



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:08 PM GMT

PDB ID : 1SP3  
Title : Crystal structure of octaheme cytochrome c from *Shewanella oneidensis*  
Authors : Mowat, C.G.; Rothery, E.; Miles, C.S.; McIver, L.; Doherty, M.K.; Drewette, K.; Taylor, P.; Walkinshaw, M.D.; Chapman, S.K.; Reid, G.A.  
Deposited on : 2004-03-16  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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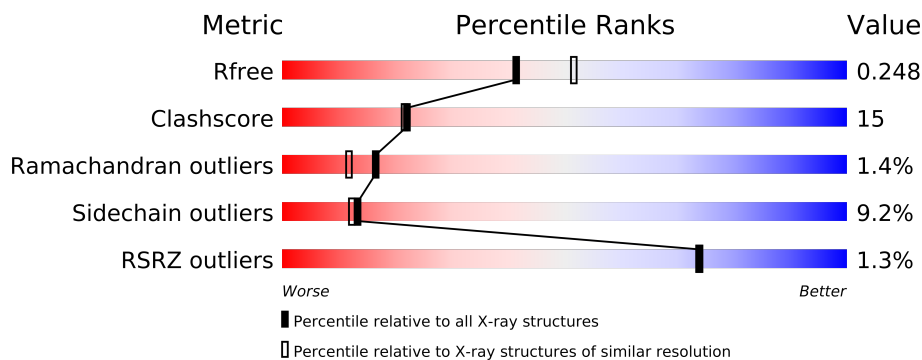
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	443	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4243 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

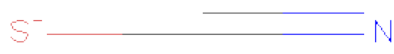
- Molecule 1 is a protein called cytochrome c, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3426	2140	598	655	33	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	ASN	GLN	CONFLICT	UNP Q8E9W8

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
2	A	1	3	1	1	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is water.

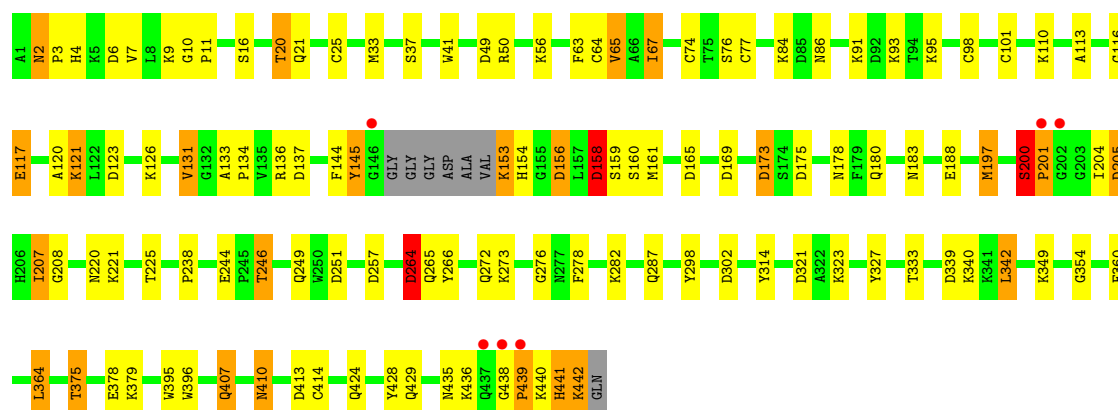
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	470	Total	O	0	0
			470	470		

### 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 ( $\text{RSRZ} > 2$ ). 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: cytochrome c, putative

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.59Å 61.77Å 185.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.77 – 2.20 23.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (23.77-2.20) 96.6 (23.76-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.155 , 0.252 0.160 , 0.248	Depositor DCC
$R_{free}$ test set	1217 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23696 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.20	4/3519 (0.1%)	1.15	22/4760 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	TYR	CD2-CE2	7.79	1.51	1.39
1	A	327	TYR	CD2-CE2	5.74	1.48	1.39
1	A	37	SER	CB-OG	-5.40	1.35	1.42
1	A	41	TRP	CB-CG	5.23	1.59	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	LEU	C-N-CA	-8.74	99.85	121.70
1	A	165	ASP	CB-CG-OD2	7.25	124.82	118.30
1	A	207	ILE	C-N-CA	-7.02	107.56	122.30
1	A	156	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	205	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	413	ASP	CB-CG-OD2	6.56	124.21	118.30
1	A	208	GLY	N-CA-C	-6.55	96.73	113.10
1	A	50	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	6	ASP	CB-CG-OD2	5.75	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	342	LEU	O-C-N	-5.64	113.67	122.70
1	A	173	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	137	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	246	THR	CB-CA-C	-5.46	96.86	111.60
1	A	158	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	131	VAL	N-CA-CB	-5.18	100.10	111.50
1	A	264	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	207	ILE	CB-CA-C	-5.07	101.46	111.60
1	A	257	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	91	LYS	CD-CE-NZ	5.05	123.32	111.70
1	A	123	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	169	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLY	Peptide
1	A	153	LYS	Peptide
1	A	264	ASP	Peptide
1	A	441	HIS	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3426	0	3243	103	0
2	A	3	0	0	0	0
3	A	344	0	240	26	0
4	A	470	0	0	24	4
All	All	4243	0	3483	104	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.



All (104) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:CYS:SG	3:A:802:HEM:HAC	1.60	1.39
1:A:74:CYS:SG	3:A:802:HEM:CAB	2.10	1.38
1:A:414:CYS:SG	3:A:808:HEM:HAC	1.61	1.38
1:A:25:CYS:HG	3:A:801:HEM:CAC	1.34	1.38
1:A:25:CYS:SG	3:A:801:HEM:HAC	1.77	1.15
1:A:429:GLN:H	1:A:439:PRO:HG3	1.17	1.07
1:A:74:CYS:HG	3:A:802:HEM:CAB	1.61	1.06
1:A:101:CYS:SG	3:A:803:HEM:HAC	1.94	1.04
1:A:101:CYS:HG	3:A:803:HEM:CAC	1.57	1.04
1:A:74:CYS:SG	3:A:802:HEM:HAB	2.00	1.00
1:A:9:LYS:HG3	4:A:1183:HOH:O	1.67	0.94
1:A:410:ASN:HA	4:A:1048:HOH:O	1.71	0.91
1:A:101:CYS:SG	3:A:803:HEM:C3C	2.69	0.85
1:A:429:GLN:H	1:A:439:PRO:CG	1.90	0.83
1:A:74:CYS:SG	3:A:802:HEM:CBB	2.68	0.82
1:A:9:LYS:CG	4:A:1183:HOH:O	2.26	0.81
1:A:429:GLN:N	1:A:439:PRO:HG3	1.95	0.81
1:A:200:SER:HB3	1:A:201:PRO:CA	2.12	0.79
1:A:200:SER:HB3	1:A:201:PRO:HA	1.64	0.79
1:A:77:CYS:SG	3:A:802:HEM:C3C	2.78	0.77
1:A:414:CYS:SG	3:A:808:HEM:C3C	2.79	0.75
1:A:439:PRO:HA	4:A:879:HOH:O	1.86	0.75
1:A:56:LYS:HE2	1:A:67:ILE:HD11	1.69	0.74
1:A:33:MET:HG2	4:A:1108:HOH:O	1.88	0.74
1:A:101:CYS:SG	3:A:803:HEM:CBC	2.77	0.71
1:A:244:GLU:HG2	4:A:848:HOH:O	1.90	0.71
1:A:439:PRO:HG2	4:A:962:HOH:O	1.91	0.71
1:A:221:LYS:HD3	4:A:1110:HOH:O	1.90	0.71
1:A:74:CYS:SG	3:A:802:HEM:C3B	2.82	0.70
1:A:441:HIS:O	1:A:442:LYS:HB2	1.91	0.70
1:A:25:CYS:HG	3:A:801:HEM:CBC	2.01	0.69
1:A:25:CYS:SG	3:A:801:HEM:C3C	2.84	0.67
1:A:414:CYS:SG	3:A:808:HEM:CBC	2.80	0.66
1:A:113:ALA:HB3	4:A:1051:HOH:O	1.94	0.66
1:A:264:ASP:HB3	1:A:266:TYR:H	1.59	0.66
1:A:197:MET:HE1	1:A:395:TRP:O	1.95	0.66
1:A:49:ASP:CB	4:A:975:HOH:O	2.44	0.65
1:A:154:HIS:CE1	1:A:396:TRP:HB3	2.30	0.65
1:A:64:CYS:SG	4:A:1263:HOH:O	2.54	0.65
1:A:287:GLN:NE2	4:A:1184:HOH:O	2.29	0.65
1:A:273:LYS:HE2	1:A:360:PHE:CE1	2.32	0.64
1:A:21:GLN:OE1	4:A:925:HOH:O	2.15	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:SER:HB3	1:A:201:PRO:O	1.98	0.64
1:A:84:LYS:HE3	4:A:1086:HOH:O	1.98	0.63
1:A:49:ASP:HB2	4:A:975:HOH:O	1.99	0.62
1:A:56:LYS:HE3	3:A:802:HEM:NA	2.14	0.62
1:A:25:CYS:SG	3:A:801:HEM:CBC	2.81	0.62
1:A:77:CYS:SG	3:A:802:HEM:CBC	2.85	0.61
1:A:74:CYS:HG	3:A:802:HEM:CBB	2.12	0.60
1:A:298:TYR:CE1	1:A:302:ASP:HB2	2.36	0.60
1:A:56:LYS:HE3	3:A:802:HEM:C4A	2.37	0.59
1:A:16:SER:O	1:A:20:THR:CG2	2.50	0.59
1:A:200:SER:HB3	1:A:201:PRO:C	2.23	0.59
1:A:56:LYS:CE	1:A:67:ILE:HD11	2.33	0.58
1:A:273:LYS:HE2	1:A:360:PHE:CZ	2.37	0.58
1:A:272:GLN:HE21	1:A:278:PHE:HE1	1.51	0.58
1:A:95:LYS:HE3	4:A:905:HOH:O	2.06	0.56
1:A:428:TYR:HA	1:A:439:PRO:CB	2.36	0.55
1:A:2:ASN:HD22	1:A:4:HIS:H	1.54	0.55
1:A:16:SER:O	1:A:20:THR:HG22	2.07	0.55
1:A:438:GLY:H	1:A:439:PRO:HD3	1.70	0.55
1:A:7:VAL:HG12	1:A:7:VAL:O	2.05	0.54
1:A:339:ASP:O	1:A:342:LEU:O	2.24	0.54
1:A:180:GLN:H	1:A:183:ASN:HD22	1.57	0.52
1:A:101:CYS:HG	3:A:803:HEM:CBC	2.16	0.51
1:A:49:ASP:HB3	4:A:975:HOH:O	2.10	0.51
1:A:354:GLY:O	1:A:364:LEU:HD13	2.11	0.51
1:A:205:ASP:HB3	1:A:207:ILE:O	2.11	0.51
1:A:56:LYS:HE2	1:A:67:ILE:CD1	2.40	0.50
1:A:438:GLY:N	1:A:439:PRO:HD3	2.26	0.50
1:A:144:PHE:CZ	1:A:161:MET:HB2	2.46	0.50
1:A:16:SER:O	1:A:20:THR:HG23	2.13	0.49
1:A:180:GLN:H	1:A:183:ASN:ND2	2.10	0.49
1:A:33:MET:CG	4:A:1108:HOH:O	2.55	0.48
1:A:375:THR:OG1	4:A:1237:HOH:O	2.20	0.48
1:A:136:ARG:HH12	1:A:178:ASN:ND2	2.11	0.48
1:A:438:GLY:N	4:A:936:HOH:O	2.46	0.47
1:A:63:PHE:HE1	1:A:396:TRP:CH2	2.33	0.47
1:A:120:ALA:O	1:A:121:LYS:HB2	2.13	0.47
1:A:429:GLN:HB2	1:A:439:PRO:HG3	1.96	0.47
1:A:428:TYR:CD2	1:A:439:PRO:HB2	2.49	0.47
1:A:156:ASP:O	1:A:161:MET:HE2	2.17	0.45
1:A:238:PRO:HG3	1:A:407:GLN:O	2.17	0.45
1:A:98:CYS:HA	3:A:803:HEM:HAB	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:ASN:HB2	1:A:3:PRO:CD	2.48	0.44
1:A:428:TYR:HA	1:A:439:PRO:HB3	2.00	0.43
1:A:158:ASP:H	1:A:161:MET:HG2	1.83	0.43
1:A:110:LYS:HE3	1:A:116:GLY:HA2	2.00	0.43
1:A:7:VAL:O	1:A:7:VAL:CG1	2.67	0.42
1:A:145:TYR:CD1	1:A:145:TYR:N	2.87	0.42
1:A:321:ASP:O	1:A:441:HIS:HE1	2.02	0.42
1:A:349:LYS:NZ	4:A:1137:HOH:O	2.18	0.42
1:A:117:GLU:OE1	4:A:845:HOH:O	2.22	0.41
1:A:249:GLN:HA	1:A:333:THR:O	2.21	0.41
1:A:220:ASN:OD1	1:A:220:ASN:C	2.58	0.41
3:A:807:HEM:HBC1	3:A:808:HEM:C2C	2.56	0.41
1:A:64:CYS:O	1:A:65:VAL:HB	2.21	0.41
1:A:197:MET:CE	4:A:1047:HOH:O	2.68	0.41
1:A:251:ASP:O	1:A:276:GLY:HA3	2.21	0.41
1:A:180:GLN:O	1:A:183:ASN:HB2	2.22	0.40
1:A:133:ALA:HA	1:A:134:PRO:HD3	1.91	0.40
1:A:204:ILE:HD11	1:A:323:LYS:O	2.22	0.40
1:A:375:THR:O	1:A:379:LYS:HG3	2.22	0.40
1:A:117:GLU:HG3	4:A:845:HOH:O	2.21	0.40

All (4) 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	Distance(Å)	Clash(Å)
4:A:975:HOH:O	4:A:1274:HOH:O[1_455]	1.49	0.71
4:A:971:HOH:O	4:A:1276:HOH:O[4_455]	1.53	0.67
4:A:1075:HOH:O	4:A:1123:HOH:O[3_545]	2.04	0.16
4:A:1044:HOH:O	4:A:1123:HOH:O[3_545]	2.07	0.13

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	432/443 (98%)	406 (94%)	20 (5%)	6 (1%)	16 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	SER
1	A	201	PRO
1	A	11	PRO
1	A	173	ASP
1	A	439	PRO
1	A	65	VAL

### 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	370/373 (99%)	336 (91%)	34 (9%)	13	12

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	20	THR
1	A	67	ILE
1	A	76	SER
1	A	86	ASN
1	A	93	LYS
1	A	117	GLU
1	A	121	LYS
1	A	126	LYS
1	A	131	VAL
1	A	145	TYR
1	A	153	LYS
1	A	158	ASP
1	A	159	SER
1	A	160	SER
1	A	188	GLU
1	A	197	MET
1	A	200	SER
1	A	225	THR
1	A	246	THR
1	A	264	ASP

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Mol	Chain	Res	Type
1	A	265	GLN
1	A	282	LYS
1	A	340	LYS
1	A	364	LEU
1	A	375	THR
1	A	378	GLU
1	A	407	GLN
1	A	410	ASN
1	A	424	GLN
1	A	435	ASN
1	A	436	LYS
1	A	440	LYS
1	A	442	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	154	HIS
1	A	177	ASN
1	A	178	ASN
1	A	183	ASN
1	A	249	GLN
1	A	272	GLN
1	A	277	ASN
1	A	363	ASN
1	A	407	GLN
1	A	429	GLN
1	A	441	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	HEM	A	801	1	49,50,50	2.72	16 (32%)	46,82,82	2.61	16 (34%)
3	HEM	A	802	1,2	49,50,50	3.51	20 (40%)	46,82,82	2.59	15 (32%)
3	HEM	A	803	1	49,50,50	3.68	18 (36%)	46,82,82	2.59	14 (30%)
3	HEM	A	804	1	49,50,50	2.39	19 (38%)	46,82,82	2.01	9 (19%)
3	HEM	A	805	1	49,50,50	2.95	15 (30%)	46,82,82	2.28	14 (30%)
3	HEM	A	806	1	49,50,50	2.70	16 (32%)	46,82,82	2.51	14 (30%)
3	HEM	A	807	1	49,50,50	2.95	19 (38%)	46,82,82	2.46	17 (36%)
3	HEM	A	808	1	49,50,50	3.43	21 (42%)	46,82,82	2.35	11 (23%)
2	SCN	A	810	3	2,2,2	0.47	0	1,1,1	0.15	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	801	1	-	0/14/114/114	0/0/8/8
3	HEM	A	802	1,2	-	0/14/114/114	0/0/8/8
3	HEM	A	803	1	-	0/14/114/114	0/0/8/8
3	HEM	A	804	1	-	0/14/114/114	0/0/8/8
3	HEM	A	805	1	-	0/14/114/114	0/0/8/8
3	HEM	A	806	1	-	0/14/114/114	0/0/8/8
3	HEM	A	807	1	-	0/14/114/114	0/0/8/8
3	HEM	A	808	1	-	0/14/114/114	0/0/8/8
2	SCN	A	810	3	-	0/0/0/0	0/0/0/0

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HEM	C2D-C1D	16.56	1.48	1.44
3	A	805	HEM	C3D-C4D	13.40	1.47	1.44
3	A	808	HEM	C3D-C4D	-13.05	1.41	1.44
3	A	803	HEM	C3D-C4D	-12.95	1.41	1.44
3	A	807	HEM	C2B-C1B	-12.54	1.41	1.44
3	A	803	HEM	C2D-C1D	-12.19	1.41	1.44
3	A	801	HEM	C2D-C1D	10.61	1.47	1.44
3	A	808	HEM	C2B-C1B	-9.82	1.42	1.44
3	A	806	HEM	C2D-C1D	8.88	1.46	1.44
3	A	806	HEM	C2B-C1B	-7.63	1.42	1.44
3	A	803	HEM	C4A-C3A	7.32	1.49	1.40
3	A	807	HEM	C3B-C2B	-6.99	1.31	1.43
3	A	808	HEM	C2D-C1D	-6.46	1.42	1.44
3	A	803	HEM	C3B-C2B	-6.25	1.32	1.43
3	A	801	HEM	C3C-CAC	6.08	1.59	1.40
3	A	801	HEM	C2B-C1B	6.07	1.46	1.44
3	A	808	HEM	C3C-C2C	-5.90	1.33	1.43
3	A	804	HEM	C3B-C2B	-5.89	1.33	1.43
3	A	802	HEM	C4A-C3A	5.87	1.47	1.40
3	A	802	HEM	C3D-C2D	5.78	1.53	1.43
3	A	803	HEM	C3C-CAC	5.75	1.58	1.40
3	A	803	HEM	C3C-C2C	-5.73	1.33	1.43
3	A	805	HEM	C3C-CAC	5.71	1.58	1.40
3	A	802	HEM	C3C-CAC	5.69	1.58	1.40
3	A	804	HEM	C3C-C2C	-5.69	1.33	1.43
3	A	808	HEM	C3C-CAC	5.67	1.58	1.40
3	A	806	HEM	C3C-CAC	5.63	1.58	1.40
3	A	803	HEM	C3D-C2D	5.63	1.53	1.43
3	A	801	HEM	C3B-C2B	-5.61	1.34	1.43
3	A	803	HEM	C3B-CAB	5.48	1.57	1.40
3	A	805	HEM	C3B-CAB	5.45	1.57	1.40
3	A	807	HEM	C3C-CAC	5.42	1.57	1.40
3	A	807	HEM	C3D-C4D	-5.40	1.43	1.44
3	A	806	HEM	C3D-C2D	5.39	1.53	1.43
3	A	808	HEM	C3B-C2B	-5.35	1.34	1.43
3	A	806	HEM	C3B-C2B	-5.27	1.34	1.43
3	A	804	HEM	C3B-CAB	5.21	1.56	1.40
3	A	804	HEM	C3D-C4D	5.13	1.45	1.44
3	A	808	HEM	C4A-C3A	4.95	1.46	1.40
3	A	806	HEM	C3B-CAB	4.89	1.55	1.40
3	A	805	HEM	C3B-C2B	-4.87	1.35	1.43
3	A	802	HEM	FE-NA	4.83	2.13	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	HEM	CAA-C2A	4.78	1.60	1.52
3	A	802	HEM	C3B-CAB	4.78	1.55	1.40
3	A	801	HEM	C3C-C2C	-4.69	1.35	1.43
3	A	808	HEM	C3B-CAB	4.65	1.55	1.40
3	A	807	HEM	C3B-CAB	4.60	1.54	1.40
3	A	805	HEM	C3C-C2C	-4.43	1.36	1.43
3	A	802	HEM	FE-NC	4.41	2.14	1.97
3	A	802	HEM	C3B-C2B	-4.33	1.36	1.43
3	A	805	HEM	CMD-C2D	4.26	1.60	1.47
3	A	805	HEM	C4A-C3A	4.25	1.45	1.40
3	A	807	HEM	C4A-C3A	4.25	1.45	1.40
3	A	803	HEM	FE-NA	4.10	2.10	1.92
3	A	806	HEM	C3D-C4D	4.10	1.45	1.44
3	A	801	HEM	C3B-CAB	4.04	1.53	1.40
3	A	804	HEM	C3C-CAC	4.01	1.53	1.40
3	A	802	HEM	FE-ND	3.98	2.12	1.97
3	A	808	HEM	CMB-C2B	3.89	1.59	1.47
3	A	802	HEM	CMA-C3A	3.76	1.59	1.51
3	A	807	HEM	C3C-C2C	-3.69	1.37	1.43
3	A	803	HEM	FE-NC	3.68	2.11	1.97
3	A	804	HEM	C2D-C1D	-3.67	1.43	1.44
3	A	807	HEM	CMD-C2D	3.61	1.58	1.47
3	A	803	HEM	CMD-C2D	3.57	1.58	1.47
3	A	802	HEM	CAA-C2A	3.51	1.58	1.52
3	A	805	HEM	CMC-C2C	3.42	1.58	1.47
3	A	808	HEM	C3D-C2D	3.40	1.49	1.43
3	A	806	HEM	C3C-C2C	-3.39	1.37	1.43
3	A	807	HEM	FE-NC	3.36	2.10	1.97
3	A	805	HEM	FE-NA	3.32	2.06	1.92
3	A	801	HEM	CMC-C2C	3.27	1.57	1.47
3	A	805	HEM	C2D-C1D	3.21	1.45	1.44
3	A	803	HEM	CMB-C2B	3.18	1.57	1.47
3	A	807	HEM	C2D-C1D	3.15	1.45	1.44
3	A	802	HEM	C3C-C2C	-3.11	1.38	1.43
3	A	801	HEM	FE-NB	3.10	2.09	1.97
3	A	808	HEM	FE-NA	3.10	2.05	1.92
3	A	808	HEM	CHA-C4D	3.10	1.40	1.35
3	A	802	HEM	CHA-C4D	3.10	1.40	1.35
3	A	804	HEM	C4A-C3A	3.08	1.44	1.40
3	A	802	HEM	CMB-C2B	3.07	1.57	1.47
3	A	801	HEM	C4A-C3A	3.06	1.44	1.40
3	A	805	HEM	CHA-C4D	3.02	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	HEM	CHB-C1B	2.98	1.40	1.35
3	A	804	HEM	C3D-C2D	2.97	1.48	1.43
3	A	805	HEM	CMB-C2B	2.93	1.56	1.47
3	A	802	HEM	CMC-C2C	2.90	1.56	1.47
3	A	808	HEM	FE-NB	2.85	2.08	1.97
3	A	801	HEM	CMD-C2D	2.84	1.56	1.47
3	A	804	HEM	FE-ND	2.79	2.08	1.97
3	A	804	HEM	CMD-C2D	2.78	1.56	1.47
3	A	801	HEM	C3D-C2D	2.69	1.48	1.43
3	A	807	HEM	FE-NA	2.67	2.03	1.92
3	A	804	HEM	CMB-C2B	2.66	1.55	1.47
3	A	806	HEM	FE-NB	2.66	2.07	1.97
3	A	804	HEM	CMC-C2C	2.64	1.55	1.47
3	A	808	HEM	CMC-C2C	2.64	1.55	1.47
3	A	802	HEM	C3D-C4D	2.64	1.45	1.44
3	A	801	HEM	FE-NA	2.64	2.03	1.92
3	A	801	HEM	CAA-C2A	2.62	1.56	1.52
3	A	801	HEM	CMB-C2B	2.60	1.55	1.47
3	A	806	HEM	FE-ND	2.59	2.07	1.97
3	A	803	HEM	CMA-C3A	2.58	1.57	1.51
3	A	806	HEM	CMD-C2D	2.55	1.55	1.47
3	A	805	HEM	FE-NC	2.51	2.07	1.97
3	A	807	HEM	CHA-C4D	2.49	1.39	1.35
3	A	808	HEM	C1A-C2A	2.47	1.47	1.43
3	A	806	HEM	C4A-C3A	2.46	1.43	1.40
3	A	805	HEM	C4C-NC	-2.45	1.34	1.38
3	A	807	HEM	O1D-CGD	2.44	1.31	1.22
3	A	804	HEM	FE-NA	2.44	2.02	1.92
3	A	803	HEM	CMC-C2C	2.41	1.54	1.47
3	A	808	HEM	C3B-C4B	-2.41	1.41	1.44
3	A	808	HEM	CMA-C3A	2.38	1.56	1.51
3	A	806	HEM	CAA-C2A	2.38	1.56	1.52
3	A	803	HEM	C1A-C2A	2.37	1.47	1.43
3	A	808	HEM	O2D-CGD	-2.36	1.21	1.30
3	A	807	HEM	CMC-C2C	2.36	1.54	1.47
3	A	807	HEM	CMB-C2B	2.33	1.54	1.47
3	A	806	HEM	FE-NA	2.28	2.02	1.92
3	A	805	HEM	CHD-C4C	2.27	1.40	1.36
3	A	802	HEM	C3B-C4B	2.26	1.47	1.44
3	A	808	HEM	O1A-CGA	2.26	1.30	1.22
3	A	807	HEM	CAD-C3D	2.26	1.59	1.51
3	A	803	HEM	CAA-C2A	2.23	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	806	HEM	CMB-C2B	2.23	1.54	1.47
3	A	802	HEM	C1A-NA	2.22	1.40	1.36
3	A	803	HEM	C3B-C4B	-2.21	1.41	1.44
3	A	806	HEM	CMC-C2C	2.21	1.54	1.47
3	A	807	HEM	CMA-C3A	2.20	1.56	1.51
3	A	808	HEM	CMD-C2D	2.17	1.54	1.47
3	A	801	HEM	C3D-C4D	-2.15	1.44	1.44
3	A	804	HEM	CMA-C3A	2.12	1.56	1.51
3	A	804	HEM	C1B-NB	-2.10	1.35	1.39
3	A	807	HEM	CHD-C1D	-2.07	1.34	1.39
3	A	804	HEM	C1C-NC	2.06	1.40	1.38
3	A	808	HEM	FE-ND	2.06	2.05	1.97
3	A	807	HEM	FE-NB	2.04	2.05	1.97
3	A	802	HEM	CBA-CGA	2.03	1.55	1.50
3	A	802	HEM	FE-NB	2.02	2.05	1.97
3	A	804	HEM	CBC-CAC	2.01	1.40	1.28
3	A	801	HEM	C4D-ND	-2.01	1.35	1.39
3	A	804	HEM	C4C-NC	2.01	1.40	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	HEM	C3B-C4B-NB	-9.17	107.44	114.00
3	A	806	HEM	C3B-C4B-NB	-8.98	107.57	114.00
3	A	801	HEM	C3B-C4B-NB	-8.77	107.72	114.00
3	A	808	HEM	C4D-ND-C1D	8.71	114.07	105.16
3	A	807	HEM	C3B-C4B-NB	-8.57	107.87	114.00
3	A	802	HEM	C4D-ND-C1D	8.11	113.46	105.16
3	A	802	HEM	C3B-C4B-NB	-8.06	108.23	114.00
3	A	804	HEM	C3B-C4B-NB	-7.96	108.30	114.00
3	A	805	HEM	C3B-C4B-NB	-7.64	108.53	114.00
3	A	808	HEM	C3B-C4B-NB	-7.62	108.54	114.00
3	A	803	HEM	CHC-C4B-NB	7.21	130.57	124.58
3	A	806	HEM	C4D-ND-C1D	7.14	112.46	105.16
3	A	801	HEM	CBA-CAA-C2A	-6.92	100.50	112.69
3	A	806	HEM	CBD-CAD-C3D	-6.70	99.74	114.37
3	A	803	HEM	C4D-ND-C1D	6.37	111.68	105.16
3	A	802	HEM	C2D-C1D-ND	-6.29	105.51	112.93
3	A	801	HEM	C4D-ND-C1D	6.09	111.40	105.16
3	A	808	HEM	C2D-C1D-ND	-5.98	105.87	112.93
3	A	804	HEM	CBD-CAD-C3D	-5.92	101.44	114.37
3	A	805	HEM	CBD-CAD-C3D	-5.38	102.63	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	CBD-CAD-C3D	-5.21	103.01	114.37
3	A	805	HEM	CBA-CAA-C2A	-4.75	104.32	112.69
3	A	802	HEM	C4C-NC-C1C	4.60	110.32	105.53
3	A	807	HEM	CBD-CAD-C3D	-4.58	104.37	114.37
3	A	807	HEM	C4C-NC-C1C	4.41	110.12	105.53
3	A	807	HEM	CBA-CAA-C2A	-4.35	105.04	112.69
3	A	806	HEM	C1B-NB-C4B	4.23	109.49	105.16
3	A	803	HEM	CBD-CAD-C3D	-4.23	105.15	114.37
3	A	801	HEM	C1B-NB-C4B	3.99	109.24	105.16
3	A	807	HEM	CHD-C4C-NC	3.97	128.18	124.73
3	A	801	HEM	CHD-C4C-NC	3.95	128.17	124.73
3	A	803	HEM	C2D-C1D-ND	-3.83	108.41	112.93
3	A	805	HEM	C4C-NC-C1C	3.80	109.48	105.53
3	A	802	HEM	CHD-C1D-ND	3.79	127.73	124.58
3	A	805	HEM	CHC-C1C-NC	3.75	127.99	124.73
3	A	802	HEM	O2D-CGD-CBD	3.68	127.22	114.22
3	A	803	HEM	CHD-C1D-ND	3.54	127.53	124.58
3	A	802	HEM	CBD-CAD-C3D	-3.53	106.66	114.37
3	A	807	HEM	C4D-ND-C1D	3.53	108.77	105.16
3	A	805	HEM	CHD-C4C-NC	3.49	127.77	124.73
3	A	804	HEM	CHD-C4C-NC	3.49	127.76	124.73
3	A	801	HEM	C2D-C1D-ND	-3.41	108.90	112.93
3	A	807	HEM	C3A-C4A-NA	-3.35	106.88	109.41
3	A	806	HEM	C2D-C1D-ND	-3.31	109.02	112.93
3	A	803	HEM	C4A-CHB-C1B	-3.25	123.19	127.47
3	A	808	HEM	CBD-CAD-C3D	-3.24	107.31	114.37
3	A	804	HEM	C4D-ND-C1D	3.18	108.41	105.16
3	A	808	HEM	C1B-NB-C4B	3.15	108.39	105.16
3	A	803	HEM	CHB-C1B-NB	3.12	128.59	124.31
3	A	803	HEM	CHA-C4D-ND	3.07	128.52	124.31
3	A	803	HEM	C1B-NB-C4B	3.06	108.29	105.16
3	A	808	HEM	CBA-CAA-C2A	-3.06	107.31	112.69
3	A	806	HEM	C4A-CHB-C1B	-3.02	123.50	127.47
3	A	805	HEM	CHD-C1D-ND	-2.99	122.10	124.58
3	A	807	HEM	CHC-C1C-NC	2.98	127.32	124.73
3	A	804	HEM	CMB-C2B-C3B	2.97	133.17	126.16
3	A	801	HEM	C3A-C4A-NA	-2.96	107.17	109.41
3	A	807	HEM	C4A-NA-C1A	2.94	110.64	106.76
3	A	803	HEM	O1A-CGA-CBA	-2.94	112.92	123.03
3	A	801	HEM	CHC-C1C-NC	2.93	127.28	124.73
3	A	802	HEM	O2A-CGA-CBA	2.92	124.53	114.22
3	A	807	HEM	C2A-C1A-NA	-2.91	105.69	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	807	HEM	CHC-C4B-NB	2.91	127.00	124.58
3	A	805	HEM	C3A-C4A-NA	-2.88	107.24	109.41
3	A	801	HEM	CHD-C1D-ND	2.83	126.93	124.58
3	A	807	HEM	C3A-C4A-CHB	2.82	131.35	126.00
3	A	802	HEM	C1B-NB-C4B	2.78	108.01	105.16
3	A	808	HEM	CHD-C4C-NC	2.78	127.15	124.73
3	A	807	HEM	CAD-CBD-CGD	-2.75	104.90	113.48
3	A	807	HEM	C1A-C2A-C3A	2.73	109.75	106.92
3	A	808	HEM	CHA-C4D-ND	2.71	128.03	124.31
3	A	805	HEM	CMC-C2C-C3C	2.70	132.52	126.16
3	A	806	HEM	C4C-NC-C1C	2.69	108.33	105.53
3	A	807	HEM	CHB-C1B-NB	2.64	127.93	124.31
3	A	806	HEM	C1A-CHA-C4D	-2.62	124.03	127.47
3	A	804	HEM	CHD-C1D-ND	-2.57	122.45	124.58
3	A	808	HEM	CMA-C3A-C4A	-2.51	124.77	128.62
3	A	802	HEM	O1D-CGD-CBD	-2.50	114.42	123.03
3	A	804	HEM	C1B-NB-C4B	2.50	107.72	105.16
3	A	805	HEM	CAA-CBA-CGA	-2.49	105.47	113.47
3	A	803	HEM	O2A-CGA-CBA	2.46	122.90	114.22
3	A	806	HEM	CHC-C4B-NB	2.39	126.57	124.58
3	A	804	HEM	O2D-CGD-CBD	2.39	122.65	114.22
3	A	802	HEM	CHB-C1B-NB	2.37	127.56	124.31
3	A	805	HEM	CHB-C1B-NB	2.34	127.52	124.31
3	A	804	HEM	C4C-NC-C1C	2.32	107.95	105.53
3	A	801	HEM	C4C-NC-C1C	2.32	107.95	105.53
3	A	808	HEM	CAD-CBD-CGD	-2.28	106.36	113.48
3	A	801	HEM	CHB-C1B-NB	2.27	127.43	124.31
3	A	801	HEM	C4A-NA-C1A	2.26	109.74	106.76
3	A	801	HEM	CMA-C3A-C4A	-2.26	125.15	128.62
3	A	807	HEM	CHD-C1D-ND	-2.22	122.74	124.58
3	A	802	HEM	O2A-CGA-O1A	-2.21	117.67	123.30
3	A	806	HEM	CHD-C4C-NC	2.19	126.64	124.73
3	A	805	HEM	CMA-C3A-C4A	-2.18	125.27	128.62
3	A	808	HEM	C1A-CHA-C4D	-2.18	124.61	127.47
3	A	803	HEM	CHD-C4C-NC	-2.17	122.85	124.73
3	A	805	HEM	CHC-C4B-NB	2.16	126.38	124.58
3	A	801	HEM	C2A-C1A-NA	-2.10	106.82	109.73
3	A	802	HEM	CMC-C2C-C3C	2.09	131.09	126.16
3	A	807	HEM	C4B-CHC-C1C	-2.07	121.11	126.57
3	A	801	HEM	CAD-C3D-C4D	2.07	128.25	124.53
3	A	806	HEM	CHA-C4D-ND	2.07	127.15	124.31
3	A	806	HEM	CMA-C3A-C4A	-2.07	125.44	128.62

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	HEM	C4C-NC-C1C	2.06	107.67	105.53
3	A	806	HEM	CHB-C1B-NB	2.06	127.13	124.31
3	A	806	HEM	O1D-CGD-CBD	-2.06	115.96	123.03
3	A	802	HEM	CAD-C3D-C4D	2.00	128.13	124.53
3	A	805	HEM	C4A-NA-C1A	2.00	109.40	106.76
3	A	802	HEM	CMB-C2B-C3B	2.00	130.88	126.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	436/443 (98%)	-0.35	6 (1%) 72 72	23, 35, 55, 79	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	GLY	10.0
1	A	146	GLY	4.9
1	A	437	GLN	4.4
1	A	201	PRO	3.4
1	A	439	PRO	3.3
1	A	438	GLY	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEM	A	804	43/43	0.11	0.47	20,24,33,34	0
3	HEM	A	806	43/43	0.12	0.17	17,29,45,56	0
3	HEM	A	801	43/43	0.11	0.11	24,32,46,59	0
3	HEM	A	803	43/43	0.12	0.07	22,29,45,49	0
3	HEM	A	807	43/43	0.12	0.02	17,27,43,45	0
3	HEM	A	808	43/43	0.12	-0.11	21,28,44,53	0
3	HEM	A	802	43/43	0.10	-0.35	24,32,47,61	0
3	HEM	A	805	43/43	0.10	-0.39	17,25,35,40	0
2	SCN	A	810	3/3	0.10	-0.46	39,39,41,42	0

## 6.5 Other polymers

There are no such residues in this entry.