



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:03 AM EDT

PDB ID : 8CPP / pdb_00008cpp
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 : 2.10 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

<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>.

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)	:	2.50

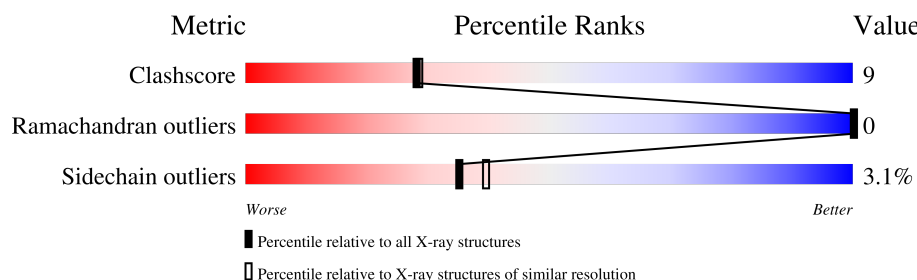
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 62% 30% . . .

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	TCM	A	422[B]	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3478 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 P450CAM.

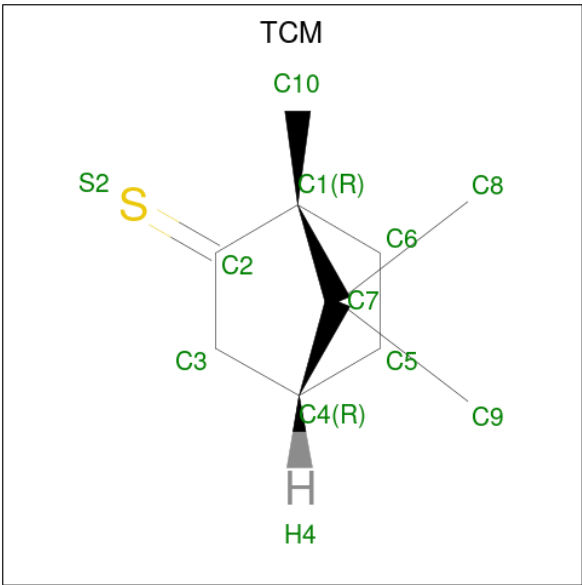
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3208	2033	560	597	18			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (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 THIOCAMPHOR (CCD ID: TCM) (formula: $C_{10}H_{16}S$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	S	0	1
			22	20	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	0
			205	205		

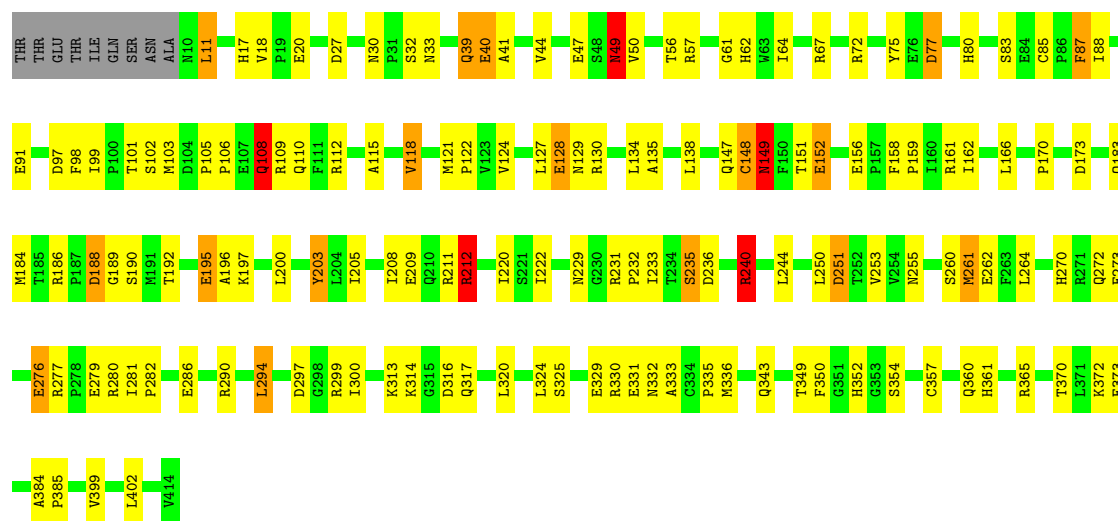
3 Residue-property plots

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 P450CAM

Chain A: 



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) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3478	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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, TCM

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	1.47	16/3287 (0.5%)	2.19	116/4465 (2.6%)

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	1	8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	PRO	CA-C	7.50	1.56	1.51
1	A	297	ASP	N-CA	6.90	1.55	1.46
1	A	399	VAL	N-CA	6.55	1.53	1.46
1	A	317	GLN	N-CA	6.14	1.53	1.45
1	A	251	ASP	C-O	5.91	1.32	1.24
1	A	18	VAL	N-CA	5.74	1.50	1.46
1	A	211	ARG	NE-CZ	-5.67	1.26	1.33
1	A	211	ARG	CD-NE	-5.57	1.38	1.46
1	A	352	HIS	CG-ND1	-5.56	1.32	1.38
1	A	349	THR	CA-CB	5.53	1.61	1.53
1	A	300	ILE	N-CA	5.41	1.52	1.46
1	A	251	ASP	C-N	-5.31	1.27	1.33
1	A	373	GLU	N-CA	-5.30	1.39	1.46
1	A	233	ILE	CA-CB	5.25	1.59	1.54
1	A	33	ASN	N-CA	5.06	1.52	1.46
1	A	112	ARG	NE-CZ	5.05	1.38	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	34.05	172.06	124.40
1	A	212	ARG	CD-NE-CZ	12.09	141.33	124.40
1	A	33	ASN	CB-CA-C	11.81	127.56	111.14
1	A	20	GLU	CA-CB-CG	11.23	136.55	114.10
1	A	152	GLU	CA-CB-CG	9.00	132.11	114.10
1	A	118	VAL	N-CA-C	8.92	120.72	111.00
1	A	195	GLU	CA-CB-CG	8.45	131.00	114.10
1	A	240	ARG	NE-CZ-NH2	-8.19	111.83	119.20
1	A	149	ASN	CA-C-O	-7.97	110.78	121.86
1	A	33	ASN	CA-CB-CG	7.74	120.34	112.60
1	A	260	SER	O-C-N	7.72	130.03	122.07
1	A	32	SER	CA-C-N	-7.71	110.15	122.95
1	A	32	SER	C-N-CA	-7.71	110.15	122.95
1	A	316	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	251	ASP	O-C-N	-7.60	113.04	122.24
1	A	240	ARG	NE-CZ-NH1	7.58	129.08	121.50
1	A	67	ARG	NE-CZ-NH2	-7.56	112.40	119.20
1	A	64	ILE	CA-C-O	-7.45	112.87	120.25
1	A	124	VAL	O-C-N	7.44	129.08	121.87
1	A	149	ASN	N-CA-CB	7.23	121.46	110.11
1	A	108	GLN	CB-CG-CD	6.98	124.46	112.60
1	A	189	GLY	N-CA-C	-6.89	104.99	114.64
1	A	115	ALA	CA-C-N	6.79	129.38	120.28
1	A	115	ALA	C-N-CA	6.79	129.38	120.28
1	A	18	VAL	N-CA-C	6.79	113.74	107.56
1	A	255	ASN	OD1-CG-ND2	6.78	129.38	122.60
1	A	250	LEU	N-CA-C	6.57	119.77	111.69
1	A	196	ALA	O-C-N	6.49	128.75	122.07
1	A	251	ASP	CB-CA-C	6.31	120.84	110.17
1	A	276	GLU	N-CA-CB	6.26	119.94	110.30
1	A	349	THR	CA-CB-OG1	-6.26	100.21	109.60
1	A	40	GLU	CB-CG-CD	6.24	123.21	112.60
1	A	109	ARG	N-CA-C	6.17	118.79	111.33
1	A	161	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	106	PRO	CA-C-N	6.09	128.44	120.28
1	A	106	PRO	C-N-CA	6.09	128.44	120.28
1	A	329	GLU	CB-CG-CD	6.05	122.89	112.60
1	A	128	GLU	N-CA-CB	6.04	118.94	109.94
1	A	277	ARG	CA-C-N	6.03	125.71	119.56
1	A	277	ARG	C-N-CA	6.03	125.71	119.56
1	A	209	GLU	CA-C-N	6.01	128.34	120.28
1	A	209	GLU	C-N-CA	6.01	128.34	120.28
1	A	320	LEU	N-CA-CB	-6.00	102.39	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	A	80	HIS	CA-CB-CG	-5.90	107.90	113.80
1	A	203	TYR	CA-C-N	5.88	128.65	120.29
1	A	203	TYR	C-N-CA	5.88	128.65	120.29
1	A	87	PHE	CA-CB-CG	5.86	119.66	113.80
1	A	280	ARG	CD-NE-CZ	5.84	132.57	124.40
1	A	253	VAL	O-C-N	5.83	127.52	121.87
1	A	85	CYS	N-CA-CB	-5.80	103.02	111.20
1	A	299	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	A	211	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	A	264	LEU	CA-C-O	-5.76	114.45	120.55
1	A	205	ILE	CA-C-N	5.70	125.38	119.05
1	A	205	ILE	C-N-CA	5.70	125.38	119.05
1	A	130	ARG	N-CA-CB	5.70	118.59	110.16
1	A	314	LYS	CA-C-O	-5.69	114.75	120.96
1	A	270	HIS	CA-CB-CG	-5.69	108.11	113.80
1	A	264	LEU	O-C-N	5.66	128.12	122.12
1	A	294	LEU	N-CA-CB	-5.65	102.19	111.01
1	A	129	ASN	CA-C-O	-5.56	114.66	120.55
1	A	108	GLN	CA-C-N	5.55	127.99	120.38
1	A	108	GLN	C-N-CA	5.55	127.99	120.38
1	A	361	HIS	CA-CB-CG	-5.55	108.25	113.80
1	A	290	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	A	64	ILE	O-C-N	5.53	128.73	123.03
1	A	11	LEU	CB-CA-C	5.52	118.75	109.48
1	A	372	LYS	CA-C-N	5.51	128.12	120.29
1	A	372	LYS	C-N-CA	5.51	128.12	120.29
1	A	235	SER	CA-C-N	5.49	127.58	120.44
1	A	235	SER	C-N-CA	5.49	127.58	120.44
1	A	281	ILE	CA-C-N	5.49	125.14	119.05
1	A	281	ILE	C-N-CA	5.49	125.14	119.05
1	A	188	ASP	N-CA-CB	-5.48	102.03	110.20
1	A	20	GLU	N-CA-CB	5.47	118.64	110.22
1	A	50	VAL	CB-CA-C	5.47	116.22	110.37
1	A	330	ARG	NE-CZ-NH1	5.44	126.94	121.50
1	A	77	ASP	CA-C-O	-5.44	112.73	120.51
1	A	361	HIS	N-CA-CB	5.43	118.11	110.12
1	A	333	ALA	CA-C-O	-5.40	115.11	121.16
1	A	149	ASN	CB-CA-C	5.38	119.96	111.72
1	A	148	CYS	CA-C-N	5.34	129.95	122.79
1	A	148	CYS	C-N-CA	5.34	129.95	122.79
1	A	360	GLN	CA-C-N	5.33	127.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	GLN	C-N-CA	5.33	127.42	120.28
1	A	72	ARG	NH1-CZ-NH2	5.32	126.21	119.30
1	A	156	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	260	SER	CA-C-O	-5.30	115.26	120.82
1	A	370	THR	CA-CB-CG2	5.29	119.50	110.50
1	A	297	ASP	CB-CA-C	5.27	120.91	110.42
1	A	280	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	A	262	GLU	CA-CB-CG	5.26	124.63	114.10
1	A	324	LEU	N-CA-C	5.25	117.91	111.82
1	A	27	ASP	CA-C-N	5.23	127.82	120.28
1	A	27	ASP	C-N-CA	5.23	127.82	120.28
1	A	20	GLU	CA-C-N	5.21	129.43	120.72
1	A	20	GLU	C-N-CA	5.21	129.43	120.72
1	A	270	HIS	N-CA-CB	5.21	117.97	110.20
1	A	286	GLU	N-CA-CB	5.21	117.78	110.12
1	A	75	TYR	N-CA-CB	5.19	118.33	110.28
1	A	49	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	102	SER	CA-CB-OG	-5.17	100.75	111.10
1	A	324	LEU	CA-C-O	-5.16	114.04	119.97
1	A	32	SER	CA-C-O	-5.15	115.41	120.82
1	A	211	ARG	CA-CB-CG	5.10	124.30	114.10
1	A	273	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	282	PRO	CA-C-N	5.09	127.51	120.29
1	A	282	PRO	C-N-CA	5.09	127.51	120.29
1	A	220	ILE	CA-C-N	5.07	127.04	120.44
1	A	220	ILE	C-N-CA	5.07	127.04	120.44
1	A	135	ALA	O-C-N	5.07	127.29	122.07
1	A	151	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	279	GLU	CA-C-N	5.05	129.97	121.14
1	A	279	GLU	C-N-CA	5.05	129.97	121.14
1	A	343	GLN	N-CA-CB	5.03	117.51	110.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	33	ASN	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	VAL	Mainchain
1	A	147	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	212	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	251	ASP	Mainchain
1	A	77	ASP	Mainchain

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	A	3208	0	3156	47	0
2	A	43	0	30	6	0
3	A	22	0	32	12	0
4	A	205	0	0	8	0
All	All	3478	0	3218	58	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 (58) 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:422[B]:TCM:C2	3:A:422[B]:TCM:S2	1.20	1.29
3:A:422[B]:TCM:S2	3:A:422[B]:TCM:C3	2.44	1.03
3:A:422[B]:TCM:S2	3:A:422[B]:TCM:C1	2.51	0.98
3:A:422[A]:TCM:S2	4:A:705:HOH:O	2.35	0.83
2:A:417:HEM:NC	4:A:705:HOH:O	2.14	0.81
2:A:417:HEM:NB	4:A:705:HOH:O	2.15	0.80
2:A:417:HEM:FE	4:A:705:HOH:O	1.35	0.79
1:A:244:LEU:HD11	3:A:422[B]:TCM:H52	1.72	0.70
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.74	0.67
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.81	0.63
1:A:99:ILE:HG12	1:A:103:MET:HE3	1.80	0.63
1:A:244:LEU:HD11	3:A:422[A]:TCM:H62	1.82	0.62
2:A:417:HEM:HBA1	3:A:422[A]:TCM:H101	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:417:HEM:NA	4:A:705:HOH:O	2.31	0.61
1:A:231:ARG:HB2	1:A:232:PRO:HD2	1.84	0.60
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.84	0.59
1:A:365:ARG:HD3	4:A:625:HOH:O	2.04	0.58
1:A:208:ILE:O	1:A:212:ARG:HG3	2.05	0.56
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.71	0.55
1:A:170:PRO:HG2	1:A:173:ASP:OD1	2.07	0.55
1:A:294:LEU:HD23	1:A:294:LEU:H	1.74	0.53
1:A:244:LEU:HD11	3:A:422[B]:TCM:C5	2.39	0.52
1:A:149:ASN:ND2	1:A:402:LEU:H	2.07	0.52
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.10	0.52
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.45	0.51
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.91	0.51
1:A:97:ASP:O	1:A:240:ARG:HD2	2.12	0.50
1:A:56:THR:O	1:A:61:GLY:HA2	2.11	0.49
1:A:11:LEU:HG	1:A:57:ARG:HB2	1.95	0.49
1:A:83:SER:HB3	1:A:101:THR:O	2.13	0.49
1:A:200:LEU:O	1:A:203:TYR:HB3	2.14	0.48
1:A:325:SER:O	1:A:331:GLU:HG3	2.14	0.48
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.95	0.48
1:A:39:GLN:NE2	1:A:39:GLN:H	2.12	0.48
1:A:87:PHE:CE2	3:A:422[B]:TCM:H92	2.48	0.47
1:A:49:ASN:HD22	1:A:49:ASN:H	1.62	0.47
1:A:41:ALA:O	1:A:44:VAL:HG22	2.14	0.47
1:A:87:PHE:CZ	3:A:422[B]:TCM:H92	2.50	0.46
1:A:183:GLN:HE22	1:A:188:ASP:HB2	1.80	0.46
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.82	0.46
1:A:261:MET:HA	1:A:261:MET:HE2	1.98	0.46
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.45	0.45
1:A:184:MET:HE2	1:A:197:LYS:HA	1.99	0.45
1:A:47:GLU:HB2	1:A:49:ASN:ND2	2.32	0.44
3:A:422[B]:TCM:S2	3:A:422[B]:TCM:C10	3.06	0.44
1:A:236:ASP:O	1:A:240:ARG:HG3	2.18	0.43
1:A:152:GLU:HB3	4:A:563:HOH:O	2.18	0.43
1:A:188:ASP:HB3	1:A:190:SER:H	1.84	0.42
1:A:30:ASN:ND2	4:A:556:HOH:O	2.37	0.42
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.50	0.42
1:A:350:PHE:HB3	1:A:357:CYS:HB3	2.01	0.42
2:A:417:HEM:HBA1	3:A:422[B]:TCM:H62	2.01	0.42
1:A:332:ASN:O	1:A:335:PRO:HD3	2.19	0.42
1:A:294:LEU:HD23	1:A:294:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HD23	1:A:162:ILE:HG13	2.01	0.41
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.36	0.41
1:A:121:MET:CB	1:A:122:PRO:HD3	2.48	0.41
1:A:17:HIS:CD2	1:A:313:LYS:HG3	2.57	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%)	386 (96%)	17 (4%)	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%)	339 (97%)	11 (3%)	35	39

All (11) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	91	GLU
1	A	108	GLN
1	A	128	GLU
1	A	138	LEU
1	A	222	ILE
1	A	235	SER
1	A	261	MET
1	A	272	GLN
1	A	276	GLU

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	21	HIS
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	108	GLN
1	A	129	ASN
1	A	149	ASN
1	A	176	HIS
1	A	213	GLN
1	A	225	ASN
1	A	229	ASN
1	A	337	HIS
1	A	388	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

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
3	TCM	A	422[B]	-	10,12,12	1.16	0	17,21,21	1.36	2 (11%)
2	HEM	A	417	1	50,50,50	1.70	10 (20%)	67,82,82	1.37	11 (16%)
3	TCM	A	422[A]	-	10,12,12	1.20	0	17,21,21	1.35	1 (5%)

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	TCM	A	422[B]	-	-	-	0/3/2/2
2	HEM	A	417	1	-	3/14/54/54	-
3	TCM	A	422[A]	-	-	-	0/3/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	FE-NB	5.62	2.12	1.94
2	A	417	HEM	FE-NC	3.13	2.05	1.95
2	A	417	HEM	FE-ND	3.05	2.04	1.94
2	A	417	HEM	CAC-C3C	3.01	1.55	1.47
2	A	417	HEM	CMC-C2C	2.71	1.56	1.50
2	A	417	HEM	CAB-C3B	2.27	1.53	1.47
2	A	417	HEM	CMD-C2D	2.23	1.55	1.50
2	A	417	HEM	CBD-CGD	2.22	1.55	1.50
2	A	417	HEM	C4C-NC	-2.06	1.35	1.39
2	A	417	HEM	C2A-C3A	-2.04	1.33	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	422[B]	TCM	C9-C7-C8	-3.84	97.95	107.67
3	A	422[A]	TCM	C9-C7-C8	-3.71	98.28	107.67
2	A	417	HEM	CBD-CAD-C3D	3.34	121.76	112.53
2	A	417	HEM	C1B-NB-C4B	3.21	109.00	105.21
2	A	417	HEM	O1D-CGD-CBD	-2.92	113.83	123.09
2	A	417	HEM	CHB-C1B-NB	2.81	127.84	124.37
3	A	422[B]	TCM	C9-C7-C1	2.68	119.02	113.05
2	A	417	HEM	CHB-C4A-NA	2.51	128.40	123.86
2	A	417	HEM	C4A-CHB-C1B	-2.45	120.49	126.25
2	A	417	HEM	CBC-CAC-C3C	-2.21	116.48	127.53
2	A	417	HEM	CHC-C4B-NB	2.11	126.69	124.42
2	A	417	HEM	C4D-ND-C1D	2.10	107.69	105.21
2	A	417	HEM	O2A-CGA-O1A	2.06	128.62	123.33
2	A	417	HEM	C3D-C4D-ND	-2.03	107.94	110.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

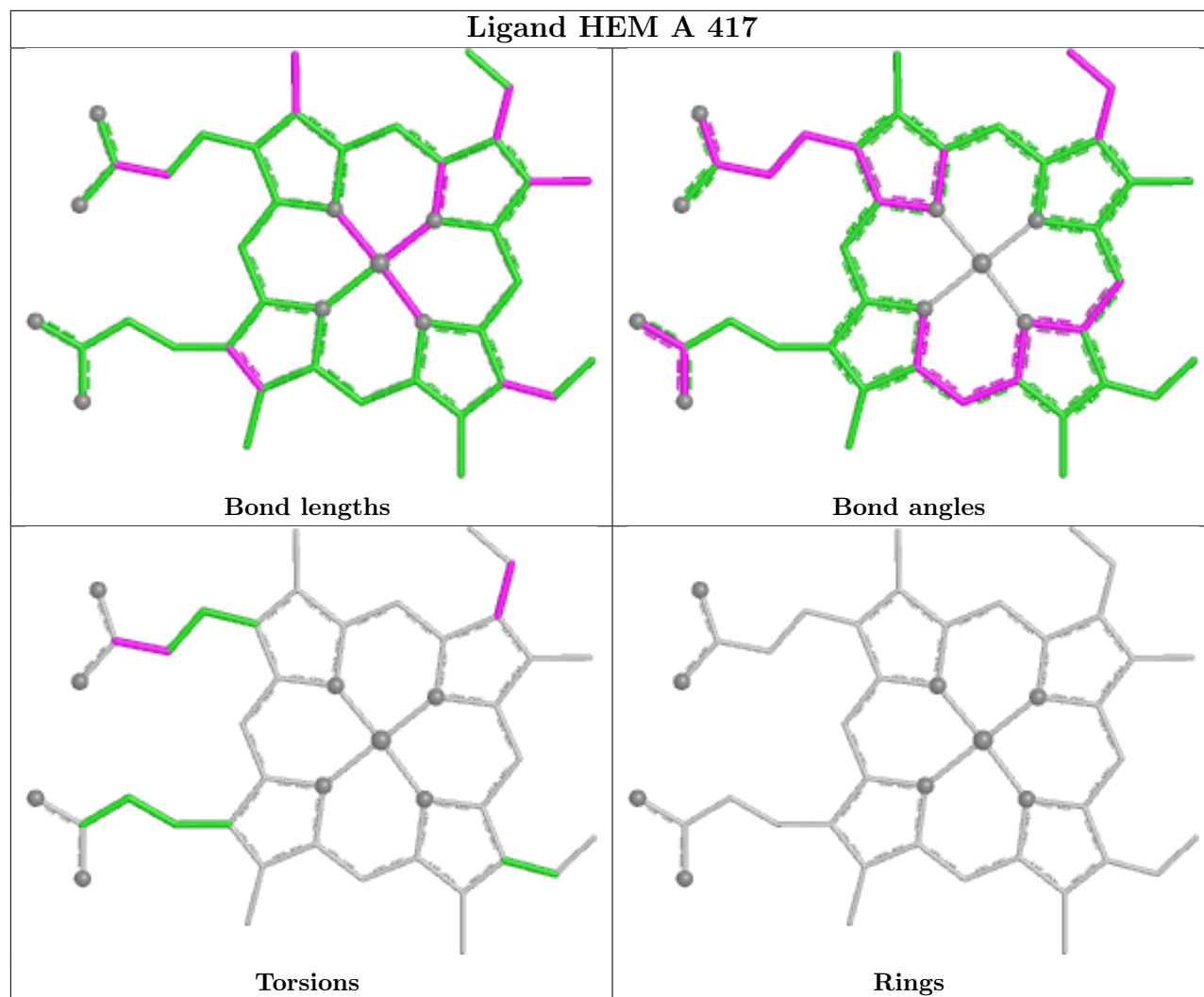
Mol	Chain	Res	Type	Atoms
2	A	417	HEM	C2C-C3C-CAC-CBC
2	A	417	HEM	C4C-C3C-CAC-CBC
2	A	417	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	422[B]	TCM	9	0
2	A	417	HEM	6	0
3	A	422[A]	TCM	3	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.