



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:24 PM UTC

PDB ID : 3CPP / pdb\_00003cpp  
Title : CRYSTAL STRUCTURE OF THE CARBON MONOXY-SUBSTRATE-CYTOCHROME P450-CAM TERNARY COMPLEX  
Authors : Raag, R.; Poulos, T.L.  
Deposited on : 1989-07-05  
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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

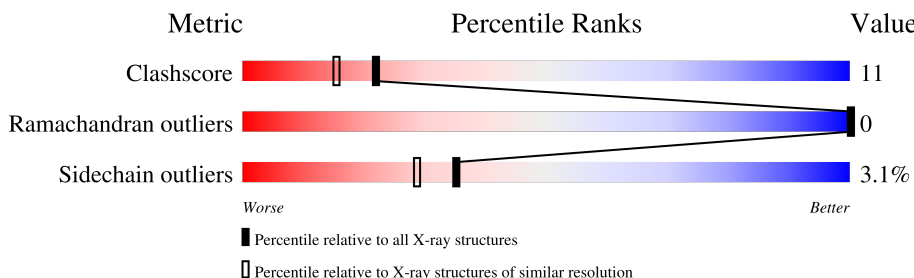
# 1 Overall quality at a glance

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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 of 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	

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
3	CMO	A	418	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3534 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.

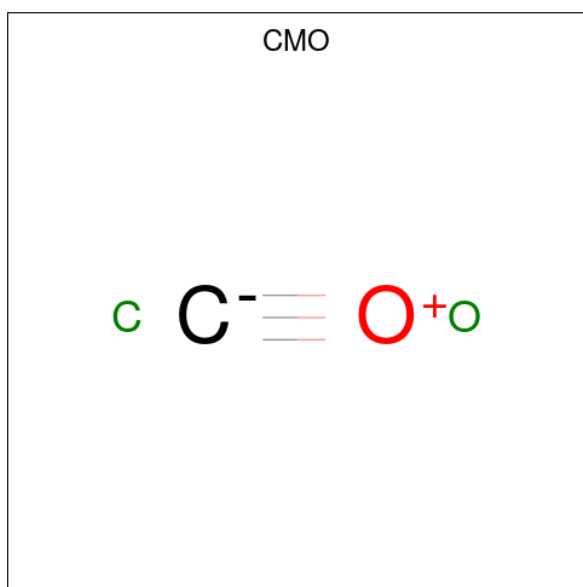
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	13	0
			3240	2051	569	600	20			

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



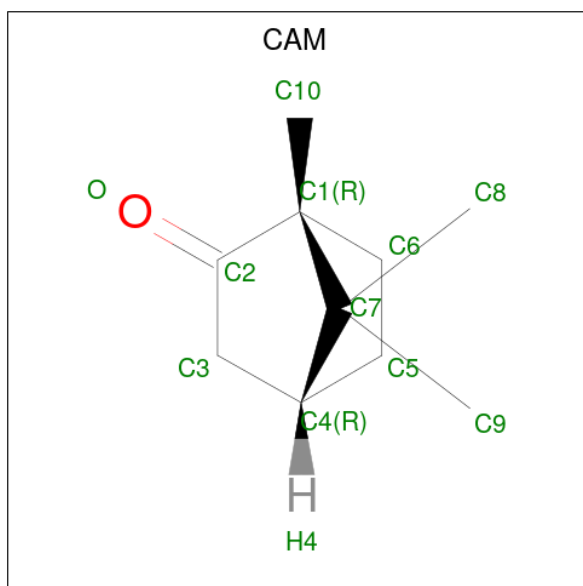
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			2	1	1		

- Molecule 4 is CAMPHOR (CCD ID: CAM) (formula: C<sub>10</sub>H<sub>16</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	10	1		

- Molecule 5 is water.

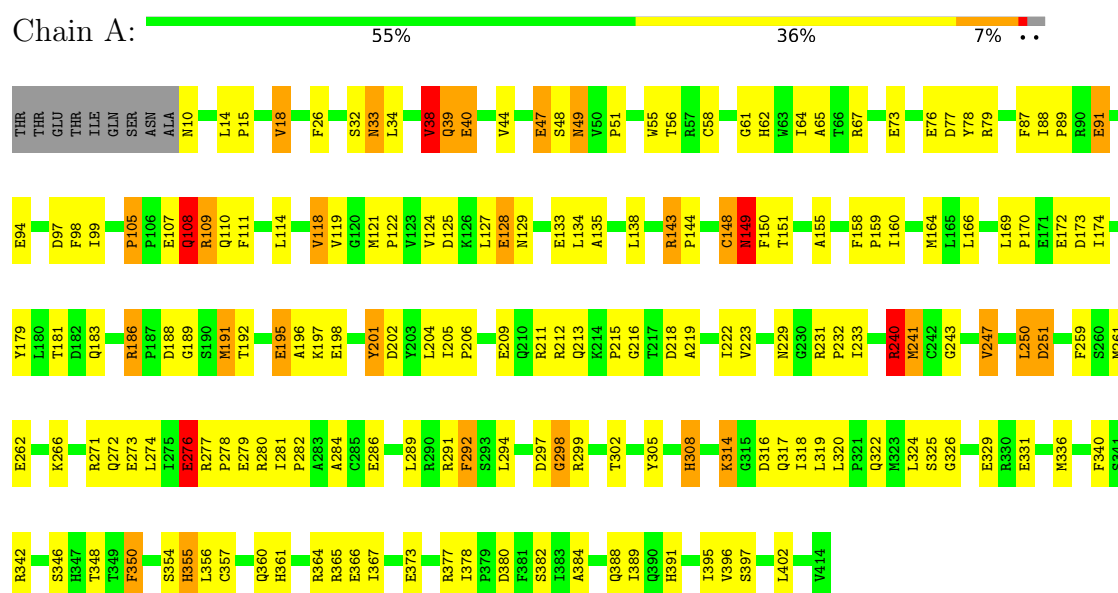
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	238	Total 238	O 238	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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) – 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	3534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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, CAM, CMO

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	1.39	16/3353 (0.5%)	2.10	127/4552 (2.8%)

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	21

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	PRO	CA-C	6.10	1.56	1.52
1	A	317	GLN	N-CA	6.05	1.53	1.46
1	A	391	HIS	CG-ND1	5.85	1.44	1.38
1	A	355	HIS	CG-ND1	5.49	1.44	1.38
1	A	105	PRO	CA-CB	-5.46	1.49	1.54
1	A	33[A]	ASN	N-CA	5.45	1.53	1.46
1	A	33[B]	ASN	N-CA	5.45	1.53	1.46
1	A	251	ASP	C-O	5.38	1.31	1.24
1	A	298	GLY	CA-C	5.35	1.58	1.51
1	A	297	ASP	N-CA	5.25	1.52	1.46
1	A	284	ALA	C-O	5.23	1.30	1.24
1	A	366	GLU	C-N	-5.23	1.27	1.33
1	A	212	ARG	NE-CZ	-5.23	1.27	1.33
1	A	276	GLU	CD-OE2	5.15	1.35	1.25
1	A	149	ASN	C-O	5.11	1.30	1.24
1	A	211	ARG	NE-CZ	-5.08	1.27	1.33

All (127) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	20.46	153.04	124.40
1	A	212	ARG	CD-NE-CZ	18.66	150.53	124.40
1	A	125	ASP	CA-CB-CG	8.85	121.45	112.60
1	A	316	ASP	CA-CB-CG	8.21	120.81	112.60
1	A	308	HIS	CA-CB-CG	-8.14	105.66	113.80
1	A	124	VAL	O-C-N	7.75	129.69	121.94
1	A	342	ARG	CD-NE-CZ	7.56	134.98	124.40
1	A	286	GLU	N-CA-CB	7.54	120.94	110.01
1	A	294	LEU	N-CA-CB	-7.43	99.42	111.01
1	A	277	ARG	CA-C-N	7.41	127.12	119.56
1	A	277	ARG	C-N-CA	7.41	127.12	119.56
1	A	211	ARG	NE-CZ-NH1	7.40	128.90	121.50
1	A	241	MET	N-CA-CB	7.36	120.74	110.07
1	A	129	ASN	CA-CB-CG	7.35	119.95	112.60
1	A	279	GLU	CB-CG-CD	7.33	125.05	112.60
1	A	105	PRO	N-CA-C	-7.30	102.77	110.58
1	A	149	ASN	N-CA-CB	7.25	122.73	110.49
1	A	38	VAL	CB-CA-C	7.24	121.24	111.97
1	A	189	GLY	N-CA-C	-7.24	105.87	114.48
1	A	149	ASN	CA-C-O	-7.16	110.28	120.51
1	A	324	LEU	CA-C-O	-7.11	111.80	119.97
1	A	271	ARG	CD-NE-CZ	6.97	134.16	124.40
1	A	396	VAL	CB-CA-C	6.84	119.65	110.42
1	A	98	PHE	N-CA-CB	6.75	119.90	110.17
1	A	18	VAL	N-CA-C	6.59	114.41	107.76
1	A	322	GLN	O-C-N	6.56	129.08	122.12
1	A	128	GLU	CB-CG-CD	6.48	123.61	112.60
1	A	391	HIS	N-CA-CB	6.45	120.62	110.56
1	A	251	ASP	O-C-N	-6.43	114.46	122.24
1	A	47	GLU	CA-CB-CG	6.43	126.95	114.10
1	A	98	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	48[A]	SER	N-CA-C	6.32	118.98	111.71
1	A	48[B]	SER	N-CA-C	6.32	118.98	111.71
1	A	291	ARG	CD-NE-CZ	6.32	133.25	124.40
1	A	361	HIS	CA-CB-CG	-6.26	107.54	113.80
1	A	133	GLU	O-C-N	6.24	128.50	122.07
1	A	299	ARG	NE-CZ-NH2	-6.24	113.59	119.20
1	A	143	ARG	CD-NE-CZ	6.23	133.13	124.40
1	A	297	ASP	CB-CA-C	6.21	122.77	110.42
1	A	172	GLU	CB-CG-CD	6.19	123.12	112.60
1	A	108	GLN	CA-C-N	6.17	130.08	120.82
1	A	108	GLN	C-N-CA	6.17	130.08	120.82
1	A	186	ARG	NE-CZ-NH2	6.15	124.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CA-C-N	6.15	128.80	120.44
1	A	125	ASP	C-N-CA	6.15	128.80	120.44
1	A	76	GLU	CA-C-N	6.13	133.25	121.54
1	A	76	GLU	C-N-CA	6.13	133.25	121.54
1	A	340	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	202	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	67	ARG	NE-CZ-NH2	-6.04	113.76	119.20
1	A	135	ALA	O-C-N	6.03	128.28	122.07
1	A	40	GLU	CB-CG-CD	6.03	122.85	112.60
1	A	350	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	89	PRO	CA-C-N	5.96	128.19	120.44
1	A	89	PRO	C-N-CA	5.96	128.19	120.44
1	A	133	GLU	CA-C-O	-5.94	114.58	120.82
1	A	250	LEU	N-CA-C	5.90	119.67	112.23
1	A	26	PHE	CA-C-N	5.89	131.86	123.14
1	A	26	PHE	C-N-CA	5.89	131.86	123.14
1	A	148	CYS	CA-C-N	5.89	132.79	121.54
1	A	148	CYS	C-N-CA	5.89	132.79	121.54
1	A	299	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	A	289	LEU	O-C-N	5.80	128.76	122.15
1	A	251	ASP	N-CA-C	5.75	121.00	113.30
1	A	324	LEU	N-CA-C	5.74	118.47	111.82
1	A	169	LEU	O-C-N	5.73	127.12	121.57
1	A	259	PHE	N-CA-CB	5.69	118.27	110.01
1	A	391	HIS	CA-CB-CG	5.67	119.47	113.80
1	A	211	ARG	CB-CG-CD	5.65	124.30	111.30
1	A	240	ARG	CA-C-O	-5.64	114.44	120.42
1	A	55	TRP	CA-C-O	-5.63	114.25	120.38
1	A	107	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	108	GLN	CB-CG-CD	5.56	122.05	112.60
1	A	274	LEU	O-C-N	5.55	128.47	122.15
1	A	305	TYR	O-C-N	5.53	129.79	123.48
1	A	32	SER	N-CA-C	5.53	117.75	111.11
1	A	151	THR	CA-CB-OG1	-5.53	101.31	109.60
1	A	33[A]	ASN	CB-CA-C	5.51	121.38	110.42
1	A	33[B]	ASN	CB-CA-C	5.51	121.38	110.42
1	A	284	ALA	N-CA-CB	-5.50	102.03	110.12
1	A	212	ARG	N-CA-C	-5.49	104.93	111.69
1	A	273	GLU	CB-CG-CD	5.47	121.90	112.60
1	A	209[A]	GLU	CA-C-N	5.47	128.05	120.29
1	A	209[A]	GLU	C-N-CA	5.47	128.05	120.29
1	A	191	MET	CA-CB-CG	5.45	125.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	VAL	CA-C-N	5.45	125.88	119.94
1	A	247	VAL	C-N-CA	5.45	125.88	119.94
1	A	243	GLY	N-CA-C	-5.42	106.23	112.73
1	A	55	TRP	O-C-N	5.38	129.64	123.29
1	A	292	PHE	CA-C-N	5.36	128.32	120.71
1	A	292	PHE	C-N-CA	5.36	128.32	120.71
1	A	319	LEU	CA-C-O	-5.36	114.43	120.43
1	A	279	GLU	CA-CB-CG	5.34	124.78	114.10
1	A	251	ASP	CB-CA-C	5.31	119.14	110.17
1	A	15	PRO	N-CA-C	-5.28	104.26	110.70
1	A	204	LEU	N-CA-C	5.28	117.11	111.36
1	A	198	GLU	CA-C-N	5.26	127.75	120.29
1	A	198	GLU	C-N-CA	5.26	127.75	120.29
1	A	233	ILE	CA-C-O	-5.25	116.33	121.58
1	A	271	ARG	CG-CD-NE	5.25	123.54	112.00
1	A	348	THR	N-CA-C	-5.24	104.06	110.61
1	A	124	VAL	N-CA-CB	5.24	116.33	110.51
1	A	51	PRO	CA-C-N	5.21	127.26	120.28
1	A	51	PRO	C-N-CA	5.21	127.26	120.28
1	A	395	ILE	O-C-N	5.19	126.90	121.87
1	A	118	VAL	N-CA-C	5.13	116.60	111.00
1	A	373	GLU	CB-CG-CD	5.13	121.32	112.60
1	A	32	SER	CA-C-O	-5.12	115.42	120.90
1	A	119	VAL	N-CA-C	5.09	118.98	113.43
1	A	314	LYS	CA-C-O	-5.09	115.41	120.96
1	A	64	ILE	CA-C-O	-5.09	114.97	120.36
1	A	298	GLY	O-C-N	5.09	129.87	123.56
1	A	329	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	216	GLY	N-CA-C	-5.08	104.14	111.20
1	A	378	ILE	CA-C-N	5.07	124.56	119.19
1	A	378	ILE	C-N-CA	5.07	124.56	119.19
1	A	10	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	38	VAL	CA-C-N	5.05	127.05	120.28
1	A	38	VAL	C-N-CA	5.05	127.05	120.28
1	A	40	GLU	CA-C-N	5.05	127.05	120.28
1	A	40	GLU	C-N-CA	5.05	127.05	120.28
1	A	87	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	384	ALA	O-C-N	5.05	125.79	121.30
1	A	94	GLU	CA-C-N	5.04	127.97	120.31
1	A	94	GLU	C-N-CA	5.04	127.97	120.31
1	A	201	TYR	CA-C-N	5.03	127.02	120.28
1	A	201	TYR	C-N-CA	5.03	127.02	120.28

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109[A]	ARG	Sidechain
1	A	109[B]	ARG	Sidechain
1	A	118	VAL	Mainchain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	186	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	280	ARG	Sidechain
1	A	292	PHE	Mainchain
1	A	298	GLY	Mainchain
1	A	33[A]	ASN	Sidechain
1	A	33[B]	ASN	Sidechain
1	A	367	ILE	Mainchain
1	A	377	ARG	Sidechain
1	A	388[A]	GLN	Sidechain
1	A	388[B]	GLN	Sidechain
1	A	77	ASP	Mainchain
1	A	79[A]	ARG	Sidechain
1	A	79[B]	ARG	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	3240	0	3180	67	0
2	A	43	0	30	1	0
3	A	2	0	0	2	0
4	A	11	0	16	2	0
5	A	238	0	0	5	0
All	All	3534	0	3226	70	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 11.

All (70) 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:183:GLN:HE22	1:A:188:ASP:HB2	1.23	1.02
1:A:360:GLN:HE21	1:A:364:ARG:HH22	1.11	0.91
3:A:418:CMO:C	4:A:422:CAM:H52	2.12	0.79
1:A:49:ASN:HD22	1:A:49:ASN:H	1.33	0.77
1:A:183:GLN:HE21	1:A:183:GLN:HA	1.49	0.76
1:A:183:GLN:NE2	1:A:188:ASP:HB2	2.01	0.74
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.57	0.69
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.77	0.67
1:A:114:LEU:HD23	1:A:241:MET:HE1	1.77	0.66
1:A:164:MET:HE2	1:A:174:ILE:HG13	1.78	0.66
1:A:183:GLN:HA	1:A:183:GLN:NE2	2.12	0.65
1:A:56:THR:O	1:A:61:GLY:HA2	1.99	0.63
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.80	0.62
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.82	0.61
1:A:109[B]:ARG:HH11	1:A:110:GLN:HG2	1.66	0.60
1:A:365:ARG:HD3	5:A:721:HOH:O	2.01	0.60
1:A:111:PHE:HD2	1:A:241:MET:HE2	1.67	0.60
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.84	0.60
1:A:170:PRO:HG2	1:A:173:ASP:OD1	2.03	0.58
1:A:114:LEU:HD23	1:A:241:MET:CE	2.35	0.57
1:A:49:ASN:H	1:A:49:ASN:ND2	2.02	0.57
1:A:262:GLU:HG2	1:A:266[A]:LYS:HE2	1.88	0.56
1:A:149:ASN:ND2	1:A:402:LEU:H	2.04	0.56
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.21	0.56
1:A:97:ASP:O	1:A:240:ARG:HD2	2.07	0.55
1:A:325:SER:O	1:A:331:GLU:HG3	2.09	0.52
1:A:302:THR:O	1:A:314:LYS:HG3	2.10	0.52
2:A:417:HEM:HMB1	2:A:417:HEM:HBB2	1.92	0.51
1:A:213:GLN:C	1:A:215:PRO:HD3	2.36	0.51
1:A:192:THR:OG1	1:A:195:GLU:HB2	2.11	0.51
1:A:34:LEU:CD1	1:A:38:VAL:HG23	2.41	0.51
1:A:181:THR:HG23	1:A:247:VAL:HG13	1.93	0.50
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.46	0.50
1:A:191:MET:HE2	1:A:196:ALA:HA	1.94	0.49
3:A:418:CMO:O	4:A:422:CAM:H52	2.12	0.48
1:A:38:VAL:HG11	1:A:397:SER:HB3	1.95	0.47
1:A:282:PRO:HD2	5:A:661:HOH:O	2.13	0.47
1:A:160:ILE:O	1:A:164:MET:HG2	2.15	0.47
1:A:355:HIS:O	1:A:356:LEU:C	2.59	0.46
1:A:39:GLN:NE2	1:A:39:GLN:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.45	0.46
1:A:149:ASN:HD21	1:A:402:LEU:H	1.65	0.45
1:A:276:GLU:C	1:A:278:PRO:HD3	2.42	0.45
1:A:65:ALA:HB3	1:A:320:LEU:HD23	1.99	0.45
1:A:73:GLU:OE1	1:A:308:HIS:NE2	2.43	0.45
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.99	0.45
1:A:326:GLY:HA2	1:A:346:SER:O	2.17	0.45
1:A:382:SER:HB2	5:A:608:HOH:O	2.17	0.44
1:A:78:TYR:CD1	1:A:105:PRO:HD2	2.52	0.44
1:A:122:PRO:HD2	5:A:701:HOH:O	2.16	0.44
1:A:40:GLU:HG3	1:A:336:MET:CE	2.48	0.44
1:A:201:TYR:O	1:A:205:ILE:HG13	2.17	0.44
1:A:150:PHE:CE2	1:A:155:ALA:HB2	2.53	0.44
1:A:99:ILE:HD11	1:A:240:ARG:CZ	2.47	0.44
1:A:179:TYR:O	1:A:183:GLN:HG2	2.18	0.44
1:A:197:LYS:HE3	1:A:201:TYR:CE2	2.54	0.43
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.99	0.43
1:A:272:GLN:NE2	1:A:276:GLU:OE1	2.50	0.43
1:A:213:GLN:O	1:A:215:PRO:HD3	2.19	0.43
1:A:281:ILE:N	1:A:282:PRO:CD	2.82	0.42
1:A:91:GLU:H	1:A:91:GLU:CD	2.27	0.42
1:A:127:LEU:HD11	1:A:166:LEU:HD13	2.02	0.42
1:A:350:PHE:HB3	1:A:357:CYS:CB	2.51	0.41
1:A:44:VAL:O	1:A:47:GLU:HG2	2.21	0.41
1:A:219:ALA:O	1:A:223:VAL:HG23	2.19	0.41
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.50	0.41
1:A:389:ILE:HA	5:A:659:HOH:O	2.21	0.41
1:A:134:LEU:O	1:A:138:LEU:HB2	2.21	0.40
1:A:318:ILE:HD13	1:A:320:LEU:HD21	2.02	0.40
1:A:218:ASP:O	1:A:222:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	411/414 (99%)	391 (95%)	20 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	358/358 (100%)	346 (97%)	12 (3%)	32	25

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	39	GLN
1	A	49	ASN
1	A	58[A]	CYS
1	A	58[B]	CYS
1	A	91	GLU
1	A	108	GLN
1	A	128	GLU
1	A	195	GLU
1	A	261	MET
1	A	276	GLU
1	A	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	149	ASN
1	A	213	GLN
1	A	225	ASN
1	A	229	ASN
1	A	311	GLN
1	A	360	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
4	CAM	A	422	-	12,12,12	1.63	2 (16%)	20,21,21	1.15	2 (10%)
3	CMO	A	418	2	0,1,1	-	-	-		
2	HEM	A	417	3,1	50,50,50	1.38	8 (16%)	67,82,82	1.14	6 (8%)



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
4	CAM	A	422	-	-	-	0/3/2/2
2	HEM	A	417	3,1	-	3/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	422	CAM	C1-C2	4.18	1.58	1.52
2	A	417	HEM	CAB-C3B	3.56	1.56	1.47
2	A	417	HEM	CAC-C3C	2.91	1.55	1.47
2	A	417	HEM	FE-NC	2.90	2.04	1.95
2	A	417	HEM	FE-NA	2.40	2.03	1.95
2	A	417	HEM	C2A-C3A	-2.31	1.32	1.38
4	A	422	CAM	C3-C2	2.22	1.57	1.51
2	A	417	HEM	C3B-C2B	-2.14	1.32	1.37
2	A	417	HEM	CMD-C2D	2.11	1.55	1.50
2	A	417	HEM	CMA-C3A	2.01	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	O1D-CGD-CBD	-3.70	111.35	123.09
4	A	422	CAM	C9-C7-C8	-2.97	100.14	107.67
2	A	417	HEM	O2A-CGA-O1A	2.92	130.84	123.33
4	A	422	CAM	C8-C7-C1	2.86	119.43	113.05
2	A	417	HEM	O2D-CGD-O1D	2.43	129.57	123.33
2	A	417	HEM	CBC-CAC-C3C	-2.15	116.78	127.53
2	A	417	HEM	C3D-C4D-ND	-2.06	107.91	110.17
2	A	417	HEM	C3B-C2B-C1B	2.03	107.93	106.41

There are no chirality outliers.

All (3) torsion outliers are listed below:

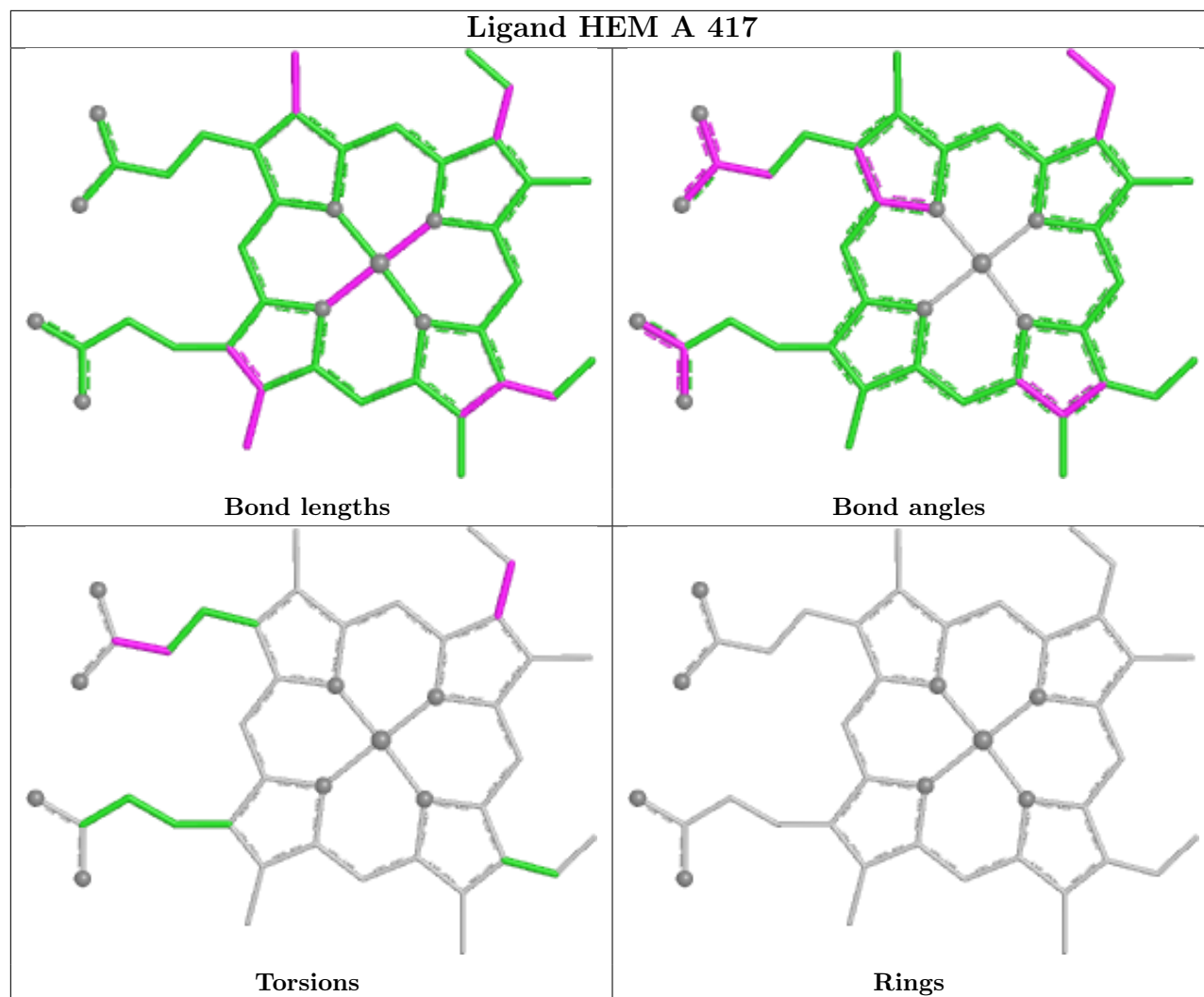
Mol	Chain	Res	Type	Atoms
2	A	417	HEM	C2C-C3C-CAC-CBC
2	A	417	HEM	C4C-C3C-CAC-CBC
2	A	417	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	422	CAM	2	0
3	A	418	CMO	2	0
2	A	417	HEM	1	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.