



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:12 pm GMT

PDB ID : 1FS9  
Title : CYTOCHROME C NITRITE REDUCTASE FROM WOLINELLA SUCCINOGENES-AZIDE COMPLEX  
Authors : Einsle, O.; Stach, P.; Messerschmidt, A.; Simon, J.; Kroeger, A.; Huber, R.; Kroneck, P.M.H.  
Deposited on : 2000-09-08  
Resolution : 2.00 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](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

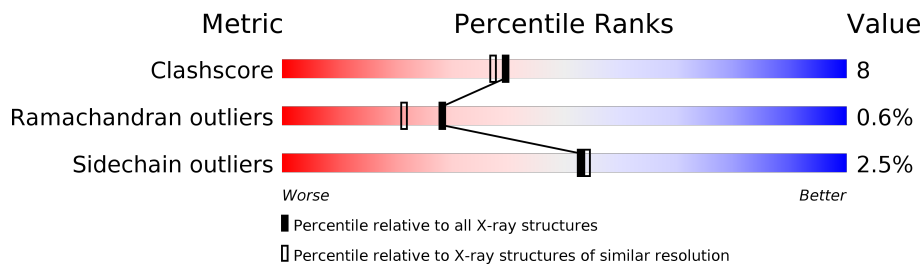
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	507	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4419 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 C NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	21	0	0
			3772	2387	648	716	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLU	LYS	CONFLICT	UNP Q9S1E5

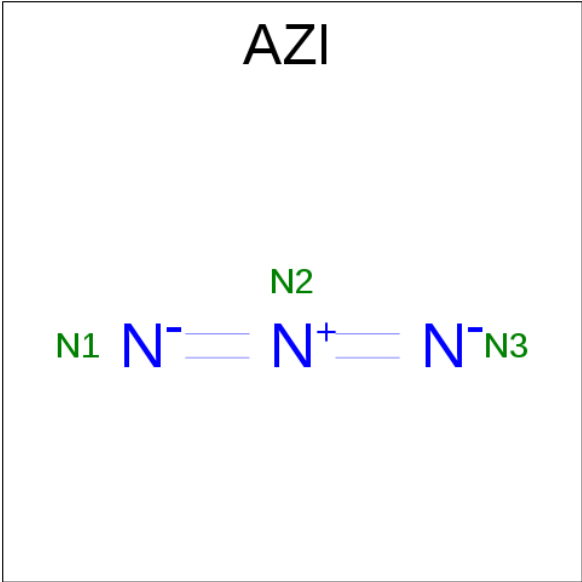
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is YTTRIUM ION (three-letter code: Y1) (formula: Y).

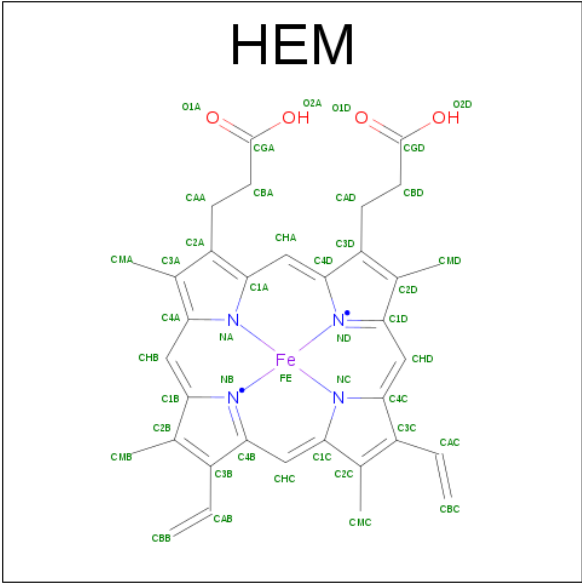
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Y	0	0
			3	3		

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	N			0	0
			3	3				

- Molecule 5 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
5	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
5	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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

- Molecule 6 is water.

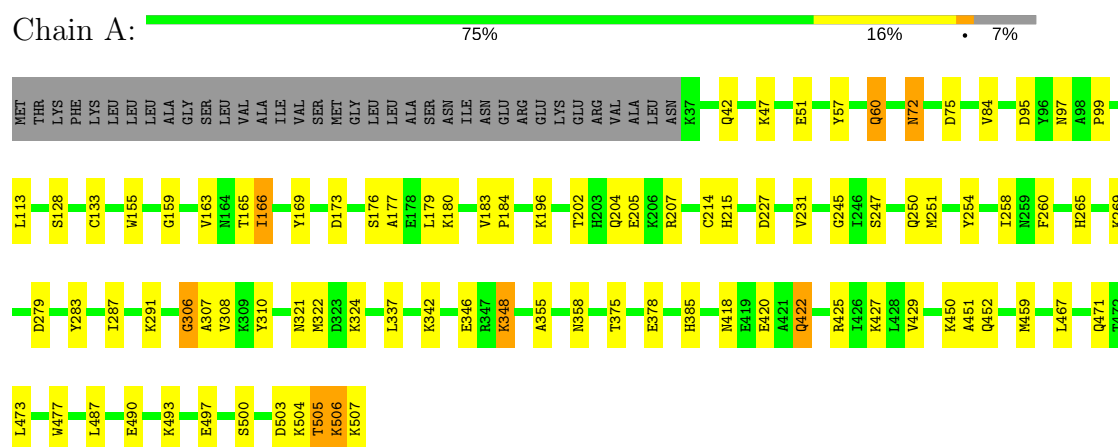
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	425	Total	O	0	0
			425	425		

### 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 the various outlier classes 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.

Note EDS was not executed.

#### • Molecule 1: CYTOCHROME C NITRITE REDUCTASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.53Å 119.53Å 186.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	5.0 (25.00-2.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.180 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4419	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 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: Y1, AZI, CA, 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	0.30	0/3863	0.56	0/5202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3772	0	3682	65	0
2	A	1	0	0	0	0
3	A	3	0	0	0	0
4	A	3	0	0	0	0
5	A	215	0	150	3	0
6	A	425	0	0	3	1
All	All	4419	0	3832	65	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 8.

All (65) 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:358:ASN:HD22	1:A:418:ASN:HD21	1.11	0.92
1:A:422:GLN:HE21	1:A:422:GLN:HA	1.48	0.79
1:A:60:GLN:H	1:A:60:GLN:NE2	1.86	0.73
1:A:346:GLU:HG2	6:A:835:HOH:O	1.91	0.71
1:A:321:ASN:ND2	1:A:324:LYS:HB2	2.07	0.69
1:A:452:GLN:HE22	1:A:459:MET:HG3	1.58	0.68
1:A:321:ASN:HD21	1:A:324:LYS:HB2	1.62	0.65
1:A:72:ASN:HB3	6:A:818:HOH:O	1.97	0.65
1:A:467:LEU:O	1:A:471:GLN:HG3	1.98	0.64
1:A:60:GLN:H	1:A:60:GLN:HE21	1.45	0.63
1:A:227:ASP:OD2	1:A:231:VAL:HB	1.97	0.63
1:A:452:GLN:NE2	1:A:459:MET:HG3	2.14	0.62
1:A:385:HIS:HE1	1:A:427:LYS:NZ	1.98	0.61
1:A:75:ASP:HA	1:A:97:ASN:HD22	1.67	0.60
1:A:385:HIS:HD2	1:A:420:GLU:OE1	1.86	0.58
1:A:179:LEU:O	1:A:180:LYS:HG2	2.03	0.58
1:A:287:ILE:O	1:A:291:LYS:HG2	2.04	0.57
1:A:196:LYS:NZ	1:A:196:LYS:HB2	2.19	0.57
1:A:245:GLY:HA3	1:A:250:GLN:NE2	2.21	0.56
1:A:179:LEU:HD11	5:A:509:HEM:HBD1	1.88	0.56
1:A:99:PRO:HG2	5:A:511:HEM:O1A	2.07	0.55
1:A:57:TYR:HB3	1:A:60:GLN:NE2	2.22	0.55
1:A:422:GLN:NE2	1:A:422:GLN:HA	2.21	0.54
1:A:506:LYS:H	1:A:506:LYS:HD3	1.71	0.54
1:A:47:LYS:HD2	1:A:169:TYR:CE1	2.44	0.53
1:A:306:GLY:O	1:A:307:ALA:HB3	2.08	0.53
1:A:358:ASN:HD22	1:A:418:ASN:ND2	1.94	0.52
1:A:247:SER:H	1:A:250:GLN:HE21	1.59	0.51
1:A:207:ARG:NH1	5:A:509:HEM:O1D	2.45	0.49
1:A:202:THR:OG1	1:A:205:GLU:HG3	2.14	0.48
1:A:490:GLU:CD	1:A:493:LYS:HE2	2.34	0.47
1:A:355:ALA:HA	1:A:418:ASN:HD22	1.79	0.47
1:A:425:ARG:O	1:A:429:VAL:HG23	2.14	0.47
1:A:165:THR:O	1:A:166:ILE:C	2.52	0.47
1:A:342:LYS:O	1:A:346:GLU:HG3	2.15	0.47
1:A:504:LYS:O	1:A:505:THR:HB	2.15	0.47
1:A:204:GLN:HA	1:A:204:GLN:HE21	1.81	0.46
1:A:450:LYS:NZ	6:A:658:HOH:O	2.49	0.46
1:A:215:HIS:HB3	1:A:279:ASP:HB2	1.98	0.46
1:A:247:SER:H	1:A:250:GLN:NE2	2.14	0.46
1:A:322:MET:HE1	1:A:337:LEU:HB3	1.98	0.46
1:A:322:MET:CE	1:A:337:LEU:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLU:OE2	1:A:493:LYS:HE2	2.17	0.45
1:A:176:SER:O	1:A:177:ALA:HB3	2.17	0.45
1:A:163:VAL:HG21	1:A:487:LEU:HB2	1.99	0.44
1:A:497:GLU:HA	1:A:504:LYS:HD2	1.99	0.44
1:A:265:HIS:O	1:A:269:LYS:HD2	2.18	0.44
1:A:97:ASN:HD21	1:A:500:SER:HB3	1.82	0.44
1:A:503:ASP:OD1	1:A:505:THR:N	2.47	0.43
1:A:348:LYS:C	1:A:348:LYS:HD2	2.39	0.43
1:A:251:MET:O	1:A:254:TYR:HB3	2.18	0.43
1:A:159:GLY:HA3	1:A:477:TRP:CE2	2.53	0.43
1:A:173:ASP:HB2	1:A:180:LYS:HG3	2.00	0.43
1:A:385:HIS:HE1	1:A:427:LYS:HZ1	1.64	0.43
1:A:183:VAL:HA	1:A:184:PRO:HD3	1.89	0.43
1:A:84:VAL:HB	1:A:451:ALA:HB1	2.00	0.43
1:A:258:ILE:HG13	1:A:260:PHE:HB2	2.00	0.43
1:A:375:THR:OG1	1:A:378:GLU:HG3	2.18	0.43
1:A:308:VAL:HG11	1:A:310:TYR:CZ	2.54	0.42
1:A:95:ASP:HB2	1:A:113:LEU:HB2	2.01	0.41
1:A:133:CYS:HB3	1:A:214:CYS:HB3	2.01	0.41
1:A:196:LYS:HB2	1:A:196:LYS:HZ3	1.83	0.41
1:A:422:GLN:HE22	1:A:425:ARG:HH11	1.68	0.41
1:A:128:SER:HA	1:A:155:TRP:HA	2.02	0.41
1:A:490:GLU:OE1	1:A:493:LYS:HE2	2.21	0.40

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)
6:A:927:HOH:O	6:A:927:HOH:O[10_565]	1.51	0.69

## 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	469/507 (92%)	452 (96%)	14 (3%)	3 (1%)	28 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ILE
1	A	505	THR
1	A	306	GLY

### 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	397/427 (93%)	387 (98%)	10 (2%)	53 54

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	51	GLU
1	A	60	GLN
1	A	72	ASN
1	A	283	TYR
1	A	348	LYS
1	A	422	GLN
1	A	473	LEU
1	A	506	LYS
1	A	507	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	60	GLN
1	A	97	ASN

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Mol	Chain	Res	Type
1	A	144	GLN
1	A	204	GLN
1	A	250	GLN
1	A	321	ASN
1	A	352	GLN
1	A	385	HIS
1	A	418	ASN
1	A	422	GLN
1	A	452	GLN
1	A	480	GLN

### 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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
5	HEM	A	508	1,6	28,50,50	1.62	4 (14%)	17,82,82	1.33	1 (5%)
5	HEM	A	509	1	28,50,50	1.57	4 (14%)	17,82,82	0.87	1 (5%)
5	HEM	A	510	1	28,50,50	1.57	5 (17%)	17,82,82	1.28	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	A	511	1	28,50,50	1.51	5 (17%)	17,82,82	1.35	2 (11%)
5	HEM	A	512	1	28,50,50	1.55	4 (14%)	17,82,82	1.02	1 (5%)
4	AZI	A	517	-	0,2,2	0.00	-	0,1,1	0.00	-

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
5	HEM	A	508	1,6	-	0/6/54/54	0/0/8/8
5	HEM	A	509	1	-	0/6/54/54	0/0/8/8
5	HEM	A	510	1	-	0/6/54/54	0/0/8/8
5	HEM	A	511	1	-	0/6/54/54	0/0/8/8
5	HEM	A	512	1	-	0/6/54/54	0/0/8/8
4	AZI	A	517	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	508	HEM	C3B-CAB	-4.05	1.39	1.47
5	A	509	HEM	C3C-CAC	-3.84	1.40	1.47
5	A	511	HEM	C3B-CAB	-3.81	1.40	1.47
5	A	509	HEM	C3C-C2C	-3.72	1.35	1.40
5	A	512	HEM	C3C-CAC	-3.67	1.40	1.47
5	A	509	HEM	C3B-CAB	-3.67	1.40	1.47
5	A	510	HEM	C3C-CAC	-3.63	1.40	1.47
5	A	512	HEM	C3B-CAB	-3.62	1.40	1.47
5	A	510	HEM	C3B-C2B	-3.45	1.35	1.40
5	A	511	HEM	C3C-C2C	-3.40	1.35	1.40
5	A	510	HEM	C3B-CAB	-3.27	1.41	1.47
5	A	508	HEM	C3C-C2C	-3.20	1.36	1.40
5	A	512	HEM	C3C-C2C	-3.17	1.36	1.40
5	A	511	HEM	C3C-CAC	-3.15	1.41	1.47
5	A	508	HEM	C3C-CAC	-3.15	1.41	1.47
5	A	508	HEM	C3B-C2B	-3.09	1.36	1.40
5	A	510	HEM	C3C-C2C	-2.98	1.36	1.40
5	A	509	HEM	C3B-C2B	-2.71	1.36	1.40
5	A	512	HEM	C3B-C2B	-2.41	1.37	1.40
5	A	511	HEM	C3B-C2B	-2.41	1.37	1.40
5	A	511	HEM	CBC-CAC	2.02	1.43	1.28
5	A	510	HEM	C4D-ND	2.17	1.39	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	511	HEM	C4C-C3C-C2C	-3.18	104.68	106.90
5	A	511	HEM	CBA-CAA-C2A	-2.54	107.62	112.48
5	A	510	HEM	C4C-C3C-C2C	-2.40	105.22	106.90
5	A	510	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
5	A	509	HEM	C3B-C4B-NB	2.11	111.94	109.21
5	A	512	HEM	CBA-CAA-C2A	2.13	116.55	112.48
5	A	510	HEM	C3B-C4B-NB	2.16	112.01	109.21
5	A	508	HEM	CBD-CAD-C3D	4.24	120.56	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	HEM	2	0
5	A	511	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.