



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 08:59 am BST

PDB ID : 4CPP  
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 : 1990-05-18  
Resolution : 2.11 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

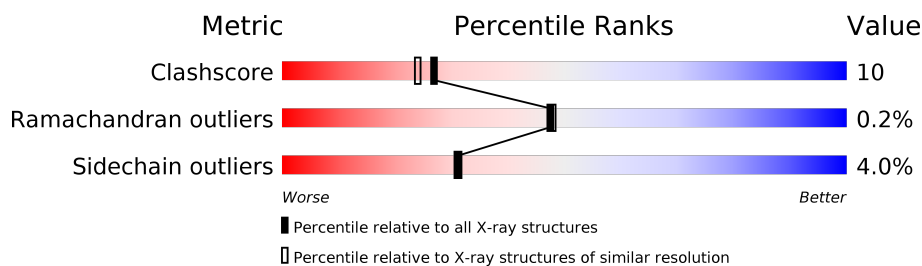
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

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 respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3476 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.

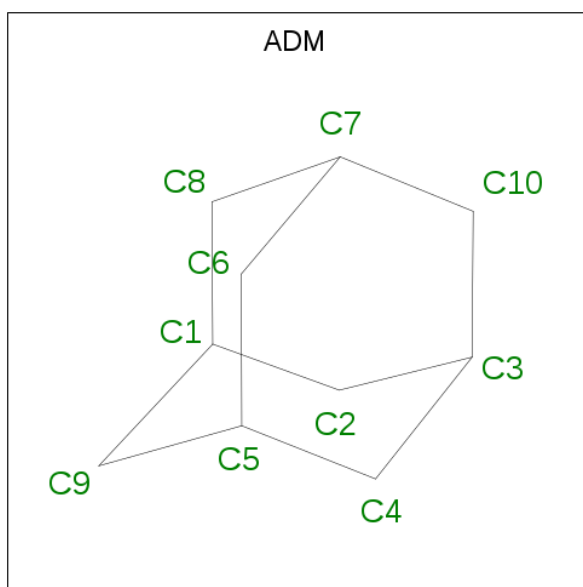
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	3	0
			3221	2044	561	597	19			

- 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 ADAMANTANE (three-letter code: ADM) (formula:  $C_{10}H_{16}$ ).



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

- Molecule 4 is water.

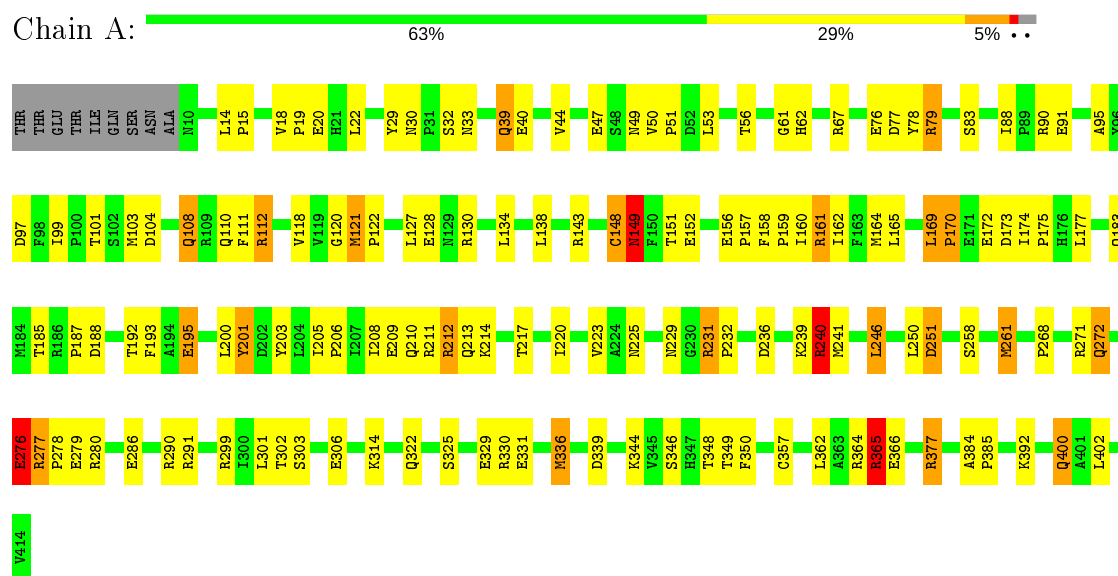
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	202	Total O 202 202	0	0

### 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. 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. 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, $\alpha$ , $\beta$ , $\gamma$	108.67Å 103.90Å 36.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.11	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.11)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3476	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: HEM, ADM

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	1.16	4/3312 (0.1%)	1.88	68/4497 (1.5%)

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	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	CD-OE2	9.94	1.36	1.25
1	A	211	ARG	CD-NE	-5.73	1.36	1.46
1	A	211	ARG	NE-CZ	-5.54	1.25	1.33
1	A	286	GLU	CD-OE1	-5.05	1.20	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	34.51	171.91	123.60
1	A	67	ARG	NE-CZ-NH2	-16.50	112.05	120.30
1	A	20	GLU	CA-CB-CG	15.30	147.06	113.40
1	A	330	ARG	NE-CZ-NH1	14.29	127.45	120.30
1	A	280	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	A	280	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	A	211	ARG	NE-CZ-NH1	12.29	126.45	120.30
1	A	67	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	210	GLN	CA-CB-CG	9.74	134.84	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	CD-NE-CZ	9.47	136.86	123.60
1	A	299	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	231	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	377	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	271	ARG	CD-NE-CZ	8.21	135.10	123.60
1	A	161	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	143	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	79	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	291	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	A	79	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	336	MET	CA-CB-CG	7.56	126.15	113.30
1	A	90	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	195	GLU	CA-CB-CG	7.29	129.44	113.40
1	A	149	ASN	N-CA-CB	7.27	123.68	110.60
1	A	32	SER	N-CA-CB	7.22	121.33	110.50
1	A	33	ASN	CB-CA-C	7.14	124.68	110.40
1	A	201	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	A	330	ARG	CD-NE-CZ	6.75	133.05	123.60
1	A	339	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	148	CYS	C-N-CA	6.60	138.19	121.70
1	A	365	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	349	THR	CA-CB-CG2	6.47	121.46	112.40
1	A	201	TYR	CB-CG-CD1	6.46	124.88	121.00
1	A	271	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	365	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	290	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	277	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	306	GLU	OE1-CD-OE2	6.23	130.78	123.30
1	A	261	MET	CG-SD-CE	6.20	110.12	100.20
1	A	400	GLN	CA-CB-CG	6.15	126.93	113.40
1	A	108	GLN	CB-CG-CD	6.13	127.54	111.60
1	A	365	ARG	CG-CD-NE	-6.06	99.08	111.80
1	A	165	LEU	CB-CG-CD1	-6.04	100.74	111.00
1	A	104	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	169	LEU	CA-CB-CG	5.99	129.09	115.30
1	A	149	ASN	CA-C-O	-5.95	107.61	120.10
1	A	112	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	121	MET	CA-CB-CG	5.77	123.11	113.30
1	A	301	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	364	ARG	CD-NE-CZ	5.59	131.42	123.60
1	A	127	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	279	GLU	CA-CB-CG	5.55	125.61	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	A	53	LEU	CB-CA-C	5.44	120.53	110.20
1	A	236	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	78	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	130	ARG	N-CA-CB	5.34	120.21	110.60
1	A	240	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	220	ILE	CB-CA-C	5.26	122.12	111.60
1	A	108	GLN	CA-CB-CG	5.22	124.89	113.40
1	A	152	GLU	CA-CB-CG	5.17	124.79	113.40
1	A	78	TYR	CB-CG-CD2	5.17	124.10	121.00
1	A	76	GLU	CB-CG-CD	5.15	128.09	114.20
1	A	251	ASP	O-C-N	-5.12	114.50	122.70
1	A	329	GLU	CA-CB-CG	5.11	124.63	113.40
1	A	271	ARG	NH1-CZ-NH2	-5.07	113.83	119.40
1	A	103	MET	CG-SD-CE	-5.06	92.11	100.20
1	A	231	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	276	GLU	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	161	ARG	Sidechain
1	A	170	PRO	Mainchain
1	A	212	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	29	TYR	Sidechain
1	A	365	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	3221	0	3176	64	0
2	A	43	0	30	2	0
3	A	10	0	16	2	0
4	A	202	0	0	5	0
All	All	3476	0	3222	66	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 10.

All (66) 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:344:LYS:HE3	1:A:346:SER:HB2	1.48	0.93
3:A:422:ADM:H5	4:A:501:HOH:O	1.70	0.92
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.68	0.75
1:A:19:PRO:HG2	1:A:22:LEU:HD12	1.72	0.72
1:A:272:GLN:HG2	4:A:700:HOH:O	1.92	0.70
1:A:170:PRO:HG2	1:A:173:ASP:OD1	1.93	0.69
1:A:392[A]:LYS:HD2	1:A:400:GLN:NE2	2.08	0.69
1:A:183:GLN:OE1	1:A:188:ASP:HB3	1.96	0.65
1:A:325:SER:O	1:A:331:GLU:HG3	1.98	0.64
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.79	0.63
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.83	0.61
1:A:149:ASN:ND2	1:A:402:LEU:H	1.99	0.59
1:A:212:ARG:HA	1:A:225:ASN:HD21	1.67	0.59
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.18	0.58
1:A:276:GLU:C	1:A:278:PRO:HD3	2.23	0.58
1:A:208:ILE:O	1:A:212:ARG:HG3	2.05	0.56
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.89	0.55
1:A:201:TYR:O	1:A:205:ILE:HG13	2.08	0.54
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.38	0.54
1:A:200:LEU:O	1:A:203:TYR:HB3	2.07	0.54
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.09	0.53
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.90	0.53
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.91	0.53
1:A:205:ILE:HD12	4:A:599:HOH:O	2.09	0.51
1:A:322:GLN:HB3	1:A:348:THR:O	2.11	0.50
1:A:39:GLN:NE2	1:A:39:GLN:H	2.10	0.50
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.42	0.49
1:A:303:SER:HA	1:A:314:LYS:HG3	1.94	0.49
1:A:302:THR:O	1:A:314:LYS:HG3	2.13	0.49
1:A:40:GLU:HG3	1:A:336:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:HG3	4:A:617:HOH:O	2.13	0.49
1:A:56:THR:O	1:A:61:GLY:HA2	2.13	0.48
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.48	0.48
1:A:118:VAL:HG11	1:A:223:VAL:HG23	1.95	0.48
1:A:277:ARG:N	1:A:278:PRO:HD3	2.28	0.48
1:A:44:VAL:O	1:A:47:GLU:HG2	2.14	0.48
1:A:156:GLU:HB2	1:A:157:PRO:HD3	1.96	0.47
1:A:169:LEU:HB3	1:A:170:PRO:HD2	1.96	0.47
1:A:160:ILE:O	1:A:164:MET:HG2	2.15	0.47
1:A:99:ILE:HD11	1:A:240:ARG:CZ	2.45	0.46
1:A:158:PHE:CE1	1:A:162[B]:ILE:HD11	2.52	0.45
1:A:392[A]:LYS:HD2	1:A:400:GLN:HE22	1.81	0.45
1:A:83:SER:HB3	1:A:101:THR:O	2.16	0.45
1:A:209:GLU:O	1:A:213:GLN:HG3	2.16	0.45
1:A:95:ALA:HB3	1:A:193:PHE:HD2	1.82	0.45
1:A:14:LEU:HD12	1:A:15:PRO:HD2	2.00	0.44
1:A:15:PRO:HG2	1:A:18:VAL:CG2	2.46	0.44
2:A:417:HEM:C1A	3:A:422:ADM:H42	2.52	0.44
1:A:91:GLU:H	1:A:91:GLU:CD	2.21	0.44
1:A:177:LEU:HD22	1:A:246:LEU:HD12	1.99	0.44
1:A:97:ASP:O	1:A:240:ARG:HD2	2.17	0.44
1:A:205:ILE:HD11	1:A:239:LYS:HD2	2.00	0.43
1:A:151:THR:HG22	1:A:258:SER:OG	2.19	0.43
1:A:302:THR:C	1:A:314:LYS:HG3	2.38	0.42
1:A:177:LEU:HD22	1:A:246:LEU:CD1	2.50	0.42
1:A:30:ASN:ND2	4:A:556:HOH:O	2.51	0.42
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.88	0.42
1:A:231:ARG:HB2	1:A:232:PRO:HD2	2.00	0.42
1:A:112:ARG:NH1	2:A:417:HEM:O1D	2.52	0.42
1:A:134:LEU:O	1:A:138:LEU:HB2	2.20	0.41
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.90	0.41
1:A:392[A]:LYS:HD2	1:A:400:GLN:HE21	1.83	0.41
1:A:362:LEU:O	1:A:366:GLU:HG3	2.21	0.41
1:A:185:THR:C	1:A:187:PRO:HD3	2.42	0.40
1:A:15:PRO:HG2	1:A:18:VAL:HG23	2.02	0.40
1:A:149:ASN:HD21	1:A:402:LEU:H	1.65	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	406/414 (98%)	385 (95%)	20 (5%)	1 (0%)	47	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	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	353/358 (99%)	339 (96%)	14 (4%)	31	31

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	ASN
1	A	79	ARG
1	A	108	GLN
1	A	128	GLU
1	A	172	GLU
1	A	214	LYS
1	A	217	THR
1	A	246	LEU
1	A	261	MET

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Mol	Chain	Res	Type
1	A	268	PRO
1	A	272	GLN
1	A	276	GLU
1	A	365	ARG

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	49	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	110	GLN
1	A	149	ASN
1	A	225	ASN
1	A	229	ASN
1	A	400	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](#)

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](#)

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
3	ADM	A	422	-	12,12,12	2.12	7 (58%)	18,18,18	0.72	0
2	HEM	A	417	1,4	27,50,50	1.78	4 (14%)	17,82,82	1.73	4 (23%)

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	ADM	A	422	-	-	-	0/4/3/3
2	HEM	A	417	1,4	-	0/6/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	C3B-C2B	-4.30	1.34	1.40
2	A	417	HEM	C3C-CAC	3.69	1.55	1.47
2	A	417	HEM	C3C-C2C	-3.59	1.35	1.40
2	A	417	HEM	C3B-CAB	3.17	1.54	1.47
3	A	422	ADM	C8-C7	3.09	1.60	1.52
3	A	422	ADM	C10-C3	2.66	1.59	1.52
3	A	422	ADM	C2-C1	2.50	1.59	1.52
3	A	422	ADM	C9-C1	2.37	1.59	1.52
3	A	422	ADM	C6-C7	2.32	1.58	1.52
3	A	422	ADM	C6-C5	2.21	1.58	1.52
3	A	422	ADM	C10-C7	2.17	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	CBD-CAD-C3D	3.38	118.71	112.48
2	A	417	HEM	CMA-C3A-C4A	-3.12	123.67	128.46
2	A	417	HEM	CMA-C3A-C2A	2.55	129.74	124.94
2	A	417	HEM	CMD-C2D-C1D	-2.53	124.58	128.46

There are no chirality outliers.

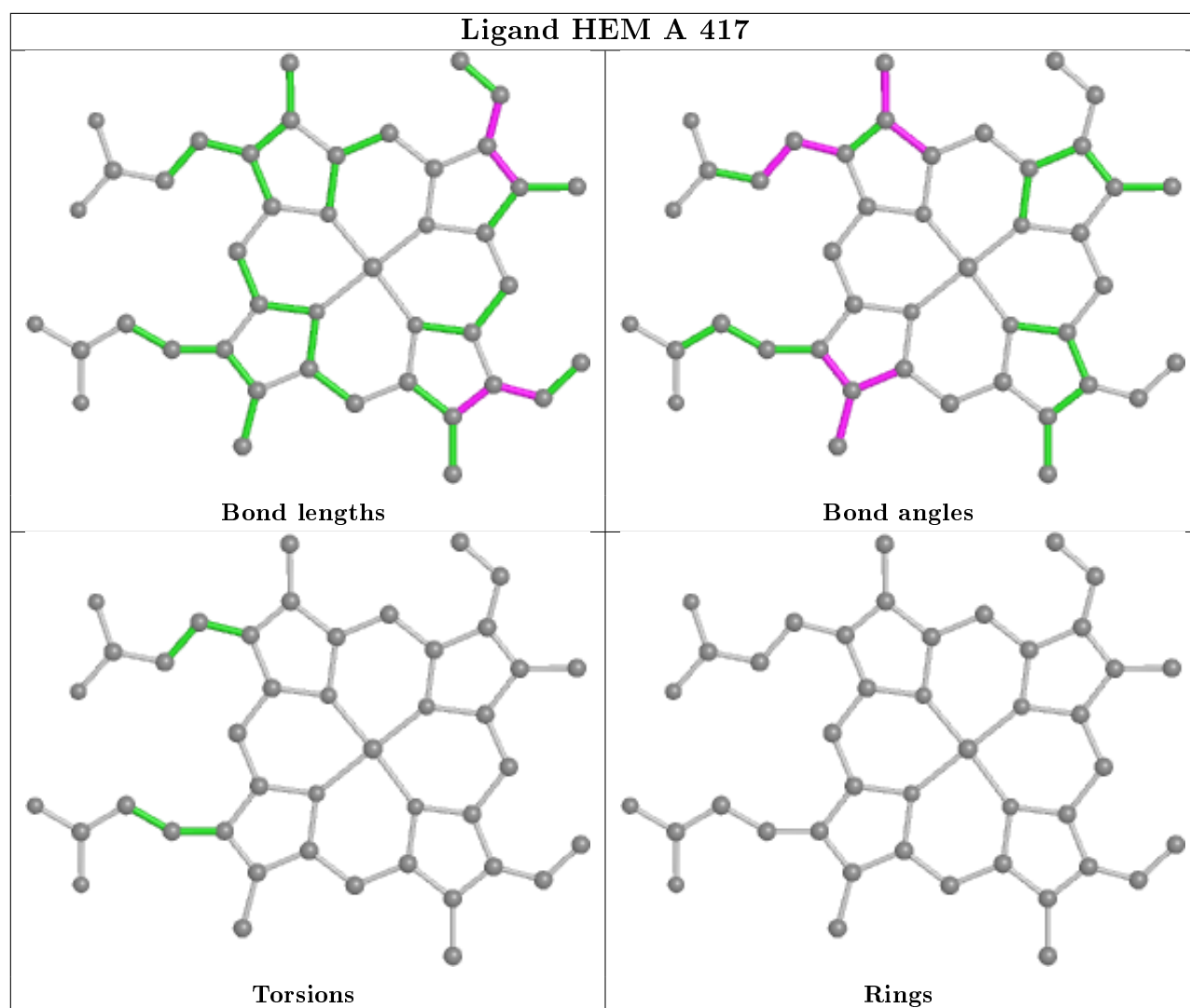
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	422	ADM	2	0
2	A	417	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.