



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:05 PM GMT

PDB ID : 1IQC
Title : Crystal structure of Di-Heme Peroxidase from Nitrosomonas europaea
Authors : Shimizu, H.
Deposited on : 2001-07-20
Resolution : 1.80 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 (RC4), CSD as536be (2015)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

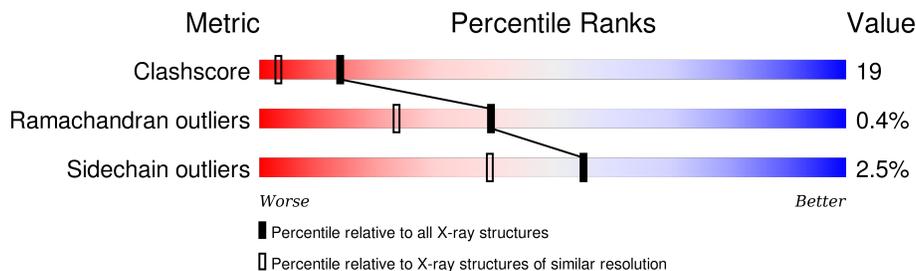
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	
1	B	308	
1	C	308	
1	D	308	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10767 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 di-heme peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	B	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	C	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	D	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			

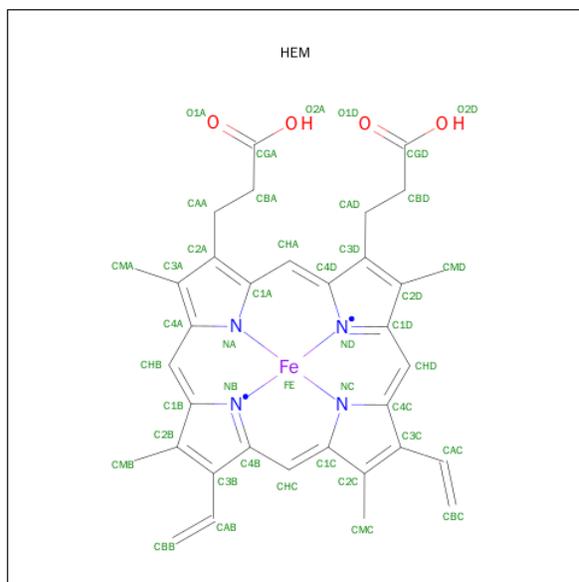
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

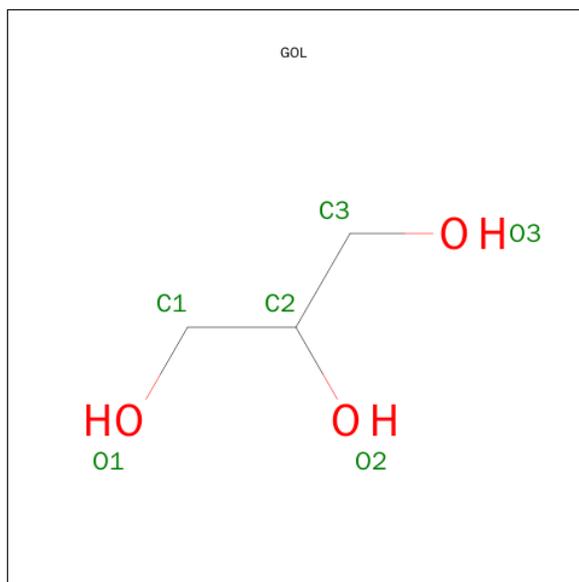
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

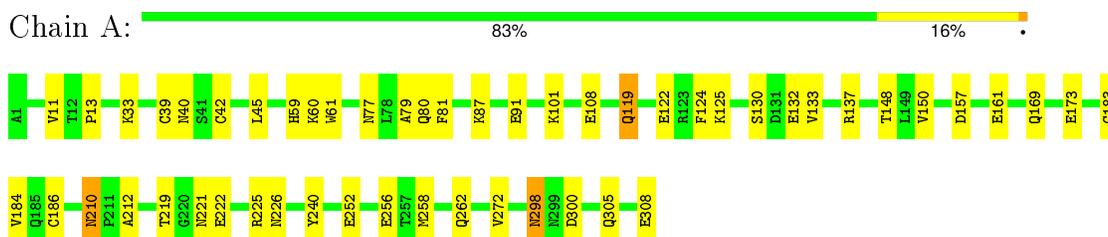
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	260	Total O 260 260	0	0
6	B	199	Total O 199 199	0	0
6	C	279	Total O 279 279	0	0
6	D	120	Total O 120 120	0	0

3 Residue-property plots

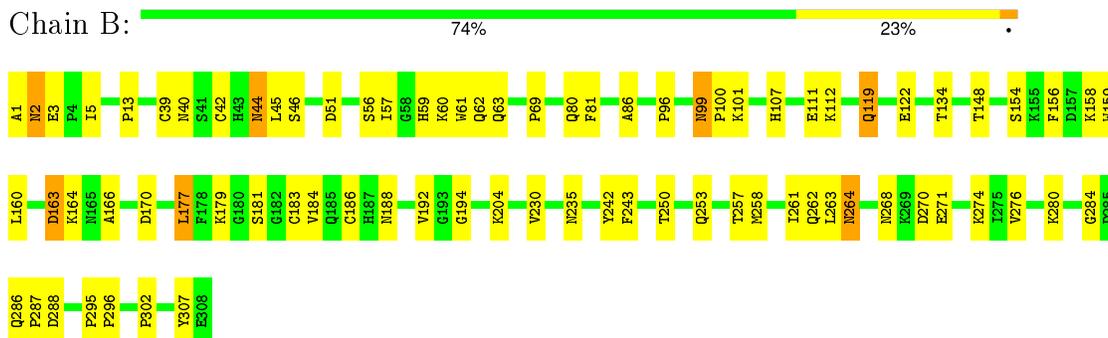
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

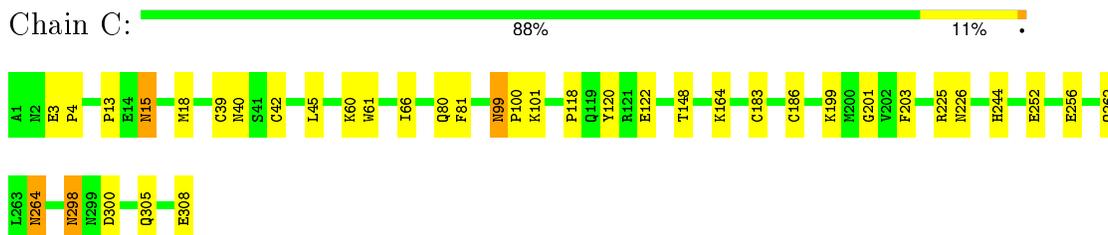
- Molecule 1: di-heme peroxidase



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A1	B83	K164	P281
M2	G84	M165	Y242
E3	R85	A166	F243
P4	A86	L167	H244
I5	P96	M168	L251
I8	P100	Q169	E286
V11	R101	D170	T287
T12	E102	E171	M288
M103	M103	E173	G289
M15	A104	L177	R260
M18	E108	C183	T281
A19	I109	V184	Q282
E20	A110	Q185	L283
L21	V113	C186	M264
G22	V114	H187	M268
K23	A115	M188	K269
M24	Q119	G189	D270
L25	Y120	V192	E271
F26	D121	G193	K274
F27	E122	S195	T281
D28	R123	S196	K290
P29	F124	Y197	L291
R30	K125	Q198	P292
L31	K126	K199	I293
S32	V127	M200	L294
S33	F128	G201	P295
S34	G129	R209	F296
G35	S130	M210	S297
F36	D131	P211	M298
I37	E132	R215	M299
S38	V133	D216	D300
C39	M134	M217	T301
M40	T134	V218	P302
S41	I135	T219	P306
C42	D136	G220	Y307
L45	R137	E221	E308
L46	I138	E222	
D51	T139	A223	
B59	T140	D224	
K60	A141	R225	
M61	I142	M226	
O62	A143	V227	
O63	Q144	F228	
O63	F145	R229	
I66	E146	V230	
L66	L149	M235	
L72	V150	L236	
M73	T151	E237	
P152	P152	L238	
M77	K155	T239	
L78	F156	Y240	
A79	D157		
Q80	E161		
F81			
M82			

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.13Å 55.11Å 144.00Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.9 (30.00-1.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, MG, 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	0.32	0/2441	0.58	0/3304
1	B	0.29	0/2441	0.56	0/3304
1	C	0.32	0/2441	0.58	0/3304
1	D	0.29	0/2441	0.52	0/3304
All	All	0.30	0/9764	0.56	0/13216

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain

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	2388	0	2331	59	0
1	B	2388	0	2331	85	0
1	C	2388	0	2331	43	0
1	D	2388	0	2331	185	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	86	0	60	18	0
4	B	86	0	60	18	0
4	C	86	0	60	15	0
4	D	86	0	60	22	0
5	B	6	0	8	0	0
6	A	260	0	0	4	0
6	B	199	0	0	4	0
6	C	279	0	0	0	0
6	D	120	0	0	6	0
All	All	10767	0	9572	360	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 19.

The worst 5 of 360 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:B:186:CYS:SG	4:B:402:HEM:HAC	1.50	1.50
1:A:39:CYS:SG	4:A:401:HEM:CAB	2.12	1.38
1:B:39:CYS:SG	4:B:401:HEM:CAB	2.13	1.37
1:A:42:CYS:SG	4:A:401:HEM:CAC	2.14	1.36
1:C:183:CYS:SG	4:C:402:HEM:CAB	2.13	1.36

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	306/308 (99%)	296 (97%)	10 (3%)	0	100	100
1	B	306/308 (99%)	287 (94%)	16 (5%)	3 (1%)	19	5
1	C	306/308 (99%)	298 (97%)	8 (3%)	0	100	100
1	D	306/308 (99%)	285 (93%)	19 (6%)	2 (1%)	26	11
All	All	1224/1232 (99%)	1166 (95%)	53 (4%)	5 (0%)	39	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	D	2	ASN
1	B	163	ASP
1	D	215	ARG
1	B	3	GLU

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	260/260 (100%)	255 (98%)	5 (2%)	65	52
1	B	260/260 (100%)	254 (98%)	6 (2%)	58	42
1	C	260/260 (100%)	255 (98%)	5 (2%)	65	52
1	D	260/260 (100%)	250 (96%)	10 (4%)	40	22
All	All	1040/1040 (100%)	1014 (98%)	26 (2%)	55	39

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ASN
1	C	264	ASN
1	D	268	ASN

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Mol	Chain	Res	Type
1	C	99	ASN
1	C	120	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	268	ASN
1	C	62	GLN
1	D	226	ASN
1	B	299	ASN
1	C	15	ASN

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 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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$
4	HEM	A	401	1,6	30,50,50	3.18	11 (36%)	24,82,82	2.13	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	402	1	30,50,50	2.89	11 (36%)	24,82,82	2.18	8 (33%)
5	GOL	B	1410	-	5,5,5	0.21	0	5,5,5	0.25	0
4	HEM	B	401	1,6	30,50,50	2.86	11 (36%)	24,82,82	2.11	6 (25%)
4	HEM	B	402	1	30,50,50	2.85	10 (33%)	24,82,82	2.06	7 (29%)
4	HEM	C	401	1,6	30,50,50	3.16	11 (36%)	24,82,82	2.13	8 (33%)
4	HEM	C	402	1	30,50,50	2.97	11 (36%)	24,82,82	2.18	7 (29%)
4	HEM	D	401	1,6	30,50,50	2.83	12 (40%)	24,82,82	2.03	6 (25%)
4	HEM	D	402	1	30,50,50	2.93	11 (36%)	24,82,82	2.13	7 (29%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	A	402	1	-	0/10/54/54	0/0/8/8
5	GOL	B	1410	-	-	0/4/4/4	0/0/0/0
4	HEM	B	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	B	402	1	-	0/10/54/54	0/0/8/8
4	HEM	C	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	C	402	1	-	0/10/54/54	0/0/8/8
4	HEM	D	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	D	402	1	-	0/10/54/54	0/0/8/8

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	HEM	C3B-C4B	-9.29	1.43	1.51
4	A	401	HEM	C3B-C4B	-8.77	1.44	1.51
4	C	402	HEM	C3B-C4B	-8.08	1.44	1.51
4	B	401	HEM	C3B-C4B	-7.95	1.44	1.51
4	D	402	HEM	C3B-C4B	-7.81	1.44	1.51

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	HEM	CAA-C2A-C1A	-3.23	123.50	127.01
4	D	402	HEM	CAA-C2A-C1A	-2.76	124.01	127.01
4	B	402	HEM	CAA-C2A-C1A	-2.34	124.47	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	402	HEM	CAA-C2A-C1A	-2.31	124.50	127.01
4	C	402	HEM	CMA-C3A-C4A	-2.26	124.62	128.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	HEM	9	0
4	A	402	HEM	9	0
4	B	401	HEM	10	0
4	B	402	HEM	8	0
4	C	401	HEM	7	0
4	C	402	HEM	8	0
4	D	401	HEM	9	0
4	D	402	HEM	13	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.