



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:21 PM UTC

PDB ID : 4CP4 / pdb_00004cp4
Title : CRYSTAL STRUCTURE OF THE CYTOCHROME P450-CAM ACTIVE
SITE MUTANT THR252ALA
Authors : Raag, R.; Poulos, T.L.
Deposited on : 1991-06-04
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) : 2.49

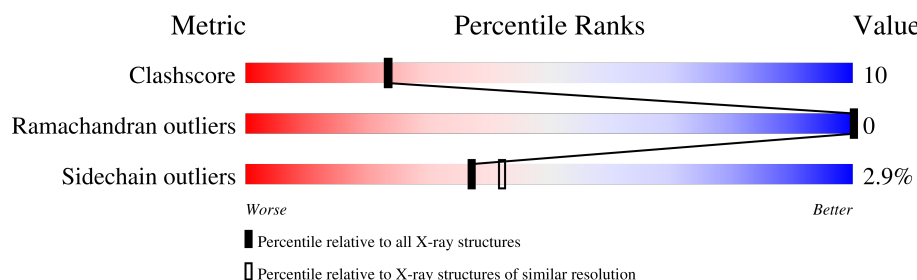
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	 48% 40% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3466 atoms, of which 0 are hydrogens and 0 are deuteriums.

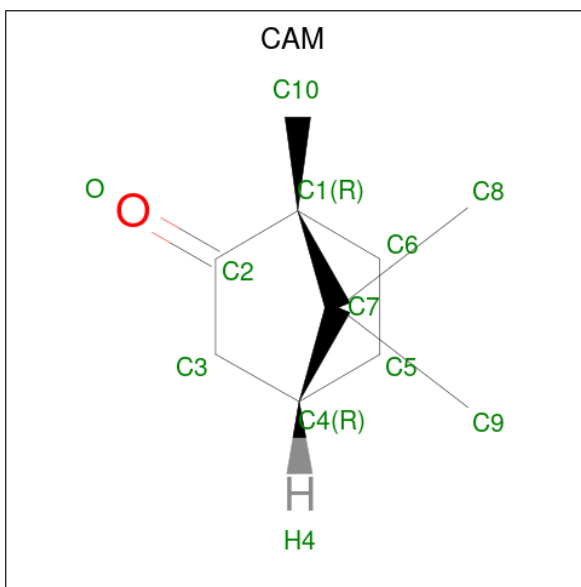
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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
			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
3	A	1	Total	C	O	0	0
			11	10	1		

- Molecule 4 is water.

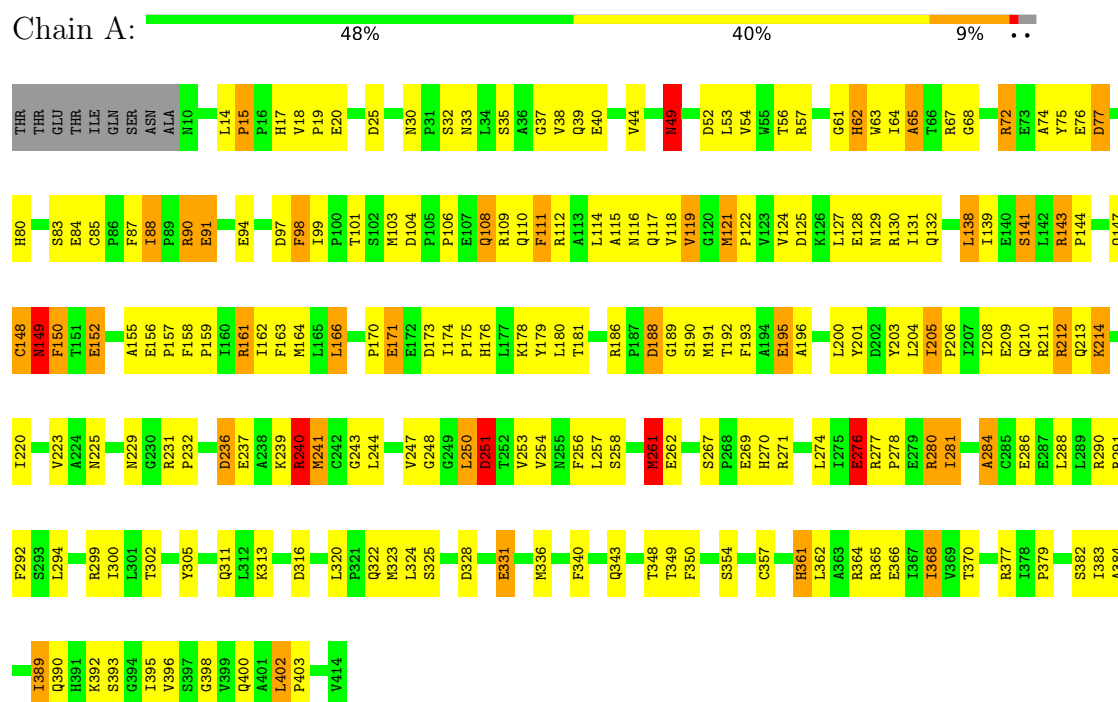
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		

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



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}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3466	wwPDB-VP
Average B, all atoms (Å ²)	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: 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	21/3287 (0.6%)	2.41	199/4465 (4.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	PHE	C-N	-10.74	1.25	1.33
1	A	211	ARG	NE-CZ	-7.48	1.24	1.33
1	A	370	THR	CA-CB	6.47	1.63	1.53
1	A	149	ASN	N-CA	-6.40	1.38	1.46
1	A	85	CYS	N-CA	6.12	1.53	1.46
1	A	251	ASP	C-O	5.97	1.32	1.23
1	A	138	LEU	N-CA	5.81	1.53	1.46
1	A	211	ARG	CD-NE	-5.76	1.38	1.46
1	A	290	ARG	CD-NE	-5.71	1.38	1.46
1	A	302	THR	CA-CB	5.50	1.62	1.53
1	A	389	ILE	C-O	5.46	1.30	1.24
1	A	74	ALA	C-N	-5.43	1.26	1.34
1	A	131	ILE	CA-CB	5.34	1.60	1.54
1	A	88	ILE	CA-C	5.32	1.56	1.52
1	A	63	TRP	C-N	-5.22	1.26	1.33
1	A	65	ALA	C-O	5.22	1.30	1.24
1	A	403	PRO	CA-CB	5.21	1.60	1.53
1	A	176	HIS	CE1-NE2	5.13	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	GLN	N-CA	5.04	1.52	1.46
1	A	132	GLN	N-CA	5.02	1.52	1.46
1	A	257	LEU	C-O	5.02	1.29	1.24

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	29.60	165.84	124.40
1	A	212	ARG	CD-NE-CZ	14.02	144.03	124.40
1	A	214	LYS	CB-CA-C	13.00	136.25	111.29
1	A	148	CYS	CA-C-N	11.80	144.07	121.54
1	A	148	CYS	C-N-CA	11.80	144.07	121.54
1	A	20	GLU	CA-CB-CG	10.06	134.21	114.10
1	A	67	ARG	NE-CZ-NH2	-10.04	110.16	119.20
1	A	364	ARG	CD-NE-CZ	9.87	138.22	124.40
1	A	195	GLU	CA-CB-CG	9.61	133.32	114.10
1	A	118	VAL	N-CA-C	9.38	121.23	111.00
1	A	98	PHE	CA-CB-CG	9.01	122.81	113.80
1	A	225	ASN	CA-CB-CG	8.82	121.42	112.60
1	A	193	PHE	O-C-N	8.39	130.72	122.07
1	A	87	PHE	CA-C-N	8.38	130.62	123.33
1	A	87	PHE	C-N-CA	8.38	130.62	123.33
1	A	209	GLU	CA-C-N	8.27	131.36	120.28
1	A	209	GLU	C-N-CA	8.27	131.36	120.28
1	A	128	GLU	N-CA-CB	8.13	122.05	109.94
1	A	286	GLU	N-CA-CB	8.12	122.18	110.16
1	A	104	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	209	GLU	CA-CB-CG	8.00	130.11	114.10
1	A	106	PRO	CA-C-N	7.96	130.95	120.28
1	A	106	PRO	C-N-CA	7.96	130.95	120.28
1	A	87	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	256	PHE	CA-C-N	7.88	130.83	120.28
1	A	256	PHE	C-N-CA	7.88	130.83	120.28
1	A	271	ARG	CD-NE-CZ	7.83	135.37	124.40
1	A	91	GLU	CB-CA-C	-7.82	97.81	110.79
1	A	366	GLU	CB-CG-CD	7.70	125.70	112.60
1	A	53	LEU	CA-C-O	-7.65	112.07	120.33
1	A	32	SER	N-CA-C	7.60	119.20	111.07
1	A	149	ASN	N-CA-CB	7.60	123.34	110.49
1	A	211	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	A	392	LYS	CA-CB-CG	7.45	129.00	114.10
1	A	74	ALA	CB-CA-C	7.42	123.12	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	348	THR	CA-CB-CG2	7.24	122.80	110.50
1	A	132	GLN	N-CA-CB	-7.23	99.50	110.12
1	A	33	ASN	OD1-CG-ND2	7.09	129.69	122.60
1	A	270	HIS	CA-CB-CG	-7.06	106.74	113.80
1	A	30	ASN	OD1-CG-ND2	-7.04	115.56	122.60
1	A	125	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	76	GLU	CB-CG-CD	6.89	124.32	112.60
1	A	189	GLY	N-CA-C	-6.86	105.04	114.64
1	A	206	PRO	CA-C-N	6.80	129.68	120.77
1	A	206	PRO	C-N-CA	6.80	129.68	120.77
1	A	349	THR	CA-CB-CG2	6.80	122.06	110.50
1	A	340	PHE	CA-CB-CG	6.78	120.58	113.80
1	A	305	TYR	O-C-N	6.77	131.20	123.48
1	A	248	GLY	CA-C-N	6.76	127.45	119.94
1	A	248	GLY	C-N-CA	6.76	127.45	119.94
1	A	67	ARG	NE-CZ-NH1	6.76	128.26	121.50
1	A	52	ASP	O-C-N	6.74	129.84	122.15
1	A	130	ARG	N-CA-CB	6.74	120.14	110.16
1	A	74	ALA	CA-C-N	6.73	129.97	120.28
1	A	74	ALA	C-N-CA	6.73	129.97	120.28
1	A	84	GLU	CA-CB-CG	6.69	127.48	114.10
1	A	396	VAL	CA-C-O	-6.68	113.53	120.27
1	A	138	LEU	CB-CA-C	6.66	122.17	110.85
1	A	251	ASP	O-C-N	-6.66	114.02	122.34
1	A	324	LEU	CA-C-O	-6.63	113.39	120.42
1	A	379	PRO	CA-C-N	6.63	132.75	123.07
1	A	379	PRO	C-N-CA	6.63	132.75	123.07
1	A	33	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	220	ILE	CB-CA-C	6.60	121.32	112.22
1	A	299	ARG	CD-NE-CZ	6.60	133.64	124.40
1	A	236	ASP	CA-C-N	6.59	129.11	120.28
1	A	236	ASP	C-N-CA	6.59	129.11	120.28
1	A	64	ILE	CA-C-O	-6.53	113.31	120.43
1	A	270	HIS	N-CA-CB	6.47	119.74	110.16
1	A	188	ASP	N-CA-CB	-6.45	100.59	110.20
1	A	186	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	A	195	GLU	CB-CG-CD	6.43	123.53	112.60
1	A	383	ILE	O-C-N	6.41	130.28	122.72
1	A	281	ILE	CA-C-N	6.39	125.96	119.19
1	A	281	ILE	C-N-CA	6.39	125.96	119.19
1	A	115	ALA	CA-C-O	6.38	127.31	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	TYR	CA-C-O	-6.38	113.66	120.42
1	A	19	PRO	CB-CA-C	6.30	119.08	111.46
1	A	237	GLU	O-C-N	6.30	128.79	122.12
1	A	288	LEU	CA-C-O	-6.29	113.76	120.42
1	A	132	GLN	CA-C-N	6.28	128.60	120.44
1	A	132	GLN	C-N-CA	6.28	128.60	120.44
1	A	276	GLU	N-CA-CB	6.26	119.94	110.30
1	A	292	PHE	CA-C-N	6.26	129.59	120.71
1	A	292	PHE	C-N-CA	6.26	129.59	120.71
1	A	143	ARG	CA-C-N	6.23	126.35	119.87
1	A	143	ARG	C-N-CA	6.23	126.35	119.87
1	A	393	SER	N-CA-C	6.13	119.70	109.95
1	A	243	GLY	N-CA-C	-6.13	105.39	112.50
1	A	20	GLU	CB-CG-CD	6.12	123.01	112.60
1	A	112	ARG	CA-C-N	6.11	128.75	120.38
1	A	112	ARG	C-N-CA	6.11	128.75	120.38
1	A	116	ASN	CA-CB-CG	-6.08	106.52	112.60
1	A	201	TYR	N-CA-CB	6.07	119.14	110.16
1	A	129	ASN	CA-C-O	-6.06	113.25	120.10
1	A	210	GLN	CA-CB-CG	6.02	126.15	114.10
1	A	150	PHE	CA-CB-CG	-6.00	107.80	113.80
1	A	30	ASN	CB-CG-ND2	5.97	125.35	116.40
1	A	35	SER	CA-C-N	5.96	130.67	120.72
1	A	35	SER	C-N-CA	5.96	130.67	120.72
1	A	400	GLN	CA-CB-CG	5.96	126.02	114.10
1	A	179	TYR	O-C-N	5.92	128.49	122.09
1	A	241	MET	CB-CA-C	-5.89	101.59	110.90
1	A	300	ILE	O-C-N	5.87	129.38	123.10
1	A	240	ARG	CA-C-O	-5.82	113.53	120.10
1	A	163	PHE	CA-C-O	-5.80	114.27	120.42
1	A	30	ASN	O-C-N	5.79	127.98	121.32
1	A	77	ASP	CA-C-N	5.79	128.83	120.38
1	A	77	ASP	C-N-CA	5.79	128.83	120.38
1	A	280	ARG	CD-NE-CZ	5.77	132.47	124.40
1	A	139	ILE	O-C-N	5.76	127.89	121.90
1	A	65	ALA	CB-CA-C	5.74	119.20	109.80
1	A	316	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	250	LEU	N-CA-C	5.70	118.70	111.69
1	A	109	ARG	N-CA-C	5.68	117.15	111.07
1	A	251	ASP	CA-C-O	-5.65	112.74	119.35
1	A	152	GLU	N-CA-CB	5.65	118.61	110.20
1	A	44	VAL	CB-CA-C	-5.64	103.41	112.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	CB-CA-C	5.64	120.16	110.79
1	A	251	ASP	CB-CA-C	5.61	119.45	110.09
1	A	62	HIS	CA-CB-CG	5.59	119.39	113.80
1	A	395	ILE	N-CA-C	-5.57	104.94	110.62
1	A	277	ARG	CA-C-N	5.55	125.22	119.56
1	A	277	ARG	C-N-CA	5.55	125.22	119.56
1	A	44	VAL	N-CA-CB	5.53	120.10	110.65
1	A	284	ALA	O-C-N	5.50	127.95	122.12
1	A	390	GLN	CB-CG-CD	-5.49	103.26	112.60
1	A	193	PHE	N-CA-C	-5.49	105.20	111.07
1	A	77	ASP	CA-C-O	-5.48	112.67	120.51
1	A	111	PHE	CB-CA-C	5.46	120.14	110.85
1	A	121	MET	CA-C-N	5.46	125.54	119.32
1	A	121	MET	C-N-CA	5.46	125.54	119.32
1	A	290	ARG	CA-C-O	-5.46	115.28	120.90
1	A	72	ARG	NH1-CZ-NH2	5.45	126.39	119.30
1	A	402	LEU	O-C-N	5.43	125.36	121.12
1	A	253	VAL	O-C-N	5.42	127.34	121.87
1	A	261	MET	CA-CB-CG	-5.41	103.28	114.10
1	A	258	SER	CB-CA-C	5.38	120.00	110.85
1	A	162	ILE	CB-CG1-CD1	-5.38	102.50	113.80
1	A	76	GLU	N-CA-CB	5.38	118.28	110.26
1	A	180	LEU	CB-CA-C	5.38	119.71	110.79
1	A	400	GLN	CB-CA-C	5.38	119.32	110.88
1	A	85	CYS	CA-C-O	5.37	127.45	121.22
1	A	156	GLU	CA-CB-CG	5.37	124.83	114.10
1	A	323	MET	N-CA-CB	-5.36	102.24	110.12
1	A	15	PRO	N-CA-C	-5.36	104.16	110.70
1	A	201	TYR	O-C-N	5.36	128.25	122.15
1	A	212	ARG	N-CA-C	-5.36	104.33	112.04
1	A	171	GLU	CA-C-N	5.35	127.99	120.28
1	A	171	GLU	C-N-CA	5.35	127.99	120.28
1	A	49	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	141	SER	CB-CA-C	5.32	120.89	110.67
1	A	75	TYR	N-CA-CB	5.30	118.38	110.22
1	A	262	GLU	O-C-N	5.28	127.79	122.09
1	A	178	LYS	CB-CA-C	5.28	120.81	110.67
1	A	398	GLY	CA-C-N	5.25	130.02	123.14
1	A	398	GLY	C-N-CA	5.25	130.02	123.14
1	A	223	VAL	N-CA-CB	5.25	116.69	110.55
1	A	119	VAL	N-CA-C	5.24	119.55	113.42
1	A	368	ILE	CA-C-O	-5.24	115.50	120.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	GLU	CA-C-N	5.23	127.24	120.44
1	A	286	GLU	C-N-CA	5.23	127.24	120.44
1	A	205	ILE	CA-C-N	5.22	124.40	118.97
1	A	205	ILE	C-N-CA	5.22	124.40	118.97
1	A	251	ASP	N-CA-C	5.22	119.75	113.17
1	A	311	GLN	CB-CA-C	5.21	118.93	110.22
1	A	213	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	400	GLN	CG-CD-NE2	-5.21	108.58	116.40
1	A	90	ARG	CD-NE-CZ	5.21	131.69	124.40
1	A	362	LEU	O-C-N	-5.21	116.71	122.07
1	A	74	ALA	N-CA-C	-5.20	105.61	111.28
1	A	37	GLY	O-C-N	5.18	129.43	122.70
1	A	322	GLN	CB-CG-CD	5.17	121.40	112.60
1	A	384	ALA	O-C-N	5.17	126.63	121.30
1	A	390	GLN	OE1-CD-NE2	5.17	127.77	122.60
1	A	166	LEU	CB-CA-C	5.14	118.95	110.88
1	A	25	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	163	PHE	N-CA-CB	5.13	117.75	110.16
1	A	178	LYS	CA-C-O	5.13	125.87	119.97
1	A	261	MET	CA-C-O	5.12	125.86	119.97
1	A	38	VAL	CA-CB-CG2	5.12	119.10	110.40
1	A	188	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	33	ASN	N-CA-CB	-5.11	101.85	110.49
1	A	267	SER	CA-CB-OG	-5.11	100.89	111.10
1	A	361	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	214	LYS	CA-C-N	5.10	125.03	119.78
1	A	214	LYS	C-N-CA	5.10	125.03	119.78
1	A	164	MET	N-CA-CB	5.10	117.61	110.12
1	A	324	LEU	N-CA-C	5.10	116.92	111.36
1	A	150	PHE	O-C-N	5.09	129.36	122.59
1	A	85	CYS	N-CA-CB	-5.09	104.78	111.09
1	A	124	VAL	O-C-N	5.09	126.81	121.87
1	A	54	VAL	CA-C-O	-5.07	116.30	121.67
1	A	343	GLN	O-C-N	5.06	127.48	122.12
1	A	80	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	143	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	A	204	LEU	N-CA-C	5.05	116.78	111.28
1	A	150	PHE	CA-C-O	-5.04	113.31	120.51

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	VAL	Mainchain
1	A	147	GLN	Mainchain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	161	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	280	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	77	ASP	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3208	0	3156	63	0
2	A	43	0	30	3	0
3	A	11	0	16	1	0
4	A	204	0	0	8	0
All	All	3466	0	3202	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:127:LEU:HD11	1:A:166:LEU:HD13	1.59	0.81
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.74	0.69
1:A:208:ILE:O	1:A:212:ARG:HG3	1.94	0.67
1:A:328:ASP:HB3	1:A:331:GLU:HG3	1.79	0.65
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.80	0.63
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.81	0.61
2:A:415:HEM:HBB2	2:A:415:HEM:HMB2	1.84	0.58
1:A:68:GLY:O	1:A:72:ARG:HG3	2.02	0.58
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:ND2	1:A:402:LEU:H	2.02	0.57
1:A:281:ILE:HG22	1:A:368:ILE:HG23	1.87	0.56
1:A:188:ASP:HB3	1:A:190:SER:H	1.72	0.55
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.37	0.54
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.89	0.54
1:A:149:ASN:HD21	1:A:402:LEU:H	1.54	0.54
1:A:254:VAL:HG23	4:A:687:HOH:O	2.07	0.54
1:A:281:ILE:CG2	1:A:368:ILE:HG23	2.37	0.53
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.07	0.53
2:A:415:HEM:C1A	3:A:416:CAM:H4	2.43	0.53
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.24	0.53
1:A:181:THR:HG22	1:A:251:ASP:HB2	1.90	0.53
1:A:49:ASN:HD22	1:A:49:ASN:H	1.57	0.53
1:A:389:ILE:HA	4:A:659:HOH:O	2.09	0.52
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.09	0.52
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.74	0.52
1:A:150:PHE:CE2	1:A:155:ALA:HB2	2.45	0.51
1:A:200:LEU:O	1:A:203:TYR:HB3	2.11	0.50
1:A:91:GLU:H	1:A:91:GLU:CD	2.20	0.50
1:A:99:ILE:HG12	1:A:103:MET:HE3	1.94	0.49
1:A:274:LEU:HD21	1:A:284:ALA:HB2	1.94	0.49
1:A:291:ARG:CZ	1:A:336:MET:HE3	2.43	0.48
1:A:294:LEU:HD23	1:A:294:LEU:N	2.28	0.48
1:A:361:HIS:HB2	4:A:560:HOH:O	2.12	0.48
1:A:97:ASP:O	1:A:240:ARG:HD2	2.13	0.48
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.42	0.47
1:A:56:THR:HG21	1:A:62:HIS:CE1	2.49	0.47
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.97	0.46
1:A:269:GLU:CD	1:A:269:GLU:H	2.23	0.46
1:A:205:ILE:HD11	1:A:239:LYS:HD2	1.95	0.46
1:A:14:LEU:HA	1:A:15:PRO:HD3	1.82	0.46
1:A:152:GLU:HB3	4:A:563:HOH:O	2.15	0.46
1:A:56:THR:O	1:A:61:GLY:HA2	2.16	0.46
1:A:382:SER:HB2	4:A:608:HOH:O	2.16	0.45
1:A:65:ALA:HB3	1:A:320:LEU:HD23	1.97	0.45
1:A:17:HIS:CD2	1:A:313:LYS:HG3	2.52	0.45
1:A:161:ARG:HD3	1:A:171:GLU:OE2	2.16	0.45
1:A:138:LEU:HD21	1:A:157:PRO:HB2	1.99	0.45
1:A:57:ARG:HG2	4:A:508:HOH:O	2.16	0.45
1:A:236:ASP:O	1:A:240:ARG:HG3	2.16	0.45
1:A:191:MET:HE2	1:A:196:ALA:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLN:CD	1:A:229:ASN:H	2.25	0.44
1:A:181:THR:HG23	1:A:247:VAL:HG13	1.98	0.44
1:A:276:GLU:C	1:A:278:PRO:HD3	2.43	0.44
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.99	0.44
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.98	0.44
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.99	0.44
1:A:114:LEU:O	1:A:117:GLN:HB2	2.18	0.44
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.49	0.43
1:A:261:MET:HA	1:A:261:MET:HE2	2.00	0.43
1:A:328:ASP:HB3	1:A:331:GLU:CG	2.46	0.42
2:A:415:HEM:HBB2	2:A:415:HEM:CMB	2.50	0.42
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.49	0.42
1:A:294:LEU:HD23	1:A:294:LEU:H	1.85	0.42
1:A:101:THR:HB	4:A:652:HOH:O	2.20	0.41
1:A:90:ARG:O	1:A:94:GLU:HG3	2.21	0.41
1:A:122:PRO:HD2	4:A:701:HOH:O	2.20	0.41

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%)	388 (96%)	15 (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%)	340 (97%)	10 (3%)	37	42

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	ASN
1	A	83	SER
1	A	108	GLN
1	A	141	SER
1	A	214	LYS
1	A	261	MET
1	A	276	GLU
1	A	325	SER
1	A	331	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	110	GLN
1	A	117	GLN
1	A	149	ASN
1	A	213	GLN
1	A	225	ASN
1	A	311	GLN
1	A	361	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	$\# Z > 2$
2	HEM	A	415	1	50,50,50	1.38	8 (16%)	67,82,82	1.19	6 (8%)
3	CAM	A	416	-	12,12,12	1.92	2 (16%)	20,21,21	1.78	3 (15%)

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	-	4/14/54/54	-
3	CAM	A	416	-	-	-	0/3/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	416	CAM	C1-C2	5.21	1.59	1.52
2	A	415	HEM	CAC-C3C	3.20	1.55	1.47
2	A	415	HEM	FE-NC	3.05	2.05	1.95
2	A	415	HEM	FE-NA	2.95	2.04	1.95
3	A	416	CAM	C3-C2	2.66	1.58	1.51
2	A	415	HEM	C4A-NA	-2.39	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	C2A-C3A	-2.23	1.33	1.38
2	A	415	HEM	CMB-C2B	2.19	1.55	1.50
2	A	415	HEM	CMD-C2D	2.15	1.55	1.50
2	A	415	HEM	FE-NB	2.09	2.01	1.94

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	416	CAM	C9-C7-C8	-5.51	93.73	107.67
3	A	416	CAM	C8-C7-C1	3.11	119.98	113.05
2	A	415	HEM	CMA-C3A-C4A	-3.03	120.80	125.42
2	A	415	HEM	CBD-CAD-C3D	2.96	120.70	112.53
2	A	415	HEM	C2A-C1A-NA	-2.78	107.07	110.15
2	A	415	HEM	CMA-C3A-C2A	2.53	130.99	125.62
3	A	416	CAM	C9-C7-C4	2.41	119.27	113.44
2	A	415	HEM	CHC-C4B-NB	-2.40	121.84	124.42
2	A	415	HEM	O2A-CGA-O1A	2.37	129.42	123.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	415	HEM	C2C-C3C-CAC-CBC
2	A	415	HEM	C4C-C3C-CAC-CBC
2	A	415	HEM	CAD-CBD-CGD-O1D
2	A	415	HEM	CAD-CBD-CGD-O2D

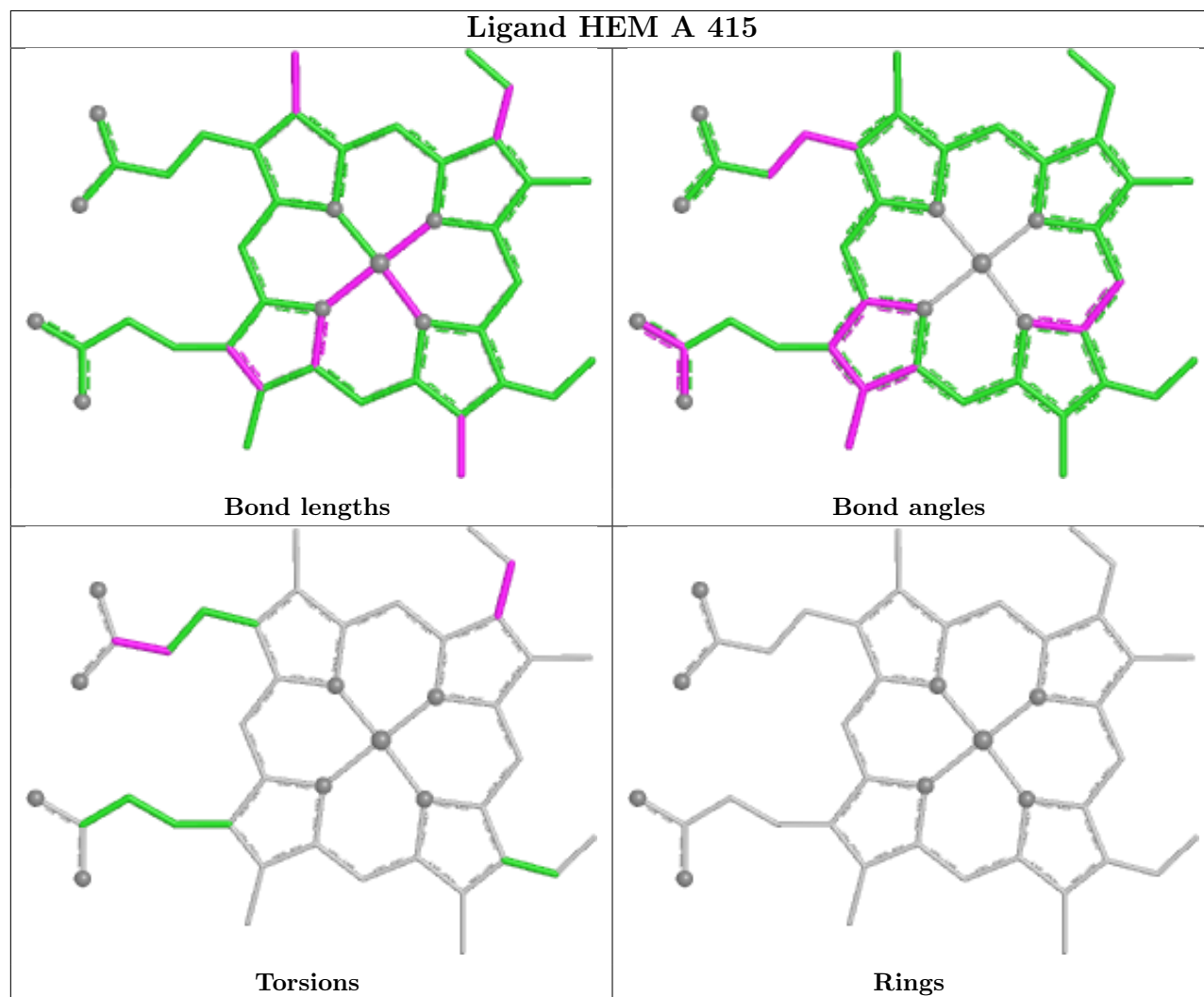
There are no ring outliers.

2 monomers are involved in 3 short contacts:

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