wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2024 – 12:53 AM EST

PDB ID	:	1SMJ
Title	:	Structure of the A264E mutant of cytochrome P450 BM3 complexed with palmitoleate
Authors	:	Joyce, M.G.; Girvan, H.M.; Munro, A.W.; Leys, D.
Deposited on	:	2004-03-09
Resolution	:	2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

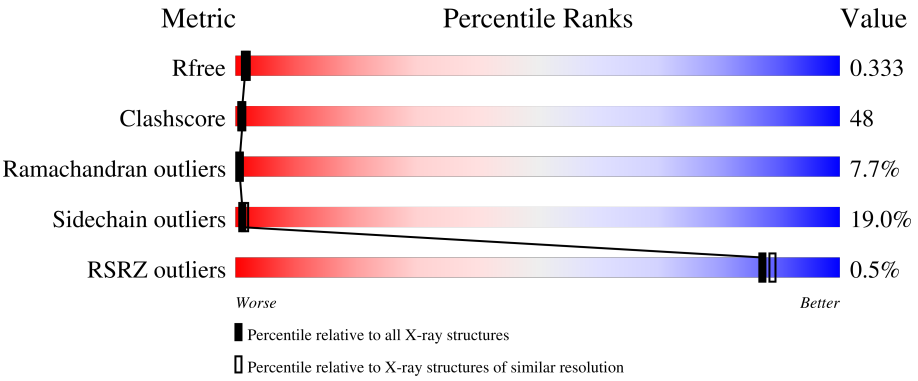
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
R_{free}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	34% 44% 16%
1	B	471	% 26% 49% 18%
1	C	471	23% 49% 20% 5%
1	D	471	% 28% 46% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14913 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.

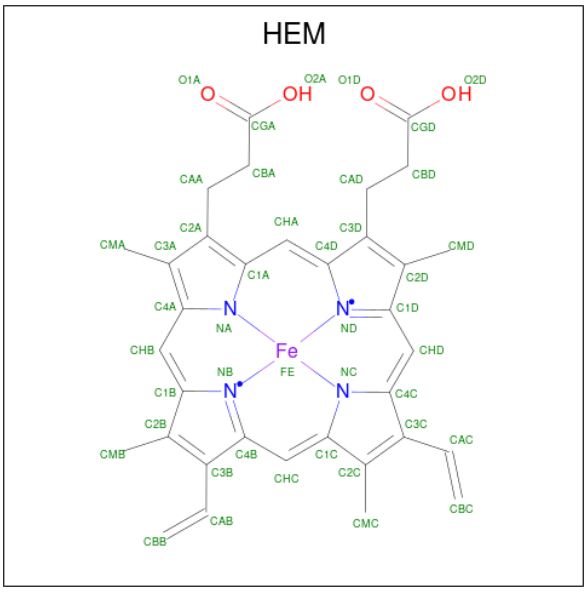
- Molecule 1 is a protein called Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3662	2340	621	684	17			
1	B	455	Total	C	N	O	S	0	0	0
			3670	2344	622	687	17			
1	C	455	Total	C	N	O	S	0	0	0
			3670	2344	622	687	17			
1	D	454	Total	C	N	O	S	0	0	0
			3667	2343	622	685	17			

There are 4 discrepancies between the modelled and reference sequences:

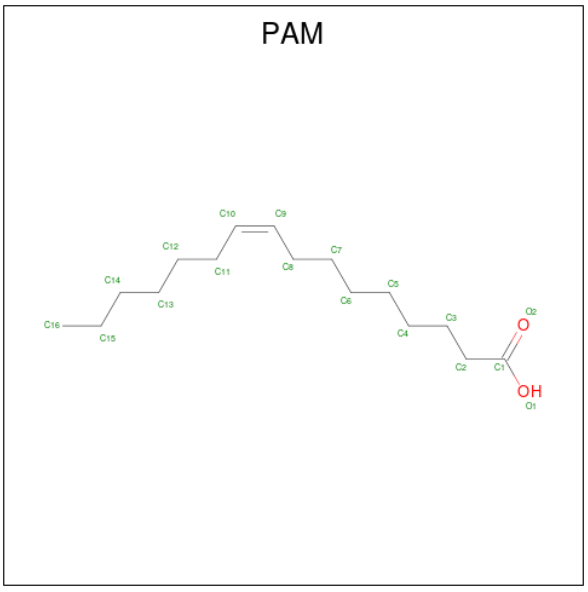
Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLU	ALA	engineered mutation	UNP P14779
B	264	GLU	ALA	engineered mutation	UNP P14779
C	264	GLU	ALA	engineered mutation	UNP P14779
D	264	GLU	ALA	engineered mutation	UNP P14779

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is PALMITOLEIC ACID (three-letter code: PAM) (formula: $C_{16}H_{30}O_2$).



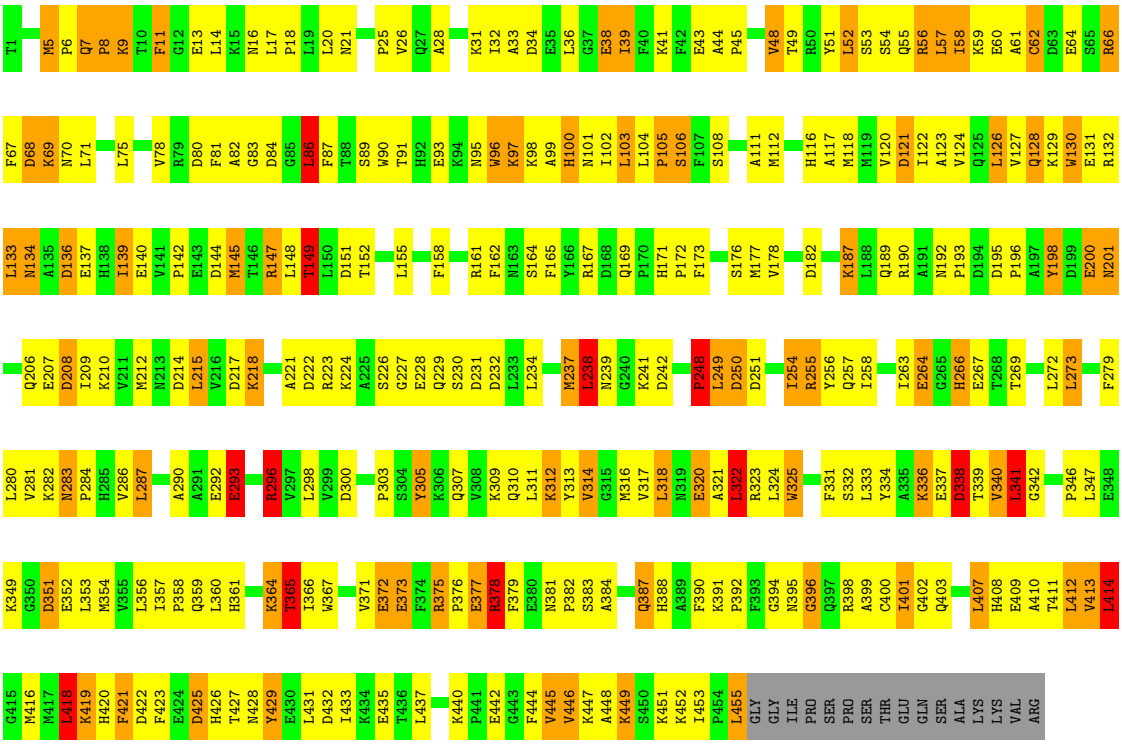
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		

3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

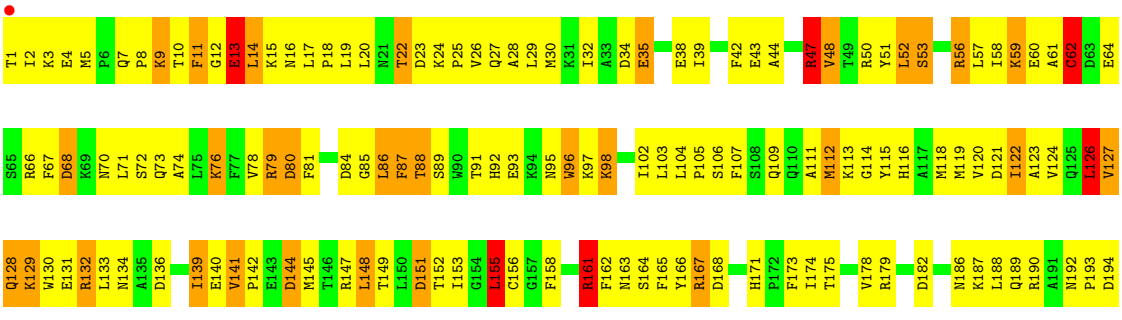
• Molecule 1: Bifunctional P-450:NADPH-P450 reductase

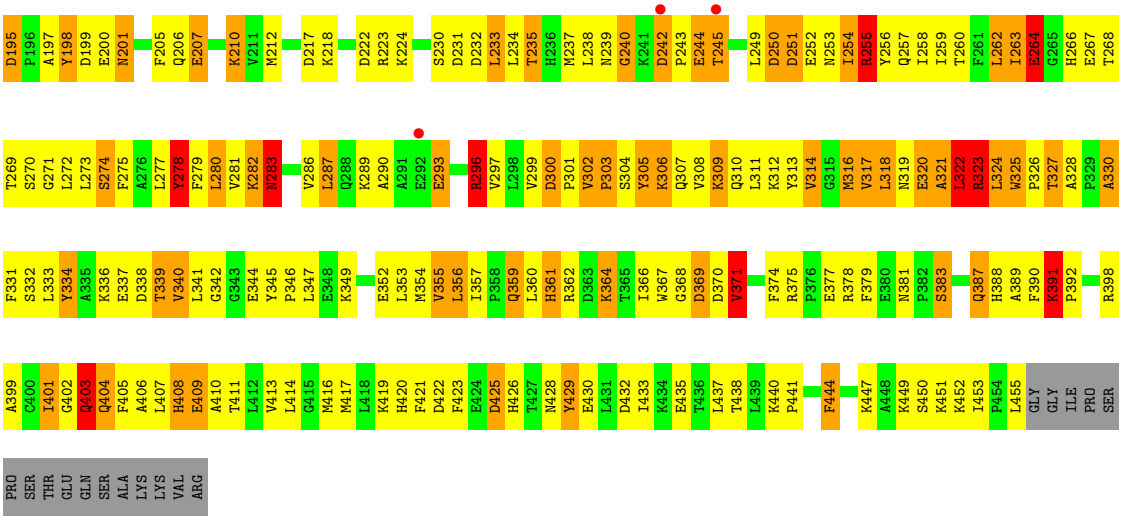
Chain A:



• Molecule 1: Bifunctional P-450:NADPH-P450 reductase

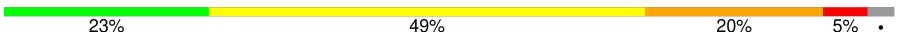
Chain B:

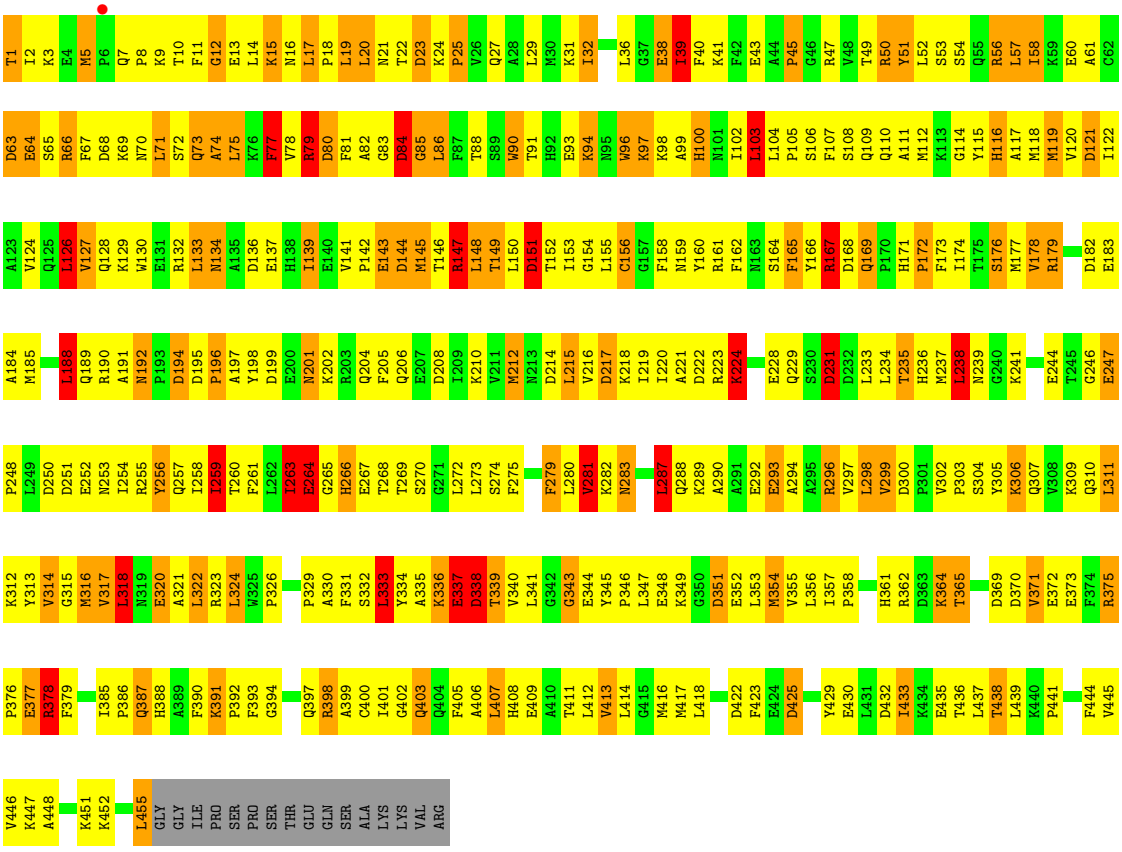




• Molecule 1: Bifunctional P-450:NADPH-P450 reductase

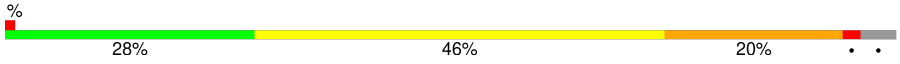
Chain C:

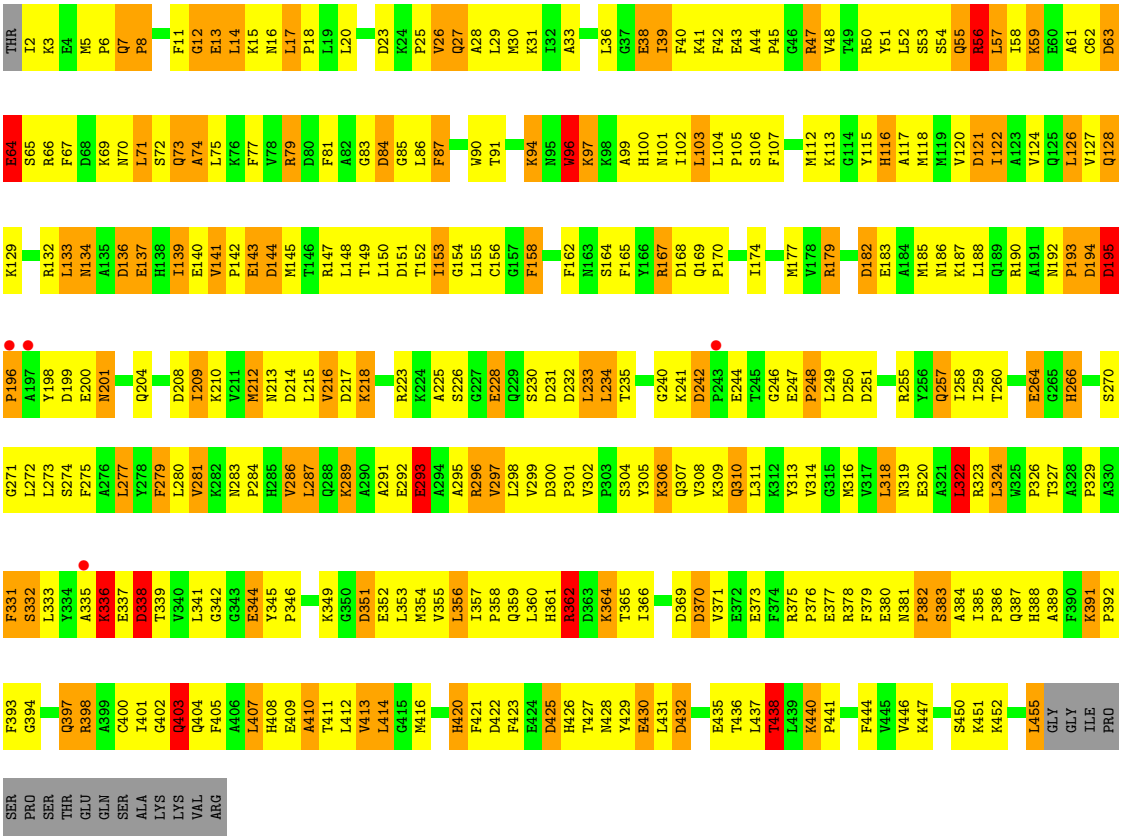




• Molecule 1: Bifunctional P-450:NADPH-P450 reductase

Chain D:




THR I2 K3 E4 M5 P6 Q7 P8 F11 G12 E13 L14 K15 N16 L17 P18 L19 L20 D23 K24 P25 V26 Q27 A28 L29 M30 K31 I32 A33 L36 G37 E38 I39 F40 K41 F42 E43 A44 P45 G46 R47 V48 T49 R50 Y51 L52 S53 S54 Q55 R56 L57 I58 K59 E60 A61 C62 D63
E64 S65 R66 F67 D68 K69 N70 L71 S72 Q73 A74 L75 K76 F77 V78 R79 D80 F81 A82 G83 D84 G85 L86 F87 W90 T91 K94 N95 W96 K97 K98 A99 H100 N101 I102 L103 L104 P105 S106 F107 M112 K113 G114 Y115 H116 A117 M118 M119 V120 D121 I122 A123 V124 Q125 L126 V127 Q128
K129 R132 L133 N134 A135 D136 E137 H138 I139 E140 V141 P142 E143 D144 M145 T146 R147 L148 T149 L150 D151 T152 I153 G154 L155 C156 G157 F158 F162 N163 S164 F165 Y166 R167 D168 Q169 P170 I174 M177 V178 R179 D182 E183 A184 M185 N186 K187 L188 Q189 R190 A191 N192 P193 D194 D195
P196 A197 Y198 D199 E200 N201 Q204 D208 I209 K210 V211 M212 N213 D214 L215 V216 D217 K218 R223 K224 A225 S226 G227 E228 Q229 S230 D231 D232 L233 L234 T235 G240 K241 D242 P243 E244 T245 G246 E247 P248 L249 D250 D251 R255 Y256 Q257 I258 I259 T260 E264 G265 H266 S270
G271 L272 L273 S274 F275 A276 L277 Y278 F279 L280 V281 K282 N283 P284 H285 V286 L287 Q288 K289 A290 A291 E292 E293 A294 A295 R296 V297 L298 V299 D300 P301 V302 P303 S304 Y305 K306 Q307 V308 K309 Q310 L311 K312 Y313 V314 G315 M316 V317 L318 N319 E320 A321 L322 R323 L324 W325 P326 T327 A328 P329 A330
F331 S332 L333 Y334 A335 K336 E337 D338 T339 V340 L341 G342 G343 E344 Y345 P346 K349 G350 D351 E352 L353 M354 V355 L356 I357 P358 Q359 L360 H361 R362 D363 K364 T365 I366 D369 D370 V371 E372 E373 F374 R375 P376 E377 R378 F379 E380 N381 P382 S383 A384 I385 P386 Q387 H388 A389 F390 K391 P392
F393 G394 Q397 R398 A399 C400 I401 G402 Q403 Q404 F405 A406 L407 H408 E409 A410 T411 L412 V413 L414 G415 M416 H420 F421 D422 F423 E424 D425 H426 T427 N428 Y429 E430 L431 D432 E435 T436 L437 T438 L439 K440 P441 F444 V445 V446 K447 S450 K451 K452 L455 GLY GLY ILE PRO
SER PRO SER THR GLU GLN SER ALA LYS LYS VAL ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.31Å 166.89Å 224.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.75 15.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.75) 98.4 (15.00-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.253 , 0.338 0.244 , 0.333	Depositor DCC
R_{free} test set	2645 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14913	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PAM, 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	1.67	36/3747 (1.0%)	1.59	47/5068 (0.9%)
1	B	1.55	23/3755 (0.6%)	1.48	39/5078 (0.8%)
1	C	1.63	38/3755 (1.0%)	1.57	57/5078 (1.1%)
1	D	1.45	14/3752 (0.4%)	1.51	49/5072 (1.0%)
All	All	1.58	111/15009 (0.7%)	1.54	192/20296 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	1
All	All	0	8

The worst 5 of 111 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	GLU	CD-OE2	13.82	1.40	1.25
1	C	373	GLU	CD-OE2	13.80	1.40	1.25
1	C	373	GLU	CD-OE1	13.44	1.40	1.25
1	B	244	GLU	CD-OE1	12.02	1.38	1.25
1	C	247	GLU	CD-OE2	10.70	1.37	1.25

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	23	ASP	CB-CG-OD2	16.00	132.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	ASP	CB-CG-OD2	14.22	131.10	118.30
1	C	23	ASP	CB-CG-OD1	-13.91	105.78	118.30
1	A	322	LEU	CB-CG-CD2	-12.58	89.62	111.00
1	C	351	ASP	CB-CG-OD2	12.05	129.15	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ASN	Peptide
1	A	292	GLU	Peptide
1	A	341	LEU	Peptide
1	B	283	ASN	Peptide
1	B	303	PRO	Peptide

5.2 Too-close contacts (i)

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	3662	0	3625	312	2
1	B	3670	0	3635	359	1
1	C	3670	0	3636	393	1
1	D	3667	0	3636	337	0
2	A	43	0	30	14	0
2	B	43	0	30	15	0
2	C	43	0	30	4	0
2	D	43	0	30	13	0
3	A	18	0	29	3	0
3	B	18	0	29	0	0
3	C	18	0	29	6	0
3	D	18	0	29	2	0
All	All	14913	0	14768	1423	2

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 48.

The worst 5 of 1423 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:C:107:PHE:CD2	1:C:401:ILE:HG22	1.45	1.49
1:C:85:GLY:HA2	1:C:257:GLN:NE2	1.50	1.24
1:C:100:HIS:CE1	1:C:104:LEU:HD22	1.72	1.22
1:B:313:TYR:HA	1:B:316:MET:CE	1.71	1.20
1:B:281:VAL:CG1	1:B:425:ASP:HB2	1.71	1.20

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD2	1:C:23:ASP:OD2[2_664]	1.70	0.50
1:A:207:GLU:OE2	1:B:207:GLU:OE2[6_664]	2.04	0.16

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	453/471 (96%)	358 (79%)	66 (15%)	29 (6%)	1	1
1	B	453/471 (96%)	326 (72%)	89 (20%)	38 (8%)	0	0
1	C	453/471 (96%)	307 (68%)	102 (22%)	44 (10%)	0	0
1	D	452/471 (96%)	351 (78%)	72 (16%)	29 (6%)	1	1
All	All	1811/1884 (96%)	1342 (74%)	329 (18%)	140 (8%)	1	0

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	GLY
1	A	365	THR
1	A	377	GLU
1	A	425	ASP
1	A	452	LYS

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	397/413 (96%)	327 (82%)	70 (18%)	1 2
1	B	399/413 (97%)	320 (80%)	79 (20%)	1 1
1	C	399/413 (97%)	327 (82%)	72 (18%)	1 2
1	D	399/413 (97%)	317 (79%)	82 (21%)	1 1
All	All	1594/1652 (96%)	1291 (81%)	303 (19%)	1 1

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	65	SER
1	D	370	ASP
1	D	121	ASP
1	D	233	LEU
1	D	438	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	310	GLN
1	D	404	GLN
1	C	134	ASN
1	D	403	GLN
1	D	171	HIS

5.3.3 RNA (i)

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)

8 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	D	472	1	42,50,50	1.87	9 (21%)	46,82,82	2.37	19 (41%)
2	HEM	A	472	1	42,50,50	1.74	13 (30%)	46,82,82	2.64	19 (41%)
3	PAM	A	1465	-	17,17,17	1.23	2 (11%)	17,17,17	1.23	1 (5%)
3	PAM	B	2465	-	17,17,17	1.29	2 (11%)	17,17,17	1.38	2 (11%)
2	HEM	C	472	1	42,50,50	1.93	13 (30%)	46,82,82	2.73	20 (43%)
3	PAM	C	3465	-	17,17,17	1.32	1 (5%)	17,17,17	1.34	3 (17%)
3	PAM	D	4465	-	17,17,17	1.22	1 (5%)	17,17,17	1.36	2 (11%)
2	HEM	B	472	1	42,50,50	2.44	14 (33%)	46,82,82	2.35	17 (36%)

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	D	472	1	-	4/12/54/54	-
2	HEM	A	472	1	-	3/12/54/54	-
3	PAM	A	1465	-	-	5/15/15/15	-
3	PAM	B	2465	-	-	12/15/15/15	-
2	HEM	C	472	1	-	5/12/54/54	-
3	PAM	C	3465	-	-	6/15/15/15	-
3	PAM	D	4465	-	-	10/15/15/15	-
2	HEM	B	472	1	-	3/12/54/54	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	472	HEM	C3D-C2D	6.41	1.50	1.36
2	B	472	HEM	C3C-C2C	-5.86	1.32	1.40
2	D	472	HEM	C3D-C2D	5.76	1.49	1.36
2	D	472	HEM	C3C-C2C	-5.62	1.32	1.40
2	B	472	HEM	C4D-ND	-5.36	1.31	1.40

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	472	HEM	C4B-CHC-C1C	-7.00	113.32	122.56
2	A	472	HEM	C4C-CHD-C1D	6.74	131.46	122.56
2	A	472	HEM	CMD-C2D-C1D	6.40	135.03	125.03
2	B	472	HEM	CBA-CAA-C2A	-6.39	101.79	112.54
2	D	472	HEM	C3B-C4B-NB	-6.08	105.10	109.47

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4465	PAM	C10-C11-C12-C13
3	A	1465	PAM	C1-C2-C3-C4
3	D	4465	PAM	C12-C13-C14-C15
3	D	4465	PAM	C1-C2-C3-C4
3	B	2465	PAM	C11-C10-C9-C8

There are no ring outliers.

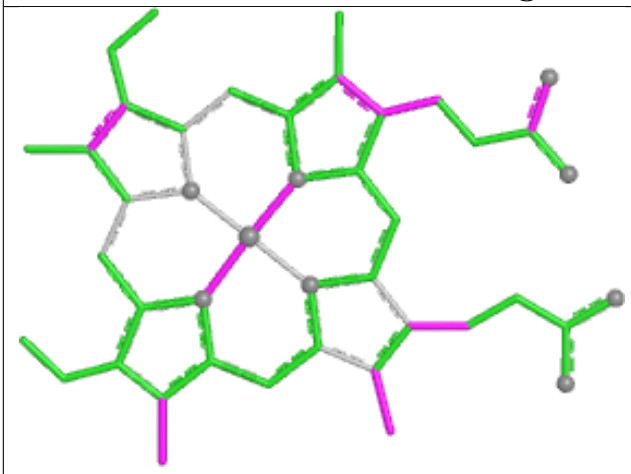
7 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	472	HEM	13	0
2	A	472	HEM	14	0
3	A	1465	PAM	3	0
2	C	472	HEM	4	0
3	C	3465	PAM	6	0
3	D	4465	PAM	2	0
2	B	472	HEM	15	0

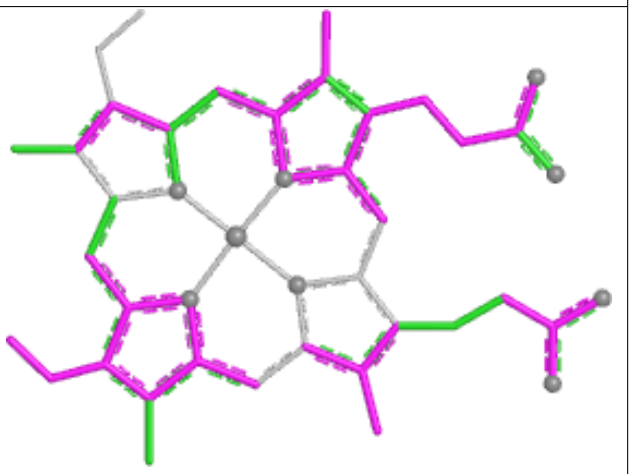
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

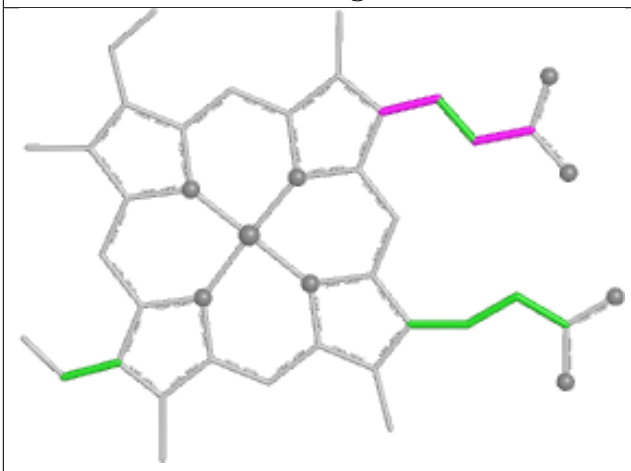
Ligand HEM D 472



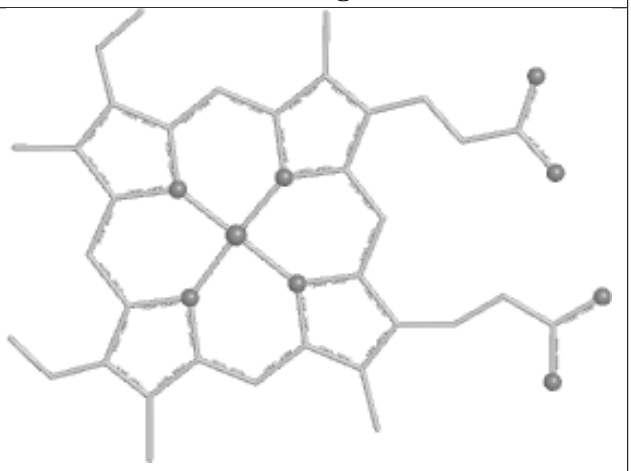
Bond lengths



Bond angles

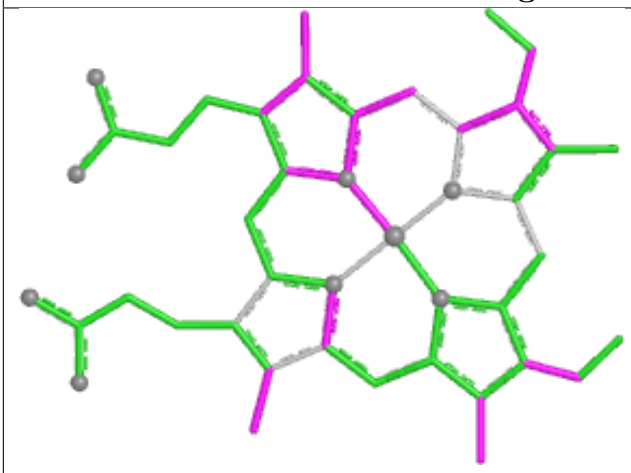


Torsions

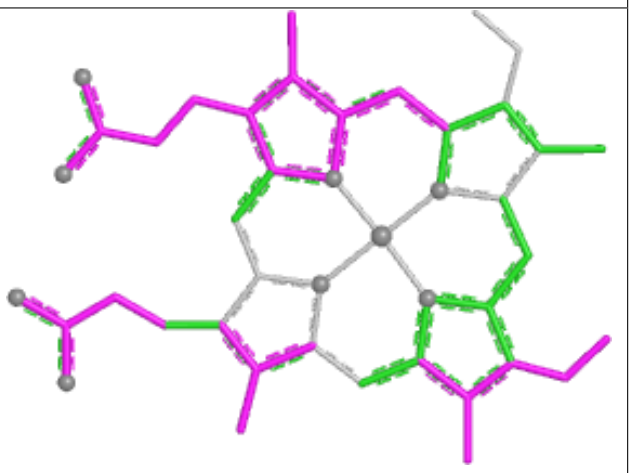


Rings

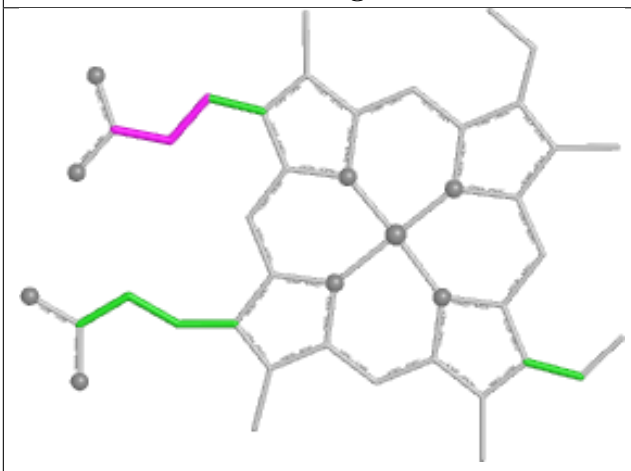
Ligand HEM A 472



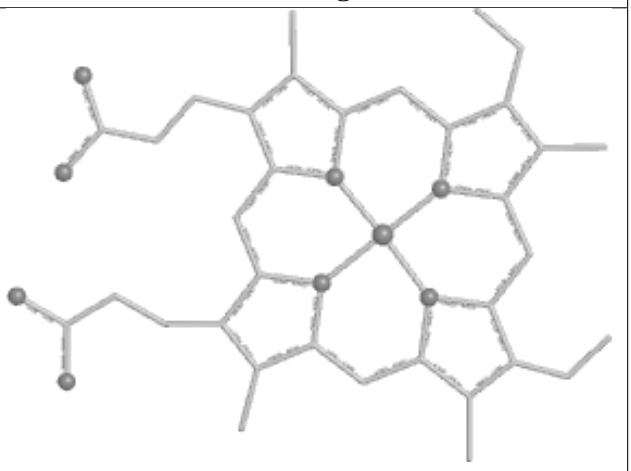
Bond lengths



Bond angles

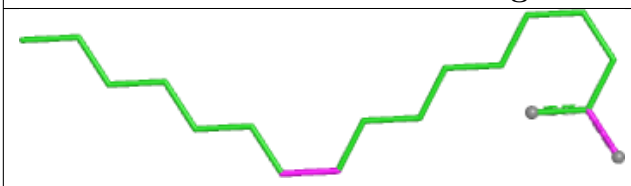


Torsions

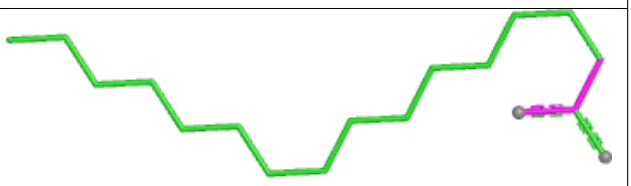


Rings

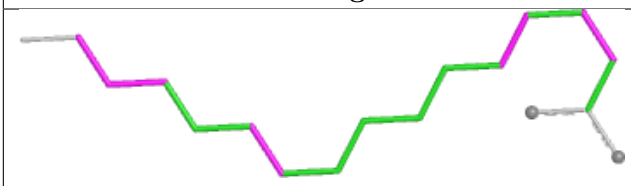
Ligand PAM A 1465



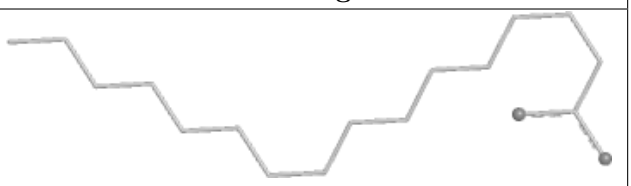
Bond lengths



Bond angles

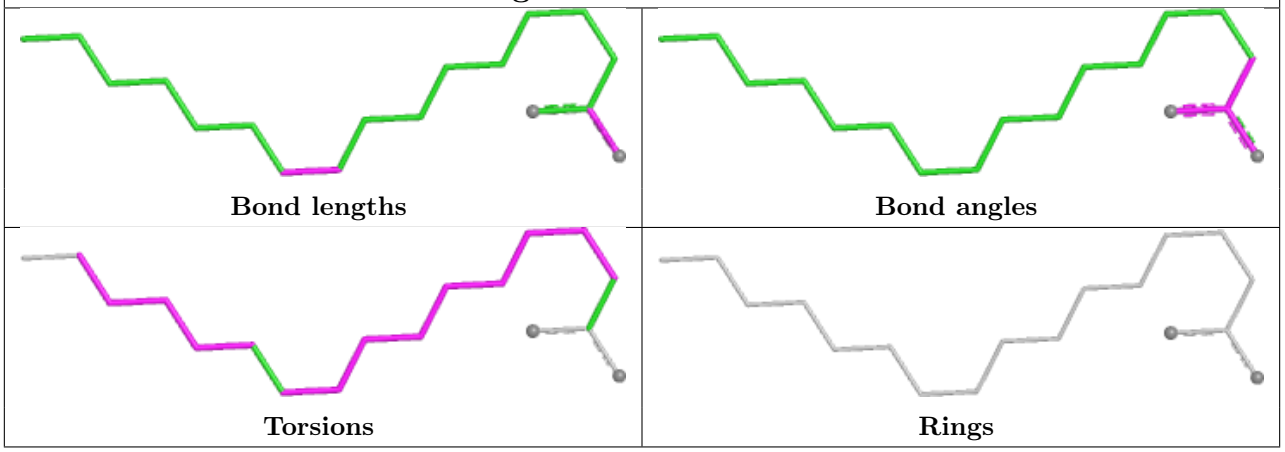


Torsions



Rings

Ligand PAM B 2465



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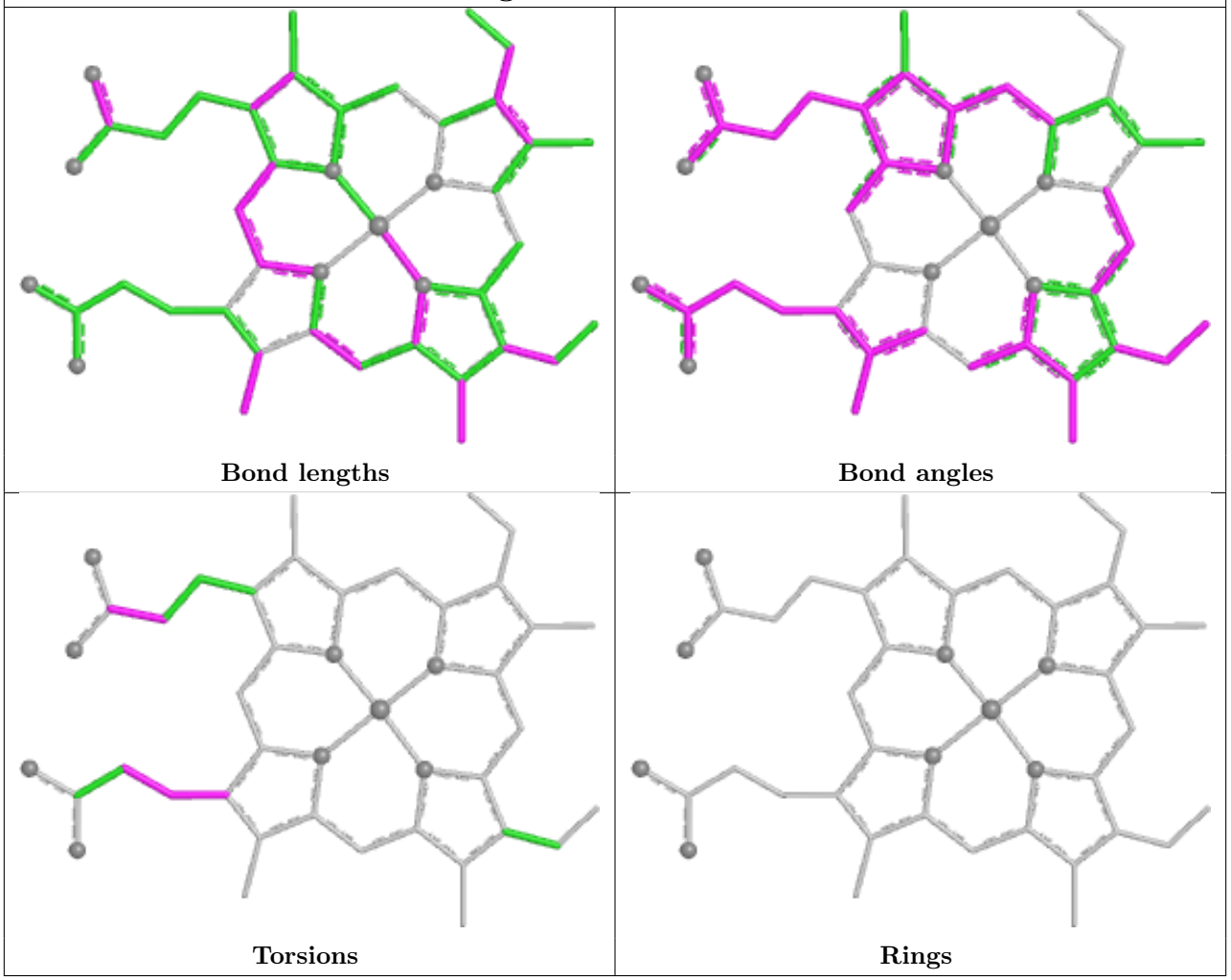
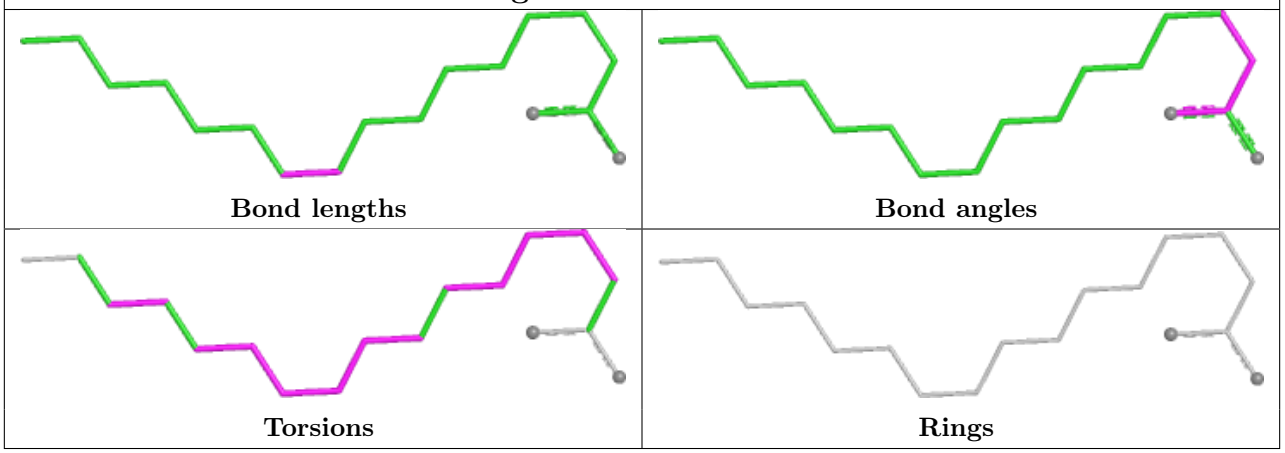
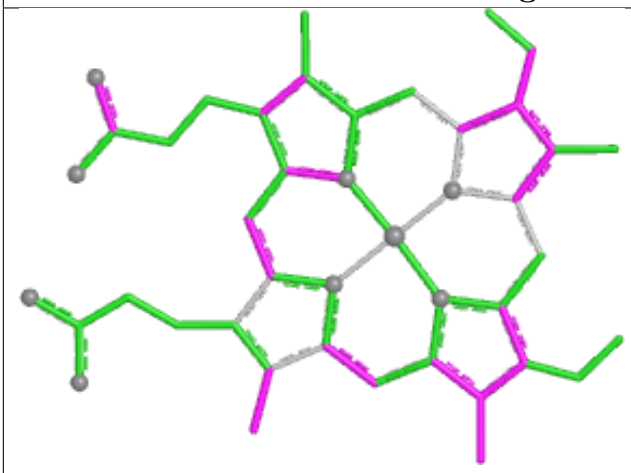


Ligand PAM C 3465

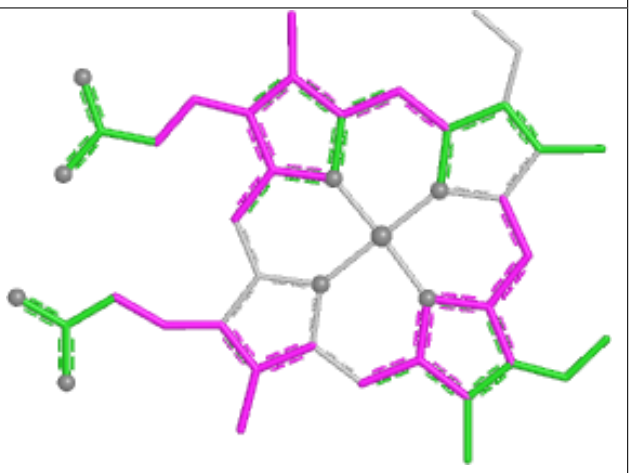
Ligand PAM D 4465



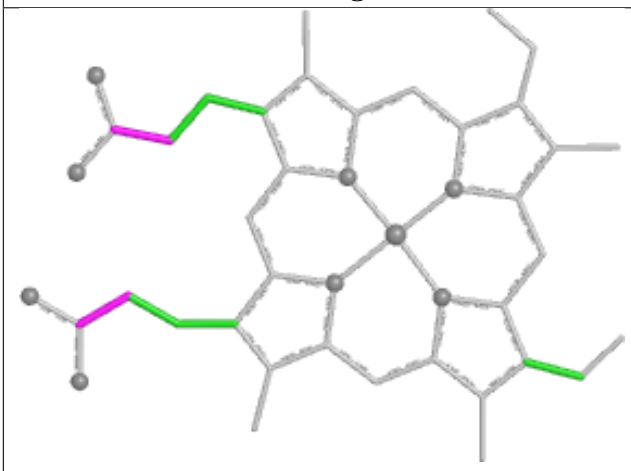
Ligand HEM B 472



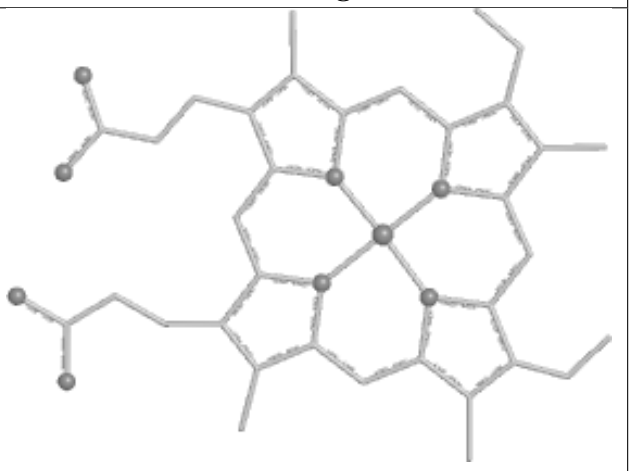
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	455/471 (96%)	-0.62	0	100	100	24, 46, 66, 87	0
1	B	455/471 (96%)	-0.31	4 (0%)	81	83	31, 58, 83, 96	0
1	C	455/471 (96%)	-0.22	1 (0%)	92	93	32, 58, 80, 90	0
1	D	454/471 (96%)	-0.22	4 (0%)	81	83	38, 62, 80, 92	0
All	All	1819/1884 (96%)	-0.34	9 (0%)	87	89	24, 56, 80, 96	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	PRO	2.6
1	B	242	ASP	2.4
1	B	245	THR	2.3
1	D	335	ALA	2.3
1	C	6	PRO	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

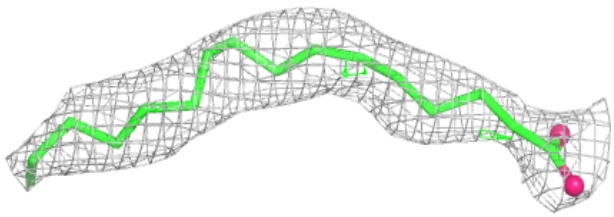
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

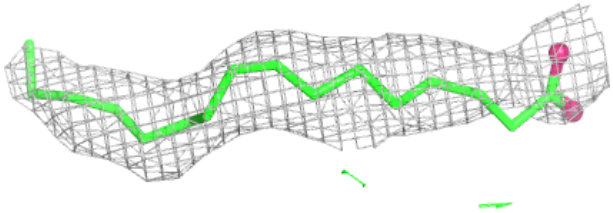
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PAM	B	2465	18/18	0.83	0.10	57,68,74,76	0
3	PAM	D	4465	18/18	0.85	0.10	45,59,78,79	0
3	PAM	C	3465	18/18	0.88	0.09	43,50,71,73	0
3	PAM	A	1465	18/18	0.90	0.07	30,45,62,64	0
2	HEM	C	472	43/43	0.96	0.07	23,30,48,54	0
2	HEM	D	472	43/43	0.96	0.07	29,40,55,60	0
2	HEM	B	472	43/43	0.96	0.07	27,35,59,68	0
2	HEM	A	472	43/43	0.98	0.06	18,27,38,43	0

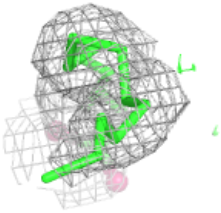
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAM B 2465:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

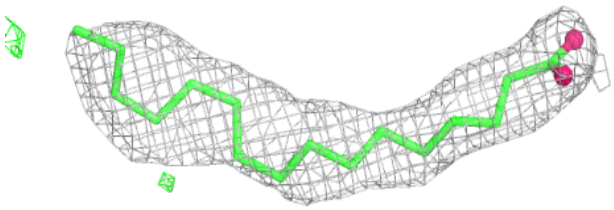


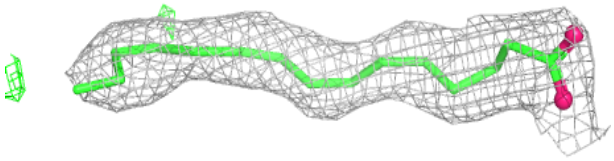


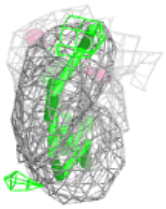


Electron density around PAM D 4465:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

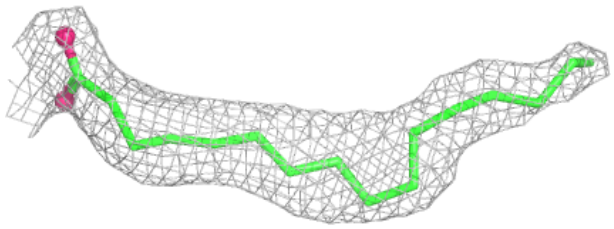


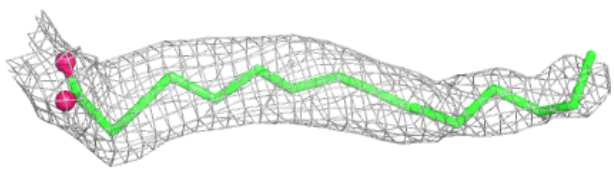


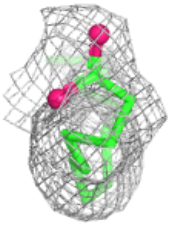


Electron density around PAM C 3465:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

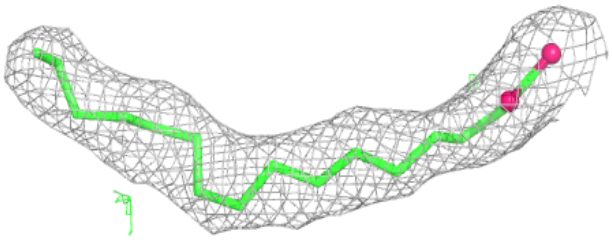


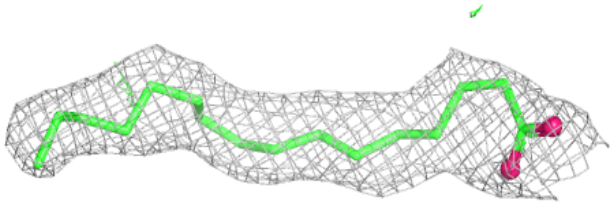


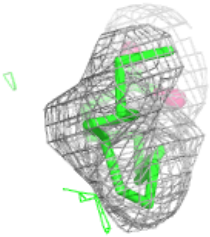


Electron density around PAM A 1465:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

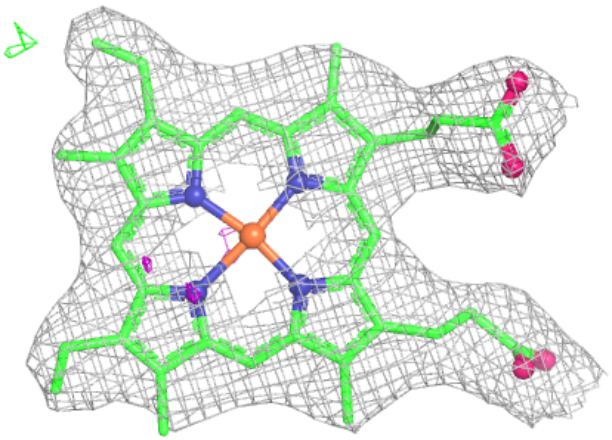


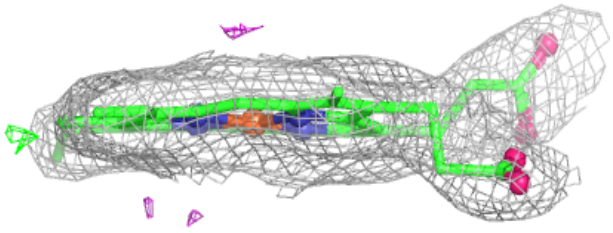


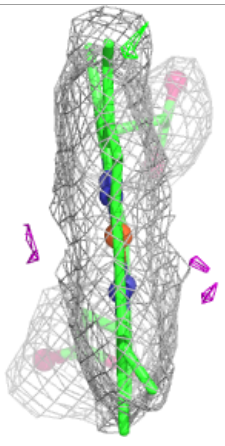


Electron density around HEM C 472:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

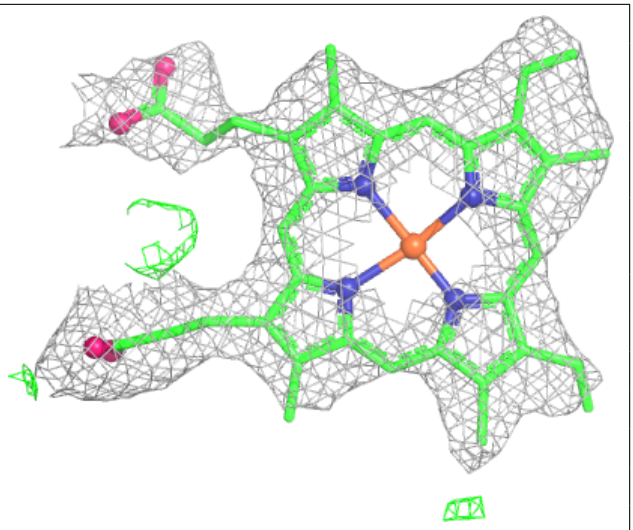


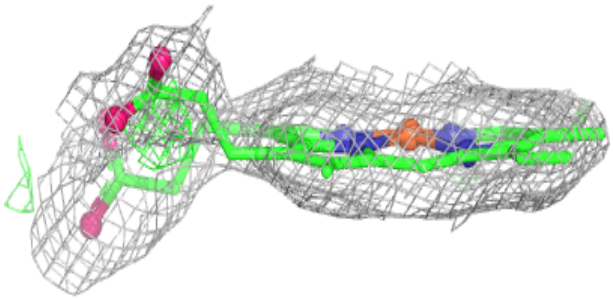


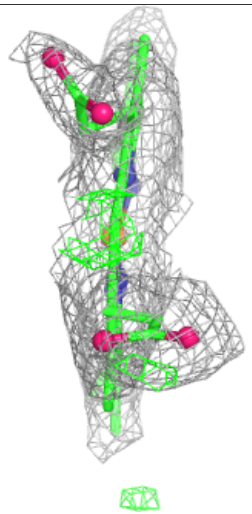


Electron density around HEM D 472:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

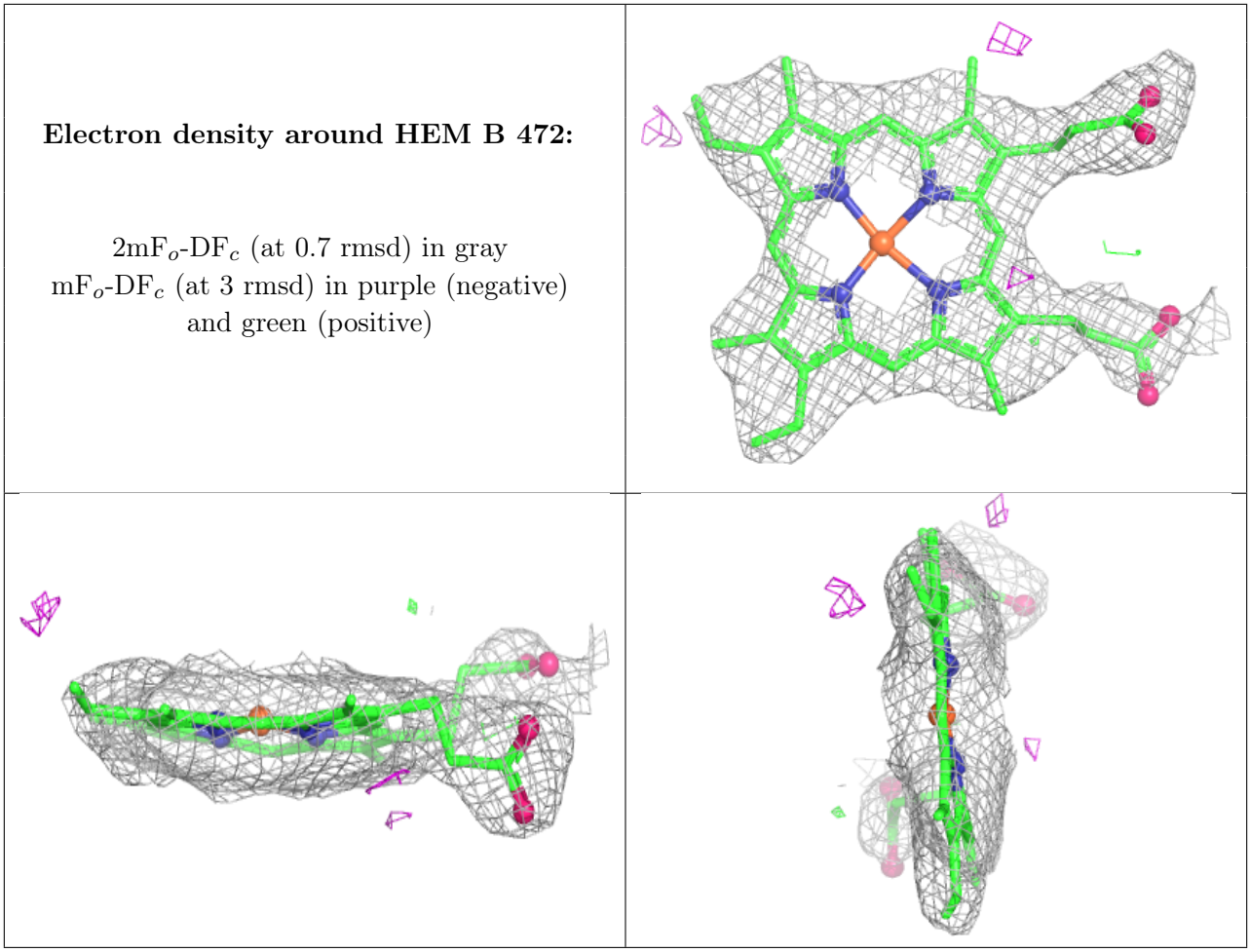






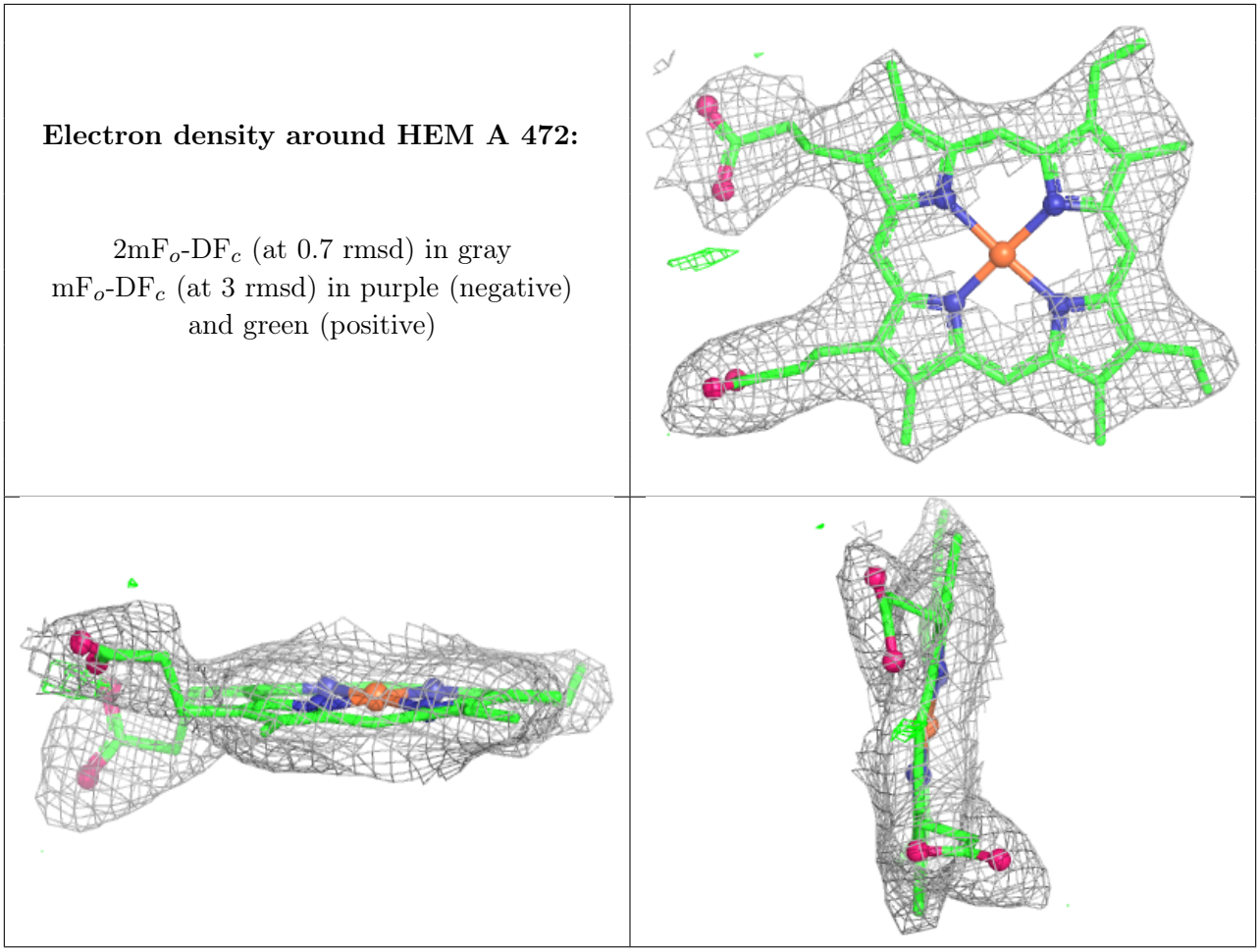
Electron density around HEM B 472:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEM A 472:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.