wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:29 AM GMT

PDB ID	:	2MTA
Title	:	CRYSTAL STRUCTURE OF A TERNARY ELECTRON TRANSFER COMPLEX BETWEEN METHYLAMINE DEHYDROGENASE, AMICYANIN AND A C-TYPE CYTOCHROME
Authors	:	Chen, L.; Mathews, F.S.
Deposited on	:	1993-10-26
Resolution	:	2.40 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 (i) symbol.

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

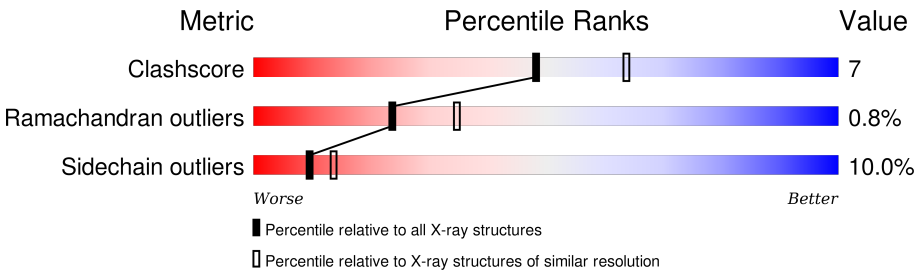
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	373	70% 24% 6% •
2	L	125	76% 19% 5%
3	A	105	76% 21% •
4	C	147	69% 19% 10% •

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	H	0	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5981 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 METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	373	2899	1840	498	553	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	299	PHE	LEU	CONFLICT	UNP P29894

- Molecule 2 is a protein called METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	125	956	590	161	192	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	TRQ	TRP	CONFLICT	UNP P22619

- Molecule 3 is a protein called AMICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	105	807	516	133	152	6	0	0	0

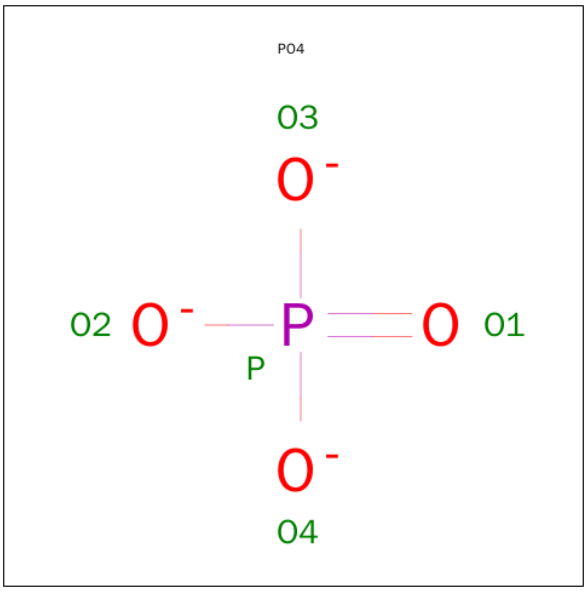
- Molecule 4 is a protein called CYTOCHROME C551I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	147	1145	724	182	231	8	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

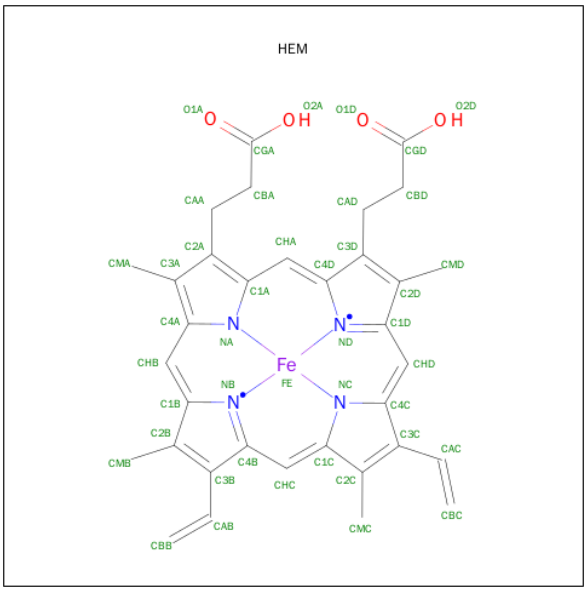
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cu 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total O P 3 2 1	0	0

- Molecule 7 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		
7	C	1	43	34	1	4	4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	14	14	14	0	0
			Total	O		
8	C	23	23	23	0	0
			Total	O		
8	H	73	73	73	0	0
			Total	O		
8	L	17	17	17	0	0

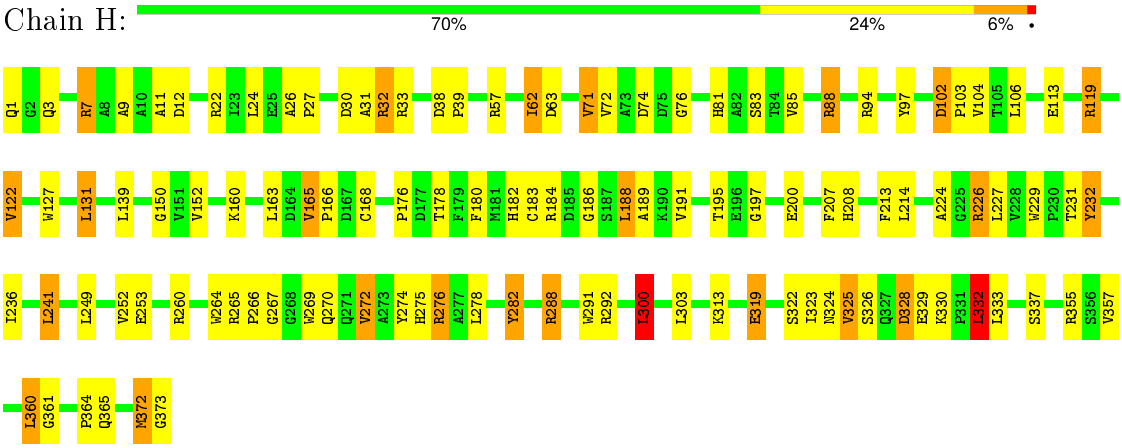
3 Residue-property plots (i)

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.

Note EDS was not executed.

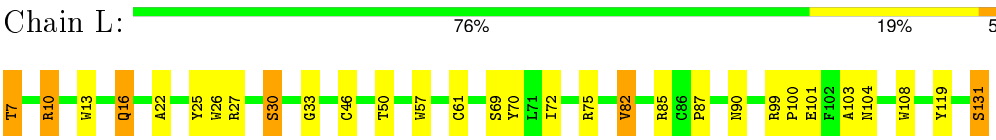
- Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

Chain H:



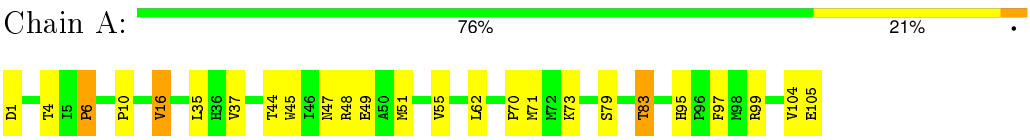
- Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain L:



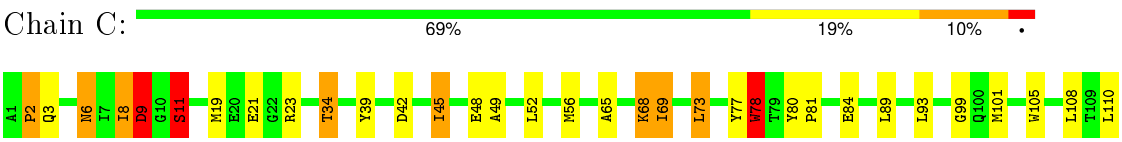
- Molecule 3: AMICYANIN

Chain A:



- Molecule 4: CYTOCHROME C551I

Chain C:



R115
T116
M117
A118
W119
V120
R121
K129
D130
A131
S132
W133
L134
Q138
P144
F145
Q146
P147

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	148.81Å 68.85Å 187.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5981	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	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: TRQ, HEM, PO4, CU

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	H	1.05	0/2976	1.84	69/4055 (1.7%)
2	L	1.04	0/964	1.87	20/1315 (1.5%)
3	A	1.04	0/828	1.79	14/1124 (1.2%)
4	C	1.05	1/1180 (0.1%)	1.92	34/1605 (2.1%)
All	All	1.05	1/5948 (0.0%)	1.85	137/8099 (1.7%)

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
4	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	78	TRP	CG-CD2	-5.24	1.34	1.43

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	119	ARG	NE-CZ-NH1	17.03	128.82	120.30
4	C	117	MET	CG-SD-CE	-15.17	75.93	100.20
1	H	119	ARG	NE-CZ-NH2	-13.32	113.64	120.30
2	L	10	ARG	NE-CZ-NH2	-13.21	113.70	120.30
3	A	99	ARG	NE-CZ-NH1	12.48	126.54	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	146	GLN	Peptide
4	C	77	TYR	Sidechain

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	H	2899	0	2792	41	0
2	L	956	0	857	15	0
3	A	807	0	794	9	0
4	C	1145	0	1038	21	0
5	A	1	0	0	0	0
6	H	3	0	0	0	2
7	C	43	0	30	0	0
8	A	14	0	0	0	0
8	C	23	0	0	3	0
8	H	73	0	0	4	0
8	L	17	0	0	2	0
All	All	5981	0	5511	83	2

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 7.

The worst 5 of 83 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)
3:A:4:THR:O	3:A:6:PRO:HD3	1.91	0.70
1:H:282:TYR:HB3	1:H:300:LEU:HD21	1.73	0.69
4:C:34:THR:HB	8:C:220:HOH:O	1.93	0.68
4:C:65:ALA:HB1	4:C:73:LEU:HB2	1.76	0.67
4:C:68:LYS:HD2	4:C:69:ILE:HD13	1.77	0.67

All (2) 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:H:0:PO4:P	6:H:0:PO4:O2[4_555]	1.52	0.68
6:H:0:PO4:P	6:H:0:PO4:O1[4_555]	1.52	0.68

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	H	371/373 (100%)	348 (94%)	23 (6%)	0	100	100
2	L	122/125 (98%)	110 (90%)	12 (10%)	0	100	100
3	A	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
4	C	145/147 (99%)	128 (88%)	11 (8%)	6 (4%)	3	3
All	All	741/750 (99%)	683 (92%)	52 (7%)	6 (1%)	24	35

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	11	SER
4	C	3	GLN
4	C	9	ASP
4	C	21	GLU
4	C	68	LYS

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	H	301/301 (100%)	272 (90%)	29 (10%)	10 15
2	L	104/104 (100%)	96 (92%)	8 (8%)	16 24
3	A	85/85 (100%)	80 (94%)	5 (6%)	24 38
4	C	118/118 (100%)	99 (84%)	19 (16%)	3 3
All	All	608/608 (100%)	547 (90%)	61 (10%)	9 14

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	333	LEU
2	L	87	PRO
4	C	121	ARG
1	H	360	LEU
2	L	16	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	271	GLN
1	H	275	HIS
2	L	104	ASN
1	H	222	GLN
1	H	365	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
2	TRQ	L	57	2	14,17,18	2.69	3 (21%)	8,24,26	3.40	4 (50%)

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
2	TRQ	L	57	2	-	0/3/19/21	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	57	TRQ	CE2-CZ2	-7.74	1.40	1.49
2	L	57	TRQ	CD1-NE1	-4.29	1.29	1.36
2	L	57	TRQ	CZ3-CH2	-3.14	1.37	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	57	TRQ	CB-CG-CD1	-7.75	118.39	127.97
2	L	57	TRQ	O-C-CA	-3.35	116.77	125.49
2	L	57	TRQ	O6-CH2-CZ3	-2.38	117.26	121.53
2	L	57	TRQ	CE3-CZ3-CH2	2.65	123.28	121.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	57	TRQ	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
7	HEM	C	200	4	30,50,50	2.91	9 (30%)	24,82,82	2.90	14 (58%)
6	PO4	H	0	-	0,2,4	0.00	-	0,1,6	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
7	HEM	C	200	4	-	0/10/54/54	0/0/8/8
6	PO4	H	0	-	-	0/0/0/0	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	200	HEM	C3B-C4B	-8.29	1.44	1.51
7	C	200	HEM	C3D-C4D	-7.06	1.42	1.51
7	C	200	HEM	C2D-C3D	-6.35	1.35	1.54
7	C	200	HEM	C2C-C1C	-4.13	1.44	1.52
7	C	200	HEM	C2B-C1B	-2.55	1.43	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	200	HEM	C3B-CAB-CBB	-7.25	113.33	124.46
7	C	200	HEM	C3C-CAC-CBC	-2.34	120.87	124.46
7	C	200	HEM	CBA-CAA-C2A	-2.33	108.35	112.53
7	C	200	HEM	CMA-C3A-C4A	-2.23	124.68	128.36
7	C	200	HEM	CAA-C2A-C1A	-2.04	124.80	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	0	PO4	0	2

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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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