



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 2CP4 / pdb_00002cp4
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

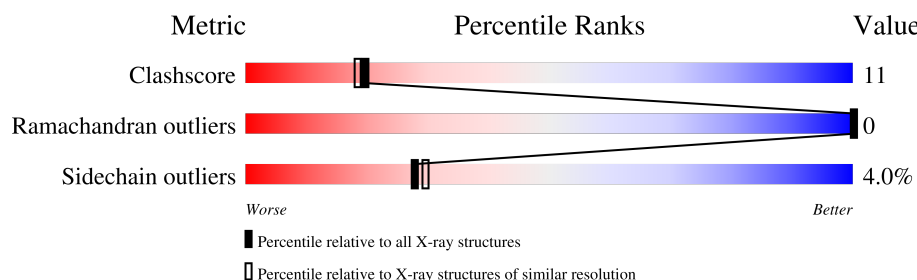
1 Overall quality at a glance

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3519 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
			Total	C	N	O	S			
1	A	405	3233	2054	561	600	18	0	7	0

There is a discrepancy between the modelled and reference sequences:

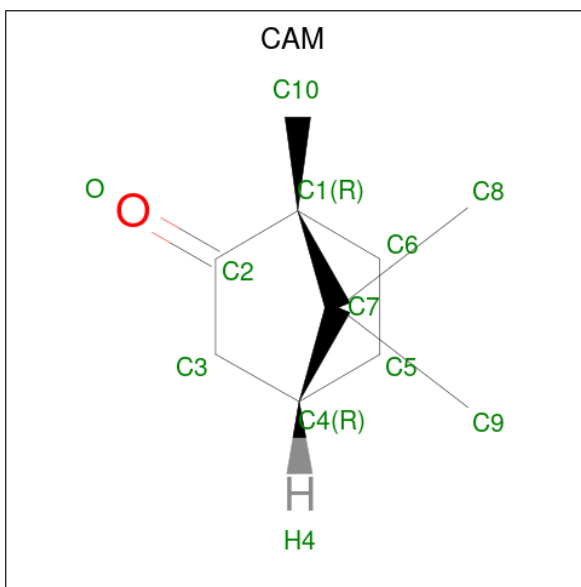
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	THR	conflict	UNP P00183

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



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

- 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.

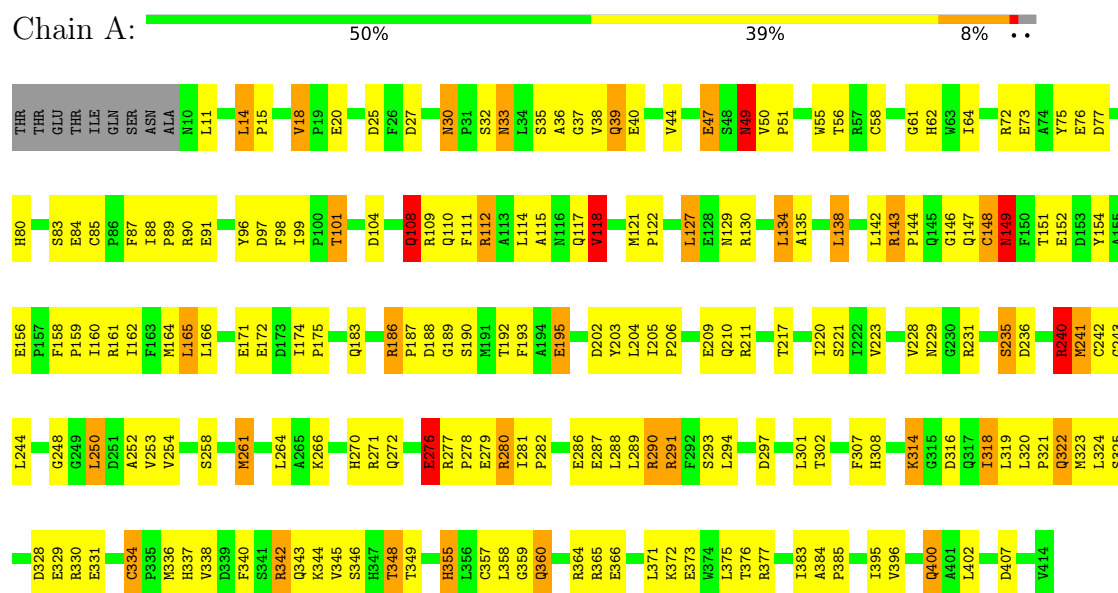
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		

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}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3519	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: 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	1.44	12/3340 (0.4%)	2.34	191/4538 (4.2%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	GLY	N-CA	7.78	1.54	1.45
1	A	33	ASN	N-CA	6.96	1.55	1.46
1	A	277	ARG	N-CA	5.96	1.53	1.46
1	A	87	PHE	C-N	-5.82	1.29	1.33
1	A	301	LEU	N-CA	5.81	1.53	1.46
1	A	355	HIS	ND1-CE1	-5.81	1.26	1.32
1	A	127	LEU	C-N	-5.55	1.26	1.33
1	A	149	ASN	N-CA	-5.45	1.39	1.46
1	A	291	ARG	NE-CZ	-5.36	1.27	1.33
1	A	211	ARG	NE-CZ	-5.35	1.27	1.33
1	A	88	ILE	CA-CB	5.30	1.58	1.54
1	A	252	ALA	C-N	-5.05	1.27	1.33

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	21.08	153.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	GLN	CA-CB-CG	12.36	138.81	114.10
1	A	148	CYS	CA-C-N	12.34	145.10	121.54
1	A	148	CYS	C-N-CA	12.34	145.10	121.54
1	A	33	ASN	CB-CA-C	11.32	127.25	111.74
1	A	365	ARG	CD-NE-CZ	10.86	139.60	124.40
1	A	290	ARG	CD-NE-CZ	10.83	139.56	124.40
1	A	279	GLU	CA-CB-CG	9.62	133.35	114.10
1	A	330	ARG	CD-NE-CZ	9.29	137.40	124.40
1	A	279	GLU	CB-CG-CD	9.12	128.10	112.60
1	A	118	VAL	N-CA-C	8.65	120.43	111.00
1	A	211	ARG	NE-CZ-NH2	8.58	126.92	119.20
1	A	329	GLU	CB-CG-CD	8.49	127.04	112.60
1	A	87	PHE	CA-C-N	8.42	130.66	123.33
1	A	87	PHE	C-N-CA	8.42	130.66	123.33
1	A	365	ARG	CA-C-N	8.28	132.04	120.29
1	A	365	ARG	C-N-CA	8.28	132.04	120.29
1	A	242	CYS	CA-C-N	8.21	129.09	119.98
1	A	242	CYS	C-N-CA	8.21	129.09	119.98
1	A	209	GLU	CA-C-N	8.15	132.70	120.31
1	A	209	GLU	C-N-CA	8.15	132.70	120.31
1	A	76	GLU	CB-CG-CD	7.98	126.16	112.60
1	A	271	ARG	CD-NE-CZ	7.90	135.46	124.40
1	A	40	GLU	CB-CG-CD	7.81	125.88	112.60
1	A	248	GLY	CA-C-N	7.80	128.58	120.00
1	A	248	GLY	C-N-CA	7.80	128.58	120.00
1	A	32	SER	N-CA-C	7.58	119.45	111.03
1	A	297	ASP	CA-CB-CG	7.58	120.18	112.60
1	A	250	LEU	N-CA-C	7.52	122.76	112.90
1	A	322	GLN	CA-C-N	7.39	130.19	120.28
1	A	322	GLN	C-N-CA	7.39	130.19	120.28
1	A	314	LYS	CA-C-O	-7.39	112.90	120.96
1	A	360	GLN	CA-C-N	7.31	130.68	120.29
1	A	360	GLN	C-N-CA	7.31	130.68	120.29
1	A	336	MET	CA-C-N	7.28	131.91	121.50
1	A	336	MET	C-N-CA	7.28	131.91	121.50
1	A	75	TYR	CA-C-N	7.25	132.98	120.58
1	A	75	TYR	C-N-CA	7.25	132.98	120.58
1	A	204	LEU	N-CA-C	7.24	118.81	111.07
1	A	85	CYS	N-CA-CB	-7.23	100.58	111.21
1	A	407	ASP	CB-CA-C	7.06	119.55	109.38
1	A	282	PRO	CA-C-N	7.04	129.59	120.44
1	A	282	PRO	C-N-CA	7.04	129.59	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	LEU	CB-CA-C	7.01	121.10	109.53
1	A	27	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	87	PHE	CA-CB-CG	6.72	120.52	113.80
1	A	316	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	109	ARG	N-CA-C	6.68	119.40	111.71
1	A	32	SER	CA-C-N	-6.66	112.52	122.24
1	A	32	SER	C-N-CA	-6.66	112.52	122.24
1	A	252	ALA	N-CA-C	6.64	118.31	111.14
1	A	49	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	395	ILE	O-C-N	6.60	128.27	121.87
1	A	328	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	115	ALA	CA-C-N	6.56	130.28	120.31
1	A	115	ALA	C-N-CA	6.56	130.28	120.31
1	A	400	GLN	CA-CB-CG	6.54	127.18	114.10
1	A	235	SER	CA-C-N	6.47	129.24	120.44
1	A	235	SER	C-N-CA	6.47	129.24	120.44
1	A	366	GLU	CA-C-N	6.46	128.83	120.56
1	A	366	GLU	C-N-CA	6.46	128.83	120.56
1	A	172[A]	GLU	CB-CG-CD	6.42	123.52	112.60
1	A	172[B]	GLU	CB-CG-CD	6.42	123.52	112.60
1	A	203	TYR	CA-C-N	6.39	128.74	120.44
1	A	203	TYR	C-N-CA	6.39	128.74	120.44
1	A	240	ARG	CA-C-O	-6.35	113.69	120.42
1	A	270	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	88	ILE	CA-C-O	-6.32	115.59	119.51
1	A	307	PHE	CA-CB-CG	6.28	120.08	113.80
1	A	55	TRP	O-C-N	6.25	130.74	123.30
1	A	187	PRO	CA-C-N	6.25	131.26	120.58
1	A	187	PRO	C-N-CA	6.25	131.26	120.58
1	A	14	LEU	O-C-N	6.22	126.72	121.31
1	A	195	GLU	CA-CB-CG	6.21	126.52	114.10
1	A	149	ASN	N-CA-CB	6.17	120.92	110.49
1	A	15	PRO	N-CA-C	-6.17	103.18	110.70
1	A	149	ASN	O-C-N	-6.16	114.40	122.59
1	A	349	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	189	GLY	N-CA-C	-6.08	106.25	115.00
1	A	118	VAL	CA-C-N	6.06	129.06	121.85
1	A	118	VAL	C-N-CA	6.06	129.06	121.85
1	A	18	VAL	N-CA-C	6.06	113.07	107.56
1	A	88	ILE	CB-CA-C	6.06	116.00	110.13
1	A	289	LEU	CA-C-N	6.05	128.67	120.44
1	A	289	LEU	C-N-CA	6.05	128.67	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ARG	N-CA-C	6.04	117.95	111.36
1	A	112	ARG	NE-CZ-NH1	6.00	127.50	121.50
1	A	30	ASN	O-C-N	5.99	125.57	121.19
1	A	301	LEU	CB-CA-C	5.98	120.09	110.29
1	A	152	GLU	CA-CB-CG	5.96	126.02	114.10
1	A	286	GLU	N-CA-CB	5.95	118.87	110.12
1	A	129	ASN	CA-C-O	-5.92	114.28	120.55
1	A	254	VAL	CA-C-N	5.91	128.20	120.28
1	A	254	VAL	C-N-CA	5.91	128.20	120.28
1	A	62	HIS	CA-CB-CG	5.88	119.68	113.80
1	A	20	GLU	CA-CB-CG	5.88	125.85	114.10
1	A	241	MET	N-CA-CB	5.88	118.59	110.07
1	A	343	GLN	N-CA-CB	5.86	119.36	110.28
1	A	395	ILE	N-CA-CB	5.82	118.45	110.54
1	A	365	ARG	N-CA-CB	5.81	118.77	110.16
1	A	280	ARG	CD-NE-CZ	5.78	132.50	124.40
1	A	221	SER	O-C-N	5.78	128.24	122.12
1	A	18	VAL	O-C-N	5.77	125.65	121.55
1	A	64	ILE	CA-C-O	-5.77	114.14	120.43
1	A	186	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A	135	ALA	O-C-N	5.77	128.32	122.09
1	A	342	ARG	CD-NE-CZ	5.74	132.44	124.40
1	A	165[A]	LEU	CA-C-N	5.74	127.90	120.44
1	A	165[A]	LEU	C-N-CA	5.74	127.90	120.44
1	A	165[B]	LEU	CA-C-N	5.74	127.90	120.44
1	A	165[B]	LEU	C-N-CA	5.74	127.90	120.44
1	A	88	ILE	CB-CG1-CD1	5.73	125.83	113.80
1	A	90	ARG	CD-NE-CZ	5.72	132.41	124.40
1	A	358	LEU	O-C-N	5.71	130.47	122.36
1	A	89	PRO	CA-C-N	5.69	128.22	120.54
1	A	89	PRO	C-N-CA	5.69	128.22	120.54
1	A	80	HIS	CA-CB-CG	-5.68	108.12	113.80
1	A	324	LEU	N-CA-C	5.66	118.39	111.82
1	A	15	PRO	O-C-N	5.65	128.12	121.46
1	A	290	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	348	THR	CA-CB-CG2	5.61	120.03	110.50
1	A	243	GLY	N-CA-C	-5.57	106.04	112.73
1	A	33	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	49	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	108	GLN	CB-CG-CD	5.54	122.02	112.60
1	A	187	PRO	CA-C-O	5.54	127.36	121.32
1	A	151	THR	N-CA-CB	5.52	117.97	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	ASP	CA-C-N	5.52	125.61	119.32
1	A	407	ASP	C-N-CA	5.52	125.61	119.32
1	A	72	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	A	127	LEU	CA-C-N	5.44	127.89	120.54
1	A	127	LEU	C-N-CA	5.44	127.89	120.54
1	A	149	ASN	CB-CA-C	5.42	121.20	110.42
1	A	376	THR	CA-CB-CG2	5.41	119.69	110.50
1	A	373	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	291	ARG	CD-NE-CZ	5.39	131.94	124.40
1	A	40	GLU	CA-C-N	5.38	127.50	120.28
1	A	40	GLU	C-N-CA	5.38	127.50	120.28
1	A	142	LEU	CA-C-N	5.38	134.93	121.80
1	A	142	LEU	C-N-CA	5.38	134.93	121.80
1	A	276	GLU	N-CA-CB	5.38	118.59	110.30
1	A	334	CYS	CA-C-N	5.37	125.19	119.28
1	A	334	CYS	C-N-CA	5.37	125.19	119.28
1	A	193	PHE	CA-C-N	5.36	127.47	120.28
1	A	193	PHE	C-N-CA	5.36	127.47	120.28
1	A	223	VAL	CB-CA-C	5.34	119.02	112.02
1	A	340	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	38	VAL	N-CA-CB	5.33	117.39	110.57
1	A	195	GLU	CB-CA-C	-5.33	102.52	110.88
1	A	44	VAL	CA-C-N	5.30	128.12	120.38
1	A	44	VAL	C-N-CA	5.30	128.12	120.38
1	A	75	TYR	N-CA-C	5.30	117.96	111.82
1	A	277	ARG	CA-C-N	5.29	124.96	119.56
1	A	277	ARG	C-N-CA	5.29	124.96	119.56
1	A	281	ILE	CA-C-N	5.27	124.59	118.85
1	A	281	ILE	C-N-CA	5.27	124.59	118.85
1	A	349	THR	CA-CB-CG2	5.26	119.44	110.50
1	A	156	GLU	CA-C-N	5.26	124.44	118.97
1	A	156	GLU	C-N-CA	5.26	124.44	118.97
1	A	288	LEU	O-C-N	5.23	128.11	122.15
1	A	329	GLU	CA-CB-CG	5.21	124.52	114.10
1	A	375	LEU	CA-C-N	5.21	127.52	120.44
1	A	375	LEU	C-N-CA	5.21	127.52	120.44
1	A	358	LEU	N-CA-C	-5.20	106.09	112.90
1	A	253	VAL	O-C-N	5.19	127.18	121.83
1	A	221	SER	CA-C-O	-5.19	115.05	120.55
1	A	39	GLN	CB-CG-CD	5.19	121.42	112.60
1	A	236	ASP	CA-CB-CG	-5.17	107.43	112.60
1	A	104	ASP	O-C-N	5.17	125.85	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LEU	N-CA-C	5.16	119.57	113.28
1	A	258	SER	CB-CA-C	5.14	119.33	110.79
1	A	58	CYS	O-C-N	5.13	128.68	122.94
1	A	15	PRO	CB-CA-C	-5.13	104.67	110.92
1	A	241	MET	CB-CA-C	-5.11	102.83	110.90
1	A	47	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	220	ILE	CA-C-N	5.08	127.09	120.28
1	A	220	ILE	C-N-CA	5.08	127.09	120.28
1	A	118	VAL	CA-CB-CG2	5.07	119.03	110.40
1	A	130	ARG	N-CA-CB	5.06	118.12	110.28
1	A	364	ARG	N-CA-CB	5.06	117.56	110.12
1	A	138	LEU	N-CA-CB	-5.05	102.69	110.16
1	A	25	ASP	N-CA-C	5.04	117.41	109.39
1	A	396	VAL	CB-CA-C	5.04	118.09	110.63
1	A	84	GLU	O-C-N	5.04	127.46	122.12
1	A	202	ASP	CA-C-N	5.03	127.47	120.63
1	A	202	ASP	C-N-CA	5.03	127.47	120.63
1	A	108	GLN	CA-C-N	5.01	127.50	120.28
1	A	108	GLN	C-N-CA	5.01	127.50	120.28
1	A	328	ASP	CB-CA-C	5.01	118.51	110.29
1	A	365	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	A	372	LYS	CB-CG-CD	5.01	122.82	111.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	VAL	Mainchain
1	A	143	ARG	Sidechain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	154	TYR	Mainchain
1	A	186	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	377	ARG	Sidechain
1	A	77	ASP	Mainchain
1	A	96	TYR	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	3233	0	3187	74	0
2	A	43	0	30	3	0
3	A	11	0	16	1	0
4	A	232	0	0	3	0
All	All	3519	0	3233	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (75) 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:110:GLN:HB3	1:A:228[A]:VAL:HG13	1.51	0.90
1:A:183:GLN:HE22	1:A:188:ASP:HB2	1.34	0.90
1:A:261:MET:HE2	1:A:264:LEU:HD12	1.62	0.80
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.72	0.72
1:A:110:GLN:HG3	1:A:229[A]:ASN:HB3	1.73	0.70
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.73	0.69
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.75	0.69
1:A:110:GLN:HG3	1:A:229[B]:ASN:HB2	1.74	0.68
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.77	0.65
1:A:158:PHE:CE1	1:A:162[B]:ILE:HD11	2.36	0.61
1:A:134:LEU:HD22	1:A:138:LEU:HD22	1.83	0.60
1:A:112:ARG:NH1	2:A:415:HEM:O1D	2.32	0.59
1:A:261:MET:HE2	1:A:261:MET:HA	1.85	0.59
1:A:261:MET:CE	1:A:264:LEU:HD12	2.31	0.58
1:A:183:GLN:NE2	1:A:188:ASP:HB2	2.13	0.58
1:A:146:GLY:O	1:A:147:GLN:HB3	2.04	0.57
1:A:160:ILE:O	1:A:164:MET:HG2	2.05	0.56
1:A:276:GLU:C	1:A:278:PRO:HD3	2.30	0.56
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.06	0.54
1:A:33:ASN:O	1:A:36:ALA:HB3	2.10	0.51
1:A:30:ASN:HB2	4:A:730:HOH:O	2.10	0.51
2:A:415:HEM:HBB2	2:A:415:HEM:HMB2	1.93	0.50
1:A:291:ARG:HG2	1:A:338:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HD2	1:A:383:ILE:HD12	1.93	0.50
1:A:73:GLU:OE1	1:A:308:HIS:NE2	2.39	0.49
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.95	0.49
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.48	0.49
1:A:344:LYS:HE3	1:A:346:SER:HB2	1.94	0.48
1:A:56:THR:O	1:A:61:GLY:HA2	2.13	0.48
1:A:359:GLY:HA3	2:A:415:HEM:C3C	2.49	0.48
1:A:325:SER:O	1:A:331:GLU:HG3	2.13	0.48
1:A:97:ASP:O	1:A:240:ARG:HD2	2.14	0.47
1:A:114:LEU:HD23	1:A:241:MET:HE3	1.97	0.47
1:A:110:GLN:HB2	4:A:707:HOH:O	2.13	0.47
1:A:30:ASN:ND2	4:A:555:HOH:O	2.47	0.47
1:A:134:LEU:HD12	1:A:162[A]:ILE:HG12	1.97	0.47
1:A:91:GLU:H	1:A:91:GLU:CD	2.24	0.46
1:A:111:PHE:HD1	1:A:241:MET:HE2	1.80	0.46
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.98	0.46
1:A:158:PHE:O	1:A:162[B]:ILE:HG13	2.16	0.46
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.97	0.45
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.98	0.45
1:A:319:LEU:HG	1:A:321:PRO:HG3	1.97	0.45
1:A:261:MET:HA	1:A:261:MET:CE	2.45	0.45
1:A:318:ILE:HD13	1:A:320:LEU:HD21	1.97	0.45
1:A:99:ILE:HG13	1:A:240:ARG:HB3	1.99	0.45
1:A:302:THR:O	1:A:314:LYS:HG3	2.16	0.45
1:A:110:GLN:CB	1:A:228[A]:VAL:HG13	2.36	0.45
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.79	0.45
1:A:302:THR:C	1:A:314:LYS:HG3	2.43	0.44
1:A:127:LEU:CD1	1:A:166:LEU:HD13	2.43	0.44
1:A:114:LEU:HD23	1:A:241:MET:CE	2.47	0.44
1:A:334:CYS:O	1:A:337:HIS:HB3	2.16	0.44
1:A:101[B]:THR:HG21	3:A:416:CAM:H31	2.00	0.44
1:A:114:LEU:O	1:A:117:GLN:HB2	2.18	0.43
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.47	0.43
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.90	0.43
1:A:188:ASP:HB3	1:A:190:SER:H	1.83	0.43
1:A:121:MET:CB	1:A:122:PRO:HD3	2.41	0.43
1:A:322:GLN:HB3	1:A:348:THR:O	2.18	0.43
1:A:294:LEU:HD23	1:A:294:LEU:H	1.84	0.42
1:A:293:SER:O	1:A:323:MET:HG3	2.20	0.42
1:A:47:GLU:HB2	1:A:49:ASN:ND2	2.34	0.42
1:A:266:LYS:HD2	1:A:383:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:ND2	1:A:402:LEU:H	2.18	0.42
1:A:287:GLU:OE1	1:A:342:ARG:HD2	2.20	0.42
1:A:161:ARG:HD3	1:A:171:GLU:OE2	2.19	0.42
1:A:357:CYS:HB3	1:A:360:GLN:HB3	2.02	0.41
1:A:39:GLN:NE2	1:A:39:GLN:H	2.19	0.41
1:A:231:ARG:H	1:A:231:ARG:HG3	1.75	0.41
1:A:134:LEU:O	1:A:138:LEU:HB2	2.21	0.40
1:A:272:GLN:NE2	1:A:276:GLU:OE2	2.52	0.40
1:A:278:PRO:C	1:A:280:ARG:H	2.30	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	410/414 (99%)	392 (96%)	18 (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	356/357 (100%)	339 (95%)	17 (5%)	23	23

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	49	ASN
1	A	101[A]	THR
1	A	101[B]	THR
1	A	108	GLN
1	A	118	VAL
1	A	134	LEU
1	A	165[A]	LEU
1	A	165[B]	LEU
1	A	217	THR
1	A	235	SER
1	A	261	MET
1	A	276	GLU
1	A	318	ILE
1	A	371[A]	LEU
1	A	371[B]	LEU
1	A	400	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	33	ASN
1	A	39	GLN
1	A	49	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	129	ASN
1	A	149	ASN
1	A	225	ASN
1	A	337	HIS
1	A	361	HIS

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	416	-	12,12,12	1.60	3 (25%)	20,21,21	1.53	4 (20%)
2	HEM	A	415	1	50,50,50	1.54	10 (20%)	67,82,82	0.91	3 (4%)

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	416	-	-	-	0/3/2/2
2	HEM	A	415	1	-	3/14/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	FE-NB	4.36	2.08	1.94
2	A	415	HEM	FE-ND	3.51	2.05	1.94
3	A	416	CAM	C1-C2	3.40	1.57	1.52
2	A	415	HEM	CAC-C3C	3.40	1.56	1.47
2	A	415	HEM	CMC-C2C	3.25	1.57	1.50
2	A	415	HEM	CAB-C3B	2.94	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	FE-NC	2.40	2.03	1.95
2	A	415	HEM	CMB-C2B	2.26	1.55	1.50
3	A	416	CAM	C7-C4	2.26	1.61	1.54
3	A	416	CAM	C3-C4	2.23	1.58	1.53
2	A	415	HEM	CMA-C3A	2.23	1.55	1.50
2	A	415	HEM	CMD-C2D	2.14	1.55	1.50
2	A	415	HEM	C3C-C2C	-2.01	1.33	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	416	CAM	C9-C7-C8	-4.29	96.81	107.67
3	A	416	CAM	C8-C7-C1	2.82	119.33	113.05
3	A	416	CAM	C9-C7-C1	2.53	118.70	113.05
2	A	415	HEM	CBD-CAD-C3D	2.44	119.28	112.53
2	A	415	HEM	CHD-C1D-ND	-2.23	122.03	124.42
2	A	415	HEM	O1D-CGD-CBD	-2.09	116.47	123.09
3	A	416	CAM	C5-C4-C3	2.05	111.94	106.39

There are no chirality outliers.

All (3) 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-O2D

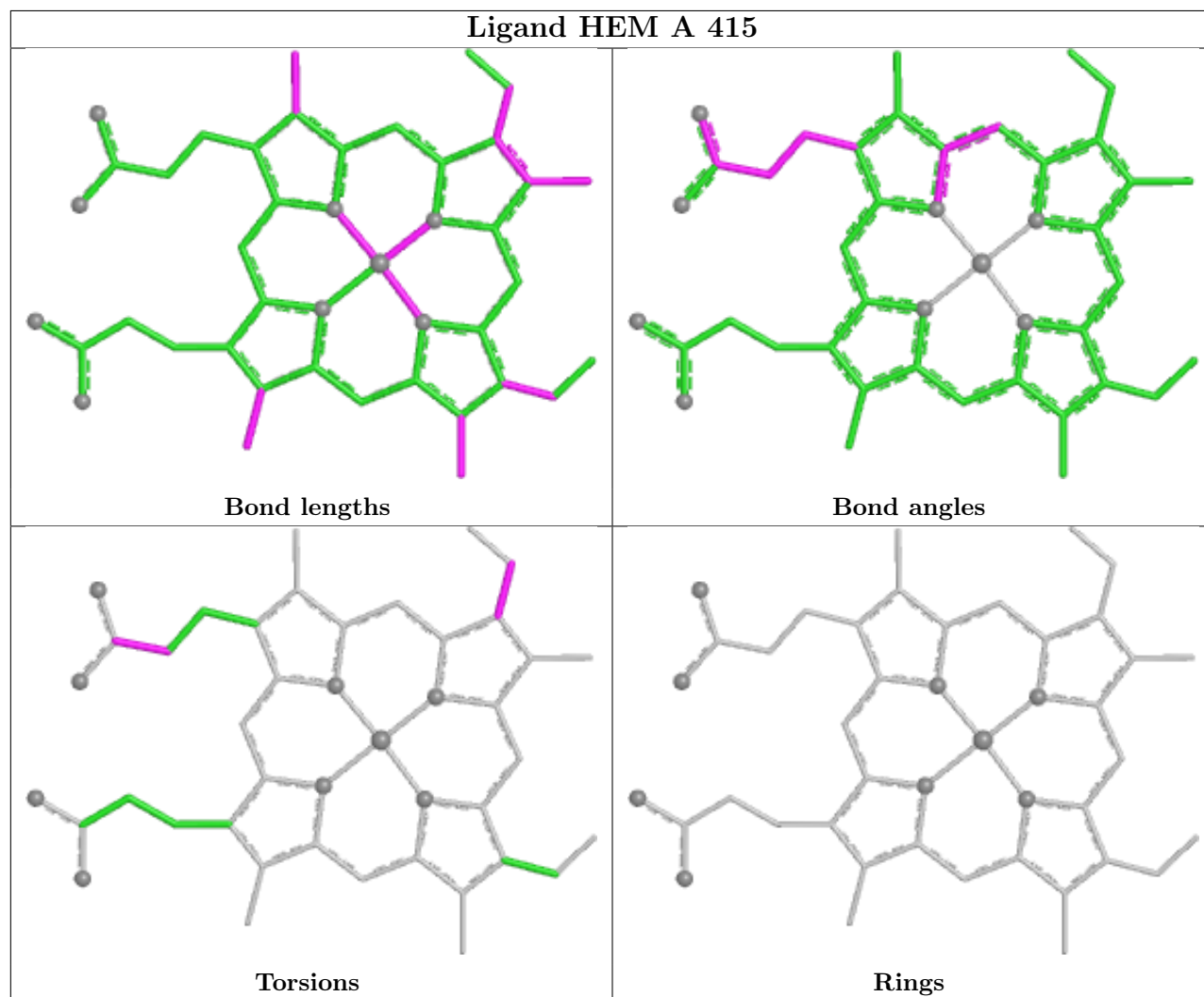
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	416	CAM	1	0
2	A	415	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.