



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:01 PM UTC

PDB ID : 2CPP / pdb_00002cpp
Title : HIGH-RESOLUTION CRYSTAL STRUCTURE OF CYTOCHROME P450-CAM
Authors : Poulos, T.L.
Deposited on : 1987-04-06
Resolution : 1.63 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)	:	2.49

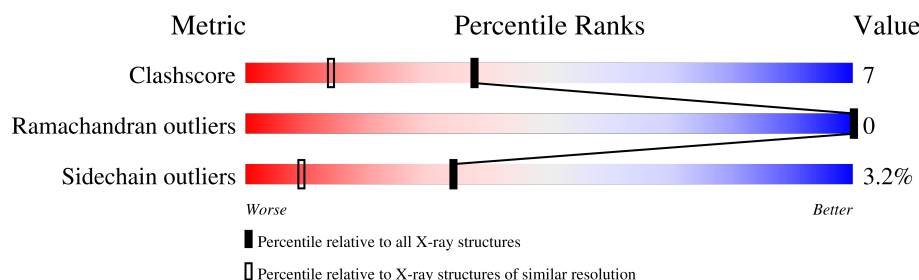
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3462 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.

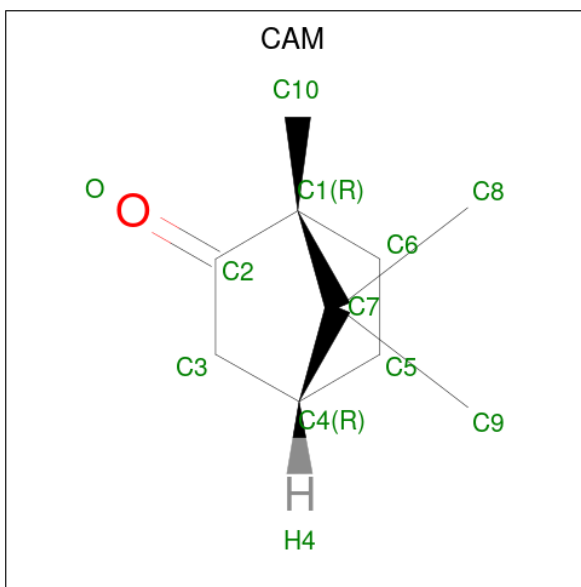
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3204	2030	559	597	18			

- 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 CAMPHOR (CCD ID: CAM) (formula: $C_{10}H_{16}O$).



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

- Molecule 4 is water.

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

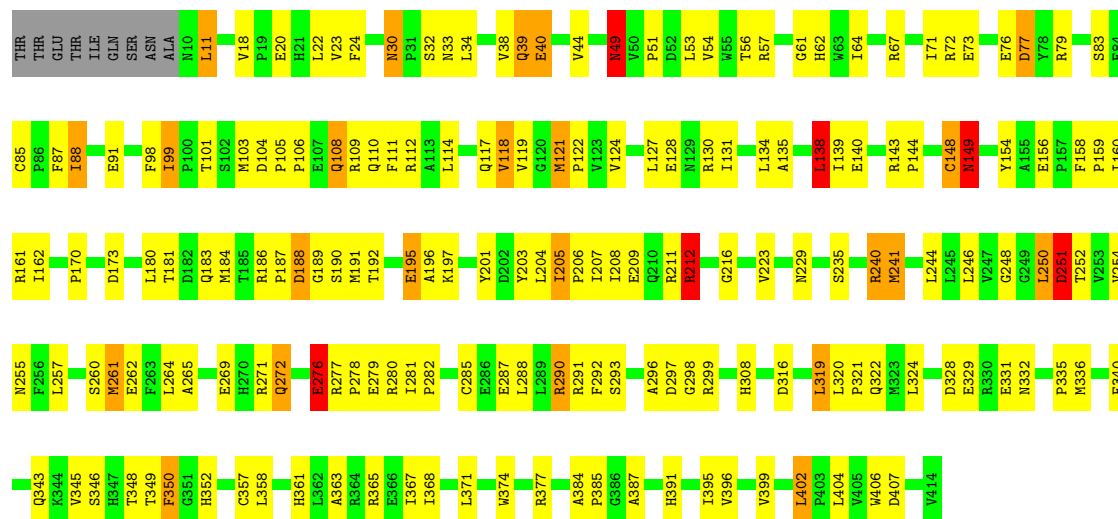
3 Residue-property plots

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 P450-CAM

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) – 1.63	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.63)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3462	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: CAM, HEM

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	1.64	26/3283 (0.8%)	2.30	175/4461 (3.9%)

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	11

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	PRO	CA-C	8.45	1.56	1.51
1	A	287	GLU	CA-C	-6.58	1.44	1.52
1	A	349	THR	CA-CB	6.54	1.64	1.53
1	A	211	ARG	NE-CZ	-6.47	1.25	1.33
1	A	367	ILE	C-N	-6.28	1.25	1.33
1	A	292	PHE	CA-CB	6.27	1.61	1.53
1	A	88	ILE	CA-CB	6.02	1.59	1.54
1	A	251	ASP	C-O	6.02	1.32	1.24
1	A	64	ILE	C-N	-5.92	1.25	1.33
1	A	77	ASP	C-O	5.86	1.31	1.24
1	A	265	ALA	C-O	5.67	1.31	1.24
1	A	149	ASN	C-N	-5.61	1.25	1.33
1	A	112	ARG	NE-CZ	5.50	1.39	1.33
1	A	293	SER	N-CA	5.39	1.52	1.46
1	A	211	ARG	CD-NE	-5.32	1.38	1.46
1	A	277	ARG	N-CA	5.31	1.52	1.46
1	A	297	ASP	N-CA	5.30	1.52	1.46
1	A	296	ALA	CA-C	5.29	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	ILE	CA-CB	5.27	1.60	1.54
1	A	287	GLU	C-O	5.24	1.30	1.24
1	A	374	TRP	C-N	-5.23	1.26	1.34
1	A	298	GLY	N-CA	5.14	1.50	1.44
1	A	396	VAL	CA-C	5.13	1.59	1.52
1	A	207	ILE	CA-CB	5.09	1.60	1.54
1	A	127	LEU	C-N	-5.06	1.27	1.33
1	A	33	ASN	N-CA	5.00	1.52	1.46

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	35.79	174.50	124.40
1	A	195	GLU	CA-CB-CG	11.23	136.57	114.10
1	A	20	GLU	CA-CB-CG	10.38	134.85	114.10
1	A	149	ASN	CA-C-O	-9.33	110.01	121.58
1	A	291	ARG	NH1-CZ-NH2	-9.32	107.18	119.30
1	A	299	ARG	NE-CZ-NH2	-9.09	111.02	119.20
1	A	287	GLU	O-C-N	-8.70	112.90	122.12
1	A	260	SER	O-C-N	8.70	131.34	122.12
1	A	349	THR	CA-CB-OG1	-8.51	96.84	109.60
1	A	88	ILE	CA-C-O	-8.13	114.47	119.51
1	A	329	GLU	CB-CG-CD	8.06	126.30	112.60
1	A	135	ALA	O-C-N	8.05	130.36	122.07
1	A	67	ARG	NE-CZ-NH2	-8.01	112.00	119.20
1	A	291	ARG	NE-CZ-NH1	7.99	129.49	121.50
1	A	51	PRO	CA-C-N	7.98	130.97	120.28
1	A	51	PRO	C-N-CA	7.98	130.97	120.28
1	A	363	ALA	CA-C-O	-7.93	112.49	120.82
1	A	187	PRO	CA-C-N	7.93	134.14	120.58
1	A	187	PRO	C-N-CA	7.93	134.14	120.58
1	A	241	MET	N-CA-CB	7.91	121.54	110.07
1	A	406	TRP	O-C-N	7.86	131.83	123.42
1	A	402	LEU	O-C-N	7.78	127.78	121.17
1	A	288	LEU	CA-C-O	-7.59	112.50	120.55
1	A	251	ASP	O-C-N	-7.54	113.12	122.24
1	A	288	LEU	O-C-N	7.51	130.09	122.12
1	A	291	ARG	N-CA-C	7.39	119.41	111.36
1	A	118	VAL	N-CA-C	7.38	119.04	111.00
1	A	124	VAL	O-C-N	7.32	128.97	121.87
1	A	33	ASN	OD1-CG-ND2	7.32	129.92	122.60
1	A	257	LEU	CA-C-O	-7.26	112.85	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ASP	N-CA-CB	-7.21	99.46	110.20
1	A	130	ARG	N-CA-CB	7.19	120.69	110.12
1	A	64	ILE	CA-C-O	-7.16	112.63	120.43
1	A	18	VAL	O-C-N	7.14	127.03	121.46
1	A	296	ALA	CA-C-N	-7.09	112.80	122.16
1	A	296	ALA	C-N-CA	-7.09	112.80	122.16
1	A	255	ASN	OD1-CG-ND2	6.97	129.57	122.60
1	A	367	ILE	CA-C-O	-6.96	113.32	121.05
1	A	39	GLN	N-CA-CB	6.87	119.97	110.01
1	A	154	TYR	O-C-N	6.81	131.65	122.59
1	A	264	LEU	CA-C-O	-6.80	112.15	119.97
1	A	292	PHE	CA-CB-CG	-6.72	107.08	113.80
1	A	319	LEU	O-C-N	-6.68	115.22	123.04
1	A	285	CYS	O-C-N	6.64	128.91	122.07
1	A	404	LEU	O-C-N	6.61	131.79	123.19
1	A	340	PHE	CA-CB-CG	6.58	120.38	113.80
1	A	291	ARG	CD-NE-CZ	6.57	133.60	124.40
1	A	251	ASP	CA-C-O	-6.45	111.64	119.32
1	A	316	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	396	VAL	O-C-N	6.43	130.21	123.26
1	A	280	ARG	CD-NE-CZ	6.43	133.40	124.40
1	A	33	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	54	VAL	O-C-N	6.40	130.14	123.04
1	A	23	VAL	N-CA-CB	6.31	117.41	110.53
1	A	212	ARG	CD-NE-CZ	6.30	133.22	124.40
1	A	290	ARG	NE-CZ-NH1	6.22	127.72	121.50
1	A	87	PHE	CA-CB-CG	6.21	120.01	113.80
1	A	322	GLN	O-C-N	6.20	128.69	122.12
1	A	128	GLU	N-CA-CB	6.19	119.17	109.94
1	A	241	MET	O-C-N	6.16	128.75	122.09
1	A	30	ASN	O-C-N	6.15	125.68	121.19
1	A	76	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	139	ILE	O-C-N	6.09	128.23	121.90
1	A	121	MET	CA-C-N	6.04	125.92	119.28
1	A	121	MET	C-N-CA	6.04	125.92	119.28
1	A	361	HIS	CA-C-N	6.00	128.24	120.44
1	A	361	HIS	C-N-CA	6.00	128.24	120.44
1	A	260	SER	CA-C-O	-5.94	114.25	120.55
1	A	240	ARG	CD-NE-CZ	5.92	132.69	124.40
1	A	368	ILE	CA-C-O	-5.91	114.81	120.95
1	A	296	ALA	O-C-N	5.90	131.03	123.24
1	A	396	VAL	N-CA-C	-5.90	99.85	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	VAL	CA-C-N	5.89	128.10	120.44
1	A	38	VAL	C-N-CA	5.89	128.10	120.44
1	A	49	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	371	LEU	CA-C-O	-5.88	114.65	120.82
1	A	277	ARG	CA-C-N	5.86	125.54	119.56
1	A	277	ARG	C-N-CA	5.86	125.54	119.56
1	A	71	ILE	CA-C-N	5.86	128.06	120.44
1	A	71	ILE	C-N-CA	5.86	128.06	120.44
1	A	287	GLU	CA-C-N	5.86	128.13	120.28
1	A	287	GLU	C-N-CA	5.86	128.13	120.28
1	A	387	ALA	N-CA-C	-5.84	100.16	109.96
1	A	367	ILE	O-C-N	5.83	127.97	121.90
1	A	204	LEU	N-CA-C	5.82	117.42	111.14
1	A	160	ILE	N-CA-CB	5.80	116.94	110.62
1	A	189	GLY	N-CA-C	-5.80	106.52	114.64
1	A	38	VAL	CA-CB-CG2	-5.79	100.55	110.40
1	A	240	ARG	NE-CZ-NH1	5.79	127.28	121.50
1	A	271	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	A	148	CYS	CA-C-N	5.77	131.89	123.12
1	A	148	CYS	C-N-CA	5.77	131.89	123.12
1	A	195	GLU	CB-CG-CD	5.75	122.38	112.60
1	A	119	VAL	CB-CA-C	5.71	117.11	110.88
1	A	282	PRO	CA-C-N	5.71	127.87	120.44
1	A	282	PRO	C-N-CA	5.71	127.87	120.44
1	A	279	GLU	CB-CG-CD	5.70	122.30	112.60
1	A	292	PHE	O-C-N	5.69	129.49	122.20
1	A	205	ILE	CA-C-N	5.68	125.36	119.05
1	A	205	ILE	C-N-CA	5.68	125.36	119.05
1	A	387	ALA	O-C-N	5.65	129.72	123.16
1	A	72	ARG	O-C-N	5.64	127.88	122.07
1	A	106	PRO	CA-C-N	5.63	128.10	120.38
1	A	106	PRO	C-N-CA	5.63	128.10	120.38
1	A	322	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	A	39	GLN	CA-C-O	5.59	126.69	120.82
1	A	216	GLY	N-CA-C	-5.59	106.08	112.79
1	A	203	TYR	CA-C-N	5.59	128.04	120.44
1	A	203	TYR	C-N-CA	5.59	128.04	120.44
1	A	320	LEU	N-CA-CB	-5.59	103.00	111.21
1	A	346	SER	CB-CA-C	5.58	119.22	110.19
1	A	44	VAL	N-CA-CB	5.55	120.14	110.65
1	A	358	LEU	O-C-N	5.50	130.05	122.46
1	A	195	GLU	CB-CA-C	-5.48	102.23	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	HIS	O-C-N	5.43	129.31	123.56
1	A	343	GLN	N-CA-CB	5.43	118.10	110.12
1	A	53	LEU	CA-C-O	-5.43	114.49	120.24
1	A	350	PHE	O-C-N	5.42	128.84	122.34
1	A	108	GLN	CA-C-N	5.40	127.78	120.38
1	A	108	GLN	C-N-CA	5.40	127.78	120.38
1	A	209	GLU	CA-C-N	5.39	127.50	120.28
1	A	209	GLU	C-N-CA	5.39	127.50	120.28
1	A	33	ASN	N-CA-CB	-5.36	103.16	110.56
1	A	262	GLU	CA-C-N	5.36	127.41	120.44
1	A	262	GLU	C-N-CA	5.36	127.41	120.44
1	A	281	ILE	O-C-N	5.34	123.84	120.42
1	A	395	ILE	O-C-N	5.34	127.45	121.90
1	A	391	HIS	CA-CB-CG	5.33	119.13	113.80
1	A	108	GLN	CA-CB-CG	5.32	124.74	114.10
1	A	404	LEU	CA-C-O	-5.29	115.13	121.11
1	A	22	LEU	CA-C-O	-5.29	113.17	119.35
1	A	23	VAL	O-C-N	5.29	128.68	122.81
1	A	85	CYS	N-CA-CB	-5.28	103.75	111.20
1	A	180	LEU	O-C-N	5.28	127.71	122.12
1	A	324	LEU	N-CA-C	5.27	118.97	112.54
1	A	211	ARG	NH1-CZ-NH2	-5.27	112.45	119.30
1	A	395	ILE	N-CA-C	-5.26	105.58	110.53
1	A	399	VAL	N-CA-CB	-5.26	104.09	111.25
1	A	279	GLU	CA-CB-CG	5.26	124.62	114.10
1	A	72	ARG	NH1-CZ-NH2	5.26	126.14	119.30
1	A	156	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	109	ARG	N-CA-C	5.25	117.68	111.33
1	A	20	GLU	N-CA-CB	5.23	119.21	110.32
1	A	254	VAL	N-CA-CB	-5.23	104.71	110.51
1	A	34	LEU	CB-CA-C	5.22	119.56	110.68
1	A	272	GLN	CB-CG-CD	5.22	121.47	112.60
1	A	76	GLU	O-C-N	5.22	128.10	122.15
1	A	87	PHE	CA-C-N	5.20	127.86	123.33
1	A	87	PHE	C-N-CA	5.20	127.86	123.33
1	A	365	ARG	CA-C-O	-5.19	114.92	120.42
1	A	329	GLU	CA-CB-CG	5.18	124.46	114.10
1	A	40	GLU	CA-C-N	5.14	127.12	120.44
1	A	40	GLU	C-N-CA	5.14	127.12	120.44
1	A	248	GLY	N-CA-C	-5.12	106.56	112.50
1	A	252	THR	O-C-N	5.12	127.65	121.76
1	A	250	LEU	N-CA-C	5.12	118.68	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CA-C	5.11	120.59	110.42
1	A	407	ASP	CB-CA-C	5.11	116.74	109.38
1	A	140	GLU	CA-C-N	5.11	127.64	120.28
1	A	140	GLU	C-N-CA	5.11	127.64	120.28
1	A	162	ILE	O-C-N	5.11	126.82	121.87
1	A	131	ILE	O-C-N	5.10	126.90	121.91
1	A	138	LEU	O-C-N	5.09	127.96	122.15
1	A	276	GLU	N-CA-CB	5.09	118.14	110.30
1	A	261	MET	CG-SD-CE	5.08	112.07	100.90
1	A	104	ASP	O-C-N	5.08	127.35	121.21
1	A	49	ASN	CA-C-N	-5.05	117.87	123.43
1	A	49	ASN	C-N-CA	-5.05	117.87	123.43
1	A	348	THR	N-CA-C	-5.04	104.39	110.44
1	A	319	LEU	CA-C-N	5.03	129.34	123.16
1	A	319	LEU	C-N-CA	5.03	129.34	123.16
1	A	24	PHE	CB-CA-C	5.02	117.77	110.79
1	A	32	SER	N-CA-C	5.02	116.75	111.28
1	A	223	VAL	CA-C-O	-5.01	115.85	121.17
1	A	257	LEU	N-CA-C	-5.01	105.81	111.28

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	VAL	Mainchain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	161	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
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	3204	0	3145	44	0
2	A	43	0	30	3	0
3	A	11	0	16	0	0
4	A	204	0	0	2	0
All	All	3462	0	3191	45	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 7.

All (45) 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:208:ILE:O	1:A:212:ARG:HG3	1.93	0.67
1:A:192:THR:OG1	1:A:195:GLU:HG2	1.96	0.65
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.78	0.64
1:A:149:ASN:ND2	1:A:402:LEU:H	1.95	0.64
1:A:99:ILE:HG12	1:A:103:MET:HE3	1.78	0.63
1:A:191:MET:HE2	1:A:196:ALA:HA	1.80	0.62
1:A:188:ASP:HB3	1:A:190:SER:H	1.66	0.59
1:A:111:PHE:HD2	1:A:241:MET:HE2	1.73	0.53
1:A:170:PRO:HG2	1:A:173:ASP:OD1	2.08	0.53
1:A:91:GLU:H	1:A:91:GLU:CD	2.17	0.52
1:A:122:PRO:HD2	4:A:701:HOH:O	2.11	0.50
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.93	0.50
1:A:56:THR:O	1:A:61:GLY:HA2	2.11	0.50
1:A:149:ASN:HD21	1:A:402:LEU:H	1.57	0.50
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.94	0.49
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.42	0.49
1:A:83:SER:HB3	1:A:101:THR:O	2.12	0.49
1:A:134:LEU:O	1:A:138:LEU:HB2	2.13	0.49
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.28	0.49
1:A:184:MET:HE2	1:A:197:LYS:HA	1.94	0.49
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.94	0.49
2:A:417:HEM:HMB1	2:A:417:HEM:HBB2	1.94	0.48
1:A:183:GLN:HE22	1:A:188:ASP:HB2	1.80	0.47
1:A:328:ASP:HB3	1:A:331:GLU:HG3	1.96	0.47
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.97	0.46
1:A:30:ASN:ND2	4:A:556:HOH:O	2.45	0.46
1:A:49:ASN:HD22	1:A:49:ASN:H	1.65	0.45
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:C	1:A:278:PRO:HD3	2.42	0.45
1:A:101:THR:HG22	2:A:417:HEM:O2D	2.17	0.44
1:A:114:LEU:O	1:A:117:GLN:HB2	2.17	0.44
1:A:101:THR:HG23	1:A:244:LEU:HD21	1.99	0.44
1:A:319:LEU:HG	1:A:321:PRO:HG3	2.00	0.44
1:A:269:GLU:CD	1:A:269:GLU:H	2.26	0.43
1:A:11:LEU:HG	1:A:57:ARG:HB2	2.00	0.43
1:A:332:ASN:O	1:A:335:PRO:HD3	2.19	0.43
1:A:181:THR:HG22	1:A:251:ASP:HB2	2.00	0.43
1:A:114:LEU:HD23	1:A:241:MET:CE	2.48	0.43
1:A:350:PHE:HB3	1:A:357:CYS:HB3	2.01	0.43
1:A:73:GLU:OE1	1:A:308:HIS:NE2	2.39	0.42
1:A:290:ARG:HD3	1:A:345:VAL:HG13	2.02	0.41
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.55	0.41
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.90	0.41
1:A:101:THR:HG22	2:A:417:HEM:HAD2	2.02	0.41
1:A:201:TYR:O	1:A:205:ILE:HG13	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	403/414 (97%)	388 (96%)	15 (4%)	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	349/358 (98%)	338 (97%)	11 (3%)	34 9

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

Mol	Chain	Res	Type
1	A	11	LEU
1	A	39	GLN
1	A	49	ASN
1	A	79	ARG
1	A	108	GLN
1	A	138	LEU
1	A	235	SER
1	A	246	LEU
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	21	HIS
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	110	GLN
1	A	145	GLN
1	A	149	ASN
1	A	213	GLN
1	A	225	ASN
1	A	337	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 [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](#)

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	CAM	A	422	-	12,12,12	1.94	1 (8%)	20,21,21	1.04	1 (5%)
2	HEM	A	417	1	50,50,50	1.78	10 (20%)	67,82,82	1.61	12 (17%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	422	CAM	C1-C2	5.54	1.60	1.52
2	A	417	HEM	FE-NB	4.34	2.08	1.94
2	A	417	HEM	FE-ND	4.17	2.07	1.94
2	A	417	HEM	CBD-CGD	4.06	1.60	1.50
2	A	417	HEM	CAC-C3C	3.57	1.56	1.47
2	A	417	HEM	CAB-C3B	3.01	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	C3B-C2B	-2.91	1.31	1.37
2	A	417	HEM	CBA-CGA	2.80	1.57	1.50
2	A	417	HEM	CMC-C2C	2.53	1.56	1.50
2	A	417	HEM	FE-NC	2.40	2.03	1.95
2	A	417	HEM	CMD-C2D	2.09	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	O2D-CGD-O1D	4.66	135.33	123.33
2	A	417	HEM	O2A-CGA-O1A	4.05	133.75	123.33
2	A	417	HEM	O1D-CGD-CBD	-3.98	110.48	123.09
2	A	417	HEM	C4D-ND-C1D	3.39	109.23	105.21
2	A	417	HEM	C3D-C4D-ND	-2.99	106.89	110.17
2	A	417	HEM	CHB-C4A-NA	2.87	129.06	123.86
2	A	417	HEM	CHA-C4D-ND	2.75	127.77	124.37
2	A	417	HEM	CHD-C1D-ND	2.68	127.31	124.42
2	A	417	HEM	CBC-CAC-C3C	-2.44	115.33	127.53
2	A	417	HEM	O2A-CGA-CBA	-2.43	106.32	114.00
2	A	417	HEM	CMA-C3A-C2A	2.27	130.44	125.62
2	A	417	HEM	C4A-CHB-C1B	-2.14	121.20	126.25
3	A	422	CAM	O-C2-C3	2.13	130.78	126.39

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

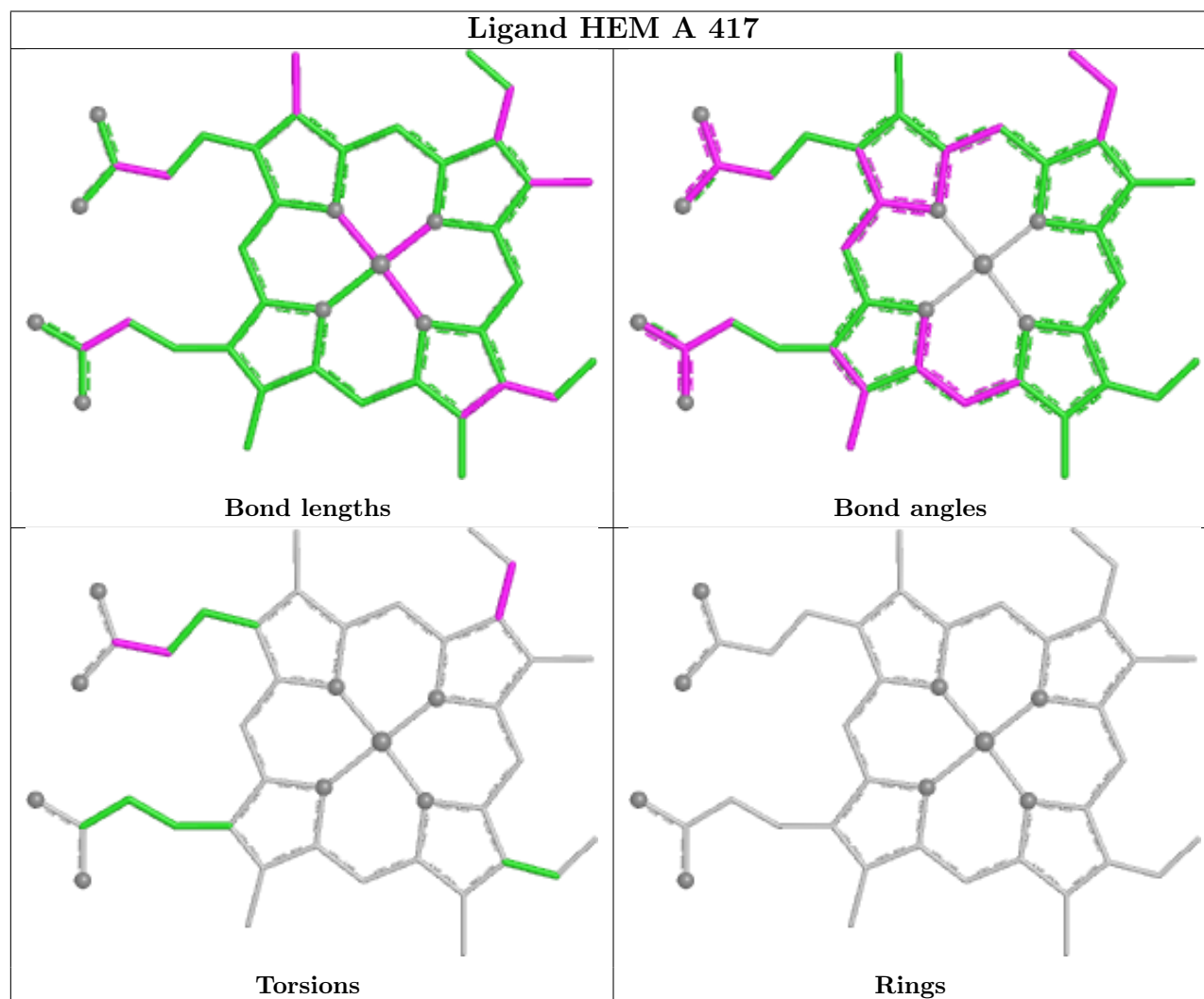
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	417	HEM	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.