



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:54 PM GMT

PDB ID : 4N4N  
Title : Nitrosomonas europea HAO  
Authors : Maalcke, W.J.; Dietl, A.; Marritt, S.J.; Butt, J.N.; Jetten, M.S.M.; Keltjens, J.T.; Barends, T.R.M.B.; Kartal, B.  
Deposited on : 2013-10-08  
Resolution : 2.20 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](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.

---

The following versions of software and data (see [references ⓘ](#)) 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

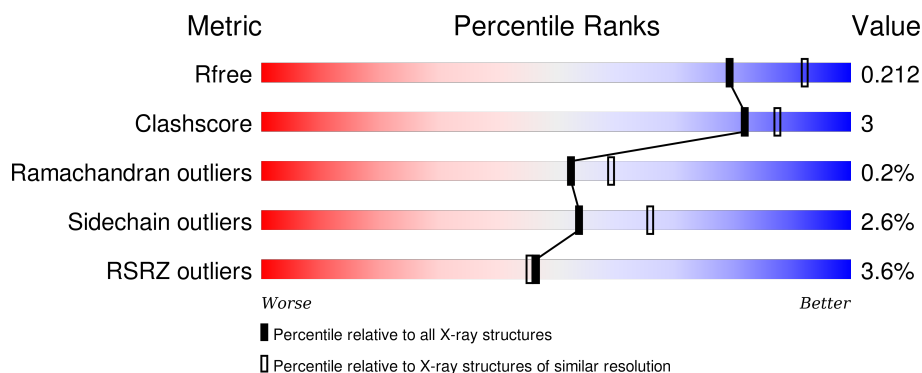
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	546	<div> <div></div> <div>86% 5% 8%</div> </div>
1	C	546	<div> <div></div> <div>85% 6% 8%</div> </div>
1	E	546	<div> <div></div> <div>82% 9% 8%</div> </div>
2	B	57	<div> <div>26%</div> <div>93% 5%</div> </div>
2	D	57	<div> <div>19%</div> <div>89% 9%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	57	<div><div></div><div>26%</div><div>89%</div><div>7%</div><div>••</div></div>

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
6	PO4	E	609	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15450 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 Hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4018	2499	713	774	32			
1	C	502	Total	C	N	O	S	0	0	0
			4005	2491	710	772	32			
1	E	503	Total	C	N	O	S	0	1	0
			4018	2499	713	774	32			

- Molecule 2 is a protein called hydroxylamine oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	56	Total	C	N	O	S	0	0	0
			423	263	75	82	3			
2	D	57	Total	C	N	O	S	0	0	0
			429	266	76	84	3			
2	F	56	Total	C	N	O	S	0	0	0
			425	264	75	83	3			

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



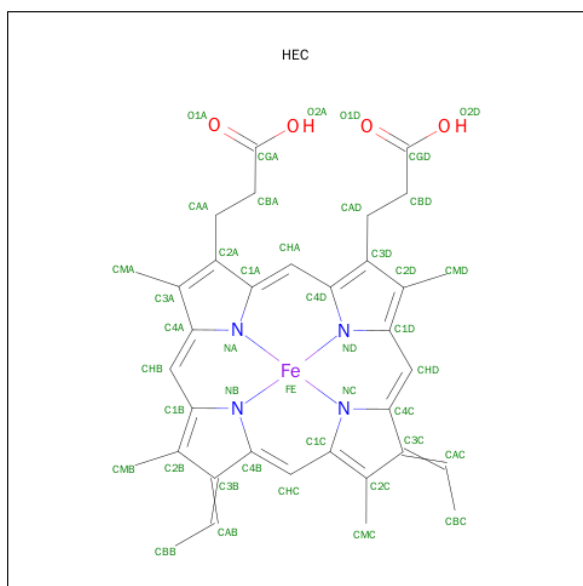
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0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

Continued on next page...

Continued from previous page...

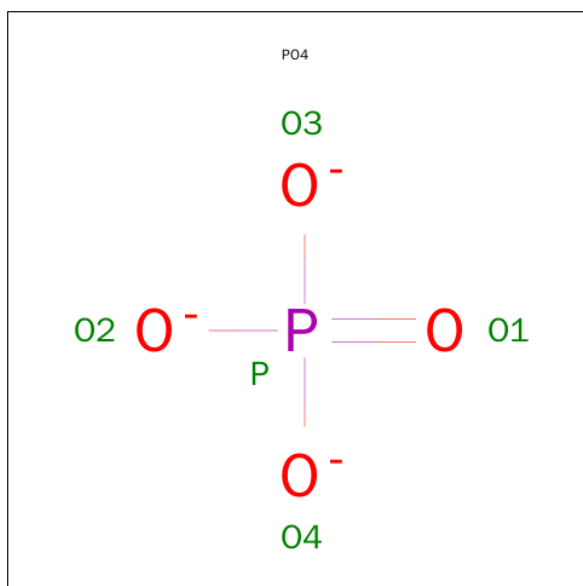
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



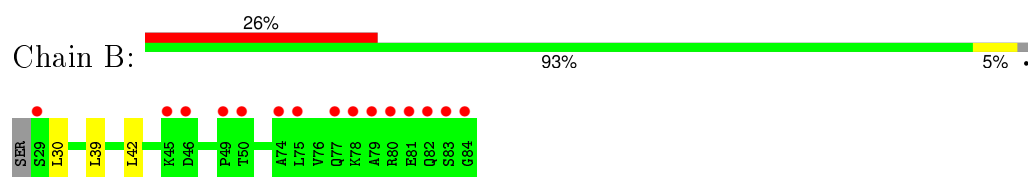
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

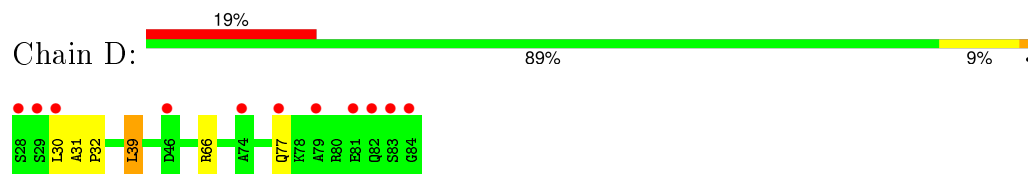
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	330	Total O 330 330	0	0
7	B	42	Total O 42 42	0	0
7	C	328	Total O 328 328	0	0
7	D	37	Total O 37 37	0	0
7	E	314	Total O 314 314	0	0
7	F	43	Total O 43 43	0	0



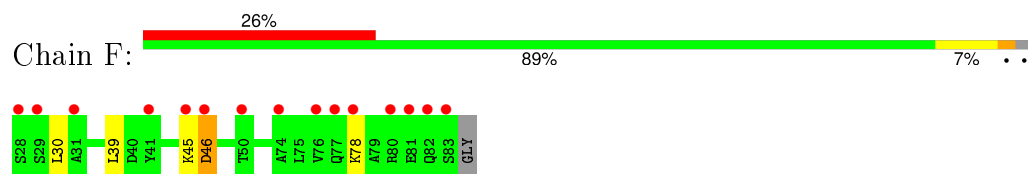




- Molecule 2: hydroxylamine oxidoreductase



- Molecule 2: hydroxylamine oxidoreductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.72Å 141.97Å 106.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.40 – 2.20 47.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.40-2.20) 99.6 (47.07-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.179 , 0.213 0.179 , 0.212	Depositor DCC
$R_{free}$ test set	10263 reflections (10.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.0	EDS
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 108386 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>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: HEM, K, PO4, HEC

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	0.35	0/4121	0.50	0/5583
1	C	0.35	0/4108	0.51	0/5567
1	E	0.35	0/4121	0.51	0/5583
2	B	0.33	0/426	0.53	0/571
2	D	0.33	0/432	0.57	0/579
2	F	0.32	0/428	0.53	0/574
All	All	0.35	0/13636	0.51	0/18457

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	4018	0	3821	20	0
1	C	4005	0	3805	22	0
1	E	4018	0	3820	38	0
2	B	423	0	444	0	0
2	D	429	0	449	2	0
2	F	425	0	446	1	0
3	A	301	0	210	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	301	0	210	5	0
3	E	301	0	210	7	0
4	A	43	0	29	2	0
4	C	43	0	29	3	0
4	E	43	0	29	2	0
5	A	1	0	0	0	0
6	E	5	0	0	0	0
7	A	330	0	0	1	0
7	B	42	0	0	0	0
7	C	328	0	0	0	0
7	D	37	0	0	0	0
7	E	314	0	0	1	0
7	F	43	0	0	0	0
All	All	15450	0	13502	90	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 3.

The worst 5 of 90 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:179[B]:LYS:HD3	1:E:179[B]:LYS:N	1.62	1.10
1:E:179[B]:LYS:CD	1:E:179[B]:LYS:H	1.69	1.03
1:E:179[B]:LYS:HD3	1:E:179[B]:LYS:H	0.81	0.94
2:F:45:LYS:O	2:F:46:ASP:HB2	1.82	0.78
1:C:37:LEU:HD11	1:C:53:LEU:HD13	1.66	0.78

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	502/546 (92%)	487 (97%)	14 (3%)	1 (0%)	52	59
1	C	500/546 (92%)	485 (97%)	14 (3%)	1 (0%)	52	59
1	E	502/546 (92%)	488 (97%)	14 (3%)	0	100	100
2	B	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	D	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
2	F	54/57 (95%)	52 (96%)	1 (2%)	1 (2%)	10	6
All	All	1667/1809 (92%)	1619 (97%)	45 (3%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	46	ASP
1	C	292	HIS
1	A	292	HIS

### 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	430/459 (94%)	421 (98%)	9 (2%)	61	74
1	C	429/459 (94%)	419 (98%)	10 (2%)	58	71
1	E	430/459 (94%)	421 (98%)	9 (2%)	61	74
2	B	48/49 (98%)	45 (94%)	3 (6%)	22	24
2	D	49/49 (100%)	45 (92%)	4 (8%)	14	13
2	F	49/49 (100%)	46 (94%)	3 (6%)	23	26
All	All	1435/1524 (94%)	1397 (97%)	38 (3%)	54	66

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	312	ASP
1	C	474	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	30	LEU
1	C	320	LEU
2	D	30	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	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 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	601	1	30,50,50	2.19	10 (33%)	24,82,82	2.48	10 (41%)
3	HEM	A	602	1	30,50,50	2.17	10 (33%)	24,82,82	2.34	10 (41%)
3	HEM	A	603	1	30,50,50	2.18	7 (23%)	24,82,82	2.35	11 (45%)
3	HEM	A	604	1	30,50,50	2.28	9 (30%)	24,82,82	2.35	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	A	605	1	30,50,50	2.20	8 (26%)	24,82,82	2.53	13 (54%)
3	HEM	A	606	1	30,50,50	2.14	9 (30%)	24,82,82	2.39	11 (45%)
3	HEM	A	607	1	30,50,50	2.15	8 (26%)	24,82,82	2.47	12 (50%)
4	HEC	A	608	1,7	24,50,50	3.82	8 (33%)	19,82,82	2.69	10 (52%)
4	HEC	C	601	1	24,50,50	3.84	8 (33%)	19,82,82	2.66	8 (42%)
3	HEM	C	602	1	30,50,50	2.18	9 (30%)	24,82,82	2.42	10 (41%)
3	HEM	C	603	1	30,50,50	2.15	9 (30%)	24,82,82	2.48	10 (41%)
3	HEM	C	604	1	30,50,50	2.13	10 (33%)	24,82,82	2.40	11 (45%)
3	HEM	C	605	1	30,50,50	2.33	8 (26%)	24,82,82	2.38	10 (41%)
3	HEM	C	606	1	30,50,50	2.21	9 (30%)	24,82,82	2.49	13 (54%)
3	HEM	C	607	1	30,50,50	2.15	10 (33%)	24,82,82	2.42	12 (50%)
3	HEM	C	608	1	30,50,50	2.22	8 (26%)	24,82,82	2.44	12 (50%)
4	HEC	E	601	1,7	24,50,50	3.85	9 (37%)	19,82,82	2.90	13 (68%)
3	HEM	E	602	1	30,50,50	2.23	9 (30%)	24,82,82	2.45	10 (41%)
3	HEM	E	603	1	30,50,50	2.17	8 (26%)	24,82,82	2.48	13 (54%)
3	HEM	E	604	1	30,50,50	2.19	9 (30%)	24,82,82	2.35	11 (45%)
3	HEM	E	605	1	30,50,50	2.29	8 (26%)	24,82,82	2.36	10 (41%)
3	HEM	E	606	1	30,50,50	2.24	8 (26%)	24,82,82	2.47	13 (54%)
3	HEM	E	607	1	30,50,50	2.19	9 (30%)	24,82,82	2.46	12 (50%)
3	HEM	E	608	1	30,50,50	2.22	6 (20%)	24,82,82	2.50	12 (50%)
6	PO4	E	609	-	4,4,4	0.49	0	6,6,6	0.27	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	601	1	-	0/10/54/54	0/0/8/8
3	HEM	A	602	1	-	0/10/54/54	0/0/8/8
3	HEM	A	603	1	-	0/10/54/54	0/0/8/8
3	HEM	A	604	1	-	0/10/54/54	0/0/8/8
3	HEM	A	605	1	-	0/10/54/54	0/0/8/8
3	HEM	A	606	1	-	0/10/54/54	0/0/8/8
3	HEM	A	607	1	-	0/10/54/54	0/0/8/8
4	HEC	A	608	1,7	-	0/6/54/54	0/0/8/8
4	HEC	C	601	1	-	0/6/54/54	0/0/8/8
3	HEM	C	602	1	-	0/10/54/54	0/0/8/8

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	603	1	-	0/10/54/54	0/0/8/8
3	HEM	C	604	1	-	0/10/54/54	0/0/8/8
3	HEM	C	605	1	-	0/10/54/54	0/0/8/8
3	HEM	C	606	1	-	0/10/54/54	0/0/8/8
3	HEM	C	607	1	-	0/10/54/54	0/0/8/8
3	HEM	C	608	1	-	0/10/54/54	0/0/8/8
4	HEC	E	601	1,7	-	0/6/54/54	0/0/8/8
3	HEM	E	602	1	-	0/10/54/54	0/0/8/8
3	HEM	E	603	1	-	0/10/54/54	0/0/8/8
3	HEM	E	604	1	-	0/10/54/54	0/0/8/8
3	HEM	E	605	1	-	0/10/54/54	0/0/8/8
3	HEM	E	606	1	-	0/10/54/54	0/0/8/8
3	HEM	E	607	1	-	0/10/54/54	0/0/8/8
3	HEM	E	608	1	-	0/10/54/54	0/0/8/8
6	PO4	E	609	-	-	0/0/0/0	0/0/0/0

The worst 5 of 206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	605	HEM	C3B-C4B	-7.98	1.44	1.51
3	E	606	HEM	C3B-C4B	-7.79	1.44	1.51
3	C	605	HEM	C3B-C4B	-7.75	1.44	1.51
3	A	604	HEM	C3B-C4B	-7.74	1.45	1.51
3	E	603	HEM	C3B-C4B	-7.64	1.45	1.51

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	HEC	CBC-CAC-C3C	-6.40	113.12	127.35
4	C	601	HEC	CBC-CAC-C3C	-6.22	113.52	127.35
4	A	608	HEC	CBC-CAC-C3C	-6.22	113.54	127.35
4	C	601	HEC	CBB-CAB-C3B	-4.98	116.29	127.35
4	A	608	HEC	CBB-CAB-C3B	-4.67	116.97	127.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	HEM	1	0
3	A	605	HEM	2	0
3	A	606	HEM	4	0
3	A	607	HEM	1	0
4	A	608	HEC	2	0
4	C	601	HEC	3	0
3	C	602	HEM	1	0
3	C	603	HEM	1	0
3	C	604	HEM	1	0
3	C	605	HEM	2	0
3	C	606	HEM	2	0
3	C	607	HEM	2	0
4	E	601	HEC	2	0
3	E	602	HEM	1	0
3	E	603	HEM	1	0
3	E	605	HEM	1	0
3	E	606	HEM	3	0
3	E	607	HEM	4	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, 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	504/546 (92%)	-0.30	7 (1%) 78 77	18, 26, 38, 61	0
1	C	502/546 (91%)	-0.28	5 (0%) 84 83	18, 26, 40, 56	0
1	E	503/546 (92%)	-0.34	8 (1%) 74 73	18, 26, 39, 54	0
2	B	56/57 (98%)	0.96	15 (26%) 1 1	28, 40, 67, 68	0
2	D	57/57 (100%)	0.51	11 (19%) 2 1	26, 32, 63, 65	0
2	F	56/57 (98%)	1.04	15 (26%) 1 1	29, 41, 69, 70	0
All	All	1678/1809 (92%)	-0.19	61 (3%) 46 45	18, 27, 44, 70	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	84	GLY	7.4
2	D	83	SER	5.9
2	B	79	ALA	5.6
2	F	81	GLU	5.1
2	F	28	SER	4.9

### 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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	PO4	E	609	5/5	0.98	0.19	2.84	53,53,53,54	0
3	HEM	C	607	43/43	0.98	0.13	1.01	17,20,24,26	0
3	HEM	A	606	43/43	0.98	0.13	0.67	18,19,23,24	0
3	HEM	A	601	43/43	0.97	0.11	0.54	19,21,23,23	0
4	HEC	C	601	43/43	0.96	0.14	0.42	21,22,24,25	0
3	HEM	E	605	43/43	0.97	0.10	0.32	22,24,26,27	0
3	HEM	E	602	43/43	0.97	0.11	0.30	19,21,22,23	0
3	HEM	C	608	43/43	0.98	0.12	0.25	18,19,22,25	0
3	HEM	E	608	43/43	0.98	0.10	0.16	19,21,22,23	0
3	HEM	C	606	43/43	0.97	0.14	0.15	17,19,22,24	0
3	HEM	E	607	43/43	0.98	0.11	0.15	18,19,22,24	0
3	HEM	A	605	43/43	0.98	0.12	0.07	17,19,22,23	0
4	HEC	E	601	43/43	0.97	0.12	0.04	21,23,25,26	0
3	HEM	E	606	43/43	0.98	0.12	0.01	17,18,19,20	0
3	HEM	E	603	43/43	0.97	0.10	-0.11	22,24,24,25	0
3	HEM	C	605	43/43	0.97	0.10	-0.11	21,22,24,24	0
3	HEM	C	603	43/43	0.98	0.09	-0.12	19,22,24,24	0
3	HEM	A	603	43/43	0.97	0.10	-0.22	22,24,25,26	0
3	HEM	A	607	43/43	0.98	0.11	-0.24	19,21,22,24	0
3	HEM	A	604	43/43	0.98	0.10	-0.25	16,21,22,23	0
3	HEM	C	602	43/43	0.98	0.10	-0.29	19,21,23,23	0
3	HEM	E	604	43/43	0.97	0.10	-0.32	26,31,34,34	0
4	HEC	A	608	43/43	0.97	0.12	-0.38	20,22,23,24	0
3	HEM	A	602	43/43	0.98	0.09	-0.50	22,23,24,24	0
3	HEM	C	604	43/43	0.98	0.09	-0.62	23,28,29,31	0
5	K	A	609	1/1	0.88	0.15	-	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.