



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:16 PM GMT

PDB ID : 5D8X
Title : 1.50Å resolution structure of BfrB (L68A E81A) from *Pseudomonas aeruginosa*
Authors : Lovell, S.; Battaile, K.P.; Wang, Y.; Yao, H.; Rivera, M.
Deposited on : 2015-08-18
Resolution : 1.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

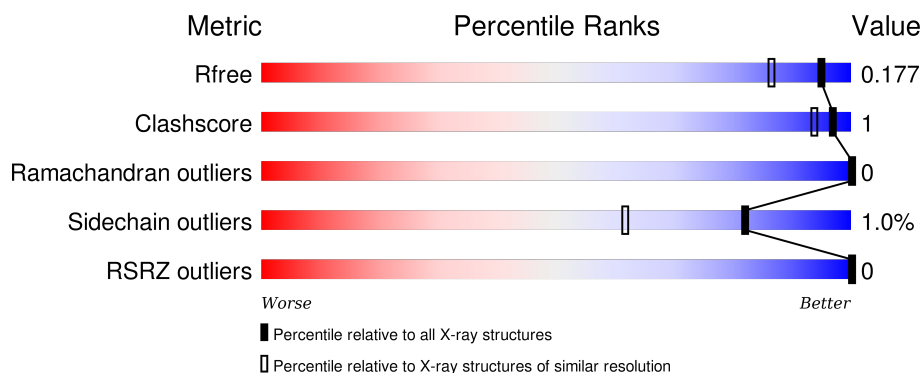
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	158	<div> <div>95%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	B	158	<div> <div>95%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	C	158	<div> <div>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	D	158	<div> <div>95%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	E	158	<div> <div>97%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	158	97% ..
1	G	158	96% ...
1	H	158	98% ..
1	I	158	97% ..
1	J	158	96% ..
1	K	158	96% ..
1	L	158	95% ..
1	M	158	95% ..
1	N	158	94% 5% .
1	O	158	96% ...
1	P	158	95% ..
1	Q	158	96% ..
1	R	158	97% ...
1	S	158	97% ..
1	T	158	95% ...
1	U	158	95% ..
1	V	158	96% ..
1	W	158	97% ...
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	HEM	A	201	-	-	-	X
2	HEM	C	202	-	-	-	X
2	HEM	E	201	-	-	-	X
2	HEM	G	201	-	-	-	X
2	HEM	I	203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEM	K	201	-	-	-	X
2	HEM	M	201	-	-	-	X
2	HEM	O	202	-	-	-	X
2	HEM	Q	201	-	-	-	X
2	HEM	S	204	-	-	-	X
2	HEM	U	201	-	-	-	X
2	HEM	W	201	-	-	-	X
3	K	D	201	-	-	-	X
4	MRD	A	203	-	-	-	X
4	MRD	B	202	-	-	-	X
4	MRD	D	202	-	-	-	X
4	MRD	E	203	-	-	-	X
4	MRD	F	201	-	-	-	X
4	MRD	G	203	-	-	-	X
4	MRD	H	201	-	-	-	X
4	MRD	I	201	-	-	-	X
4	MRD	J	202	-	-	-	X
4	MRD	K	202	-	-	-	X
4	MRD	M	202	-	-	-	X
4	MRD	M	203	-	-	-	X
4	MRD	N	201	-	-	-	X
4	MRD	N	202	-	-	-	X
4	MRD	O	201	-	-	-	X
4	MRD	P	201	-	-	-	X
4	MRD	R	202	-	-	-	X
4	MRD	S	202	-	-	-	X
4	MRD	T	201	-	-	-	X
4	MRD	U	202	-	-	-	X
4	MRD	V	201	-	-	-	X
4	MRD	W	202	-	-	-	X
4	MRD	X	201	-	-	-	X
6	MPD	C	201	-	-	-	X
6	MPD	I	202	-	-	-	X
6	MPD	J	201	-	-	-	X
6	MPD	K	203	-	-	-	X
6	MPD	L	202	-	-	-	X
6	MPD	Q	202	-	-	-	X
6	MPD	Q	203	-	-	-	X
6	MPD	R	201	-	-	-	X
6	MPD	S	201	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35653 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	5	0
			1293	817	220	249	7			
1	B	156	Total	C	N	O	S	0	2	0
			1270	802	216	245	7			
1	C	156	Total	C	N	O	S	0	3	0
			1278	807	218	246	7			
1	D	156	Total	C	N	O	S	0	3	0
			1281	809	219	246	7			
1	E	156	Total	C	N	O	S	0	2	0
			1271	802	217	245	7			
1	F	156	Total	C	N	O	S	0	2	0
			1269	802	218	242	7			
1	G	156	Total	C	N	O	S	0	4	0
			1285	812	219	247	7			
1	H	156	Total	C	N	O	S	0	1	0
			1264	798	216	243	7			
1	I	156	Total	C	N	O	S	0	2	0
			1269	801	217	244	7			
1	J	156	Total	C	N	O	S	0	1	0
			1260	796	215	242	7			
1	K	156	Total	C	N	O	S	0	1	0
			1267	800	217	243	7			
1	L	156	Total	C	N	O	S	0	2	0
			1277	807	219	244	7			
1	M	156	Total	C	N	O	S	0	3	0
			1281	810	218	246	7			
1	N	156	Total	C	N	O	S	0	2	0
			1272	803	217	245	7			
1	O	156	Total	C	N	O	S	0	4	0
			1281	809	218	247	7			
1	P	156	Total	C	N	O	S	0	2	0
			1272	803	218	244	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	156	Total	C	N	O	S	0	2	0
			1272	803	217	245	7			
1	R	156	Total	C	N	O	S	0	2	0
			1273	804	218	244	7			
1	S	156	Total	C	N	O	S	0	2	0
			1275	805	218	245	7			
1	T	156	Total	C	N	O	S	0	2	0
			1272	803	218	244	7			
1	U	156	Total	C	N	O	S	0	2	0
			1266	800	216	243	7			
1	V	156	Total	C	N	O	S	0	2	0
			1272	803	218	244	7			
1	W	156	Total	C	N	O	S	0	3	0
			1276	806	218	245	7			
1	X	156	Total	C	N	O	S	0	2	0
			1272	803	217	245	7			

There are 48 discrepancies between the modelled and reference sequences:

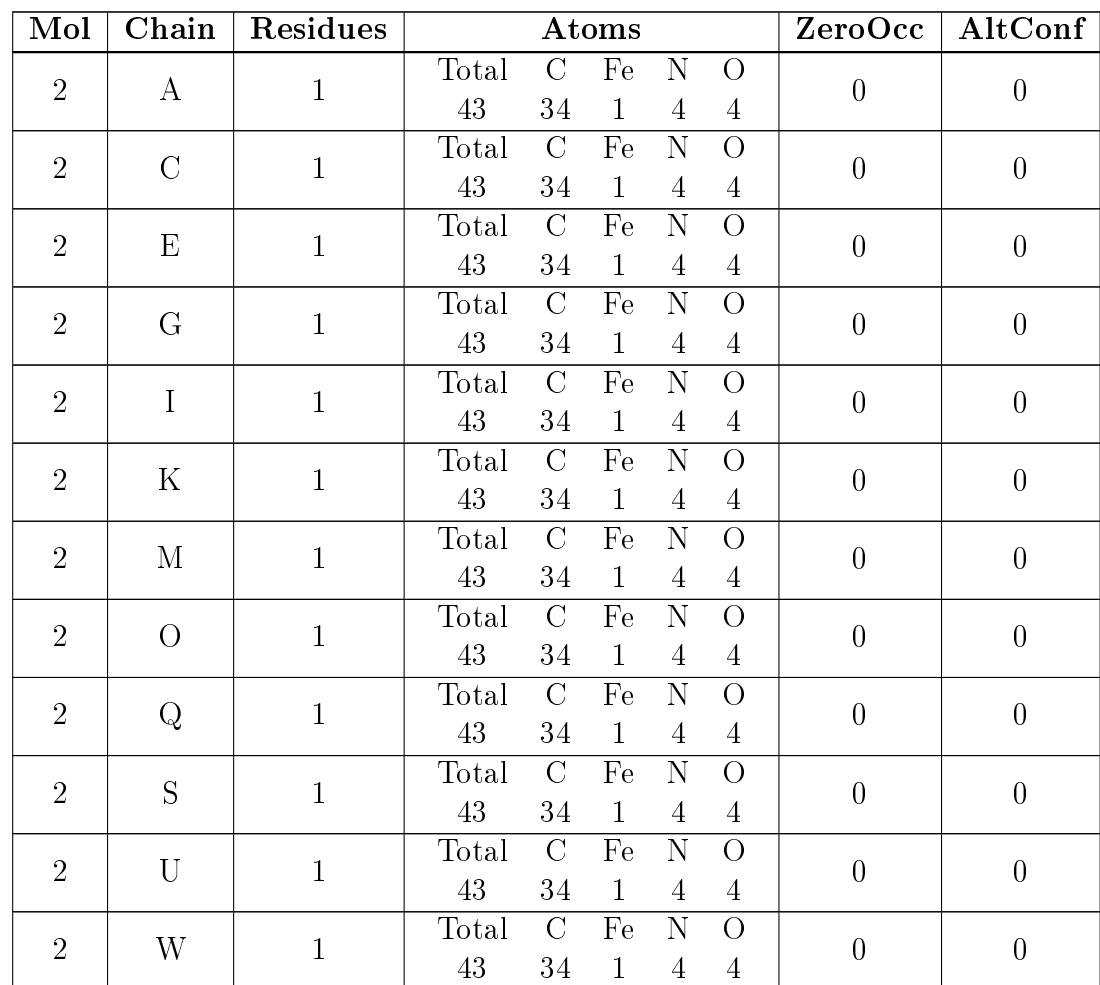
Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	LEU	engineered mutation	UNP Q9HY79
A	81	ALA	GLU	engineered mutation	UNP Q9HY79
B	68	ALA	LEU	engineered mutation	UNP Q9HY79
B	81	ALA	GLU	engineered mutation	UNP Q9HY79
C	68	ALA	LEU	engineered mutation	UNP Q9HY79
C	81	ALA	GLU	engineered mutation	UNP Q9HY79
D	68	ALA	LEU	engineered mutation	UNP Q9HY79
D	81	ALA	GLU	engineered mutation	UNP Q9HY79
E	68	ALA	LEU	engineered mutation	UNP Q9HY79
E	81	ALA	GLU	engineered mutation	UNP Q9HY79
F	68	ALA	LEU	engineered mutation	UNP Q9HY79
F	81	ALA	GLU	engineered mutation	UNP Q9HY79
G	68	ALA	LEU	engineered mutation	UNP Q9HY79
G	81	ALA	GLU	engineered mutation	UNP Q9HY79
H	68	ALA	LEU	engineered mutation	UNP Q9HY79
H	81	ALA	GLU	engineered mutation	UNP Q9HY79
I	68	ALA	LEU	engineered mutation	UNP Q9HY79
I	81	ALA	GLU	engineered mutation	UNP Q9HY79
J	68	ALA	LEU	engineered mutation	UNP Q9HY79
J	81	ALA	GLU	engineered mutation	UNP Q9HY79
K	68	ALA	LEU	engineered mutation	UNP Q9HY79
K	81	ALA	GLU	engineered mutation	UNP Q9HY79
L	68	ALA	LEU	engineered mutation	UNP Q9HY79

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Chain	Residue	Modelled	Actual	Comment	Reference
L	81	ALA	GLU	engineered mutation	UNP Q9HY79
M	68	ALA	LEU	engineered mutation	UNP Q9HY79
M	81	ALA	GLU	engineered mutation	UNP Q9HY79
N	68	ALA	LEU	engineered mutation	UNP Q9HY79
N	81	ALA	GLU	engineered mutation	UNP Q9HY79
O	68	ALA	LEU	engineered mutation	UNP Q9HY79
O	81	ALA	GLU	engineered mutation	UNP Q9HY79
P	68	ALA	LEU	engineered mutation	UNP Q9HY79
P	81	ALA	GLU	engineered mutation	UNP Q9HY79
Q	68	ALA	LEU	engineered mutation	UNP Q9HY79
Q	81	ALA	GLU	engineered mutation	UNP Q9HY79
R	68	ALA	LEU	engineered mutation	UNP Q9HY79
R	81	ALA	GLU	engineered mutation	UNP Q9HY79
S	68	ALA	LEU	engineered mutation	UNP Q9HY79
S	81	ALA	GLU	engineered mutation	UNP Q9HY79
T	68	ALA	LEU	engineered mutation	UNP Q9HY79
T	81	ALA	GLU	engineered mutation	UNP Q9HY79
U	68	ALA	LEU	engineered mutation	UNP Q9HY79
U	81	ALA	GLU	engineered mutation	UNP Q9HY79
V	68	ALA	LEU	engineered mutation	UNP Q9HY79
V	81	ALA	GLU	engineered mutation	UNP Q9HY79
W	68	ALA	LEU	engineered mutation	UNP Q9HY79
W	81	ALA	GLU	engineered mutation	UNP Q9HY79
X	68	ALA	LEU	engineered mutation	UNP Q9HY79
X	81	ALA	GLU	engineered mutation	UNP Q9HY79

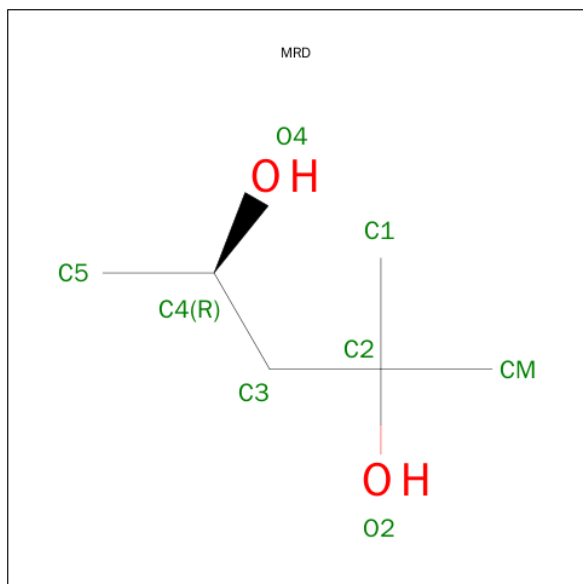
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0
3	A	1	Total K 1 1	0	0
3	L	1	Total K 1 1	0	0

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	O	1	Total	C	O	0	0
			8	6	2		
4	P	1	Total	C	O	0	0
			8	6	2		
4	R	1	Total	C	O	0	0
			8	6	2		
4	S	1	Total	C	O	0	0
			8	6	2		
4	T	1	Total	C	O	0	0
			8	6	2		
4	U	1	Total	C	O	0	0
			8	6	2		
4	V	1	Total	C	O	0	0
			8	6	2		
4	W	1	Total	C	O	0	0
			8	6	2		
4	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	2	Total Na 2 2	0	0
5	J	1	Total Na 1 1	0	0
5	D	2	Total Na 2 2	0	0
5	K	1	Total Na 1 1	0	0
5	E	2	Total Na 2 2	0	0
5	H	1	Total Na 1 1	0	0
5	B	2	Total Na 2 2	0	0
5	I	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	V	1	Total Na 1 1	0	0
5	A	2	Total Na 2 2	0	0
5	T	1	Total Na 1 1	0	0
5	N	1	Total Na 1 1	0	0
5	R	1	Total Na 1 1	0	0
5	L	2	Total Na 2 2	0	0
5	S	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0
5	M	1	Total Na 1 1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			8	6	2		
6	I	1	Total	C	O	0	0
			8	6	2		
6	J	1	Total	C	O	0	0
			8	6	2		
6	K	1	Total	C	O	0	0
			8	6	2		
6	L	1	Total	C	O	0	0
			8	6	2		
6	Q	1	Total	C	O	0	0
			8	6	2		
6	Q	1	Total	C	O	0	0
			8	6	2		
6	R	1	Total	C	O	0	0
			8	6	2		
6	S	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	179	Total	O	0	0
			179	179		
7	B	180	Total	O	0	0
			180	180		
7	C	182	Total	O	0	0
			182	182		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	183	Total 183	O 183	0	0
7	E	178	Total 178	O 178	0	0
7	F	167	Total 167	O 167	0	0
7	G	181	Total 181	O 181	0	0
7	H	184	Total 184	O 184	0	0
7	I	171	Total 171	O 171	0	0
7	J	165	Total 165	O 165	0	0
7	K	175	Total 175	O 175	0	0
7	L	173	Total 173	O 173	0	0
7	M	195	Total 195	O 195	0	0
7	N	191	Total 191	O 191	0	0
7	O	177	Total 177	O 177	0	0
7	P	163	Total 163	O 163	0	0
7	Q	200	Total 200	O 200	0	0
7	R	166	Total 166	O 166	0	0
7	S	188	Total 188	O 188	0	0
7	T	181	Total 181	O 181	0	0
7	U	168	Total 168	O 168	0	0
7	V	172	Total 172	O 172	0	0
7	W	176	Total 176	O 176	0	0
7	X	180	Total 180	O 180	0	0

3 Residue-property plots

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: Ferroxidase

Chain A: 



- Molecule 1: Ferroxidase

Chain B: 



- Molecule 1: Ferroxidase

Chain C: 



- Molecule 1: Ferroxidase

Chain D: 



- Molecule 1: Ferroxidase

Chain E: 



- Molecule 1: Ferroxidase

Chain F: 



- Molecule 1: Ferroxidase

Chain G:  96%



- Molecule 1: Ferroxidase

Chain H:  98%



- Molecule 1: Ferroxidase

Chain I:  97%



- Molecule 1: Ferroxidase

Chain J:  96%



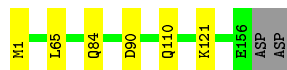
- Molecule 1: Ferroxidase

Chain K:  96%



- Molecule 1: Ferroxidase

Chain L:  95%



- Molecule 1: Ferroxidase

Chain M:  95%



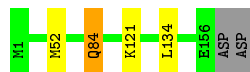
- Molecule 1: Ferroxidase

Chain N:  94% 5%



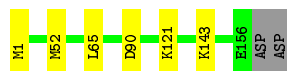
- Molecule 1: Ferroxidase

Chain O:  96%



- Molecule 1: Ferroxidase

Chain P:  95%



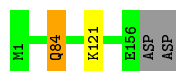
- Molecule 1: Ferroxidase

Chain Q:  96%



- Molecule 1: Ferroxidase

Chain R:  97%



- Molecule 1: Ferroxidase

Chain S:  97%



- Molecule 1: Ferroxidase

Chain T:  95%



- Molecule 1: Ferroxidase

Chain U:  95%



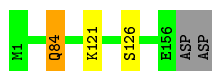
- Molecule 1: Ferroxidase

Chain V:  96% ..



- Molecule 1: Ferroxidase

Chain W:  97% ...



- Molecule 1: Ferroxidase

Chain X:  96% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	125.27Å 125.27Å 274.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.01 – 1.50 46.65 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.01-1.50) 99.9 (46.65-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.50Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.152 , 0.173 0.157 , 0.177	Depositor DCC
R_{free} test set	39693 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
Estimated twinning fraction	0.005 for -h,-k,l 0.019 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 770228 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, NA, MPD, K, 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	0.43	0/1329	0.57	0/1791
1	B	0.39	0/1297	0.55	1/1750 (0.1%)
1	C	0.38	0/1308	0.55	0/1764
1	D	0.40	0/1311	0.55	1/1767 (0.1%)
1	E	0.42	0/1298	0.56	0/1751
1	F	0.41	0/1296	0.57	1/1748 (0.1%)
1	G	0.37	0/1318	0.56	1/1777 (0.1%)
1	H	0.38	0/1288	0.55	0/1738
1	I	0.39	0/1296	0.56	1/1749 (0.1%)
1	J	0.40	0/1284	0.55	0/1733
1	K	0.38	0/1291	0.55	0/1741
1	L	0.40	0/1304	0.58	1/1757 (0.1%)
1	M	0.41	0/1311	0.58	1/1767 (0.1%)
1	N	0.42	0/1299	0.56	1/1752 (0.1%)
1	O	0.40	0/1314	0.57	0/1773
1	P	0.38	0/1299	0.55	1/1752 (0.1%)
1	Q	0.40	0/1299	0.55	0/1752
1	R	0.39	0/1300	0.57	0/1753
1	S	0.39	0/1302	0.55	0/1755
1	T	0.40	0/1299	0.58	1/1752 (0.1%)
1	U	0.40	0/1293	0.53	1/1745 (0.1%)
1	V	0.40	0/1299	0.55	0/1752
1	W	0.38	0/1306	0.56	0/1762
1	X	0.39	0/1299	0.55	0/1752
All	All	0.40	0/31240	0.56	11/42133 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	90	ASP	CB-CG-OD1	6.44	124.10	118.30
1	M	90	ASP	CB-CG-OD1	6.16	123.84	118.30
1	P	90	ASP	CB-CG-OD1	5.99	123.69	118.30
1	F	90	ASP	CB-CG-OD1	5.90	123.61	118.30
1	L	90	ASP	CB-CG-OD1	5.69	123.42	118.30

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	1293	0	1270	4	0
1	B	1270	0	1232	2	0
1	C	1278	0	1247	3	0
1	D	1281	0	1256	2	0
1	E	1271	0	1237	2	0
1	F	1269	0	1239	0	0
1	G	1285	0	1257	3	0
1	H	1264	0	1226	0	0
1	I	1269	0	1232	0	0
1	J	1260	0	1220	3	0
1	K	1267	0	1235	2	0
1	L	1277	0	1254	3	0
1	M	1281	0	1253	4	0
1	N	1272	0	1239	7	0
1	O	1281	0	1246	3	0
1	P	1272	0	1241	4	0
1	Q	1272	0	1239	2	0
1	R	1273	0	1243	1	0
1	S	1275	0	1248	3	0
1	T	1272	0	1241	4	0
1	U	1266	0	1228	3	0
1	V	1272	0	1241	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1276	0	1242	2	0
1	X	1272	0	1239	3	0
2	A	43	0	30	1	0
2	C	43	0	30	1	0
2	E	43	0	30	1	0
2	G	43	0	30	2	0
2	I	43	0	30	2	0
2	K	43	0	30	1	0
2	M	43	0	30	2	0
2	O	43	0	30	3	0
2	Q	43	0	30	2	0
2	S	43	0	30	1	0
2	U	43	0	30	2	0
2	W	43	0	30	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	L	1	0	0	0	0
4	A	8	0	14	0	0
4	B	8	0	14	0	0
4	D	8	0	14	0	0
4	E	16	0	28	0	0
4	F	8	0	14	0	0
4	G	8	0	14	0	0
4	H	8	0	14	0	0
4	I	8	0	14	0	0
4	J	8	0	14	0	0
4	K	8	0	14	0	0
4	M	16	0	28	0	0
4	N	16	0	28	5	0
4	O	8	0	14	0	0
4	P	8	0	14	0	0
4	R	8	0	14	0	0
4	S	8	0	14	3	0
4	T	8	0	14	0	0
4	U	8	0	14	0	0
4	V	8	0	14	0	0
4	W	8	0	14	0	0
4	X	8	0	14	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	2	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
5	V	1	0	0	0	0
6	C	8	0	14	1	0
6	I	8	0	14	0	0
6	J	8	0	14	4	0
6	K	8	0	14	1	0
6	L	8	0	14	0	0
6	Q	16	0	28	2	0
6	R	8	0	14	1	0
6	S	8	0	14	0	0
7	A	179	0	0	3	1
7	B	180	0	0	0	0
7	C	182	0	0	1	0
7	D	183	0	0	1	0
7	E	178	0	0	2	0
7	F	167	0	0	0	0
7	G	181	0	0	2	0
7	H	184	0	0	0	0
7	I	171	0	0	0	0
7	J	165	0	0	1	0
7	K	175	0	0	2	0
7	L	173	0	0	2	0
7	M	195	0	0	4	1
7	N	191	0	0	2	0
7	O	177	0	0	2	0
7	P	163	0	0	2	0
7	Q	200	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	166	0	0	1	0
7	S	188	0	0	1	0
7	T	181	0	0	4	0
7	U	168	0	0	1	0
7	V	172	0	0	2	0
7	W	176	0	0	2	0
7	X	180	0	0	1	0
All	All	35653	0	30627	81	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 81 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:E:50[B]:ASP:OD2	7:E:301:HOH:O	1.90	0.90
1:M:50[B]:ASP:OD2	7:M:301:HOH:O	1.90	0.88
1:N:50[B]:ASP:OD2	7:N:301:HOH:O	1.91	0.87
6:J:201:MPD:H13	7:J:331:HOH:O	1.75	0.86
1:T:126[A]:SER:OG	7:T:301:HOH:O	2.08	0.71

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:360:HOH:O	7:M:405:HOH:O[2_554]	2.00	0.20

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	159/158 (101%)	158 (99%)	1 (1%)	0	100	100
1	B	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	C	157/158 (99%)	157 (100%)	0	0	100	100
1	D	157/158 (99%)	157 (100%)	0	0	100	100
1	E	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	F	156/158 (99%)	156 (100%)	0	0	100	100
1	G	158/158 (100%)	158 (100%)	0	0	100	100
1	H	155/158 (98%)	155 (100%)	0	0	100	100
1	I	156/158 (99%)	156 (100%)	0	0	100	100
1	J	155/158 (98%)	155 (100%)	0	0	100	100
1	K	155/158 (98%)	155 (100%)	0	0	100	100
1	L	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	M	157/158 (99%)	155 (99%)	2 (1%)	0	100	100
1	N	156/158 (99%)	156 (100%)	0	0	100	100
1	O	158/158 (100%)	158 (100%)	0	0	100	100
1	P	156/158 (99%)	156 (100%)	0	0	100	100
1	Q	156/158 (99%)	156 (100%)	0	0	100	100
1	R	156/158 (99%)	156 (100%)	0	0	100	100
1	S	156/158 (99%)	156 (100%)	0	0	100	100
1	T	156/158 (99%)	156 (100%)	0	0	100	100
1	U	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	V	156/158 (99%)	156 (100%)	0	0	100	100
1	W	157/158 (99%)	157 (100%)	0	0	100	100
1	X	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
All	All	3752/3792 (99%)	3744 (100%)	8 (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	141/142 (99%)	140 (99%)	1 (1%)	88	73
1	B	136/142 (96%)	135 (99%)	1 (1%)	88	73
1	C	138/142 (97%)	138 (100%)	0	100	100
1	D	139/142 (98%)	137 (99%)	2 (1%)	74	47
1	E	137/142 (96%)	136 (99%)	1 (1%)	88	73
1	F	136/142 (96%)	135 (99%)	1 (1%)	88	73
1	G	139/142 (98%)	136 (98%)	3 (2%)	60	25
1	H	135/142 (95%)	134 (99%)	1 (1%)	88	73
1	I	136/142 (96%)	135 (99%)	1 (1%)	88	73
1	J	134/142 (94%)	133 (99%)	1 (1%)	88	73
1	K	136/142 (96%)	135 (99%)	1 (1%)	88	73
1	L	138/142 (97%)	137 (99%)	1 (1%)	88	73
1	M	138/142 (97%)	137 (99%)	1 (1%)	88	73
1	N	137/142 (96%)	135 (98%)	2 (2%)	72	44
1	O	138/142 (97%)	135 (98%)	3 (2%)	60	25
1	P	137/142 (96%)	136 (99%)	1 (1%)	88	73
1	Q	137/142 (96%)	135 (98%)	2 (2%)	72	44
1	R	137/142 (96%)	134 (98%)	3 (2%)	60	25
1	S	138/142 (97%)	137 (99%)	1 (1%)	88	73
1	T	137/142 (96%)	135 (98%)	2 (2%)	72	44
1	U	135/142 (95%)	134 (99%)	1 (1%)	88	73
1	V	137/142 (96%)	135 (98%)	2 (2%)	72	44
1	W	137/142 (96%)	134 (98%)	3 (2%)	60	25
1	X	137/142 (96%)	136 (99%)	1 (1%)	88	73
All	All	3290/3408 (96%)	3254 (99%)	36 (1%)	82	58

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	121	LYS
1	P	121	LYS
1	W	84[B]	GLN
1	O	84[B]	GLN

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Mol	Chain	Res	Type
1	Q	121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	155	HIS
1	T	46	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 30 are monoatomic - leaving 45 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	$\# Z > 2$
2	HEM	A	201	1	24,50,50	1.98	7 (29%)	16,82,82	2.08	7 (43%)
4	MRD	A	203	-	6,7,7	0.36	0	6,10,10	0.35	0
4	MRD	B	202	-	6,7,7	0.30	0	6,10,10	0.36	0
6	MPD	C	201	-	6,7,7	0.29	0	6,10,10	0.40	0
2	HEM	C	202	1	24,50,50	1.93	5 (20%)	16,82,82	2.17	7 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MRD	D	202	-	6,7,7	0.31	0	6,10,10	0.31	0
2	HEM	E	201	1	24,50,50	1.98	5 (20%)	16,82,82	1.95	6 (37%)
4	MRD	E	203	-	6,7,7	0.34	0	6,10,10	0.41	0
4	MRD	E	204	-	6,7,7	0.45	0	6,10,10	0.60	0
4	MRD	F	201	-	6,7,7	0.34	0	6,10,10	0.52	0
2	HEM	G	201	1	24,50,50	2.00	5 (20%)	16,82,82	1.92	7 (43%)
4	MRD	G	203	-	6,7,7	0.36	0	6,10,10	0.26	0
4	MRD	H	201	-	6,7,7	0.35	0	6,10,10	0.34	0
4	MRD	I	201	-	6,7,7	0.29	0	6,10,10	0.40	0
6	MPD	I	202	-	6,7,7	0.32	0	6,10,10	0.57	0
2	HEM	I	203	1	24,50,50	2.02	6 (25%)	16,82,82	1.93	4 (25%)
6	MPD	J	201	-	6,7,7	0.47	0	6,10,10	0.38	0
4	MRD	J	202	-	6,7,7	0.51	0	6,10,10	0.64	0
2	HEM	K	201	1	24,50,50	1.96	6 (25%)	16,82,82	2.03	5 (31%)
4	MRD	K	202	-	6,7,7	0.35	0	6,10,10	0.35	0
6	MPD	K	203	-	6,7,7	0.37	0	6,10,10	0.51	0
6	MPD	L	202	-	6,7,7	0.33	0	6,10,10	0.46	0
2	HEM	M	201	1	24,50,50	2.06	6 (25%)	16,82,82	2.04	6 (37%)
4	MRD	M	202	-	6,7,7	0.29	0	6,10,10	0.35	0
4	MRD	M	203	-	6,7,7	0.50	0	6,10,10	0.53	0
4	MRD	N	201	-	6,7,7	0.34	0	6,10,10	0.49	0
4	MRD	N	202	-	6,7,7	0.44	0	6,10,10	0.60	0
4	MRD	O	201	-	6,7,7	0.41	0	6,10,10	0.23	0
2	HEM	O	202	1	24,50,50	1.94	5 (20%)	16,82,82	2.17	6 (37%)
4	MRD	P	201	-	6,7,7	0.31	0	6,10,10	0.39	0
2	HEM	Q	201	1	24,50,50	2.06	6 (25%)	16,82,82	1.88	6 (37%)
6	MPD	Q	202	-	6,7,7	0.38	0	6,10,10	0.54	0
6	MPD	Q	203	-	6,7,7	0.36	0	6,10,10	0.46	0
6	MPD	R	201	-	6,7,7	0.34	0	6,10,10	0.38	0
4	MRD	R	202	-	6,7,7	0.40	0	6,10,10	0.43	0
6	MPD	S	201	-	6,7,7	0.42	0	6,10,10	0.40	0
4	MRD	S	202	-	6,7,7	0.40	0	6,10,10	0.50	0
2	HEM	S	204	1	24,50,50	1.92	5 (20%)	16,82,82	2.03	6 (37%)
4	MRD	T	201	-	6,7,7	0.33	0	6,10,10	0.29	0
2	HEM	U	201	1	24,50,50	1.97	5 (20%)	16,82,82	2.07	6 (37%)
4	MRD	U	202	-	6,7,7	0.35	0	6,10,10	0.45	0
4	MRD	V	201	-	6,7,7	0.29	0	6,10,10	0.34	0
2	HEM	W	201	1	24,50,50	1.94	8 (33%)	16,82,82	1.98	6 (37%)
4	MRD	W	202	-	6,7,7	0.28	0	6,10,10	0.30	0
4	MRD	X	201	-	6,7,7	0.33	0	6,10,10	0.34	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
2	HEM	A	201	1	-	0/6/54/54	0/0/8/8
4	MRD	A	203	-	-	0/5/5/5	0/0/0/0
4	MRD	B	202	-	-	0/5/5/5	0/0/0/0
6	MPD	C	201	-	-	0/5/5/5	0/0/0/0
2	HEM	C	202	1	-	0/6/54/54	0/0/8/8
4	MRD	D	202	-	-	0/5/5/5	0/0/0/0
2	HEM	E	201	1	-	0/6/54/54	0/0/8/8
4	MRD	E	203	-	-	0/5/5/5	0/0/0/0
4	MRD	E	204	-	-	0/5/5/5	0/0/0/0
4	MRD	F	201	-	-	0/5/5/5	0/0/0/0
2	HEM	G	201	1	-	0/6/54/54	0/0/8/8
4	MRD	G	203	-	-	0/5/5/5	0/0/0/0
4	MRD	H	201	-	-	0/5/5/5	0/0/0/0
4	MRD	I	201	-	-	0/5/5/5	0/0/0/0
6	MPD	I	202	-	-	0/5/5/5	0/0/0/0
2	HEM	I	203	1	-	0/6/54/54	0/0/8/8
6	MPD	J	201	-	-	0/5/5/5	0/0/0/0
4	MRD	J	202	-	-	0/5/5/5	0/0/0/0
2	HEM	K	201	1	-	0/6/54/54	0/0/8/8
4	MRD	K	202	-	-	0/5/5/5	0/0/0/0
6	MPD	K	203	-	-	0/5/5/5	0/0/0/0
6	MPD	L	202	-	-	0/5/5/5	0/0/0/0
2	HEM	M	201	1	-	0/6/54/54	0/0/8/8
4	MRD	M	202	-	-	0/5/5/5	0/0/0/0
4	MRD	M	203	-	-	0/5/5/5	0/0/0/0
4	MRD	N	201	-	-	0/5/5/5	0/0/0/0
4	MRD	N	202	-	-	0/5/5/5	0/0/0/0
4	MRD	O	201	-	-	0/5/5/5	0/0/0/0
2	HEM	O	202	1	-	0/6/54/54	0/0/8/8
4	MRD	P	201	-	-	0/5/5/5	0/0/0/0
2	HEM	Q	201	1	-	0/6/54/54	0/0/8/8
6	MPD	Q	202	-	-	0/5/5/5	0/0/0/0
6	MPD	Q	203	-	-	0/5/5/5	0/0/0/0
6	MPD	R	201	-	-	0/5/5/5	0/0/0/0
4	MRD	R	202	-	-	0/5/5/5	0/0/0/0
6	MPD	S	201	-	-	0/5/5/5	0/0/0/0
4	MRD	S	202	-	-	0/5/5/5	0/0/0/0
2	HEM	S	204	1	-	0/6/54/54	0/0/8/8
4	MRD	T	201	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	U	201	1	-	0/6/54/54	0/0/8/8
4	MRD	U	202	-	-	0/5/5/5	0/0/0/0
4	MRD	V	201	-	-	0/5/5/5	0/0/0/0
2	HEM	W	201	1	-	0/6/54/54	0/0/8/8
4	MRD	W	202	-	-	0/5/5/5	0/0/0/0
4	MRD	X	201	-	-	0/5/5/5	0/0/0/0

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	201	HEM	C3B-C2B	-5.46	1.33	1.40
2	O	202	HEM	C3B-C2B	-5.42	1.33	1.40
2	Q	201	HEM	C3B-C2B	-5.36	1.33	1.40
2	Q	201	HEM	C3C-C2C	-5.04	1.34	1.40
2	G	201	HEM	C3B-C2B	-4.93	1.34	1.40

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	201	HEM	CBA-CAA-C2A	-4.47	104.63	112.49
2	E	201	HEM	CBA-CAA-C2A	-3.92	105.60	112.49
2	C	202	HEM	C3B-CAB-CBB	-3.77	118.82	126.40
2	I	203	HEM	CBD-CAD-C3D	-3.67	106.02	112.47
2	K	201	HEM	CBA-CAA-C2A	-3.64	106.09	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	HEM	1	0
6	C	201	MPD	1	0
2	C	202	HEM	1	0
2	E	201	HEM	1	0
2	G	201	HEM	2	0
2	I	203	HEM	2	0
6	J	201	MPD	4	0
2	K	201	HEM	1	0
6	K	203	MPD	1	0
2	M	201	HEM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	201	MRD	1	0
4	N	202	MRD	4	0
2	O	202	HEM	3	0
2	Q	201	HEM	2	0
6	Q	202	MPD	1	0
6	Q	203	MPD	1	0
6	R	201	MPD	1	0
4	S	202	MRD	3	0
2	S	204	HEM	1	0
2	U	201	HEM	2	0
2	W	201	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/158 (98%)	-0.03	0 100 100	10, 14, 23, 35	0
1	B	156/158 (98%)	-0.17	0 100 100	11, 15, 24, 40	0
1	C	156/158 (98%)	-0.07	0 100 100	13, 17, 27, 38	0
1	D	156/158 (98%)	-0.10	0 100 100	13, 16, 24, 34	0
1	E	156/158 (98%)	-0.05	0 100 100	12, 16, 25, 37	0
1	F	156/158 (98%)	-0.09	0 100 100	12, 16, 25, 34	0
1	G	156/158 (98%)	-0.07	0 100 100	13, 17, 25, 37	0
1	H	156/158 (98%)	-0.08	0 100 100	12, 16, 25, 35	0
1	I	156/158 (98%)	-0.08	0 100 100	13, 17, 26, 38	0
1	J	156/158 (98%)	-0.08	0 100 100	13, 17, 26, 39	0
1	K	156/158 (98%)	-0.07	0 100 100	13, 16, 26, 38	0
1	L	156/158 (98%)	-0.14	0 100 100	12, 16, 25, 34	0
1	M	156/158 (98%)	0.01	0 100 100	11, 14, 23, 39	0
1	N	156/158 (98%)	-0.11	0 100 100	11, 15, 24, 34	0
1	O	156/158 (98%)	-0.02	0 100 100	13, 17, 25, 37	0
1	P	156/158 (98%)	-0.08	0 100 100	14, 17, 26, 36	0
1	Q	156/158 (98%)	-0.16	0 100 100	12, 15, 24, 34	0
1	R	156/158 (98%)	-0.10	0 100 100	12, 16, 24, 36	0
1	S	156/158 (98%)	-0.14	0 100 100	11, 15, 25, 36	0
1	T	156/158 (98%)	-0.11	0 100 100	12, 15, 26, 35	0
1	U	156/158 (98%)	-0.15	0 100 100	13, 17, 25, 38	0
1	V	156/158 (98%)	-0.10	0 100 100	14, 17, 26, 35	0
1	W	156/158 (98%)	-0.06	0 100 100	14, 17, 24, 35	0
1	X	156/158 (98%)	-0.06	0 100 100	12, 16, 25, 36	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3744/3792 (98%)	-0.09	0 100 100	10, 16, 25, 40	0

There are no RSRZ outliers to report.

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
4	MRD	A	203	8/8	0.82	0.21	12.62	24,28,36,41	0
6	MPD	L	202	8/8	0.88	0.22	12.14	22,30,41,48	0
4	MRD	E	203	8/8	0.82	0.18	11.34	19,27,34,37	0
4	MRD	V	201	8/8	0.87	0.16	9.98	24,27,33,36	0
4	MRD	I	201	8/8	0.86	0.20	8.65	23,30,38,39	0
4	MRD	B	202	8/8	0.86	0.15	7.96	20,24,33,34	0
4	MRD	T	201	8/8	0.90	0.16	7.92	22,29,35,37	0
4	MRD	D	202	8/8	0.91	0.17	7.77	19,27,32,34	0
6	MPD	R	201	8/8	0.81	0.26	7.10	24,34,44,50	0
2	HEM	E	201	43/43	0.95	0.15	6.91	14,18,28,32	0
4	MRD	M	203	8/8	0.86	0.21	6.82	21,30,41,41	0
4	MRD	P	201	8/8	0.88	0.14	5.94	24,30,37,38	0
6	MPD	S	201	8/8	0.89	0.15	5.87	22,27,36,47	0
2	HEM	U	201	43/43	0.94	0.16	5.58	16,19,31,31	0
6	MPD	Q	202	8/8	0.88	0.15	5.57	22,28,35,44	0
2	HEM	M	201	43/43	0.95	0.14	5.33	13,16,26,31	0
2	HEM	S	204	43/43	0.96	0.13	5.20	13,16,29,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MPD	C	201	8/8	0.84	0.16	5.18	22,30,35,45	0
4	MRD	S	202	8/8	0.80	0.21	5.00	27,32,42,42	0
4	MRD	N	202	8/8	0.79	0.22	4.86	25,34,45,46	0
4	MRD	H	201	8/8	0.88	0.14	4.62	22,30,34,35	0
4	MRD	J	202	8/8	0.82	0.18	4.43	23,30,39,40	0
4	MRD	G	203	8/8	0.89	0.14	4.41	21,27,35,36	0
2	HEM	A	201	43/43	0.96	0.13	4.40	13,16,27,28	0
4	MRD	O	201	8/8	0.88	0.14	4.39	25,28,37,37	0
2	HEM	C	202	43/43	0.95	0.14	4.35	15,19,32,35	0
4	MRD	W	202	8/8	0.88	0.16	4.28	20,27,32,33	0
2	HEM	W	201	43/43	0.95	0.12	4.13	15,18,30,35	0
4	MRD	R	202	8/8	0.86	0.18	4.06	24,33,39,41	0
2	HEM	K	201	43/43	0.95	0.13	4.00	14,19,31,33	0
2	HEM	I	203	43/43	0.95	0.14	3.95	15,20,32,34	0
6	MPD	J	201	8/8	0.92	0.15	3.88	17,25,40,41	0
4	MRD	F	201	8/8	0.83	0.15	3.85	22,30,33,39	0
6	MPD	I	202	8/8	0.86	0.17	3.79	26,34,43,45	0
4	MRD	X	201	8/8	0.88	0.15	3.76	24,32,36,37	0
6	MPD	K	203	8/8	0.86	0.20	3.62	23,35,41,42	0
4	MRD	K	202	8/8	0.90	0.15	3.52	21,23,34,34	0
4	MRD	U	202	8/8	0.90	0.12	3.47	20,25,30,33	0
4	MRD	N	201	8/8	0.90	0.12	3.06	24,27,37,38	0
2	HEM	G	201	43/43	0.95	0.12	2.77	14,18,31,32	0
2	HEM	O	202	43/43	0.94	0.12	2.60	15,18,30,33	0
3	K	D	201	1/1	1.00	0.09	2.37	13,13,13,13	0
2	HEM	Q	201	43/43	0.96	0.11	2.37	13,16,30,34	0
6	MPD	Q	203	8/8	0.84	0.16	2.30	25,32,39,40	0
4	MRD	M	202	8/8	0.90	0.12	2.29	23,24,34,36	0
4	MRD	E	204	8/8	0.83	0.16	1.88	23,29,40,43	0
3	K	L	201	1/1	1.00	0.08	0.13	12,12,12,12	0
3	K	G	202	1/1	0.99	0.08	0.07	13,13,13,13	0
3	K	A	202	1/1	1.00	0.09	0.05	11,11,11,11	0
3	K	E	202	1/1	0.99	0.07	-1.41	14,14,14,14	0
3	K	B	201	1/1	0.99	0.07	-1.59	15,15,15,15	0
5	NA	K	204	1/1	0.89	0.12	-	27,27,27,27	0
5	NA	B	204	1/1	0.90	0.10	-	27,27,27,27	0
5	NA	R	203	1/1	0.89	0.12	-	26,26,26,26	0
5	NA	L	203	1/1	0.93	0.10	-	26,26,26,26	0
5	NA	T	202	1/1	0.90	0.14	-	26,26,26,26	0
5	NA	J	203	1/1	0.87	0.14	-	28,28,28,28	0
5	NA	V	202	1/1	0.91	0.15	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NA	G	205	1/1	0.92	0.10	-	28,28,28,28	0
5	NA	D	204	1/1	0.93	0.10	-	28,28,28,28	0
5	NA	G	204	1/1	0.92	0.12	-	26,26,26,26	0
5	NA	N	203	1/1	0.93	0.10	-	23,23,23,23	0
5	NA	H	202	1/1	0.94	0.10	-	26,26,26,26	0
5	NA	F	202	1/1	0.95	0.12	-	27,27,27,27	0
5	NA	C	203	1/1	0.97	0.10	-	29,29,29,29	0
5	NA	M	204	1/1	0.93	0.12	-	24,24,24,24	0
5	NA	E	205	1/1	0.91	0.14	-	28,28,28,28	0
5	NA	E	206	1/1	0.89	0.14	-	26,26,26,26	0
5	NA	L	204	1/1	0.94	0.12	-	29,29,29,29	0
5	NA	A	204	1/1	0.94	0.13	-	28,28,28,28	0
5	NA	S	203	1/1	0.94	0.11	-	26,26,26,26	0
5	NA	D	203	1/1	0.87	0.16	-	26,26,26,26	0
5	NA	A	205	1/1	0.95	0.12	-	22,22,22,22	0
5	NA	B	203	1/1	0.96	0.15	-	24,24,24,24	0
5	NA	I	204	1/1	0.88	0.10	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.