2	P	206	1/1	0.95	0.23	-	55,55,55,55	0
2	FE2	A	204	1/1	0.98	0.11	-	36,36,36,36	0
2	FE2	W	204	1/1	0.91	0.33	-	65,65,65,65	0
2	FE2	U	205	1/1	0.86	0.35	-	71,71,71,71	0
2	FE2	C	206	1/1	0.69	0.23	-	70,70,70,70	0
2	FE2	F	202	1/1	0.97	0.13	-	30,30,30,30	0
2	FE2	G	204	1/1	0.96	0.16	-	43,43,43,43	0
2	FE2	M	206	1/1	0.94	0.24	-	61,61,61,61	0
2	FE2	B	207	1/1	0.81	0.27	-	64,64,64,64	0
2	FE2	E	203	1/1	0.99	0.11	-	26,26,26,26	0
2	FE2	W	206	1/1	0.87	0.28	-	60,60,60,60	0
2	FE2	R	206	1/1	0.85	0.34	-	70,70,70,70	0
2	FE2	W	202	1/1	0.99	0.14	-	39,39,39,39	0
2	FE2	S	205	1/1	0.90	0.19	-	51,51,51,51	0
2	FE2	I	203	1/1	0.96	0.14	-	40,40,40,40	0
2	FE2	D	205	1/1	0.86	0.30	-	65,65,65,65	0
2	FE2	O	201	1/1	0.99	0.11	-	25,25,25,25	0
2	FE2	H	203	1/1	0.98	0.13	-	35,35,35,35	0
2	FE2	F	205	1/1	0.81	0.40	-	72,72,72,72	0
2	FE2	C	203	1/1	0.99	0.13	-	30,30,30,30	0
2	FE2	T	205	1/1	0.88	0.29	-	68,68,68,68	0
2	FE2	P	205	1/1	0.82	0.34	-	73,73,73,73	0
2	FE2	J	201	1/1	0.99	0.10	-	26,26,26,26	0
2	FE2	Q	206	1/1	0.93	0.24	-	58,58,58,58	0
2	FE2	R	207	1/1	0.89	0.17	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE2	G	201	1/1	0.99	0.07	-	26,26,26,26	0
2	FE2	N	202	1/1	0.99	0.11	-	24,24,24,24	0
2	FE2	V	205	1/1	0.80	0.21	-	67,67,67,67	0
2	FE2	L	205	1/1	0.91	0.50	-	69,69,69,69	0
2	FE2	R	202	1/1	0.99	0.15	-	28,28,28,28	0
2	FE2	X	203	1/1	0.98	0.14	-	35,35,35,35	0
2	FE2	J	205	1/1	0.93	0.33	-	61,61,61,61	0
2	FE2	U	206	1/1	0.92	0.32	-	63,63,63,63	0
2	FE2	Q	201	1/1	0.99	0.14	-	33,33,33,33	0
2	FE2	F	204	1/1	0.98	0.08	-	25,25,25,25	0
2	FE2	I	206	1/1	0.87	0.16	-	57,57,57,57	0
2	FE2	G	203	1/1	0.99	0.09	-	26,26,26,26	0
2	FE2	F	201	1/1	0.99	0.11	-	29,29,29,29	0
2	FE2	N	203	1/1	0.99	0.11	-	26,26,26,26	0
2	FE2	X	201	1/1	0.99	0.14	-	27,27,27,27	0
2	FE2	U	204	1/1	0.65	0.39	-	74,74,74,74	0
2	FE2	K	203	1/1	0.99	0.15	-	27,27,27,27	0
2	FE2	M	205	1/1	0.90	0.32	-	57,57,57,57	0
2	FE2	U	202	1/1	0.99	0.19	-	33,33,33,33	0
2	FE2	L	202	1/1	0.98	0.12	-	27,27,27,27	0
2	FE2	O	206	1/1	0.91	0.17	-	57,57,57,57	0
2	FE2	W	201	1/1	0.98	0.19	-	32,32,32,32	0
2	FE2	K	205	1/1	0.74	0.41	-	72,72,72,72	0
2	FE2	J	203	1/1	0.99	0.14	-	36,36,36,36	0
2	FE2	F	206	1/1	0.83	0.28	-	64,64,64,64	0
2	FE2	E	206	1/1	0.73	0.25	-	66,66,66,66	0
2	FE2	P	204	1/1	0.98	0.17	-	47,47,47,47	0
2	FE2	S	204	1/1	0.99	0.11	-	31,31,31,31	0
2	FE2	L	204	1/1	0.98	0.12	-	35,35,35,35	0
2	FE2	O	204	1/1	0.99	0.13	-	32,32,32,32	0
2	FE2	O	205	1/1	0.91	0.37	-	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.