Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	3CAR
Title	:	REDUCED STRUCTURE OF THE ACIDIC CYTOCHROME C3 FROM DESULFOVIBRIO AFRICANUS
Authors	:	Norager, S.; Legrand, P.; Pieulle, L.; Hatchikian, C.; Roth, M.
Deposited on	:	1998-11-17
Resolution	:	1.90 Å(reported)

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

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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution
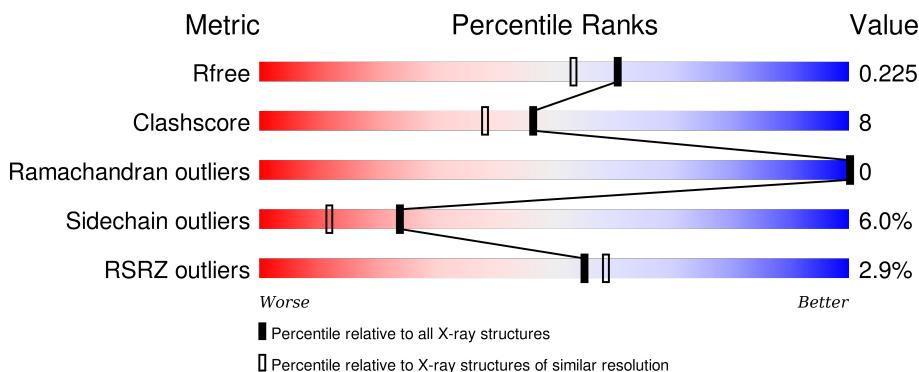
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	103	3% ... 74% ... 24% ... •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1124 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 CYTOCHROME C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	103	786	474	141	161	10	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	4	4	4	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
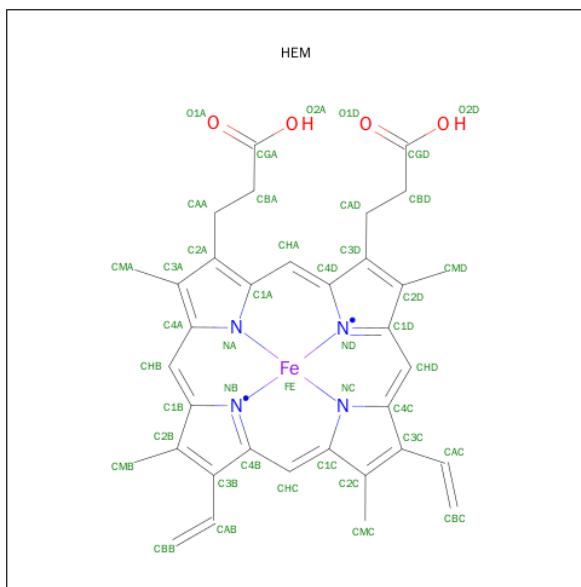
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
3	A	1	43	34	1	4	4	0	0

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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		

- Molecule 4 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	As	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	159	Total	O	0	0
			159	159		

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: CYTOCHROME C3
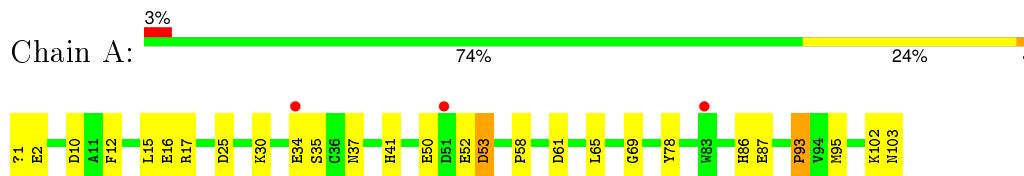
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	107.66Å 107.66Å 107.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 26.91 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-1.90) 97.9 (26.91-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.245 0.189 , 0.225	Depositor DCC
R_{free} test set	832 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.7	EDS
Estimated twinning fraction	0.022 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Outliers	0 of 17499 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1124	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.63	0/798	1.33	6/1082 (0.6%)

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	12

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ASP	CB-CG-OD2	-11.35	108.09	118.30
1	A	78	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	A	17	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	A	25	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	87	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	A	53	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ASP	Mainchain
1	A	12	PHE	Mainchain
1	A	15	LEU	Mainchain
1	A	16	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	34	GLU	Mainchain
1	A	35	SER	Mainchain
1	A	52	GLU	Mainchain
1	A	58	PRO	Mainchain
1	A	61	ASP	Mainchain
1	A	69	GLY	Mainchain
1	A	93	PRO	Mainchain
1	A	95	MET	Mainchain

5.2 Too-close contacts (i)

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	786	0	685	12	0
2	A	4	0	0	0	0
3	A	172	0	120	1	0
4	A	3	0	0	0	0
5	A	159	0	0	2	0
All	All	1124	0	805	13	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 8.

All (13) 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:A:1:CGN:CB	1:A:1:CGN:CA	1.80	1.56
1:A:1:CGN:CG	1:A:1:CGN:CD	1.80	1.54
1:A:1:CGN:N	1:A:1:CGN:CA	1.77	1.45
1:A:1:CGN:CB	1:A:1:CGN:CD	2.22	1.18
1:A:1:CGN:N	1:A:1:CGN:CB	2.23	1.01
1:A:1:CGN:CB	1:A:1:CGN:C	2.40	1.00
1:A:1:CGN:CA	1:A:1:CGN:CD	2.46	0.93
1:A:37:ASN:HB3	1:A:53:ASP:HB3	1.76	0.66
1:A:1:CGN:CG	1:A:1:CGN:OE1	2.42	0.65
1:A:103:ASN:HA	5:A:265:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:HIS:CE1	1:A:93:PRO:HD2	2.42	0.55
3:A:106:HEM:HBA2	5:A:268:HOH:O	2.13	0.48
1:A:1:CGN:N	1:A:2:GLU:N	2.64	0.46

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	101/103 (98%)	96 (95%)	5 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/84 (100%)	79 (94%)	5 (6%)	24	12

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	41	HIS
1	A	50	GLU

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Mol	Chain	Res	Type
1	A	65	LEU
1	A	102	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	104	1	30,50,50	2.65	10 (33%)	24,82,82	3.40	11 (45%)
3	HEM	A	105	1,2	30,50,50	2.70	8 (26%)	24,82,82	3.68	14 (58%)
3	HEM	A	106	1	30,50,50	2.58	8 (26%)	24,82,82	3.27	11 (45%)
3	HEM	A	107	1	30,50,50	2.36	10 (33%)	24,82,82	3.24	11 (45%)

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	104	1	-	0/10/54/54	0/0/8/8
3	HEM	A	105	1,2	-	0/10/54/54	0/0/8/8
3	HEM	A	106	1	-	0/10/54/54	0/0/8/8
3	HEM	A	107	1	-	0/10/54/54	0/0/8/8

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	105	HEM	C3B-C4B	-7.90	1.44	1.51
3	A	106	HEM	C3B-C4B	-7.54	1.45	1.51
3	A	105	HEM	C2D-C3D	-7.49	1.32	1.54
3	A	106	HEM	C2D-C3D	-7.49	1.32	1.54
3	A	104	HEM	C2D-C3D	-7.44	1.32	1.54
3	A	107	HEM	C2D-C3D	-7.14	1.33	1.54
3	A	104	HEM	C3B-C4B	-6.32	1.46	1.51
3	A	105	HEM	C3D-C4D	-5.78	1.44	1.51
3	A	104	HEM	C3D-C4D	-5.42	1.44	1.51
3	A	106	HEM	C3D-C4D	-4.72	1.45	1.51
3	A	107	HEM	C2C-C1C	-4.58	1.43	1.52
3	A	107	HEM	C3B-C4B	-3.93	1.48	1.51
3	A	107	HEM	C3D-C4D	-3.87	1.46	1.51
3	A	104	HEM	C2C-C1C	-3.69	1.45	1.52
3	A	105	HEM	C2C-C1C	-3.47	1.46	1.52
3	A	106	HEM	C2C-C1C	-2.99	1.46	1.52
3	A	104	HEM	C2B-C1B	-2.38	1.44	1.51
3	A	107	HEM	C2D-C1D	-2.03	1.45	1.51
3	A	106	HEM	C3B-CAB	2.02	1.55	1.51
3	A	104	HEM	C3C-CAC	2.03	1.55	1.51
3	A	105	HEM	CAA-C2A	2.05	1.55	1.52
3	A	107	HEM	CBC-CAC	2.06	1.41	1.29
3	A	104	HEM	C3B-CAB	2.13	1.55	1.51
3	A	107	HEM	C1C-NC	2.20	1.38	1.36
3	A	107	HEM	CMA-C3A	2.23	1.56	1.51
3	A	104	HEM	C4C-NC	2.31	1.38	1.36
3	A	106	HEM	CAA-C2A	2.50	1.56	1.52
3	A	106	HEM	C3C-CAC	2.54	1.56	1.51
3	A	105	HEM	C3B-CAB	2.55	1.56	1.51
3	A	105	HEM	C1C-NC	2.65	1.39	1.36
3	A	104	HEM	CAA-C2A	2.71	1.56	1.52
3	A	107	HEM	C3C-CAC	2.94	1.56	1.51
3	A	105	HEM	C3C-CAC	3.01	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	106	HEM	C4C-NC	3.11	1.39	1.36
3	A	104	HEM	C1C-NC	3.66	1.40	1.36
3	A	107	HEM	C4C-NC	3.82	1.40	1.36

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	107	HEM	C3C-CAC-CBC	-8.56	111.33	124.46
3	A	105	HEM	C3B-CAB-CBB	-8.46	111.47	124.46
3	A	104	HEM	C3C-CAC-CBC	-8.06	112.10	124.46
3	A	106	HEM	C3B-CAB-CBB	-7.70	112.65	124.46
3	A	105	HEM	C3C-CAC-CBC	-7.33	113.21	124.46
3	A	104	HEM	C3B-CAB-CBB	-7.17	113.45	124.46
3	A	107	HEM	C3B-CAB-CBB	-5.43	116.13	124.46
3	A	106	HEM	C3C-CAC-CBC	-5.18	116.52	124.46
3	A	105	HEM	CAA-C2A-C1A	-4.66	121.95	127.01
3	A	105	HEM	CMA-C3A-C4A	-3.84	122.01	128.36
3	A	105	HEM	C1D-CHD-C4C	-3.71	119.63	125.82
3	A	104	HEM	CAA-C2A-C1A	-3.68	123.01	127.01
3	A	107	HEM	C4B-CHC-C1C	-3.57	119.86	125.82
3	A	106	HEM	CAA-C2A-C1A	-3.50	123.21	127.01
3	A	107	HEM	CAA-C2A-C1A	-3.44	123.27	127.01
3	A	104	HEM	CMA-C3A-C4A	-3.15	123.15	128.36
3	A	106	HEM	C1D-CHD-C4C	-3.09	120.66	125.82
3	A	107	HEM	CMA-C3A-C4A	-3.01	123.38	128.36
3	A	106	HEM	CMA-C3A-C4A	-2.76	123.79	128.36
3	A	105	HEM	CBD-CAD-C3D	-2.41	106.53	113.55
3	A	105	HEM	CMA-C3A-C2A	2.28	130.00	125.24
3	A	106	HEM	CAD-C3D-C4D	2.31	120.60	112.47
3	A	107	HEM	CAD-C3D-C4D	2.59	121.60	112.47
3	A	105	HEM	C3B-C4B-CHC	2.74	127.02	123.16
3	A	104	HEM	CAD-C3D-C4D	2.86	122.54	112.47
3	A	107	HEM	CMD-C2D-C3D	2.98	127.52	114.35
3	A	105	HEM	CAD-C3D-C4D	3.08	123.35	112.47
3	A	104	HEM	CAA-CBA-CGA	3.11	118.45	112.75
3	A	104	HEM	CMD-C2D-C3D	3.20	128.49	114.35
3	A	106	HEM	CMD-C2D-C3D	3.21	128.55	114.35
3	A	105	HEM	CMD-C2D-C3D	3.53	129.95	114.35
3	A	107	HEM	C2D-C3D-C4D	3.70	107.77	101.50
3	A	104	HEM	C2D-C3D-C4D	3.89	108.09	101.50
3	A	107	HEM	CMC-C2C-C3C	4.21	127.04	116.53
3	A	106	HEM	C2D-C3D-C4D	4.38	108.92	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed($^\circ$)	Ideal($^\circ$)
3	A	105	HEM	CMC-C2C-C3C	4.56	127.91	116.53
3	A	104	HEM	CMB-C2B-C3B	4.59	127.99	116.53
3	A	105	HEM	C2D-C3D-C4D	4.69	109.46	101.50
3	A	107	HEM	CMB-C2B-C3B	4.72	128.32	116.53
3	A	105	HEM	CAD-C3D-C2D	4.77	126.92	113.22
3	A	106	HEM	CMC-C2C-C3C	5.06	129.16	116.53
3	A	104	HEM	CMC-C2C-C3C	5.41	130.04	116.53
3	A	104	HEM	CAD-C3D-C2D	5.42	128.81	113.22
3	A	106	HEM	CMB-C2B-C3B	5.52	130.31	116.53
3	A	105	HEM	CMB-C2B-C3B	5.86	131.15	116.53
3	A	107	HEM	CAD-C3D-C2D	5.99	130.45	113.22
3	A	106	HEM	CAD-C3D-C2D	6.00	130.46	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	106	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	102/103 (99%)	-0.14	3 (2%)	55	59	17, 27, 44, 56	12 (11%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	ASP	2.5
1	A	83	TRP	2.3
1	A	34	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
3	HEM	A	104	43/43	0.98	0.09	0.31	17,20,45,51	0
3	HEM	A	107	43/43	0.98	0.11	0.07	15,20,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	HEM	A	105	43/43	0.98	0.08	-0.15	16,22,25,29	0
3	HEM	A	106	43/43	0.98	0.09	-0.44	15,19,33,34	3
4	ARS	A	110	1/1	0.79	0.10	-	48,48,48,48	1
2	ZN	A	114	1/1	0.97	0.03	-	42,42,42,42	0
4	ARS	A	108	1/1	0.82	0.07	-	59,59,59,59	1
2	ZN	A	112	1/1	0.98	0.05	-	50,50,50,50	0
2	ZN	A	111	1/1	0.99	0.06	-	25,25,25,25	0
2	ZN	A	113	1/1	0.94	0.07	-	61,61,61,61	0
4	ARS	A	109	1/1	0.95	0.15	-	59,59,59,59	1

6.5 Other polymers (i)

There are no such residues in this entry.