



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 07:24 AM EST

PDB ID : 6CPP
Title : CRYSTAL STRUCTURES OF CYTOCHROME P450-CAM COMPLEXED
WITH CAMPHANE, THIOCAMPHOR, AND ADAMANTANE: FACTORS
CONTROLLING P450 SUBSTRATE HYDROXYLATION
Authors : Raag, R.; Poulos, T.L.
Deposited on : unknown
Resolution : 1.90 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

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 : 1.7.2 (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) : rb-20030345

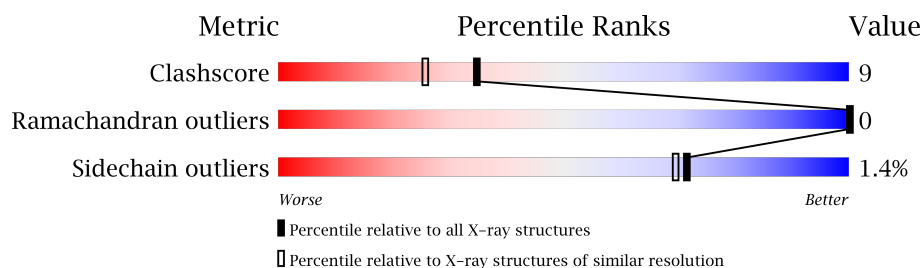
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (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 $\leq 5\%$. 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	414	 <div style="display: flex; justify-content: space-between; width: 100%;"> 68% 26% ... </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3465 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 P450-CAM.

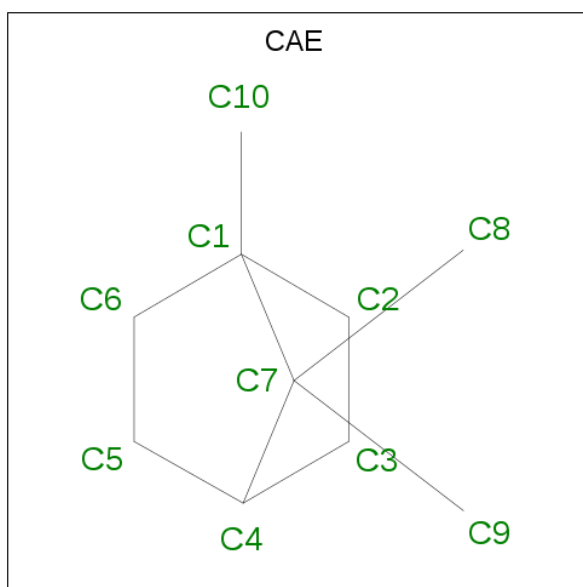
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3208	2033	560	597	18			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is CAMPHANE (three-letter code: CAE) (formula: $C_{10}H_{18}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 10 10	0	1

- Molecule 4 is water.

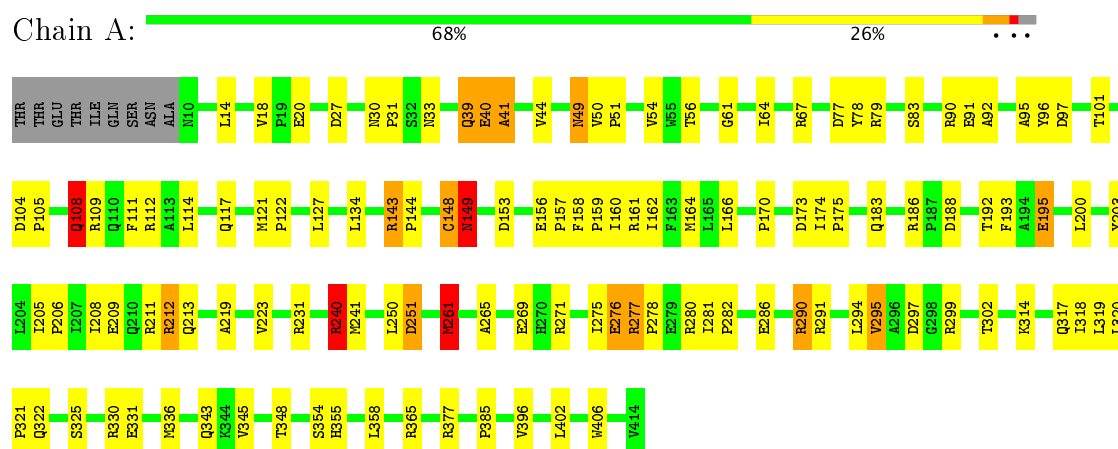
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	204	Total O 204 204	0	0

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 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 P450-CAM



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.67Å 103.90Å 36.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3465	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: HEM, CAE

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	1.12	3/3287 (0.1%)	1.78	54/4465 (1.2%)

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	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	CD-OE2	7.05	1.33	1.25
1	A	211	ARG	NE-CZ	-5.81	1.25	1.33
1	A	286	GLU	CD-OE1	-5.71	1.19	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	37.12	175.56	123.60
1	A	271	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	A	299	ARG	NE-CZ-NH2	-12.64	113.98	120.30
1	A	271	ARG	CD-NE-CZ	12.22	140.71	123.60
1	A	67	ARG	NE-CZ-NH2	-11.48	114.56	120.30
1	A	280	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	A	112	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	A	240	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	A	365	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	A	161	ARG	NE-CZ-NH2	-9.17	115.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	112	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	A	211	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	291	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	A	261	MET	CG-SD-CE	7.81	112.70	100.20
1	A	195	GLU	CA-CB-CG	7.54	129.99	113.40
1	A	212	ARG	CD-NE-CZ	7.23	133.72	123.60
1	A	251	ASP	O-C-N	-7.09	111.35	122.70
1	A	161	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	277	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	A	40	GLU	OE1-CD-OE2	-6.88	115.05	123.30
1	A	108	GLN	CB-CG-CD	6.84	129.39	111.60
1	A	153	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	79	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	143	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	365	ARG	CD-NE-CZ	6.07	132.10	123.60
1	A	297	ASP	CB-CA-C	6.04	122.48	110.40
1	A	27	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	108	GLN	CA-CB-CG	6.00	126.59	113.40
1	A	265	ALA	N-CA-CB	5.88	118.33	110.10
1	A	280	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	295	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	A	358	LEU	O-C-N	5.73	132.94	123.20
1	A	148	CYS	C-N-CA	5.61	135.71	121.70
1	A	290	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	212	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	290	ARG	CD-NE-CZ	5.51	131.32	123.60
1	A	79	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	294	LEU	N-CA-CB	-5.42	99.57	110.40
1	A	280	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	90	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	20	GLU	CA-CB-CG	5.28	125.02	113.40
1	A	104	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	231	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	33	ASN	CB-CA-C	5.23	120.86	110.40
1	A	343	GLN	N-CA-CB	5.20	119.95	110.60
1	A	330	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	186	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	41	ALA	N-CA-CB	5.16	117.33	110.10
1	A	271	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
1	A	64	ILE	CA-C-O	-5.13	109.32	120.10
1	A	149	ASN	N-CA-CB	5.12	119.82	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	406	TRP	O-C-N	5.07	130.80	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	277	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	77	ASP	Mainchain

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	3208	0	3156	59	0
2	A	43	0	30	1	0
3	A	10	0	18	3	0
4	A	204	0	0	7	0
All	All	3465	0	3204	61	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 9.

All (61) 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:121:MET:HB2	1:A:122:PRO:HD3	1.70	0.71
1:A:101:THR:HG21	3:A:422[B]:CAE:H31	1.82	0.62
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:417:HEM:C1A	3:A:422[B]:CAE:H4	2.38	0.58
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.84	0.57
1:A:49:ASN:H	1:A:49:ASN:HD22	1.52	0.57
1:A:160:ILE:O	1:A:164:MET:HG2	2.05	0.56
1:A:56:THR:O	1:A:61:GLY:HA2	2.04	0.56
1:A:39:GLN:NE2	1:A:39:GLN:H	2.04	0.56
1:A:325:SER:O	1:A:331:GLU:HG3	2.07	0.55
1:A:149:ASN:ND2	1:A:402:LEU:H	2.04	0.55
3:A:422[B]:CAE:H52	4:A:697:HOH:O	2.07	0.55
1:A:134:LEU:HB2	4:A:589:HOH:O	2.06	0.54
1:A:261:MET:HA	1:A:261:MET:HE2	1.91	0.52
1:A:114:LEU:HB3	1:A:241:MET:HE1	1.92	0.52
1:A:95:ALA:HB3	1:A:193:PHE:HD2	1.74	0.52
1:A:183:GLN:OE1	1:A:188:ASP:HB3	2.09	0.51
1:A:322:GLN:HB3	1:A:348:THR:O	2.10	0.51
1:A:30:ASN:ND2	4:A:555:HOH:O	2.40	0.51
1:A:302:THR:O	1:A:314:LYS:HG3	2.12	0.50
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.12	0.50
1:A:208:ILE:O	1:A:212:ARG:HG3	2.12	0.50
1:A:78:TYR:CD1	1:A:105:PRO:HD2	2.46	0.50
1:A:174:ILE:N	1:A:175:PRO:HD2	2.28	0.49
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.79	0.48
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.96	0.47
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.95	0.47
1:A:209:GLU:O	1:A:213:GLN:HG3	2.15	0.47
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.95	0.46
1:A:276:GLU:C	1:A:278:PRO:HD3	2.36	0.46
1:A:114:LEU:O	1:A:117:GLN:HB2	2.16	0.46
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.46	0.46
1:A:269:GLU:H	1:A:269:GLU:CD	2.19	0.46
1:A:275:ILE:HG21	4:A:691:HOH:O	2.15	0.46
1:A:319:LEU:O	1:A:321:PRO:HD3	2.16	0.46
1:A:83:SER:HB3	1:A:101:THR:O	2.17	0.45
1:A:149:ASN:HD21	1:A:402:LEU:H	1.65	0.45
1:A:97:ASP:O	1:A:240:ARG:HD2	2.17	0.45
1:A:51:PRO:HD2	1:A:54:VAL:CG1	2.47	0.45
1:A:295:VAL:HG22	1:A:396:VAL:HG22	1.99	0.44
1:A:158:PHE:CE1	1:A:162:ILE:HD11	2.52	0.44
1:A:111:PHE:HB3	1:A:241:MET:HE2	2.00	0.44
1:A:31:PRO:HA	4:A:502:HOH:O	2.17	0.44
1:A:41:ALA:O	1:A:44:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HD13	1:A:320:LEU:HD21	1.99	0.44
1:A:156:GLU:HB2	1:A:157:PRO:HD3	1.99	0.43
1:A:317:GLN:NE2	4:A:646:HOH:O	2.51	0.43
1:A:319:LEU:HG	1:A:321:PRO:HG3	2.01	0.43
1:A:281:ILE:N	1:A:282:PRO:CD	2.82	0.43
1:A:30:ASN:ND2	4:A:554:HOH:O	2.51	0.43
1:A:219:ALA:O	1:A:223:VAL:HG23	2.18	0.43
1:A:170:PRO:HG2	1:A:173:ASP:OD1	2.18	0.42
1:A:200:LEU:O	1:A:203:TYR:HB3	2.20	0.42
1:A:319:LEU:C	1:A:321:PRO:HD3	2.40	0.42
1:A:40:GLU:HG3	1:A:336:MET:CE	2.50	0.42
1:A:160:ILE:HG21	1:A:174:ILE:HG23	2.02	0.41
1:A:91:GLU:H	1:A:91:GLU:CD	2.23	0.41
1:A:92:ALA:O	1:A:96:TYR:HB2	2.21	0.41
1:A:290:ARG:HD3	1:A:345:VAL:HG13	2.01	0.41
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.56	0.41
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.82	0.40

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	403/414 (97%)	384 (95%)	19 (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	350/358 (98%)	345 (99%)	5 (1%)	71 69

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

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	ASN
1	A	108	GLN
1	A	261	MET
1	A	385	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	69	GLN
1	A	108	GLN
1	A	129	ASN
1	A	149	ASN
1	A	225	ASN
1	A	361	HIS
1	A	388	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

2 ligands are 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	HEM	A	417	1,4	28,50,50	1.88	5 (17%)	17,82,82	2.25	5 (29%)
3	CAE	A	422[B]	-	11,11,11	1.75	4 (36%)	16,19,19	2.69	6 (37%)

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	HEM	A	417	1,4	-	0/6/54/54	0/0/8/8
3	CAE	A	422[B]	-	-	0/0/27/27	0/0/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	C3C-C2C	-5.51	1.33	1.40
2	A	417	HEM	C3B-C2B	-4.88	1.33	1.40
3	A	422[B]	CAE	C10-C1	-2.90	1.47	1.53
3	A	422[B]	CAE	C7-C4	2.00	1.60	1.54
2	A	417	HEM	C4D-ND	2.25	1.39	1.36
3	A	422[B]	CAE	C5-C4	2.40	1.60	1.53
2	A	417	HEM	C3B-CAB	2.42	1.52	1.47
3	A	422[B]	CAE	C2-C1	2.70	1.61	1.55
2	A	417	HEM	C3C-CAC	2.96	1.53	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	CMA-C3A-C4A	-4.67	121.28	128.46
3	A	422[B]	CAE	C9-C7-C8	-3.75	98.10	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	CMD-C2D-C1D	-3.73	122.73	128.46
3	A	422[B]	CAE	C5-C4-C7	-3.28	97.01	102.85
3	A	422[B]	CAE	C3-C4-C7	-2.97	97.56	102.85
3	A	422[B]	CAE	C2-C3-C4	2.08	106.42	103.17
2	A	417	HEM	CMD-C2D-C3D	2.53	129.71	124.94
2	A	417	HEM	CMA-C3A-C2A	3.80	132.10	124.94
2	A	417	HEM	CBD-CAD-C3D	4.03	120.15	112.47
3	A	422[B]	CAE	C10-C1-C6	4.97	122.11	110.98
3	A	422[B]	CAE	C1-C7-C4	6.00	100.81	93.17

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
2	A	417	HEM	1	0
3	A	422[B]	CAE	3	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.