



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:39 pm BST

PDB ID : 3CP4
Title : CRYSTAL STRUCTURE OF THE CYTOCHROME P450-CAM ACTIVE
SITE MUTANT THR252ALA
Authors : Raag, R.; Poulos, T.L.
Deposited on : 1991-06-04
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

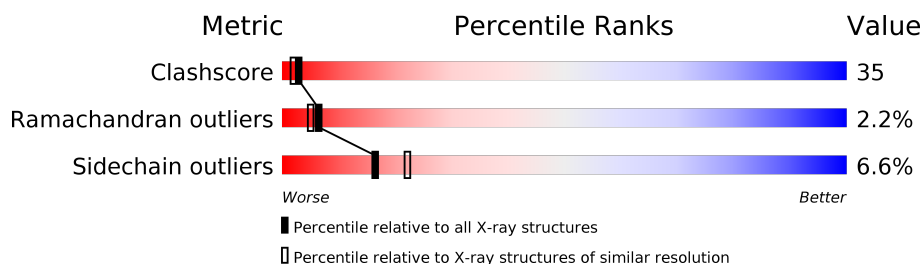
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 on 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	<div> <div style="width: 35%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 14%; background-color: orange;"></div> <div style="width: 5%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>35% 46% 14% . .</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADM	A	416	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3465 atoms, of which 0 are hydrogens and 0 are deuteriums.

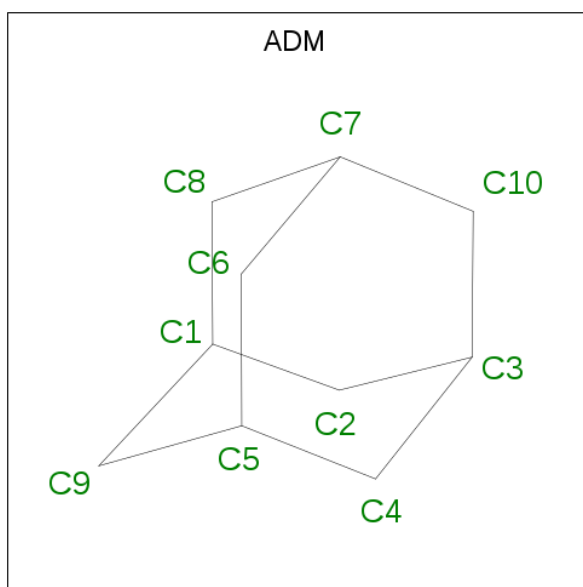
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





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

- Molecule 4 is water.

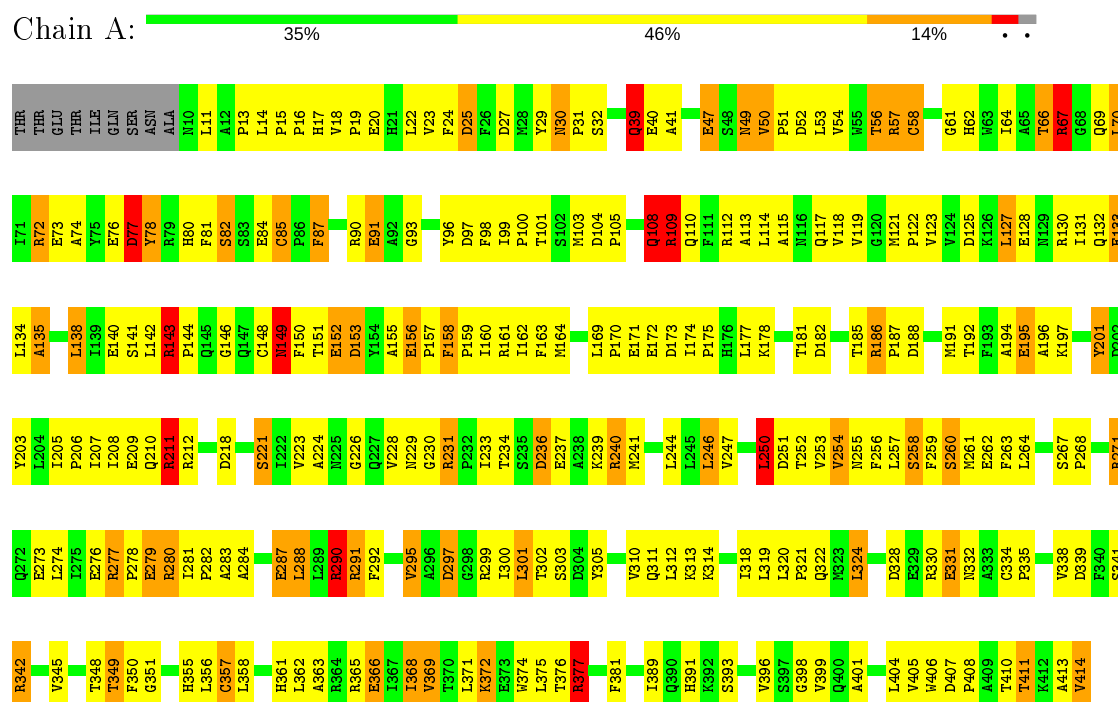
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	204	Total O 204 204	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.163 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3465	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, ADM

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	1.18	1/3287 (0.0%)	2.04	114/4465 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	CD-OE1	9.14	1.35	1.25

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	A	231	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	A	90	ARG	NE-CZ-NH1	13.43	127.01	120.30
1	A	271	ARG	NE-CZ-NH1	13.30	126.95	120.30
1	A	138	LEU	CA-CB-CG	13.20	145.65	115.30
1	A	143	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	A	377	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	A	211	ARG	CD-NE-CZ	12.03	140.45	123.60
1	A	52	ASP	CB-CG-OD1	11.70	128.83	118.30
1	A	211	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	A	143	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	A	195	GLU	CA-CB-CG	10.19	135.82	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	LEU	CA-CB-CG	10.05	138.41	115.30
1	A	209	GLU	CA-CB-CG	9.57	134.46	113.40
1	A	67	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	A	271	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	330	ARG	NE-CZ-NH2	8.90	124.75	120.30
1	A	112	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	280	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	132	GLN	CA-CB-CG	8.69	132.51	113.40
1	A	201	TYR	CB-CG-CD1	8.44	126.06	121.00
1	A	186	ARG	CD-NE-CZ	8.42	135.39	123.60
1	A	366	GLU	OE1-CD-OE2	-8.22	113.43	123.30
1	A	291	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	A	211	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	90	ARG	CD-NE-CZ	8.04	134.86	123.60
1	A	130	ARG	CD-NE-CZ	7.99	134.78	123.60
1	A	377	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	369	VAL	CA-CB-CG1	7.93	122.80	110.90
1	A	342	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	104	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	153	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	260	SER	N-CA-CB	7.34	121.52	110.50
1	A	290	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	223	VAL	CB-CA-C	7.28	125.23	111.40
1	A	84	GLU	CA-CB-CG	7.13	129.09	113.40
1	A	156	GLU	OE1-CD-OE2	-7.13	114.75	123.30
1	A	108	GLN	CA-CB-CG	7.11	129.05	113.40
1	A	209	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	A	210	GLN	CA-CB-CG	7.00	128.79	113.40
1	A	201	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	A	115	ALA	CB-CA-C	6.96	120.54	110.10
1	A	133	GLU	OE1-CD-OE2	-6.90	115.02	123.30
1	A	287	GLU	OE1-CD-OE2	-6.89	115.03	123.30
1	A	287	GLU	CA-CB-CG	6.87	128.52	113.40
1	A	301	LEU	CA-CB-CG	6.84	131.03	115.30
1	A	152	GLU	CA-CB-CG	6.72	128.19	113.40
1	A	374	TRP	CB-CA-C	6.69	123.79	110.40
1	A	109	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	113	ALA	N-CA-CB	6.62	119.36	110.10
1	A	256	PHE	CB-CG-CD1	-6.58	116.19	120.80
1	A	135	ALA	CB-CA-C	6.56	119.94	110.10
1	A	299	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	212	ARG	NE-CZ-NH1	6.39	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	GLU	OE1-CD-OE2	6.34	130.91	123.30
1	A	299	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	366	GLU	CB-CG-CD	6.27	131.14	114.20
1	A	280	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	47	GLU	CA-CB-CG	6.21	127.06	113.40
1	A	152	GLU	N-CA-CB	6.19	121.74	110.60
1	A	257	LEU	CB-CG-CD1	6.18	121.51	111.00
1	A	414	VAL	CA-CB-CG1	6.15	120.12	110.90
1	A	221	SER	N-CA-CB	6.14	119.72	110.50
1	A	240	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	72	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	158	PHE	N-CA-CB	6.00	121.40	110.60
1	A	57	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	195	GLU	CG-CD-OE2	5.92	130.13	118.30
1	A	133	GLU	CB-CG-CD	5.88	130.06	114.20
1	A	58	CYS	CB-CA-C	5.86	122.12	110.40
1	A	279	GLU	CA-CB-CG	5.84	126.26	113.40
1	A	149	ASN	N-CA-CB	5.79	121.03	110.60
1	A	209	GLU	CG-CD-OE1	5.79	129.89	118.30
1	A	297	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	110	GLN	CA-CB-CG	5.77	126.09	113.40
1	A	40	GLU	CA-CB-CG	5.77	126.09	113.40
1	A	250	LEU	CA-CB-CG	5.73	128.49	115.30
1	A	236	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	251	ASP	CB-CA-C	5.66	121.72	110.40
1	A	262	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	A	264	LEU	CB-CA-C	5.66	120.95	110.20
1	A	342	ARG	NH1-CZ-NH2	-5.65	113.19	119.40
1	A	357	CYS	C-N-CA	5.65	135.82	121.70
1	A	194	ALA	CB-CA-C	5.64	118.56	110.10
1	A	87	PHE	CB-CG-CD1	5.61	124.72	120.80
1	A	405	VAL	CA-CB-CG1	5.58	119.28	110.90
1	A	372	LYS	N-CA-CB	5.57	120.62	110.60
1	A	130	ARG	N-CA-CB	5.56	120.61	110.60
1	A	231	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
1	A	262	GLU	CA-CB-CG	5.53	125.56	113.40
1	A	66	THR	OG1-CB-CG2	5.47	122.57	110.00
1	A	254	VAL	CA-CB-CG1	5.46	119.09	110.90
1	A	70	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	211	ARG	CA-CB-CG	5.39	125.25	113.40
1	A	127	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	371	LEU	CB-CA-C	5.35	120.36	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	VAL	CA-CB-CG2	5.32	118.88	110.90
1	A	101	THR	N-CA-CB	5.31	120.38	110.30
1	A	143	ARG	CD-NE-CZ	5.29	131.00	123.60
1	A	39	GLN	N-CA-CB	5.28	120.10	110.60
1	A	77	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	398	GLY	N-CA-C	5.24	126.19	113.10
1	A	90	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
1	A	104	ASP	CB-CA-C	5.21	120.82	110.40
1	A	218	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	A	87	PHE	CA-CB-CG	5.14	126.23	113.90
1	A	349	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	411	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	39	GLN	CA-CB-CG	5.07	124.55	113.40
1	A	50	VAL	CG1-CB-CG2	-5.04	102.83	110.90
1	A	324	LEU	N-CA-C	5.04	124.61	111.00
1	A	295	VAL	CB-CA-C	5.02	120.94	111.40
1	A	277	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	A	27	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	119	VAL	Mainchain
1	A	135	ALA	Mainchain
1	A	149	ASN	Mainchain
1	A	250	LEU	Mainchain
1	A	290	ARG	Sidechain
1	A	339	ASP	Mainchain
1	A	377	ARG	Sidechain
1	A	67	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	223	0
2	A	43	0	30	8	0
3	A	10	0	16	6	0
4	A	204	0	0	28	0
All	All	3465	0	3202	224	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 35.

All (224) 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:39:GLN:HE21	1:A:39:GLN:H	1.15	0.91
1:A:260:SER:HB3	1:A:288:LEU:HD13	1.60	0.83
1:A:131:ILE:HG22	1:A:369:VAL:HG11	1.66	0.78
1:A:159:PRO:HA	1:A:162:ILE:HD12	1.67	0.77
1:A:181:THR:HG23	1:A:247:VAL:HG22	1.67	0.75
1:A:39:GLN:NE2	1:A:39:GLN:H	1.85	0.74
1:A:114:LEU:O	1:A:117:GLN:HB2	1.90	0.72
1:A:281:ILE:HG22	1:A:368:ILE:HG23	1.72	0.71
1:A:319:LEU:HG	1:A:321:PRO:HD3	1.72	0.70
1:A:178:LYS:HZ3	1:A:254:VAL:HG11	1.57	0.70
1:A:177:LEU:HD13	1:A:246:LEU:HD11	1.73	0.70
1:A:203:TYR:O	1:A:206:PRO:HD2	1.91	0.70
1:A:143:ARG:NH2	1:A:413:ALA:HB2	2.06	0.70
1:A:322:GLN:HB3	1:A:348:THR:O	1.92	0.69
1:A:407:ASP:HB3	1:A:410:THR:HG23	1.74	0.68
1:A:82:SER:O	1:A:300:ILE:HG22	1.94	0.68
1:A:281:ILE:CG2	1:A:368:ILE:HG23	2.24	0.68
1:A:156:GLU:HB2	1:A:157:PRO:HD3	1.76	0.67
1:A:178:LYS:NZ	1:A:254:VAL:HG11	2.09	0.67
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.59	0.67
1:A:82:SER:HB2	4:A:581:HOH:O	1.96	0.65
1:A:362:LEU:O	1:A:366:GLU:HG3	1.96	0.65
1:A:128:GLU:HA	1:A:131:ILE:HD12	1.78	0.65
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.79	0.65
1:A:134:LEU:HB2	4:A:590:HOH:O	1.97	0.64
1:A:78:TYR:CE2	1:A:105:PRO:HG2	2.32	0.64
1:A:233:ILE:HG12	1:A:234:THR:O	1.97	0.64
1:A:229:ASN:O	1:A:231:ARG:HG3	1.98	0.63
1:A:169:LEU:HD13	1:A:203:TYR:OH	1.99	0.63
1:A:146:GLY:HA2	1:A:406:TRP:CE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:O	1:A:301:LEU:HA	1.98	0.62
1:A:186:ARG:HH12	1:A:255:ASN:ND2	1.97	0.62
1:A:143:ARG:HG3	1:A:411:THR:HG21	1.82	0.61
1:A:142:LEU:HD22	1:A:148:CYS:HB3	1.81	0.61
1:A:252:THR:HB	2:A:415:HEM:HBB2	1.83	0.61
1:A:303:SER:HA	1:A:314:LYS:HB2	1.83	0.61
1:A:143:ARG:HH21	1:A:413:ALA:HB2	1.65	0.60
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.32	0.60
1:A:56:THR:O	1:A:61:GLY:HA2	2.01	0.60
1:A:376:THR:HG22	1:A:414:VAL:HG21	1.82	0.60
1:A:197:LYS:HE3	1:A:201:TYR:HE2	1.66	0.60
1:A:234:THR:OG1	1:A:237:GLU:HG3	2.02	0.59
1:A:208:ILE:HD12	1:A:239:LYS:HA	1.83	0.59
1:A:149:ASN:C	1:A:149:ASN:HD22	2.05	0.59
1:A:14:LEU:HD21	1:A:18:VAL:O	2.02	0.59
1:A:177:LEU:HD21	1:A:203:TYR:CE1	2.38	0.59
1:A:25:ASP:OD1	1:A:57:ARG:HB2	2.02	0.59
1:A:29:TYR:O	1:A:30:ASN:HB2	2.03	0.59
1:A:381:PHE:HD2	1:A:404:LEU:HD13	1.68	0.58
1:A:151:THR:HA	1:A:155:ALA:HB3	1.86	0.58
1:A:254:VAL:HG12	4:A:571:HOH:O	2.02	0.57
1:A:169:LEU:HD21	1:A:207:ILE:HG21	1.84	0.57
1:A:97:ASP:O	1:A:240:ARG:HD2	2.04	0.57
1:A:109:ARG:HB2	4:A:623:HOH:O	2.04	0.57
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.05	0.57
1:A:99:ILE:HG23	1:A:103:MET:CE	2.35	0.57
1:A:205:ILE:HD11	1:A:239:LYS:CD	2.34	0.57
1:A:407:ASP:HB3	1:A:410:THR:CG2	2.34	0.56
1:A:15:PRO:HG2	1:A:18:VAL:HG23	1.86	0.56
1:A:186:ARG:HH12	1:A:255:ASN:HD21	1.53	0.56
1:A:259:PHE:HB3	1:A:292:PHE:CD2	2.41	0.56
1:A:151:THR:OG1	1:A:401:ALA:HA	2.06	0.56
1:A:20:GLU:HA	1:A:23:VAL:HG23	1.88	0.56
1:A:186:ARG:NH1	1:A:255:ASN:ND2	2.54	0.55
1:A:319:LEU:O	1:A:320:LEU:HD23	2.06	0.55
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.89	0.55
1:A:234:THR:HB	4:A:604:HOH:O	2.07	0.55
1:A:332:ASN:HA	4:A:693:HOH:O	2.06	0.55
1:A:159:PRO:HG3	1:A:254:VAL:HG22	1.88	0.55
1:A:376:THR:CG2	1:A:414:VAL:HG21	2.37	0.54
1:A:51:PRO:HB2	1:A:54:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:ADM:H5	4:A:801:HOH:O	2.07	0.54
1:A:381:PHE:CD2	1:A:404:LEU:HD13	2.43	0.54
1:A:268:PRO:HB3	1:A:271:ARG:NH2	2.23	0.54
1:A:169:LEU:HD22	1:A:207:ILE:HD13	1.90	0.53
1:A:328:ASP:O	1:A:331:GLU:HB2	2.08	0.53
1:A:358:LEU:HD12	2:A:415:HEM:HMD3	1.90	0.53
1:A:53:LEU:HD23	1:A:310:VAL:HG21	1.90	0.53
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.91	0.53
1:A:302:THR:O	1:A:314:LYS:HE3	2.09	0.53
1:A:67:ARG:HB3	4:A:541:HOH:O	2.08	0.53
1:A:205:ILE:HD11	1:A:239:LYS:HD3	1.91	0.52
1:A:303:SER:HA	1:A:314:LYS:CB	2.39	0.52
1:A:191:MET:HE1	1:A:196:ALA:HA	1.91	0.52
1:A:31:PRO:HB2	1:A:41:ALA:HB1	1.91	0.52
1:A:322:GLN:HG2	1:A:351:GLY:HA2	1.91	0.52
1:A:67:ARG:NH1	1:A:328:ASP:OD1	2.42	0.52
1:A:160:ILE:O	1:A:164:MET:HG2	2.10	0.52
1:A:87:PHE:HB2	1:A:93:GLY:HA2	1.92	0.51
1:A:99:ILE:HD11	1:A:237:GLU:HA	1.93	0.51
1:A:39:GLN:N	1:A:39:GLN:HE21	1.95	0.51
1:A:278:PRO:C	1:A:280:ARG:H	2.14	0.51
1:A:99:ILE:HG23	1:A:103:MET:SD	2.50	0.51
1:A:163:PHE:CE1	1:A:246:LEU:HD22	2.45	0.51
1:A:181:THR:HG23	1:A:247:VAL:HG13	1.93	0.51
1:A:393:SER:HB3	4:A:528:HOH:O	2.09	0.51
1:A:49:ASN:HD22	1:A:49:ASN:H	1.59	0.51
1:A:140:GLU:OE2	1:A:143:ARG:NH2	2.39	0.51
1:A:349:THR:HG23	4:A:536:HOH:O	2.11	0.51
1:A:252:THR:HG21	2:A:415:HEM:C1B	2.46	0.51
1:A:15:PRO:HG2	1:A:18:VAL:CG2	2.41	0.50
1:A:69:GLN:HB3	4:A:580:HOH:O	2.10	0.50
1:A:149:ASN:C	1:A:149:ASN:ND2	2.65	0.50
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.10	0.50
1:A:87:PHE:HZ	3:A:416:ADM:H81	1.77	0.50
1:A:159:PRO:HG2	1:A:160:ILE:H	1.77	0.50
1:A:363:ALA:HB1	2:A:415:HEM:HAB	1.93	0.50
1:A:263:PHE:CE2	1:A:338:VAL:HG11	2.47	0.49
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.48	0.49
1:A:205:ILE:CB	1:A:206:PRO:HD3	2.42	0.49
1:A:236:ASP:OD1	1:A:239:LYS:HE2	2.12	0.49
1:A:118:VAL:O	1:A:123:VAL:HG11	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:MET:CE	1:A:196:ALA:HA	2.43	0.49
1:A:127:LEU:HA	4:A:587:HOH:O	2.11	0.49
1:A:244:LEU:HD11	3:A:416:ADM:H21	1.94	0.49
1:A:181:THR:CG2	1:A:247:VAL:HA	2.41	0.49
1:A:291:ARG:HG3	1:A:291:ARG:NH1	2.23	0.49
1:A:334:CYS:N	1:A:335:PRO:HD3	2.27	0.49
1:A:177:LEU:HD21	1:A:203:TYR:CD1	2.48	0.49
1:A:295:VAL:HG11	2:A:415:HEM:HMA2	1.94	0.48
1:A:93:GLY:O	1:A:96:TYR:HB3	2.13	0.48
1:A:15:PRO:HB2	1:A:17:HIS:CE1	2.48	0.48
1:A:174:ILE:N	1:A:175:PRO:HD2	2.28	0.48
1:A:321:PRO:CG	1:A:324:LEU:HD12	2.43	0.48
1:A:295:VAL:HG22	1:A:396:VAL:HG22	1.94	0.48
1:A:99:ILE:HG13	1:A:240:ARG:HB3	1.95	0.48
1:A:350:PHE:O	1:A:356:LEU:HD12	2.14	0.48
1:A:361:HIS:HB2	4:A:560:HOH:O	2.14	0.48
1:A:22:LEU:HD22	1:A:53:LEU:O	2.14	0.48
1:A:181:THR:HG23	1:A:247:VAL:HA	1.96	0.48
1:A:303:SER:HA	1:A:314:LYS:CG	2.43	0.48
1:A:56:THR:HG21	1:A:64:ILE:HD11	1.96	0.48
1:A:260:SER:HB3	1:A:288:LEU:CD1	2.37	0.48
1:A:211:ARG:HG3	1:A:221:SER:OG	2.14	0.47
1:A:134:LEU:HD12	1:A:134:LEU:O	2.14	0.47
1:A:47:GLU:HB2	1:A:49:ASN:ND2	2.29	0.47
1:A:72:ARG:O	1:A:76:GLU:HG3	2.14	0.47
1:A:100:PRO:HG2	2:A:415:HEM:CGD	2.45	0.47
1:A:274:LEU:HD12	1:A:375:LEU:HD11	1.96	0.47
1:A:87:PHE:HE1	3:A:416:ADM:H102	1.79	0.47
1:A:197:LYS:HE3	1:A:201:TYR:CE2	2.49	0.47
1:A:53:LEU:HD23	1:A:310:VAL:CG2	2.45	0.47
1:A:287:GLU:OE1	1:A:342:ARG:HD2	2.15	0.47
1:A:121:MET:HB2	1:A:122:PRO:CD	2.45	0.47
1:A:151:THR:HG22	1:A:258:SER:OG	2.14	0.47
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.96	0.46
1:A:25:ASP:HB2	4:A:550:HOH:O	2.16	0.46
1:A:186:ARG:NH1	1:A:255:ASN:HD21	2.13	0.46
1:A:14:LEU:HD11	1:A:18:VAL:HB	1.98	0.46
1:A:160:ILE:HG21	1:A:174:ILE:HG12	1.98	0.46
1:A:197:LYS:HG2	1:A:201:TYR:CE2	2.50	0.46
1:A:302:THR:O	1:A:314:LYS:HG3	2.16	0.46
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:O	1:A:254:VAL:HG21	2.16	0.46
1:A:271:ARG:NH1	1:A:381:PHE:O	2.49	0.46
1:A:187:PRO:HA	4:A:681:HOH:O	2.15	0.45
1:A:357:CYS:HB2	2:A:415:HEM:C1A	2.51	0.45
1:A:143:ARG:HB3	1:A:144:PRO:CD	2.45	0.45
1:A:185:THR:C	1:A:187:PRO:HD3	2.36	0.45
1:A:377:ARG:O	1:A:411:THR:HB	2.16	0.45
1:A:128:GLU:O	1:A:131:ILE:HB	2.17	0.45
1:A:188:ASP:HB2	4:A:597:HOH:O	2.16	0.45
1:A:305:TYR:O	1:A:312:LEU:N	2.47	0.45
1:A:377:ARG:NH2	1:A:414:VAL:HB	2.32	0.45
1:A:133:GLU:HG2	1:A:133:GLU:O	2.17	0.45
1:A:178:LYS:HE3	1:A:182:ASP:OD1	2.16	0.45
1:A:74:ALA:HB3	1:A:320:LEU:HD13	1.97	0.45
1:A:87:PHE:CE1	3:A:416:ADM:H102	2.51	0.45
1:A:32:SER:N	4:A:513:HOH:O	2.48	0.44
1:A:372:LYS:HD3	4:A:561:HOH:O	2.17	0.44
1:A:281:ILE:N	1:A:282:PRO:CD	2.80	0.44
1:A:391:HIS:CD2	1:A:399:VAL:HG22	2.52	0.44
1:A:85:CYS:HB3	1:A:300:ILE:HD13	2.00	0.44
1:A:302:THR:HA	4:A:538:HOH:O	2.17	0.44
1:A:51:PRO:HD2	1:A:54:VAL:CG1	2.47	0.44
1:A:57:ARG:HG2	4:A:508:HOH:O	2.18	0.44
1:A:152:GLU:HB3	4:A:563:HOH:O	2.18	0.43
1:A:226:GLY:O	1:A:233:ILE:HG22	2.18	0.43
1:A:252:THR:HG1	2:A:415:HEM:CHC	2.31	0.43
1:A:156:GLU:HB2	1:A:157:PRO:CD	2.45	0.43
1:A:161:ARG:HD2	1:A:171:GLU:OE2	2.17	0.43
1:A:99:ILE:HG22	1:A:100:PRO:HA	2.01	0.43
1:A:134:LEU:CD1	1:A:138:LEU:HD22	2.48	0.43
1:A:181:THR:HG23	1:A:247:VAL:CG2	2.42	0.43
1:A:303:SER:HA	1:A:314:LYS:HD2	2.01	0.43
1:A:319:LEU:C	1:A:320:LEU:HD23	2.38	0.43
1:A:17:HIS:CD2	1:A:313:LYS:HB2	2.54	0.43
1:A:246:LEU:O	1:A:250:LEU:HD13	2.19	0.43
1:A:401:ALA:HB2	4:A:564:HOH:O	2.19	0.42
1:A:69:GLN:NE2	4:A:580:HOH:O	2.50	0.42
1:A:205:ILE:HD11	1:A:239:LYS:HD2	2.01	0.42
1:A:208:ILE:HG23	1:A:224:ALA:HB2	2.02	0.42
1:A:297:ASP:C	1:A:319:LEU:HD12	2.40	0.42
1:A:389:ILE:HA	4:A:659:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLY:HA3	4:A:671:HOH:O	2.19	0.42
1:A:159:PRO:HG2	1:A:160:ILE:N	2.35	0.42
1:A:169:LEU:CD2	1:A:207:ILE:HD13	2.50	0.42
1:A:318:ILE:HD13	1:A:320:LEU:HD21	2.01	0.42
1:A:342:ARG:HD3	4:A:643:HOH:O	2.19	0.42
1:A:171:GLU:HA	1:A:174:ILE:CD1	2.50	0.42
1:A:11:LEU:HB3	1:A:57:ARG:HB3	2.01	0.41
1:A:273:GLU:OE2	1:A:280:ARG:NH1	2.53	0.41
1:A:260:SER:CB	1:A:288:LEU:HD13	2.43	0.41
1:A:244:LEU:CD1	3:A:416:ADM:H21	2.50	0.41
1:A:278:PRO:O	1:A:280:ARG:N	2.53	0.41
1:A:277:ARG:HB3	1:A:279:GLU:OE2	2.21	0.41
1:A:78:TYR:HA	1:A:81:PHE:O	2.20	0.41
1:A:172:GLU:O	1:A:175:PRO:HD2	2.19	0.41
1:A:77:ASP:OD2	1:A:80:HIS:ND1	2.51	0.41
1:A:142:LEU:O	1:A:143:ARG:C	2.58	0.41
1:A:163:PHE:HE1	1:A:246:LEU:HD22	1.85	0.41
1:A:91:GLU:CD	1:A:91:GLU:H	2.24	0.41
1:A:70:LEU:O	1:A:73:GLU:N	2.53	0.41
1:A:283:ALA:O	1:A:284:ALA:C	2.58	0.41
1:A:372:LYS:HD3	4:A:545:HOH:O	2.20	0.41
1:A:149:ASN:N	1:A:153:ASP:OD2	2.54	0.41
1:A:62:HIS:NE2	4:A:503:HOH:O	2.37	0.41
1:A:99:ILE:CD1	1:A:237:GLU:HA	2.50	0.41
1:A:290:ARG:NH2	1:A:335:PRO:O	2.52	0.40
1:A:19:PRO:HG2	1:A:22:LEU:HD12	2.03	0.40
1:A:99:ILE:O	1:A:241:MET:HG2	2.21	0.40
1:A:177:LEU:HD13	1:A:246:LEU:CD1	2.46	0.40
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.88	0.40
1:A:267:SER:HA	1:A:268:PRO:HD2	1.80	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%)	351 (87%)	43 (11%)	9 (2%)	6	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	PHE
1	A	230	GLY
1	A	24	PHE
1	A	25	ASP
1	A	30	ASN
1	A	78	TYR
1	A	158	PHE
1	A	13	PRO
1	A	143	ARG

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	350/358 (98%)	327 (93%)	23 (7%)	16	22

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	39	GLN
1	A	49	ASN
1	A	56	THR
1	A	58	CYS
1	A	66	THR
1	A	82	SER
1	A	85	CYS
1	A	91	GLU
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	125	ASP
1	A	141	SER
1	A	149	ASN
1	A	211	ARG
1	A	228	VAL
1	A	246	LEU
1	A	250	LEU
1	A	258	SER
1	A	261	MET
1	A	311	GLN
1	A	341	SER
1	A	368	ILE
1	A	408	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	49	ASN
1	A	69	GLN
1	A	108	GLN
1	A	129	ASN
1	A	149	ASN
1	A	225	ASN
1	A	272	GLN
1	A	343	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 carbohydrates 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	1,4	27,50,50	1.99	4 (14%)	17,82,82	2.50	7 (41%)
3	ADM	A	416	-	12,12,12	2.07	6 (50%)	18,18,18	0.70	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	1,4	-	0/6/54/54	-
3	ADM	A	416	-	-	-	0/4/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	C3B-C2B	-5.80	1.32	1.40
2	A	415	HEM	C3C-CAC	4.42	1.56	1.47
2	A	415	HEM	C3C-C2C	-4.38	1.34	1.40
2	A	415	HEM	C3B-CAB	3.54	1.55	1.47
3	A	416	ADM	C4-C5	2.87	1.60	1.52
3	A	416	ADM	C10-C3	2.36	1.58	1.52
3	A	416	ADM	C2-C1	2.31	1.58	1.52
3	A	416	ADM	C8-C1	2.27	1.58	1.52
3	A	416	ADM	C10-C7	2.17	1.58	1.52
3	A	416	ADM	C9-C5	2.03	1.58	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	HEM	CBD-CAD-C3D	6.79	124.99	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	HEM	CBA-CAA-C2A	3.61	119.14	112.49
2	A	415	HEM	CMA-C3A-C4A	-2.92	123.98	128.46
2	A	415	HEM	CMD-C2D-C1D	-2.91	123.99	128.46
2	A	415	HEM	CMC-C2C-C3C	2.60	129.54	124.68
2	A	415	HEM	CMB-C2B-C3B	2.38	129.14	124.68
2	A	415	HEM	CMA-C3A-C2A	2.31	129.30	124.94

There are no chirality outliers.

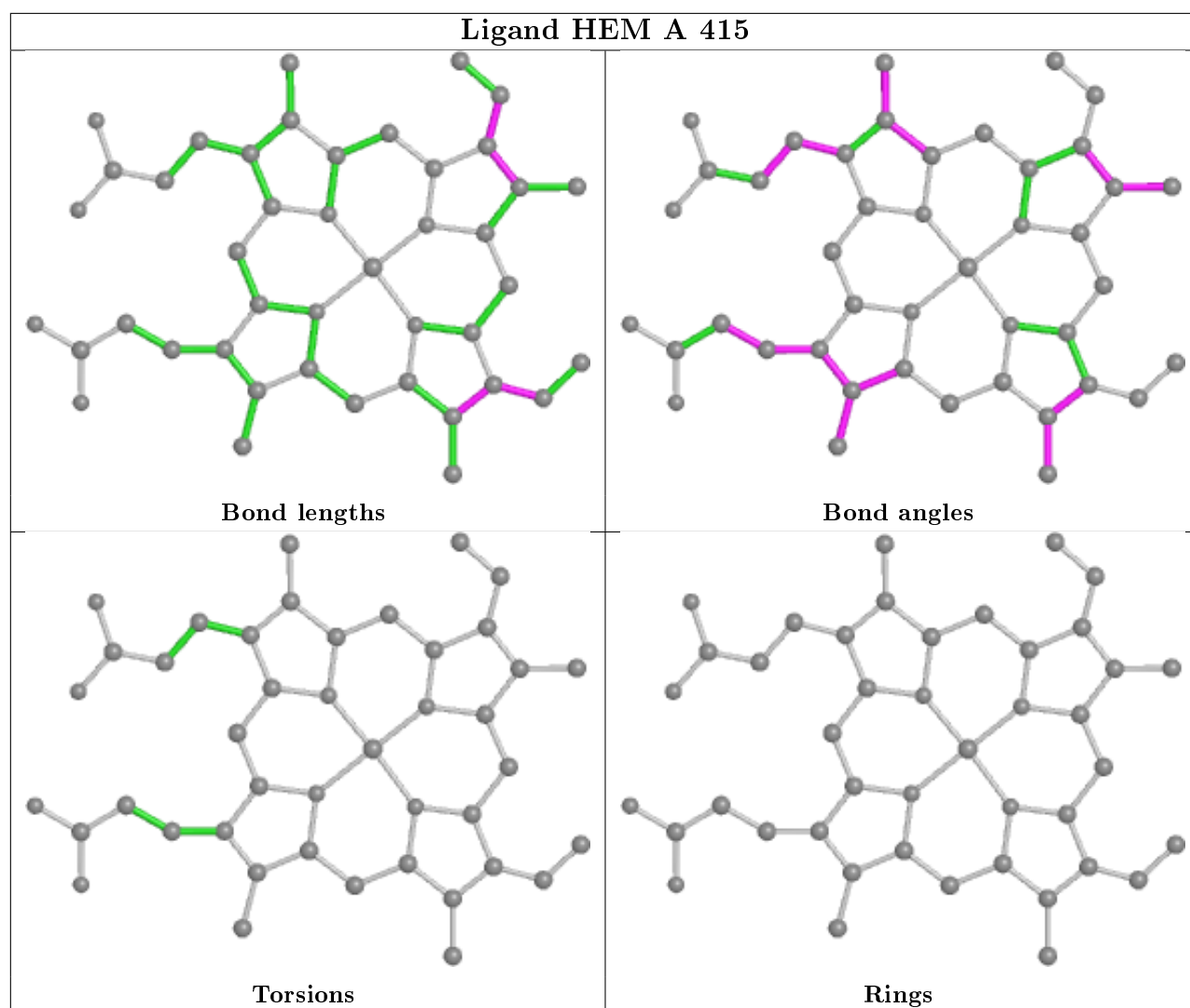
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	HEM	8	0
3	A	416	ADM	6	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.