



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:33 AM UTC

PDB ID : 1CP4 / pdb_00001cp4
Title : FORMATION, CRYSTAL STRUCTURE, AND REARRANGEMENT OF A
CYTOCHROME P450-CAM IRON-PHENYL COMPLEX
Authors : Raag, R.; Poulos, T.L.
Deposited on : 1991-06-04
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

<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

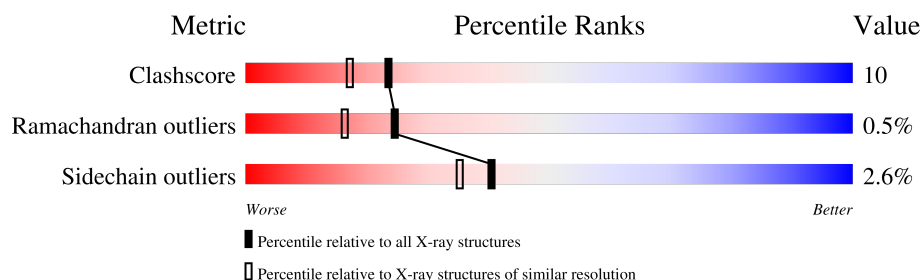
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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 ≥ 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	 57% 33% 7% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3467 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.

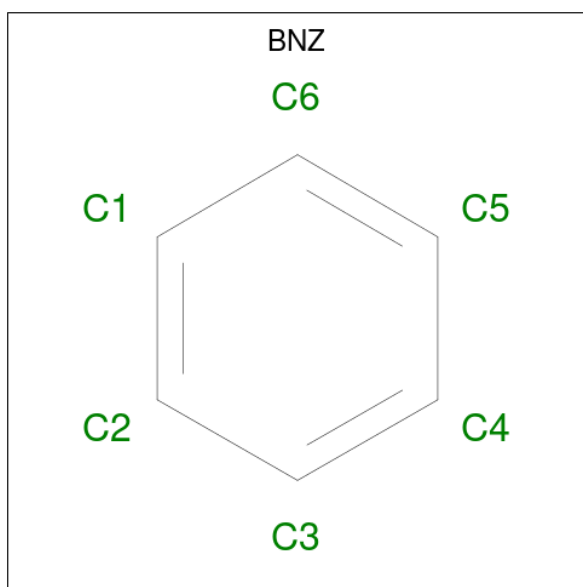
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	1	0
			3215	2037	563	597	18			

- 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 BENZENE (CCD ID: BNZ) (formula: C_6H_6).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	203	Total O 203 203	0	0

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}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3467	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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, BNZ

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	1.49	13/3298 (0.4%)	2.16	121/4479 (2.7%)

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	16

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	ILE	CA-CB	7.66	1.60	1.54
1	A	317	GLN	N-CA	7.56	1.54	1.45
1	A	281	ILE	CA-CB	6.87	1.57	1.54
1	A	99	ILE	CA-CB	6.17	1.62	1.54
1	A	211	ARG	NE-CZ	-5.97	1.26	1.33
1	A	398	GLY	CA-C	-5.87	1.46	1.52
1	A	149	ASN	C-O	5.77	1.31	1.24
1	A	312	LEU	N-CA	5.69	1.52	1.46
1	A	105	PRO	CA-CB	-5.69	1.48	1.53
1	A	66	THR	CA-CB	5.27	1.61	1.53
1	A	364	ARG	CZ-NH2	5.11	1.40	1.33
1	A	64	ILE	C-N	-5.10	1.26	1.33
1	A	41	ALA	C-O	5.00	1.29	1.24

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	26.34	161.28	124.40
1	A	195	GLU	CA-CB-CG	11.62	137.35	114.10
1	A	380	ASP	CA-CB-CG	10.78	123.38	112.60
1	A	64	ILE	CA-C-O	-10.60	109.76	120.25
1	A	149	ASN	CA-C-O	-9.99	106.22	120.51
1	A	188	ASP	CA-CB-CG	9.37	121.97	112.60
1	A	211	ARG	NE-CZ-NH2	9.28	127.55	119.20
1	A	279	GLU	CB-CG-CD	9.05	127.99	112.60
1	A	62	HIS	CA-CB-CG	8.86	122.66	113.80
1	A	241	MET	N-CA-CB	8.79	122.81	110.07
1	A	118	VAL	N-CA-C	8.41	120.17	111.00
1	A	32	SER	N-CA-C	7.54	119.28	111.14
1	A	49	ASN	CA-C-N	-7.51	115.17	123.43
1	A	49	ASN	C-N-CA	-7.51	115.17	123.43
1	A	72	ARG	CD-NE-CZ	7.46	134.85	124.40
1	A	316	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	32	SER	CA-C-O	-7.36	113.12	120.70
1	A	91	GLU	O-C-N	7.33	129.89	122.12
1	A	50	VAL	CB-CA-C	7.30	118.19	110.37
1	A	251	ASP	O-C-N	-7.28	112.89	122.42
1	A	33	ASN	CB-CA-C	7.27	124.89	110.42
1	A	108	GLN	CA-C-N	7.14	129.84	120.28
1	A	108	GLN	C-N-CA	7.14	129.84	120.28
1	A	33	ASN	CA-CB-CG	7.13	119.73	112.60
1	A	364	ARG	CD-NE-CZ	7.04	134.25	124.40
1	A	322	GLN	CB-CG-CD	7.00	124.49	112.60
1	A	80	HIS	CA-CB-CG	-6.93	106.87	113.80
1	A	40	GLU	CB-CG-CD	6.84	124.23	112.60
1	A	108	GLN	CB-CG-CD	6.83	124.21	112.60
1	A	357	CYS	N-CA-CB	6.70	119.94	109.69
1	A	209	GLU	CA-CB-CG	6.70	127.49	114.10
1	A	391	HIS	CA-CB-CG	6.68	120.48	113.80
1	A	365[A]	ARG	CA-C-N	6.64	129.18	120.28
1	A	365[A]	ARG	C-N-CA	6.64	129.18	120.28
1	A	365[B]	ARG	CA-C-N	6.64	129.18	120.28
1	A	365[B]	ARG	C-N-CA	6.64	129.18	120.28
1	A	254	VAL	N-CA-CB	-6.57	102.87	110.55
1	A	148	CYS	CA-C-N	6.53	134.00	121.54
1	A	148	CYS	C-N-CA	6.53	134.00	121.54
1	A	255	ASN	OD1-CG-ND2	6.50	129.10	122.60
1	A	282	PRO	CA-C-N	6.48	129.25	120.44
1	A	282	PRO	C-N-CA	6.48	129.25	120.44
1	A	209	GLU	CA-C-N	6.41	129.19	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	GLU	C-N-CA	6.41	129.19	120.54
1	A	303	SER	O-C-N	6.38	129.67	123.29
1	A	128	GLU	N-CA-CB	6.37	119.44	109.94
1	A	18	VAL	O-C-N	6.37	126.43	121.46
1	A	363	ALA	CA-C-N	6.32	128.75	120.28
1	A	363	ALA	C-N-CA	6.32	128.75	120.28
1	A	149	ASN	N-CA-CB	6.30	121.13	110.49
1	A	109	ARG	N-CA-C	6.20	118.03	111.28
1	A	129	ASN	CA-C-O	-6.18	114.00	120.55
1	A	295	VAL	O-C-N	6.16	129.46	122.93
1	A	251	ASP	N-CA-C	6.13	120.92	113.38
1	A	271	ARG	CD-NE-CZ	6.10	132.94	124.40
1	A	270	HIS	N-CA-CB	6.08	119.26	110.20
1	A	279	GLU	CA-CB-CG	6.07	126.25	114.10
1	A	277	ARG	CA-C-N	6.06	125.74	119.56
1	A	277	ARG	C-N-CA	6.06	125.74	119.56
1	A	164	MET	CA-C-N	6.05	128.30	120.44
1	A	164	MET	C-N-CA	6.05	128.30	120.44
1	A	322	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	210	GLN	CA-CB-CG	5.96	126.02	114.10
1	A	398	GLY	N-CA-C	5.95	119.99	111.12
1	A	287	GLU	O-C-N	-5.95	115.81	122.12
1	A	67	ARG	O-C-N	5.93	130.53	123.24
1	A	287	GLU	CA-C-O	5.92	126.83	120.55
1	A	76	GLU	CA-C-N	5.92	132.84	121.54
1	A	76	GLU	C-N-CA	5.92	132.84	121.54
1	A	156	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	407	ASP	CB-CA-C	5.91	116.02	110.17
1	A	188	ASP	N-CA-CB	-5.87	102.50	110.67
1	A	357	CYS	O-C-N	5.79	130.13	122.95
1	A	329	GLU	CB-CG-CD	5.77	122.42	112.60
1	A	105	PRO	N-CA-C	-5.75	104.95	110.47
1	A	357	CYS	CB-CA-C	-5.71	100.99	109.90
1	A	356	LEU	N-CA-CB	-5.71	100.15	109.56
1	A	328	ASP	CB-CA-C	5.70	118.80	110.26
1	A	153	ASP	N-CA-C	5.68	119.93	112.89
1	A	67	ARG	NE-CZ-NH2	-5.66	114.10	119.20
1	A	138	LEU	N-CA-CB	-5.66	101.80	110.12
1	A	62	HIS	CA-C-O	-5.66	115.18	121.23
1	A	20	GLU	CA-CB-CG	5.60	125.29	114.10
1	A	91	GLU	N-CA-CB	5.60	118.46	110.06
1	A	85	CYS	N-CA-CB	-5.58	104.17	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ARG	N-CA-C	-5.57	104.84	111.69
1	A	399	VAL	CA-C-N	5.57	127.68	120.44
1	A	399	VAL	C-N-CA	5.57	127.68	120.44
1	A	195	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	11	LEU	CB-CA-C	5.54	118.67	109.53
1	A	316	ASP	O-C-N	5.54	129.65	122.89
1	A	402	LEU	O-C-N	5.49	125.66	121.27
1	A	308	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	47	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	181	THR	CA-C-N	5.37	127.47	120.28
1	A	181	THR	C-N-CA	5.37	127.47	120.28
1	A	58	CYS	O-C-N	5.33	128.91	122.94
1	A	356	LEU	CB-CA-C	5.32	118.01	109.61
1	A	406	TRP	O-C-N	5.27	129.06	123.42
1	A	342	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	91	GLU	CB-CA-C	-5.23	101.79	110.68
1	A	149	ASN	CB-CA-C	5.20	120.77	110.42
1	A	195	GLU	CB-CA-C	-5.17	102.22	110.79
1	A	39	GLN	N-CA-CB	5.16	117.49	110.01
1	A	281	ILE	CA-C-N	5.15	124.33	118.97
1	A	281	ILE	C-N-CA	5.15	124.33	118.97
1	A	53	LEU	CA-C-N	5.15	128.30	122.48
1	A	53	LEU	C-N-CA	5.15	128.30	122.48
1	A	266	LYS	CG-CD-CE	5.14	123.13	111.30
1	A	299	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	A	251	ASP	CA-C-O	-5.11	113.33	119.15
1	A	316	ASP	CA-C-N	-5.09	113.98	122.64
1	A	316	ASP	C-N-CA	-5.09	113.98	122.64
1	A	373	GLU	CB-CG-CD	5.07	121.22	112.60
1	A	397	SER	O-C-N	5.06	128.73	123.06
1	A	71	ILE	CA-C-N	5.04	127.04	120.28
1	A	71	ILE	C-N-CA	5.04	127.04	120.28
1	A	169	LEU	O-C-N	5.02	126.44	121.57
1	A	251	ASP	CB-CA-C	5.01	118.38	109.65
1	A	286	GLU	CA-CB-CG	5.01	124.13	114.10
1	A	387	ALA	O-C-N	5.01	128.94	123.27

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	147	GLN	Mainchain
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	271	ARG	Sidechain
1	A	292	PHE	Mainchain
1	A	325	SER	Mainchain
1	A	365[A]	ARG	Sidechain
1	A	365[B]	ARG	Sidechain
1	A	375	LEU	Mainchain
1	A	377	ARG	Sidechain
1	A	72	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	3215	0	3166	65	0
2	A	43	0	30	2	0
3	A	6	0	5	1	0
4	A	203	0	0	3	0
All	All	3467	0	3201	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	1.64	0.78
1:A:49:ASN:HD22	1:A:49:ASN:H	1.43	0.67
1:A:191:MET:HE2	1:A:196:ALA:HA	1.77	0.64
1:A:160:ILE:O	1:A:164:MET:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.82	0.61
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.83	0.61
1:A:183:GLN:OE1	1:A:188:ASP:HB3	2.01	0.61
1:A:19:PRO:HG2	1:A:22:LEU:HD12	1.82	0.60
1:A:325:SER:O	1:A:331:GLU:HG3	2.02	0.59
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.03	0.58
1:A:319:LEU:O	1:A:321:PRO:HD3	2.04	0.58
1:A:17:HIS:CD2	1:A:313:LYS:HG3	2.40	0.56
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.05	0.56
1:A:181:THR:HG22	1:A:251:ASP:HB2	1.88	0.55
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.89	0.55
1:A:112:ARG:NH1	2:A:415:HEM:O1D	2.33	0.55
1:A:276:GLU:C	1:A:278:PRO:HD3	2.32	0.55
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.90	0.53
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.92	0.52
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.24	0.52
1:A:134:LEU:HD23	1:A:162:ILE:HG13	1.94	0.50
1:A:218:ASP:O	1:A:222:ILE:HG13	2.12	0.50
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.93	0.50
1:A:357:CYS:HB3	1:A:360:GLN:HB3	1.94	0.50
1:A:281:ILE:N	1:A:282:PRO:CD	2.75	0.49
1:A:40:GLU:HG3	1:A:336:MET:CE	2.43	0.49
1:A:149:ASN:ND2	1:A:402:LEU:H	2.10	0.49
1:A:319:LEU:C	1:A:321:PRO:HD3	2.39	0.48
1:A:30:ASN:ND2	4:A:555:HOH:O	2.44	0.47
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.44	0.47
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.95	0.47
1:A:149:ASN:C	1:A:149:ASN:HD22	2.22	0.47
1:A:49:ASN:H	1:A:49:ASN:ND2	2.13	0.46
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.46	0.46
1:A:90:ARG:O	1:A:94:GLU:HG3	2.16	0.46
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.81	0.46
1:A:193:PHE:HB3	4:A:690:HOH:O	2.15	0.45
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.98	0.45
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.87	0.45
1:A:41:ALA:O	1:A:44:VAL:HG22	2.17	0.44
1:A:149:ASN:ND2	1:A:149:ASN:C	2.75	0.44
1:A:39:GLN:NE2	1:A:39:GLN:H	2.16	0.44
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.53	0.44
1:A:121:MET:CB	1:A:122:PRO:HD3	2.47	0.44
1:A:201:TYR:OH	1:A:240:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:O	1:A:223:VAL:HG23	2.17	0.43
1:A:56:THR:O	1:A:61:GLY:HA2	2.18	0.43
1:A:97:ASP:O	1:A:240:ARG:HD2	2.19	0.43
1:A:181:THR:HG23	1:A:247:VAL:HG13	2.01	0.43
1:A:277:ARG:N	1:A:278:PRO:HD3	2.32	0.43
1:A:407:ASP:HA	1:A:408:PRO:HD3	1.87	0.42
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.89	0.42
1:A:127:LEU:CD1	1:A:166:LEU:HD13	2.50	0.42
1:A:322:GLN:HB3	1:A:348:THR:O	2.19	0.42
1:A:207:ILE:O	1:A:211:ARG:HD3	2.19	0.42
1:A:295:VAL:HG22	1:A:396:VAL:HG22	2.03	0.41
2:A:415:HEM:C1B	3:A:416:BNZ:H4	2.55	0.41
1:A:72:ARG:O	1:A:76:GLU:HG3	2.21	0.41
1:A:156:GLU:HB2	1:A:157:PRO:CD	2.51	0.41
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.50	0.41
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.48	0.40
1:A:184:MET:HE2	1:A:197:LYS:HA	2.03	0.40
1:A:261:MET:HE2	1:A:261:MET:HA	2.02	0.40
1:A:317:GLN:NE2	4:A:647:HOH:O	2.53	0.40
1:A:83:SER:HB3	1:A:101:THR:O	2.21	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	404/414 (98%)	386 (96%)	16 (4%)	2 (0%)	24 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	PHE

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Mol	Chain	Res	Type
1	A	120	GLY

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	351/358 (98%)	342 (97%)	9 (3%)	40	35

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	79	ARG
1	A	108	GLN
1	A	246	LEU
1	A	261	MET
1	A	272	GLN
1	A	276	GLU
1	A	357	CYS
1	A	400	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	110	GLN
1	A	129	ASN
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	176	HIS
1	A	225	ASN
1	A	311	GLN
1	A	317	GLN
1	A	388	GLN
1	A	390	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 oligosaccharides 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	415	1	50,50,50	1.56	12 (24%)	67,82,82	1.53	14 (20%)
3	BNZ	A	416	-	6,6,6	1.02	0	6,6,6	0.85	0

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	415	1	-	1/14/54/54	-
3	BNZ	A	416	-	-	-	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	FE-NB	3.26	2.04	1.94
2	A	415	HEM	C1C-NC	-3.18	1.33	1.39
2	A	415	HEM	FE-NA	3.11	2.05	1.95
2	A	415	HEM	CAC-C3C	3.05	1.55	1.47
2	A	415	HEM	FE-NC	2.95	2.04	1.95
2	A	415	HEM	CMD-C2D	2.69	1.56	1.50
2	A	415	HEM	CMB-C2B	2.55	1.56	1.50
2	A	415	HEM	C4A-C3A	2.39	1.48	1.43
2	A	415	HEM	C3C-C2C	-2.24	1.32	1.37
2	A	415	HEM	C1A-NA	-2.13	1.35	1.39
2	A	415	HEM	C3D-C2D	-2.05	1.32	1.36
2	A	415	HEM	CMA-C3A	2.01	1.54	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	HEM	CHB-C4A-NA	3.70	130.57	123.86
2	A	415	HEM	O2A-CGA-O1A	3.67	132.76	123.33
2	A	415	HEM	CMA-C3A-C4A	-3.54	120.02	125.42
2	A	415	HEM	C3B-C2B-C1B	3.29	108.89	106.41
2	A	415	HEM	CHD-C4C-NC	3.29	128.04	124.45
2	A	415	HEM	CMA-C3A-C2A	2.86	131.69	125.62
2	A	415	HEM	CAC-C3C-C4C	-2.35	119.20	124.82
2	A	415	HEM	C3A-C4A-NA	-2.27	106.50	110.14
2	A	415	HEM	C3D-C4D-ND	-2.23	107.73	110.17
2	A	415	HEM	O1A-CGA-CBA	-2.22	116.05	123.09
2	A	415	HEM	CHD-C1D-ND	-2.22	122.04	124.42
2	A	415	HEM	O1D-CGD-CBD	-2.15	116.29	123.09
2	A	415	HEM	C4C-NC-C1C	2.03	109.12	105.82
2	A	415	HEM	CHD-C1D-C2D	2.02	128.22	125.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

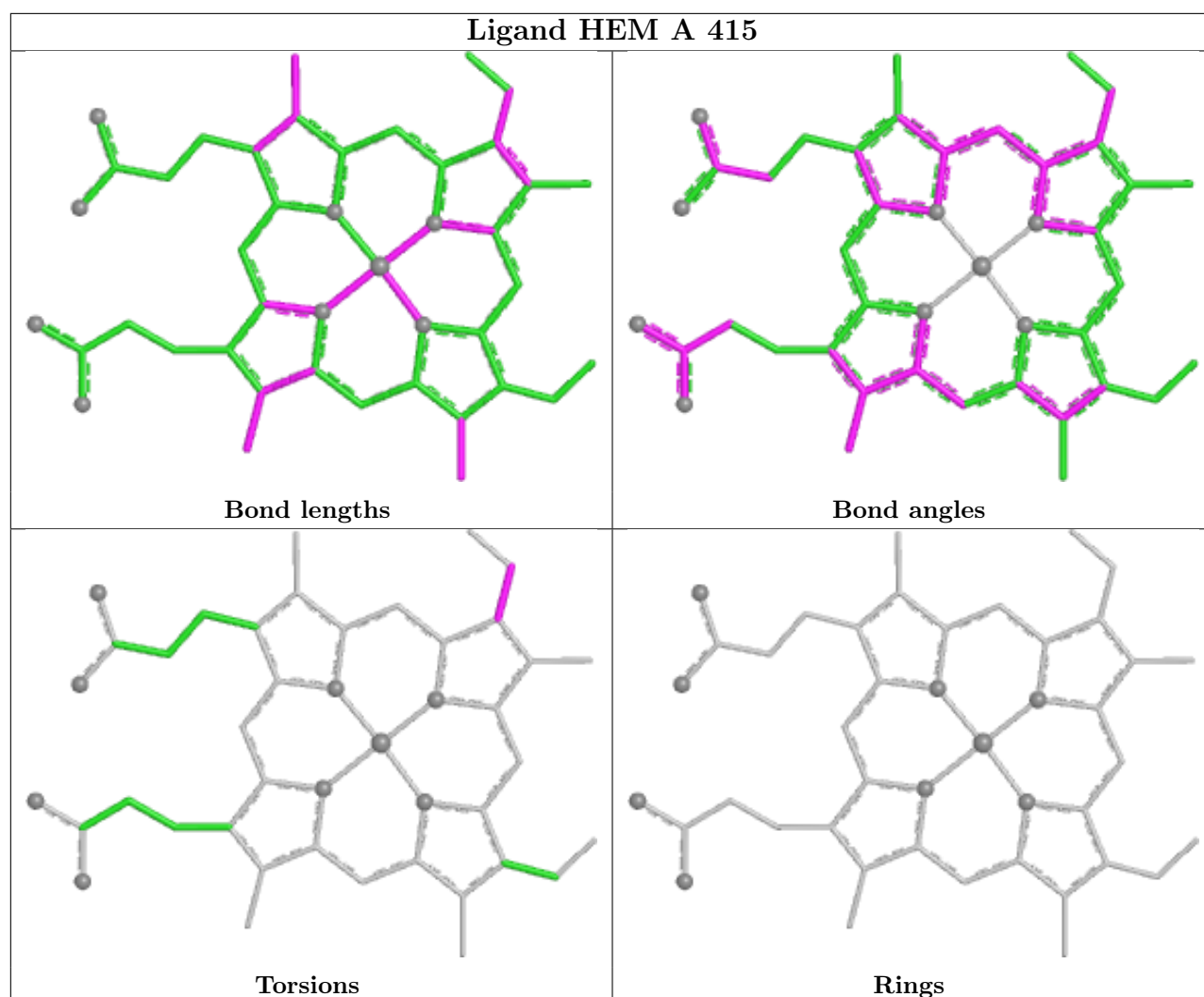
Mol	Chain	Res	Type	Atoms
2	A	415	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	HEM	2	0
3	A	416	BNZ	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.