wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2025 – 10:55 PM EDT

PDB ID	:	3QU8 / pdb_00003qu8
Title	:	Crystal structure of a human cytochrome P450 2B6 (Y226H/K262R) in complex with the inhibitor 4-(4-Nitrobenzyl)pyridine.
Authors	:	Shah, M.B.; Pascual, J.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2011-02-23
Resolution	:	2.80 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:

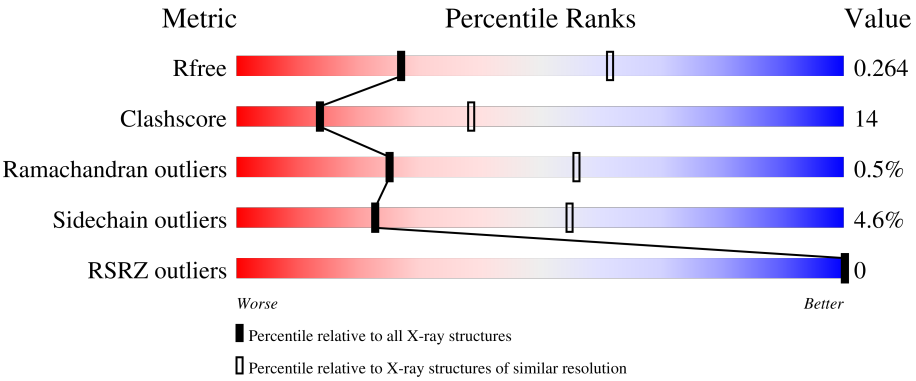
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	476	74% 20%
1	B	476	74% 20%
1	C	476	73% 21%
1	D	476	72% 21%
1	E	476	70% 24%

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Mol	Chain	Length	Quality of chain
1	F	476	68% 24% 5%

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
4	CM5	D	604	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22964 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 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total 3732	C 2416	N 641	O 658	S 17	0	0	0
1	B	459	Total 3713	C 2403	N 639	O 655	S 16	0	0	0
1	C	462	Total 3724	C 2408	N 642	O 658	S 16	0	0	0
1	D	458	Total 3693	C 2389	N 635	O 653	S 16	0	0	0
1	E	459	Total 3717	C 2406	N 640	O 655	S 16	0	0	0
1	F	453	Total 3649	C 2359	N 625	O 649	S 16	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	engineered mutation	UNP P20813
A	22	LYS	ARG	engineered mutation	UNP P20813
A	23	LYS	HIS	engineered mutation	UNP P20813
A	24	THR	PRO	engineered mutation	UNP P20813
A	25	SER	ASN	engineered mutation	UNP P20813
A	26	SER	THR	engineered mutation	UNP P20813
A	27	LYS	HIS	engineered mutation	UNP P20813
A	28	GLY	ASP	engineered mutation	UNP P20813
A	29	LYS	ARG	engineered mutation	UNP P20813
A	226	HIS	TYR	engineered mutation	UNP P20813
A	262	ARG	LYS	engineered mutation	UNP P20813
A	492	HIS	-	expression tag	UNP P20813
A	493	HIS	-	expression tag	UNP P20813
A	494	HIS	-	expression tag	UNP P20813
A	495	HIS	-	expression tag	UNP P20813
B	2	ALA	GLU	engineered mutation	UNP P20813
B	22	LYS	ARG	engineered mutation	UNP P20813

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	LYS	HIS	engineered mutation	UNP P20813
B	24	THR	PRO	engineered mutation	UNP P20813
B	25	SER	ASN	engineered mutation	UNP P20813
B	26	SER	THR	engineered mutation	UNP P20813
B	27	LYS	HIS	engineered mutation	UNP P20813
B	28	GLY	ASP	engineered mutation	UNP P20813
B	29	LYS	ARG	engineered mutation	UNP P20813
B	226	HIS	TYR	engineered mutation	UNP P20813
B	262	ARG	LYS	engineered mutation	UNP P20813
B	492	HIS	-	expression tag	UNP P20813
B	493	HIS	-	expression tag	UNP P20813
B	494	HIS	-	expression tag	UNP P20813
B	495	HIS	-	expression tag	UNP P20813
C	2	ALA	GLU	engineered mutation	UNP P20813
C	22	LYS	ARG	engineered mutation	UNP P20813
C	23	LYS	HIS	engineered mutation	UNP P20813
C	24	THR	PRO	engineered mutation	UNP P20813
C	25	SER	ASN	engineered mutation	UNP P20813
C	26	SER	THR	engineered mutation	UNP P20813
C	27	LYS	HIS	engineered mutation	UNP P20813
C	28	GLY	ASP	engineered mutation	UNP P20813
C	29	LYS	ARG	engineered mutation	UNP P20813
C	226	HIS	TYR	engineered mutation	UNP P20813
C	262	ARG	LYS	engineered mutation	UNP P20813
C	492	HIS	-	expression tag	UNP P20813
C	493	HIS	-	expression tag	UNP P20813
C	494	HIS	-	expression tag	UNP P20813
C	495	HIS	-	expression tag	UNP P20813
D	2	ALA	GLU	engineered mutation	UNP P20813
D	22	LYS	ARG	engineered mutation	UNP P20813
D	23	LYS	HIS	engineered mutation	UNP P20813
D	24	THR	PRO	engineered mutation	UNP P20813
D	25	SER	ASN	engineered mutation	UNP P20813
D	26	SER	THR	engineered mutation	UNP P20813
D	27	LYS	HIS	engineered mutation	UNP P20813
D	28	GLY	ASP	engineered mutation	UNP P20813
D	29	LYS	ARG	engineered mutation	UNP P20813
D	226	HIS	TYR	engineered mutation	UNP P20813
D	262	ARG	LYS	engineered mutation	UNP P20813
D	492	HIS	-	expression tag	UNP P20813
D	493	HIS	-	expression tag	UNP P20813
D	494	HIS	-	expression tag	UNP P20813

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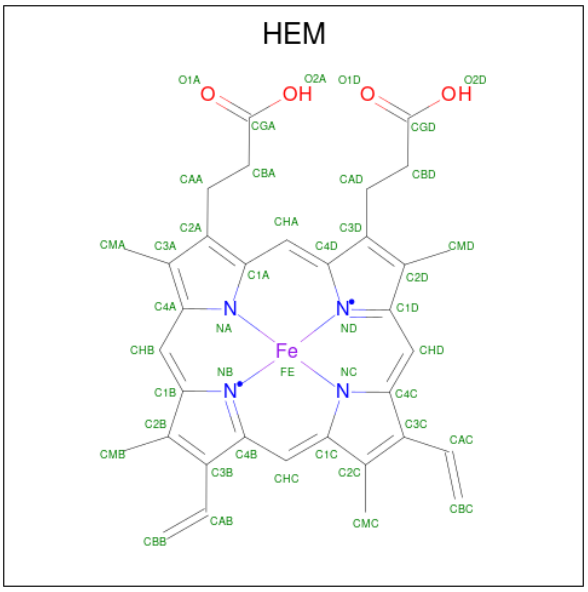
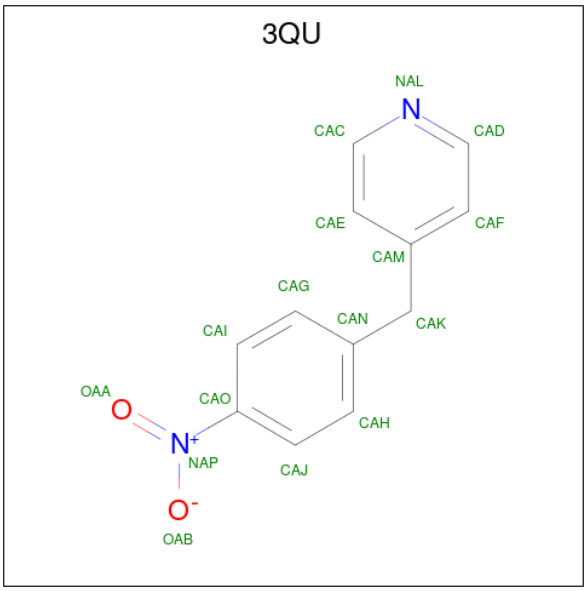
Chain	Residue	Modelled	Actual	Comment	Reference
D	495	HIS	-	expression tag	UNP P20813
E	2	ALA	GLU	engineered mutation	UNP P20813
E	22	LYS	ARG	engineered mutation	UNP P20813
E	23	LYS	HIS	engineered mutation	UNP P20813
E	24	THR	PRO	engineered mutation	UNP P20813
E	25	SER	ASN	engineered mutation	UNP P20813
E	26	SER	THR	engineered mutation	UNP P20813
E	27	LYS	HIS	engineered mutation	UNP P20813
E	28	GLY	ASP	engineered mutation	UNP P20813
E	29	LYS	ARG	engineered mutation	UNP P20813
E	226	HIS	TYR	engineered mutation	UNP P20813
E	262	ARG	LYS	engineered mutation	UNP P20813
E	492	HIS	-	expression tag	UNP P20813
E	493	HIS	-	expression tag	UNP P20813
E	494	HIS	-	expression tag	UNP P20813
E	495	HIS	-	expression tag	UNP P20813
F	2	ALA	GLU	engineered mutation	UNP P20813
F	22	LYS	ARG	engineered mutation	UNP P20813
F	23	LYS	HIS	engineered mutation	UNP P20813
F	24	THR	PRO	engineered mutation	UNP P20813
F	25	SER	ASN	engineered mutation	UNP P20813
F	26	SER	THR	engineered mutation	UNP P20813
F	27	LYS	HIS	engineered mutation	UNP P20813
F	28	GLY	ASP	engineered mutation	UNP P20813
F	29	LYS	ARG	engineered mutation	UNP P20813
F	226	HIS	TYR	engineered mutation	UNP P20813
F	262	ARG	LYS	engineered mutation	UNP P20813
F	492	HIS	-	expression tag	UNP P20813
F	493	HIS	-	expression tag	UNP P20813
F	494	HIS	-	expression tag	UNP P20813
F	495	HIS	-	expression tag	UNP P20813

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



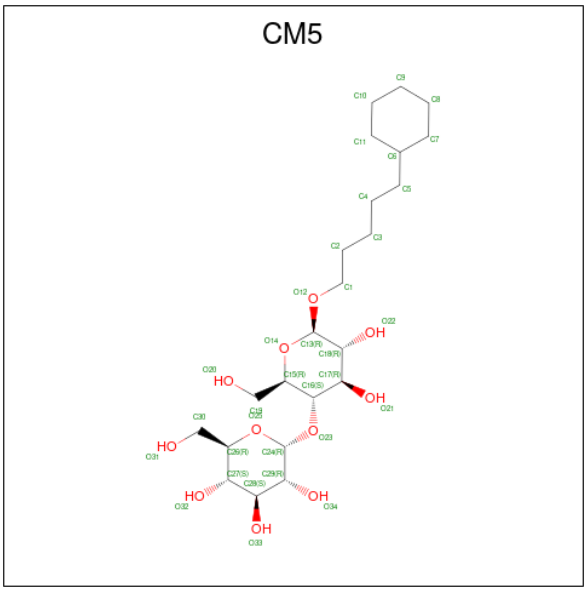
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 4-(4-nitrobenzyl)pyridine (CCD ID: 3QU) (formula: $C_{12}H_{10}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 7 6 1	0	0
3	B	1	Total C N O 16 12 2 2	0	0
3	C	1	Total C N 7 6 1	0	0
3	D	1	Total C N 13 12 1	0	0
3	E	1	Total C N 13 12 1	0	0

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (CCD ID: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 34 23 11	0	0
4	B	1	Total C O 34 23 11	0	0
4	B	1	Total C O 34 23 11	0	0
4	C	1	Total C O 34 23 11	0	0
4	D	1	Total C O 34 23 11	0	0
4	D	1	Total C O 34 23 11	0	0
4	E	1	Total C O 34 23 11	0	0
4	F	1	Total C O 34 23 11	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	B	23	Total O 23 23	0	0
5	C	29	Total O 29 29	0	0
5	D	38	Total O 38 38	0	0

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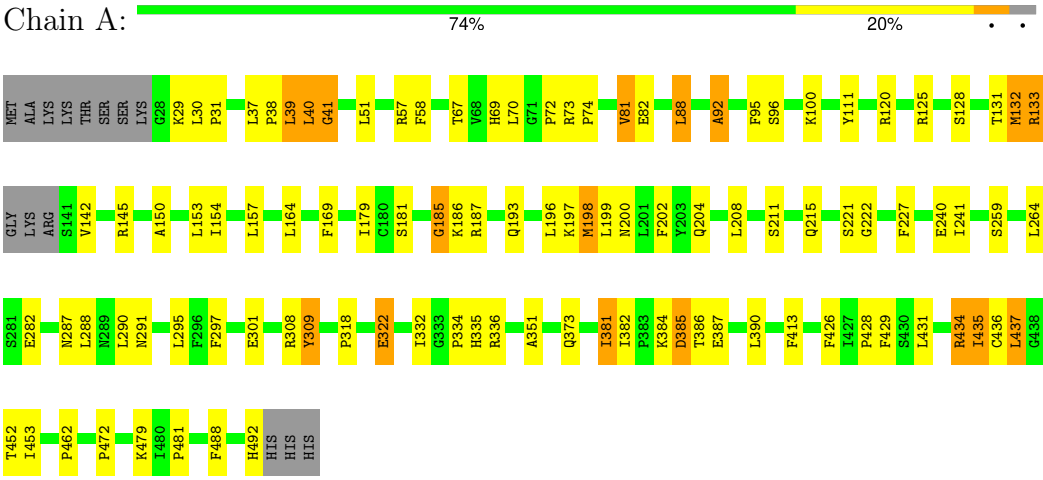
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	23	Total O 23 23	0	0
5	F	12	Total O 12 12	0	0

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.

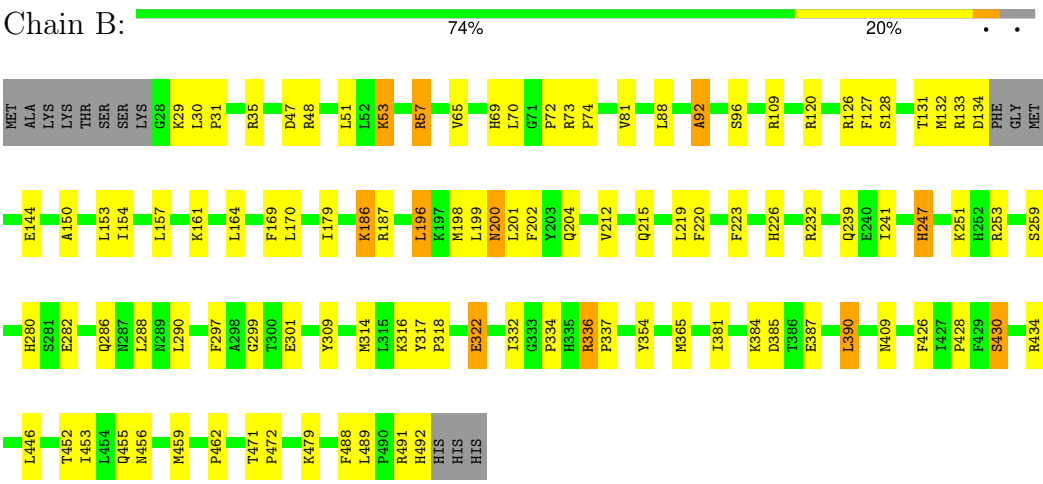
• Molecule 1: Cytochrome P450 2B6

Chain A:



• Molecule 1: Cytochrome P450 2B6

Chain B:

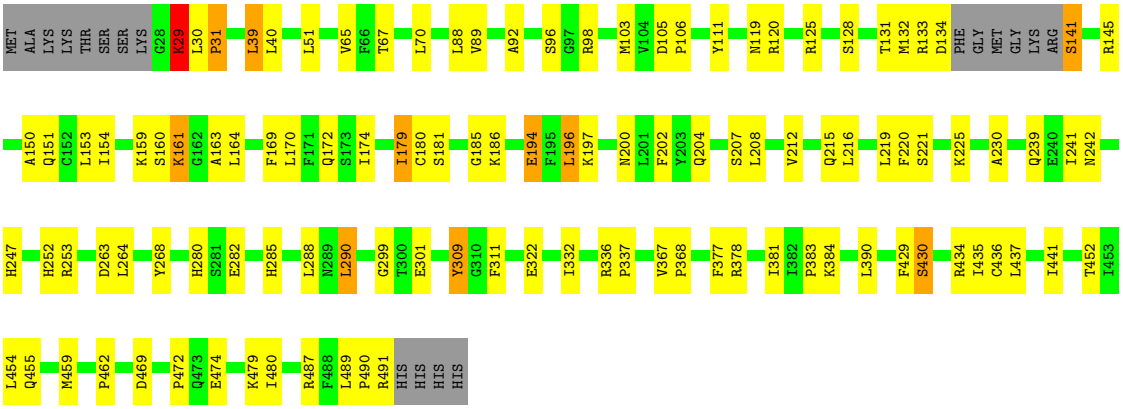


• Molecule 1: Cytochrome P450 2B6

Chain C:

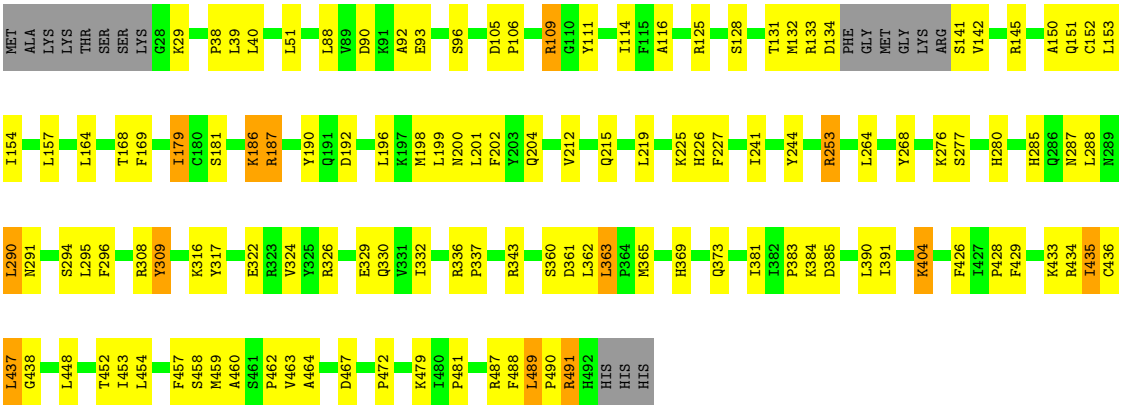
• Molecule 1: Cytochrome P450 2B6

Chain D:



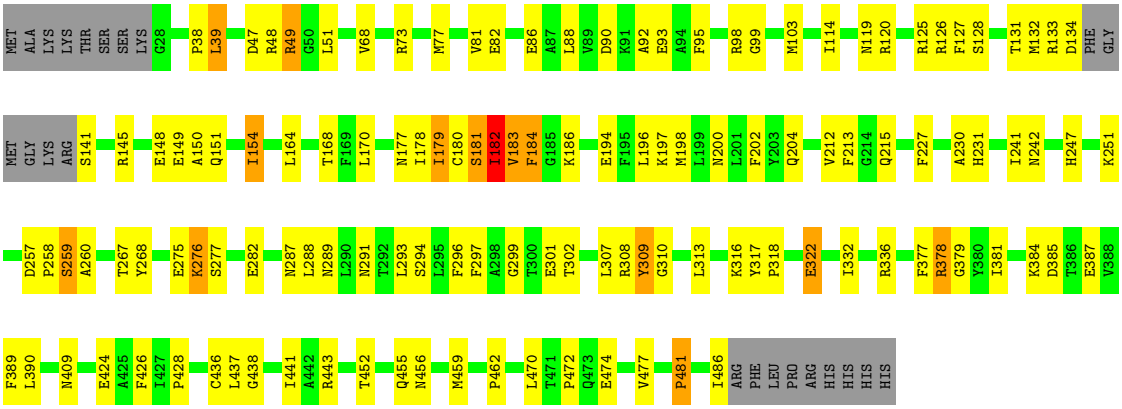
• Molecule 1: Cytochrome P450 2B6

Chain E:



• Molecule 1: Cytochrome P450 2B6

Chain F:


MET ALA LYS LYS THR SER SER LYS G28 P38 L39 D47 R48 R49 G50 L51 V68 R73 M77 V81 E82 E86 A87 L88 V89 D90 K91 A92 E93 A94 F95 R98 G99 M103 I114 N119 R120 R125 R126 F127 S128 T131 M132 R133 D134 PHE GLY
MET GLY LYS ARG S141 R145 E148 E149 A150 Q151 I154 L164 T168 F169 L170 N177 I178 I179 C180 S181 I182 V183 F184 G185 K186 E194 F195 L196 K197 M198 L199 N200 L201 F202 Y203 Q204 V212 F213 G214 Q215 F227 A230 H231 I241 N242 H247 K251
D257 P258 S259 A260 T267 Y268 E275 K276 S277 E282 N287 L288 N289 L290 N291 T292 L293 S294 L295 F296 F297 A298 G299 T300 E301 T302 L307 R308 Y309 G310 L313 K316 Y317 P318 E322 I332 R336 F377 R378 G379 Y380 I381 K384 D385 T386 E387 V388
F389 L390 N409 E424 A425 F426 I427 P428 C436 L437 G438 I441 A442 R443 T452 Q455 N456 M459 P462 L470 T471 P472 Q473 E474 V477 P481 I486 ARG PHE LEU PRO ARG HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	101.88Å 101.88Å 299.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.51 – 2.80 50.51 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (50.51-2.80) 88.9 (50.51-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.218 , 0.259 0.226 , 0.264	Depositor DCC
R_{free} test set	3810 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l 0.149 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22964	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CM5, 3QU

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	1.06	2/3833 (0.1%)	1.06	6/5185 (0.1%)
1	B	1.05	2/3813 (0.1%)	1.08	10/5158 (0.2%)
1	C	1.11	4/3822 (0.1%)	1.06	9/5167 (0.2%)
1	D	1.05	4/3791 (0.1%)	1.09	10/5129 (0.2%)
1	E	1.02	1/3817 (0.0%)	1.05	9/5162 (0.2%)
1	F	1.11	2/3745 (0.1%)	1.11	12/5067 (0.2%)
All	All	1.07	15/22821 (0.1%)	1.07	56/30868 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ALA	CA-CB	-6.19	1.43	1.53
1	E	90	ASP	N-CA	6.09	1.54	1.46
1	F	183	VAL	CA-CB	-5.83	1.48	1.55
1	C	93	GLU	CA-C	5.68	1.60	1.52
1	D	89	VAL	C-O	-5.67	1.17	1.24

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	40	LEU	N-CA-C	-9.21	103.15	114.75
1	F	183	VAL	CB-CA-C	-7.98	103.86	111.44
1	A	185	GLY	N-CA-C	7.70	126.76	114.90
1	D	480	ILE	CA-C-N	7.32	124.93	119.66
1	D	480	ILE	C-N-CA	7.32	124.93	119.66

There are no chirality outliers.

There are no planarity outliers.

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	3732	0	3712	107	0
1	B	3713	0	3702	97	0
1	C	3724	0	3711	87	0
1	D	3693	0	3682	100	0
1	E	3717	0	3713	123	0
1	F	3649	0	3635	103	0
2	A	43	0	30	10	0
2	B	43	0	30	4	0
2	C	43	0	30	9	0
2	D	43	0	30	12	0
2	E	43	0	30	9	0
2	F	43	0	30	18	0
3	A	7	0	4	0	0
3	B	16	0	10	0	0
3	C	7	0	4	0	0
3	D	13	0	10	0	0
3	E	13	0	10	1	0
4	A	34	0	35	1	0
4	B	68	0	77	34	0
4	C	34	0	40	5	0
4	D	68	0	78	12	0
4	E	34	0	40	3	0
4	F	34	0	38	5	0
5	A	25	0	0	1	0
5	B	23	0	0	12	0
5	C	29	0	0	2	0
5	D	38	0	0	5	0
5	E	23	0	0	5	0
5	F	12	0	0	5	0
All	All	22964	0	22681	652	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 14.

The worst 5 of 652 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)
4:B:608:CM5:O23	4:B:608:CM5:C16	1.64	1.42
1:D:454:LEU:CD2	1:D:459:MET:HE1	1.60	1.29
4:B:608:CM5:C24	4:B:608:CM5:H17	1.61	1.28
1:A:381:ILE:HG21	1:B:239:GLN:CG	1.65	1.25
1:A:136:GLY:HA2	1:A:142:VAL:CG2	1.65	1.24

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	458/476 (96%)	436 (95%)	18 (4%)	4 (1%)	14	42
1	B	455/476 (96%)	431 (95%)	21 (5%)	3 (1%)	19	48
1	C	456/476 (96%)	424 (93%)	30 (7%)	2 (0%)	30	61
1	D	454/476 (95%)	424 (93%)	28 (6%)	2 (0%)	30	61
1	E	455/476 (96%)	433 (95%)	22 (5%)	0	100	100
1	F	449/476 (94%)	417 (93%)	29 (6%)	3 (1%)	19	48
All	All	2727/2856 (96%)	2565 (94%)	148 (5%)	14 (0%)	25	56

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	430	SER
1	F	276	LYS
1	F	378	ARG
1	B	430	SER
1	C	190	TYR

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	404/418 (97%)	386 (96%)	18 (4%)	23	55
1	B	403/418 (96%)	380 (94%)	23 (6%)	17	46
1	C	402/418 (96%)	382 (95%)	20 (5%)	20	51
1	D	400/418 (96%)	385 (96%)	15 (4%)	28	62
1	E	404/418 (97%)	383 (95%)	21 (5%)	19	50
1	F	396/418 (95%)	381 (96%)	15 (4%)	28	62
All	All	2409/2508 (96%)	2297 (95%)	112 (5%)	23	55

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	404	LYS
1	F	441	ILE
1	D	309	TYR
1	F	381	ILE
1	F	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	233	GLN
1	E	286	GLN
1	D	485	GLN
1	E	357	GLN
1	B	172	GLN

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)

19 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	E	500	1,3	42,50,50	1.96	5 (11%)	46,82,82	1.59	6 (13%)
4	CM5	B	602	-	36,36,36	2.84	9 (25%)	49,49,49	4.88	23 (46%)
4	CM5	D	604	-	36,36,36	4.12	16 (44%)	49,49,49	6.30	24 (48%)
4	CM5	E	605	-	36,36,36	3.44	14 (38%)	49,49,49	3.20	23 (46%)
4	CM5	C	603	-	36,36,36	3.34	13 (36%)	49,49,49	5.38	22 (44%)
4	CM5	A	601	-	36,36,36	4.12	16 (44%)	49,49,49	5.41	26 (53%)
4	CM5	F	606	-	36,36,36	3.00	13 (36%)	49,49,49	4.34	25 (51%)
2	HEM	F	500	1	42,50,50	1.95	6 (14%)	46,82,82	1.58	6 (13%)
3	3QU	A	501	2	7,7,17	0.28	0	8,8,22	1.31	0
2	HEM	A	500	1,3	42,50,50	1.95	6 (14%)	46,82,82	1.59	6 (13%)
3	3QU	D	501	2	14,14,17	0.33	0	17,17,22	0.90	0
4	CM5	B	608	-	36,36,36	3.16	15 (41%)	49,49,49	5.96	27 (55%)
4	CM5	D	607	-	36,36,36	3.53	13 (36%)	49,49,49	4.99	26 (53%)
2	HEM	D	500	1,3	42,50,50	1.95	5 (11%)	46,82,82	1.60	6 (13%)
3	3QU	B	501	2	17,17,17	0.81	1 (5%)	20,22,22	1.75	7 (35%)
2	HEM	C	500	1,3	42,50,50	2.35	15 (35%)	46,82,82	2.42	15 (32%)
2	HEM	B	500	1,3	42,50,50	1.95	9 (21%)	46,82,82	1.83	13 (28%)
3	3QU	C	501	2	7,7,17	0.29	0	8,8,22	1.29	0
3	3QU	E	501	2	14,14,17	0.86	0	17,17,22	0.95	1 (5%)

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	E	500	1,3	-	2/12/54/54	-
4	CM5	B	602	-	-	9/17/65/65	0/3/3/3
4	CM5	D	604	-	1/1/11/11	9/17/65/65	0/3/3/3
4	CM5	E	605	-	-	9/17/65/65	0/3/3/3
4	CM5	C	603	-	-	11/17/65/65	0/3/3/3
4	CM5	A	601	-	-	11/17/65/65	0/3/3/3
4	CM5	F	606	-	-	5/17/65/65	0/3/3/3
2	HEM	F	500	1	-	4/12/54/54	-
3	3QU	D	501	2	-	0/4/4/8	0/2/2/2
2	HEM	A	500	1,3	-	4/12/54/54	-
3	3QU	A	501	2	-	-	0/1/1/2
4	CM5	B	608	-	-	11/17/65/65	0/3/3/3
4	CM5	D	607	-	-	13/17/65/65	0/3/3/3
2	HEM	D	500	1,3	-	5/12/54/54	-
3	3QU	B	501	2	-	0/6/8/8	0/2/2/2
2	HEM	C	500	1,3	-	6/12/54/54	-
2	HEM	B	500	1,3	-	4/12/54/54	-
3	3QU	C	501	2	-	-	0/1/1/2
3	3QU	E	501	2	-	0/4/4/8	0/2/2/2

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	CM5	O23-C24	-13.40	1.04	1.41
4	A	601	CM5	O21-C17	-12.91	1.11	1.43
4	E	605	CM5	O23-C24	-11.11	1.10	1.41
4	D	604	CM5	C29-C28	-11.05	1.23	1.52
4	D	604	CM5	O25-C26	-10.77	1.18	1.44

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	604	CM5	O23-C16-C17	19.80	157.57	107.23
4	F	606	CM5	O12-C13-C18	-17.68	81.43	108.27
4	B	608	CM5	O14-C15-C19	-17.38	63.38	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	603	CM5	O33-C28-C27	-17.27	69.67	110.38
4	B	608	CM5	O14-C13-O12	-16.72	70.54	110.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	604	CM5	C16

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C1A-C2A-CAA-CBA
2	A	500	HEM	C3A-C2A-CAA-CBA
4	B	602	CM5	C18-C13-O12-C1
4	B	602	CM5	O14-C13-O12-C1
4	E	605	CM5	O14-C13-O12-C1

There are no ring outliers.

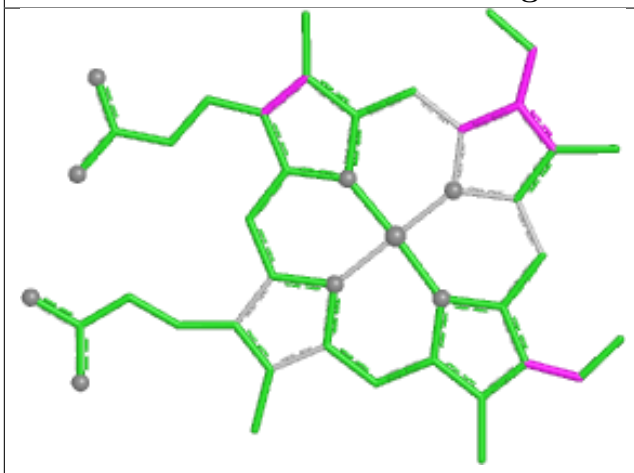
15 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	HEM	9	0
4	B	602	CM5	14	0
4	D	604	CM5	4	0
4	E	605	CM5	3	0
4	C	603	CM5	5	0
4	A	601	CM5	1	0
4	F	606	CM5	5	0
2	F	500	HEM	18	0
2	A	500	HEM	10	0
4	B	608	CM5	20	0
4	D	607	CM5	8	0
2	D	500	HEM	12	0
2	C	500	HEM	9	0
2	B	500	HEM	4	0
3	E	501	3QU	1	0

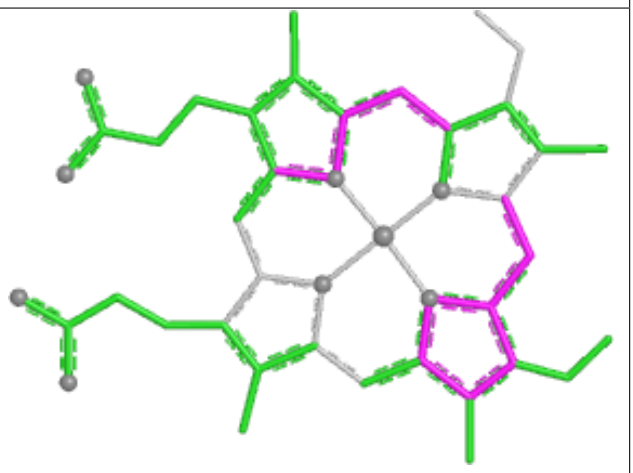
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

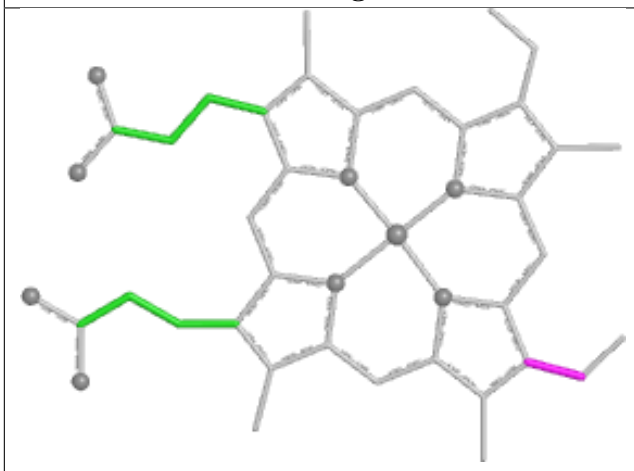
Ligand HEM E 500



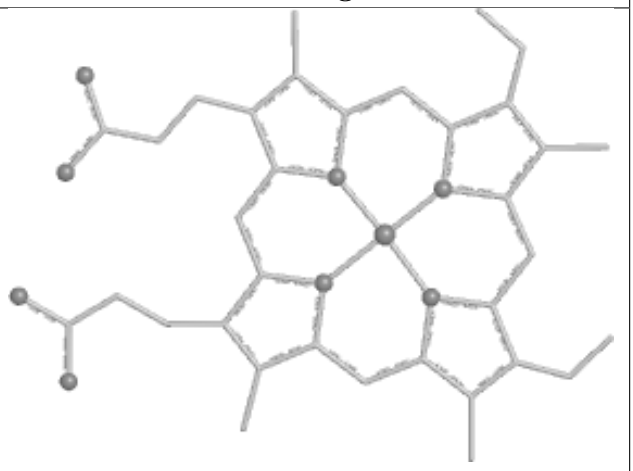
Bond lengths



Bond angles

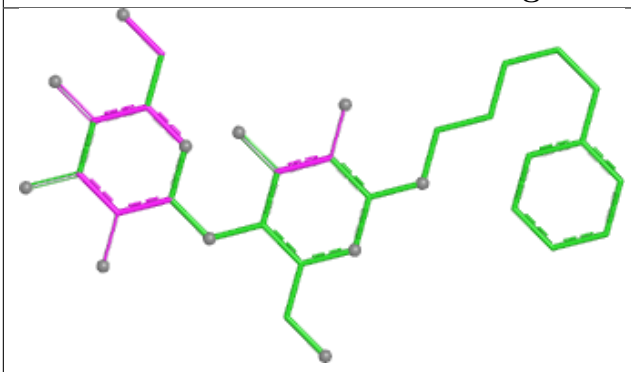


Torsions



Rings

Ligand CM5 B 602



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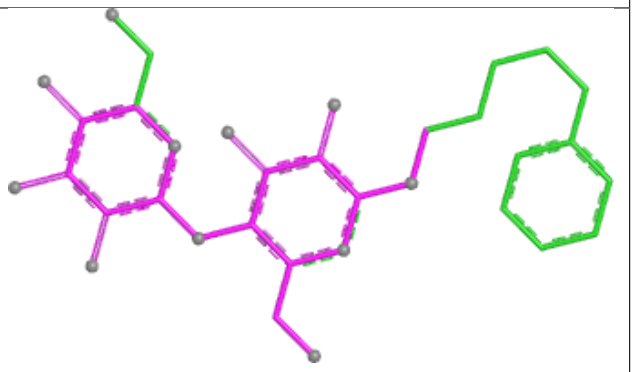

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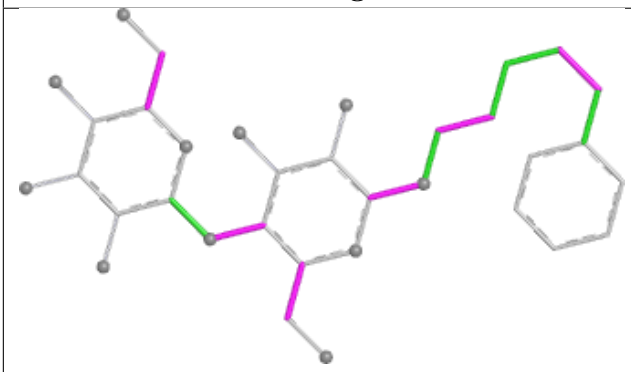

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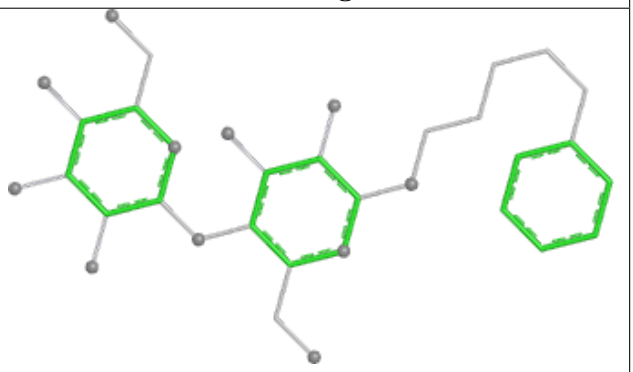
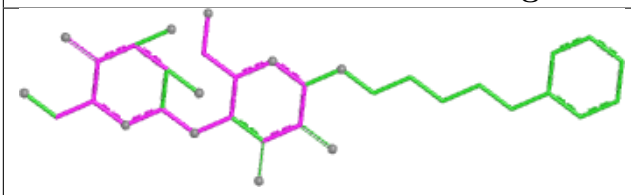


Rings

Ligand CM5 D 604



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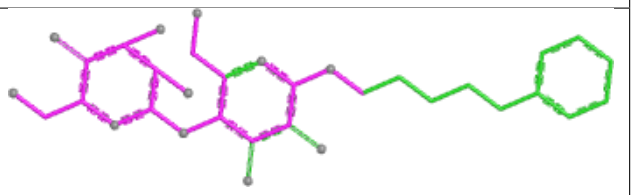

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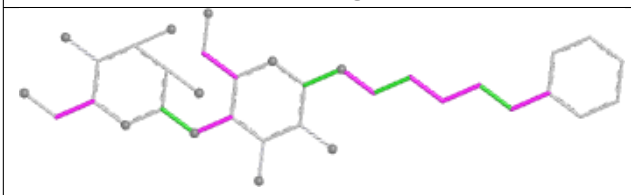

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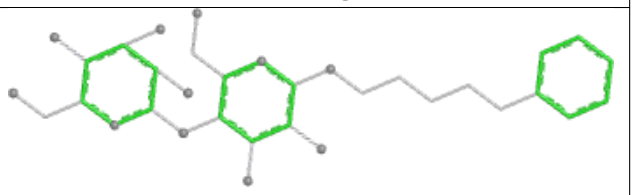
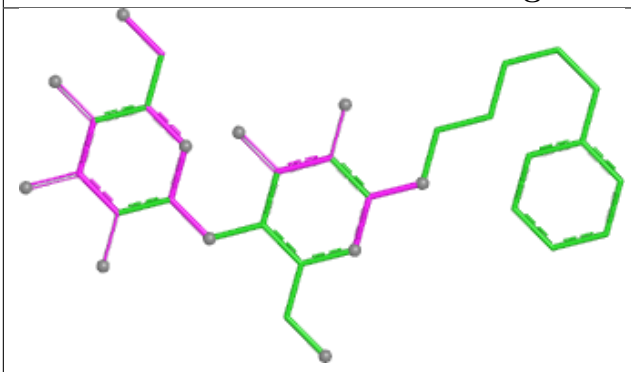


Rings

Ligand CM5 E 605



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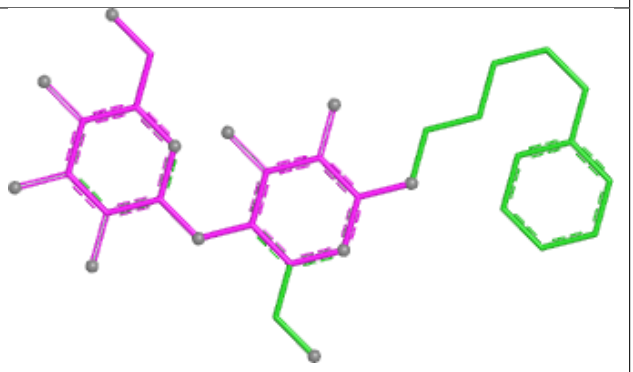

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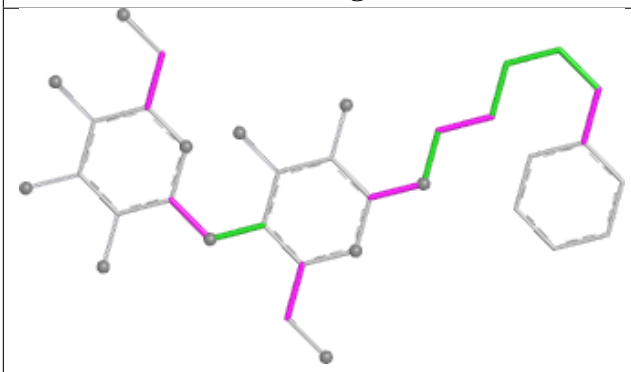

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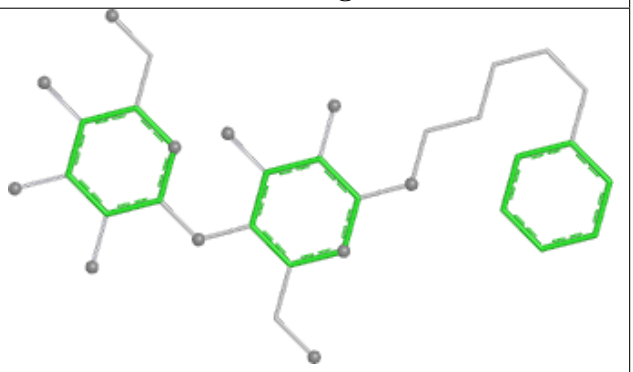
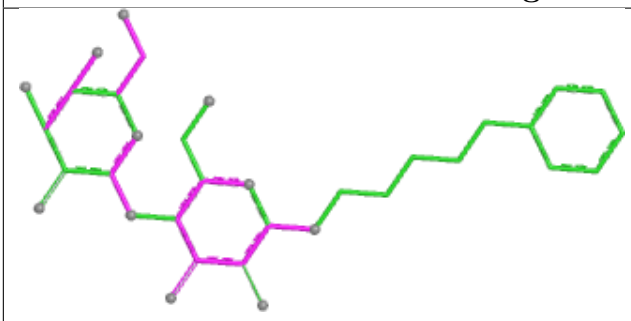


Rings

Ligand CM5 C 603



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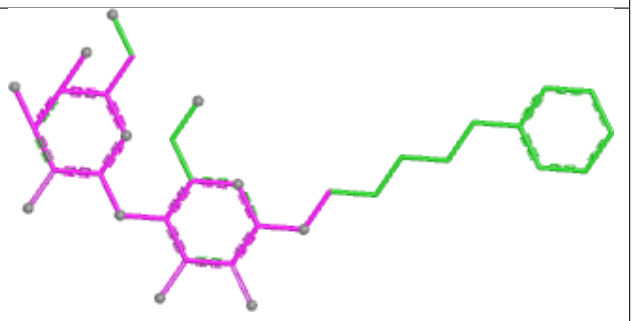

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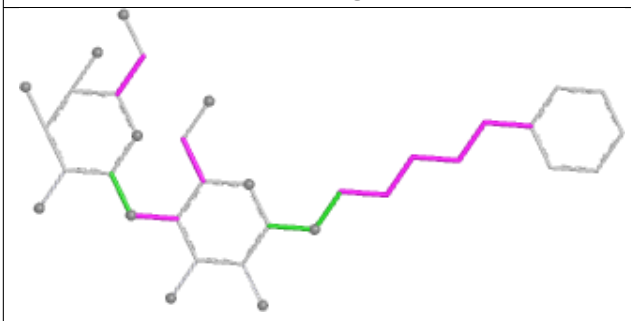

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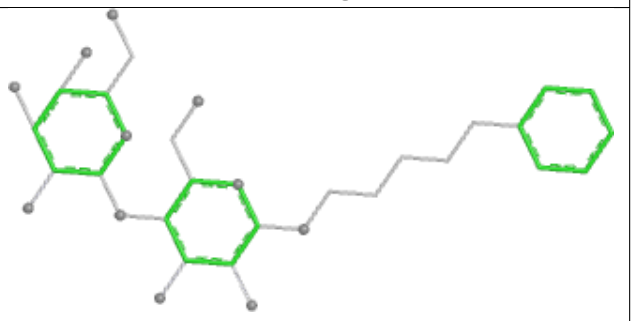
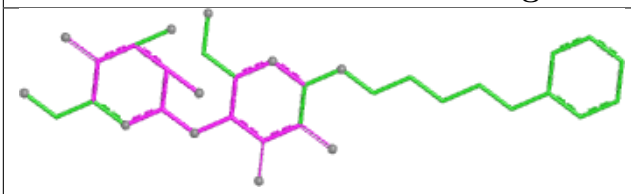


Rings

Ligand CM5 A 601



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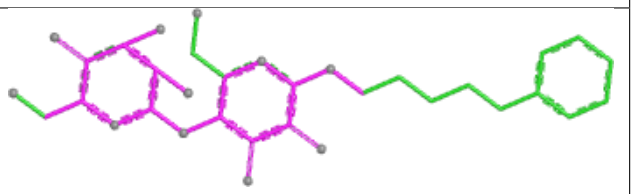

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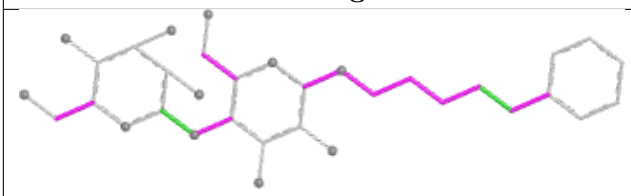

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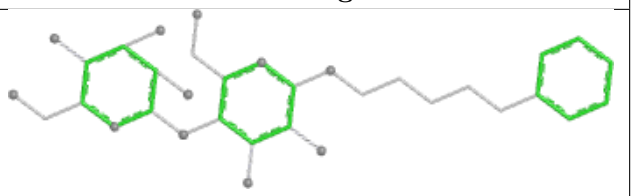
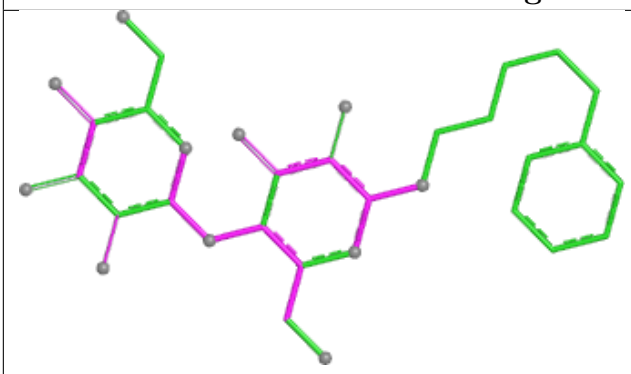


Rings

Ligand CM5 F 606



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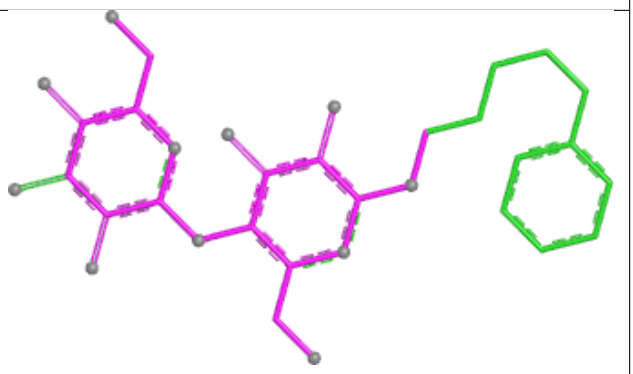

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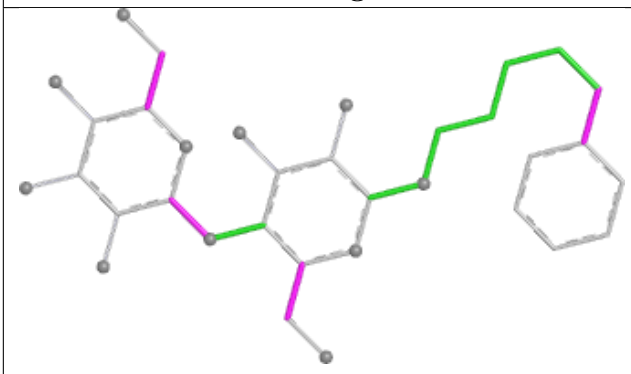

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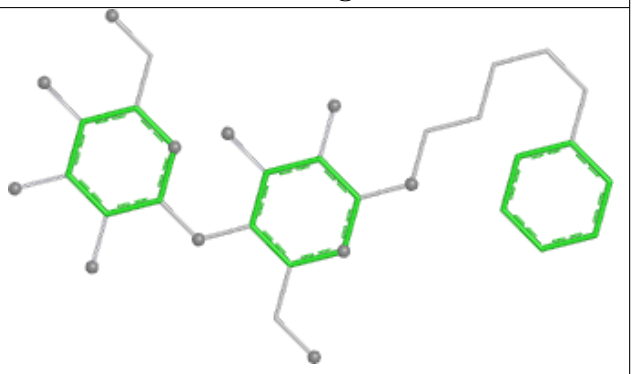
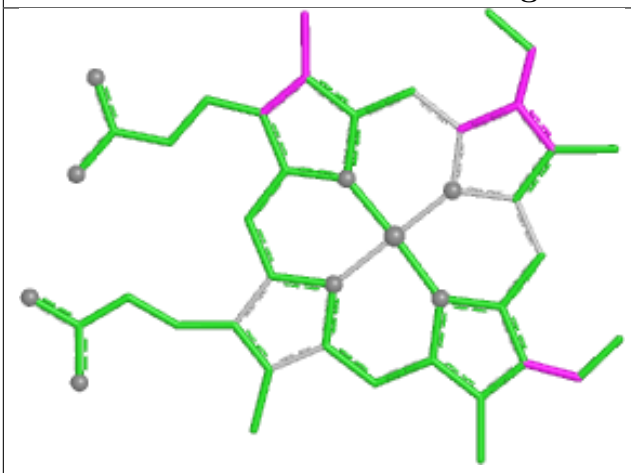


Rings

Ligand HEM F 500



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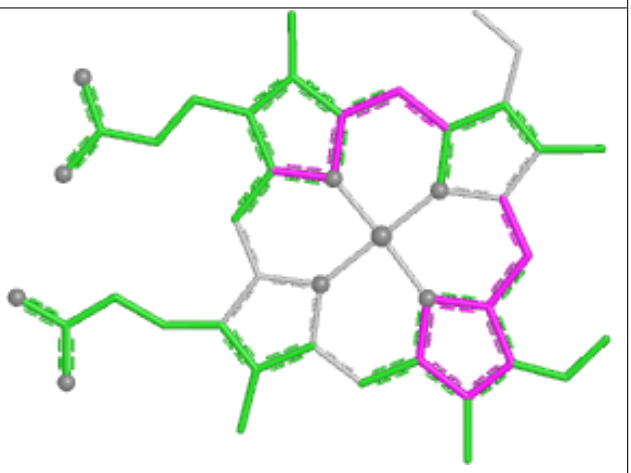

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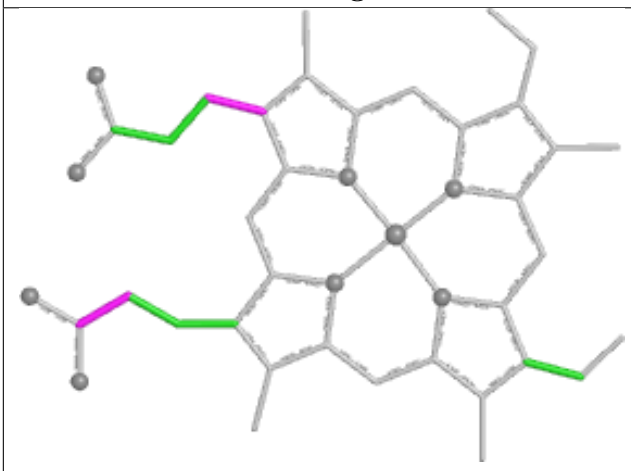

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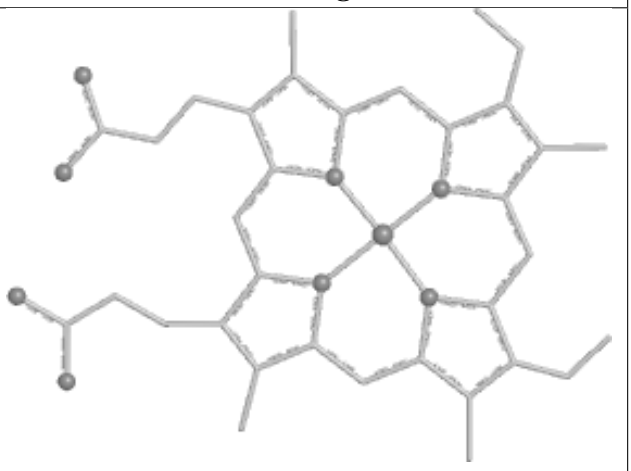
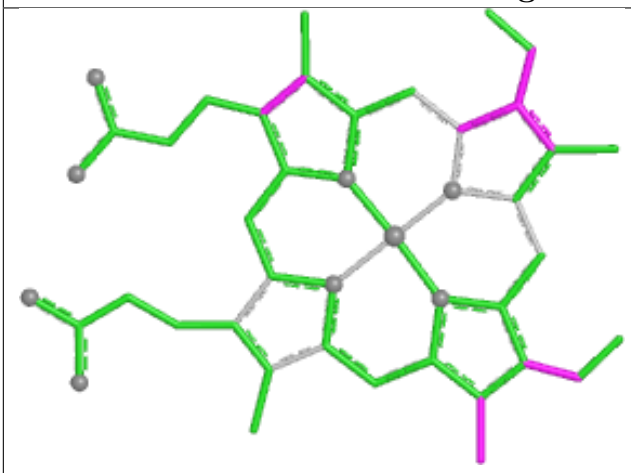
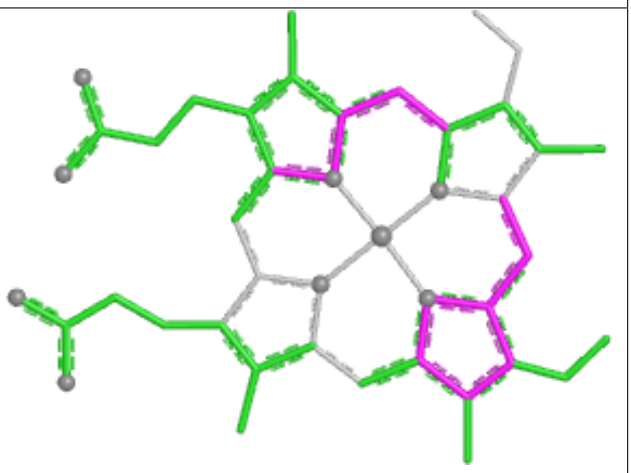


Rings

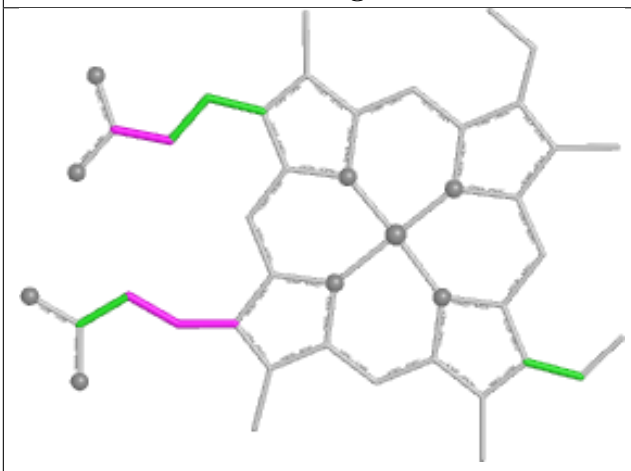
Ligand HEM A 500



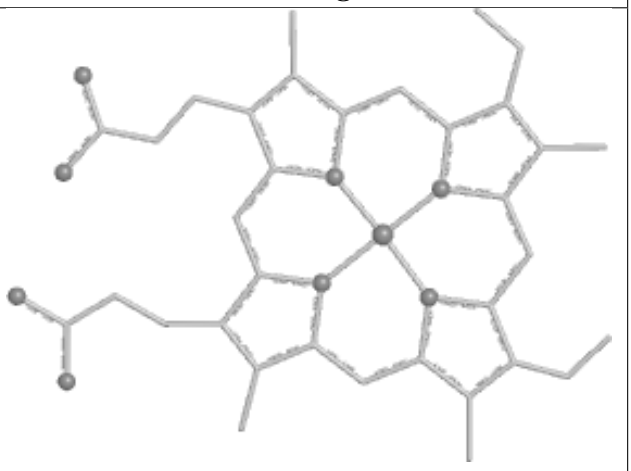
Bond lengths



Bond angles

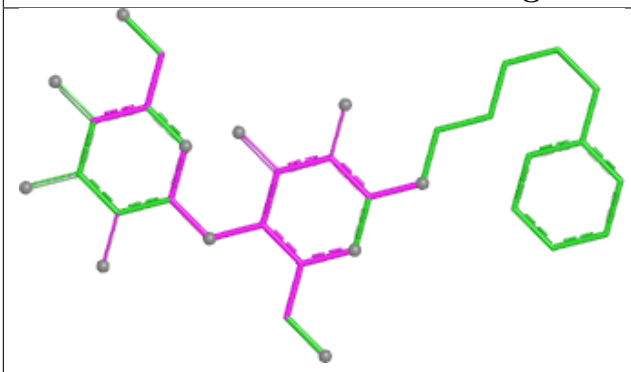


Torsions

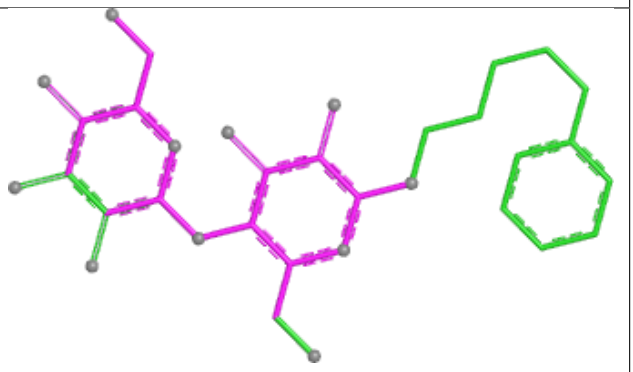


Rings

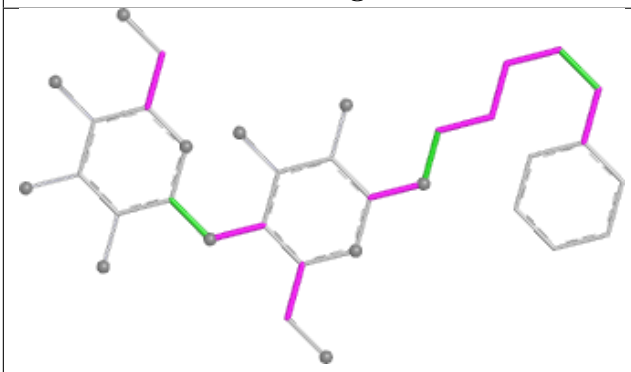
Ligand CM5 B 608



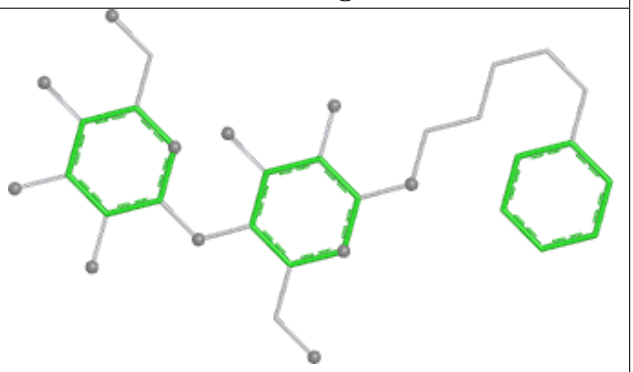
Bond lengths



Bond angles

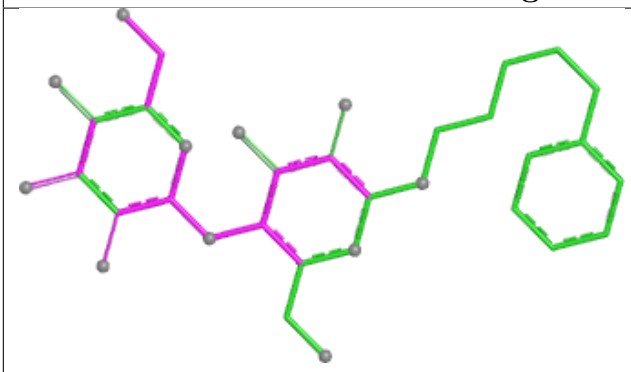


Torsions

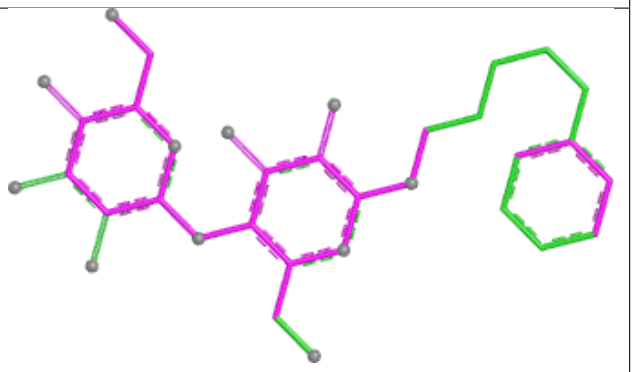


Rings

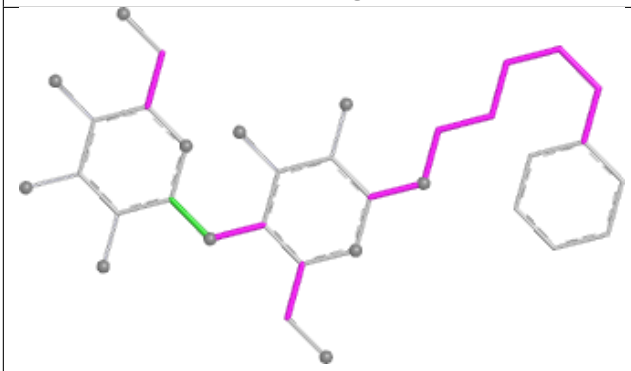
Ligand CM5 D 607



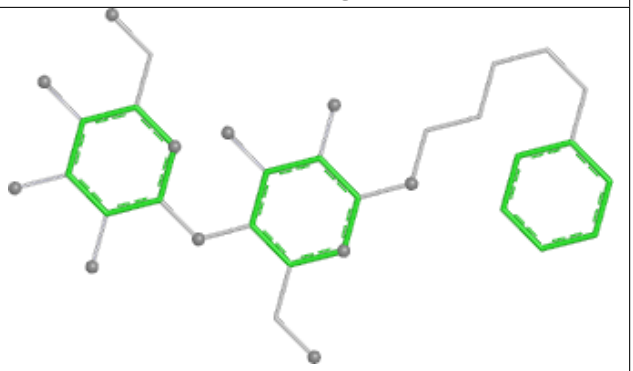
Bond lengths



Bond angles

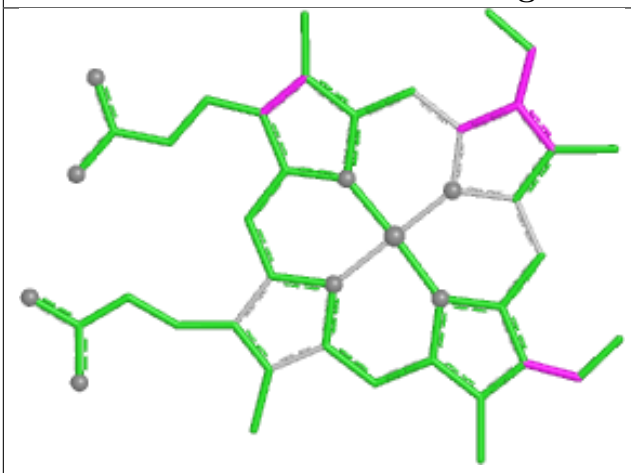


Torsions

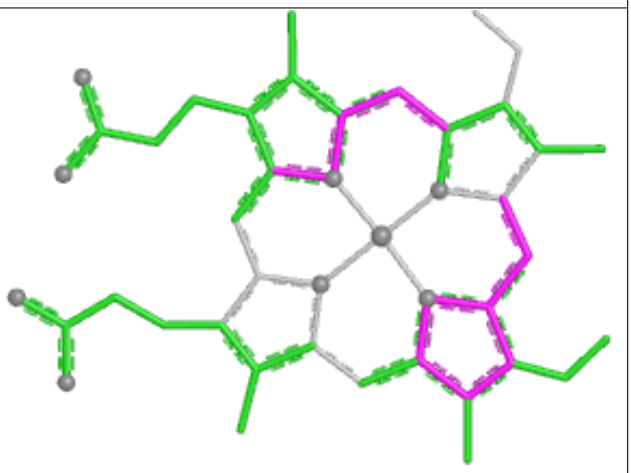


Rings

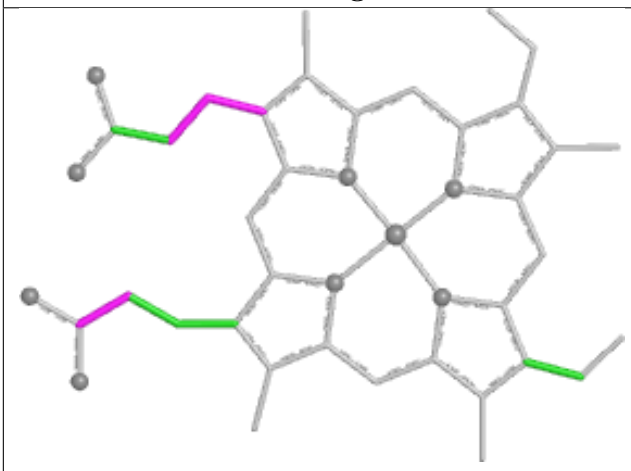
Ligand HEM D 500



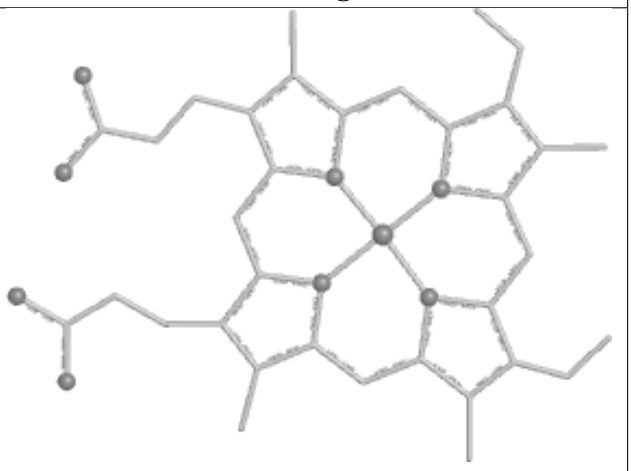
Bond lengths



Bond angles

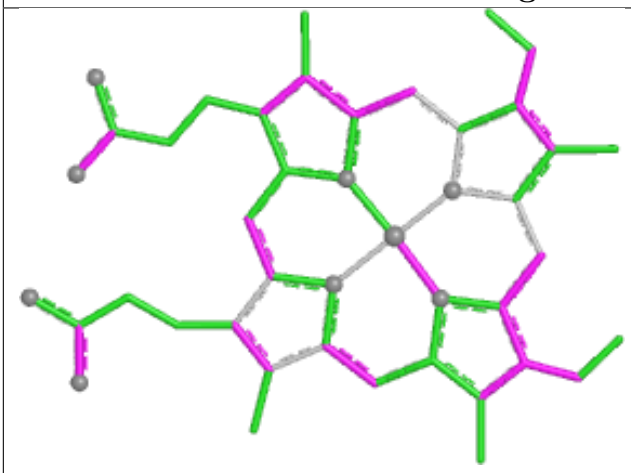


Torsions

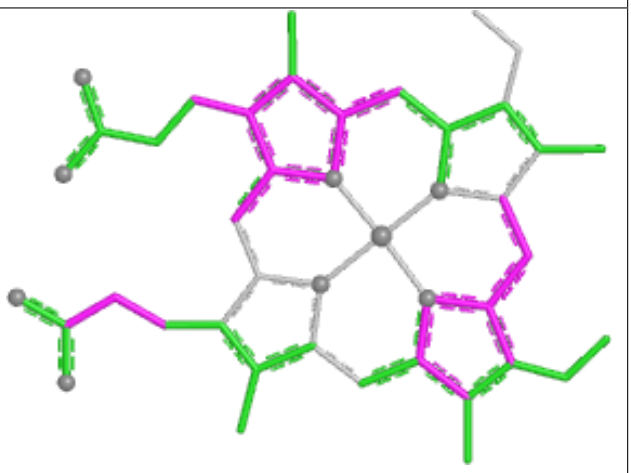


Rings

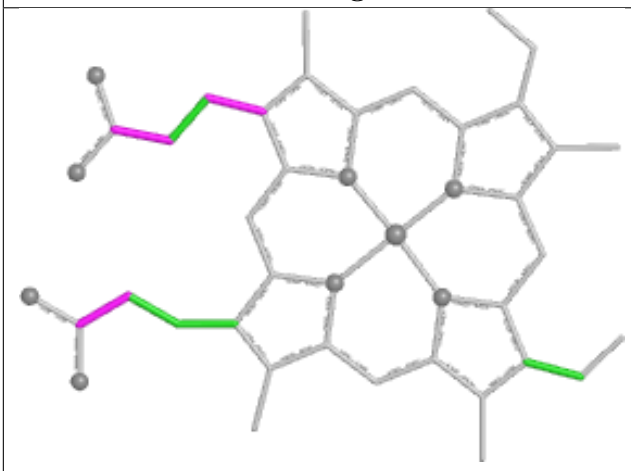
Ligand HEM C 500



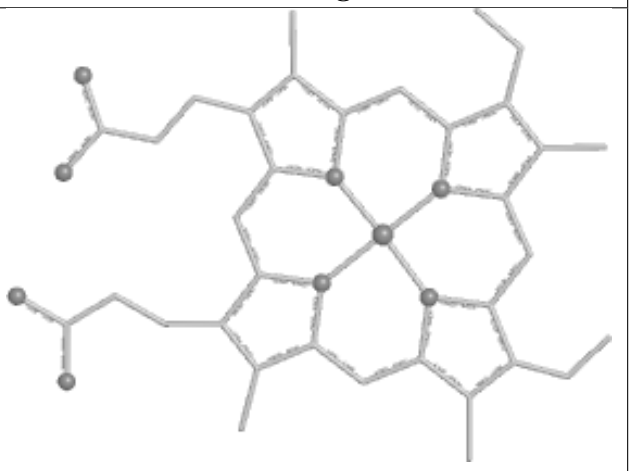
Bond lengths



Bond angles

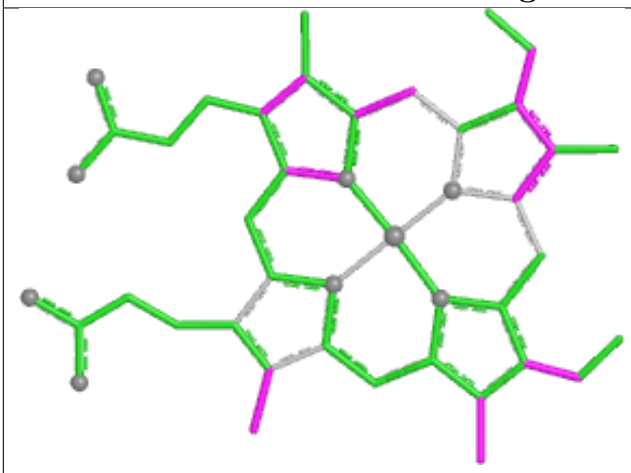


Torsions

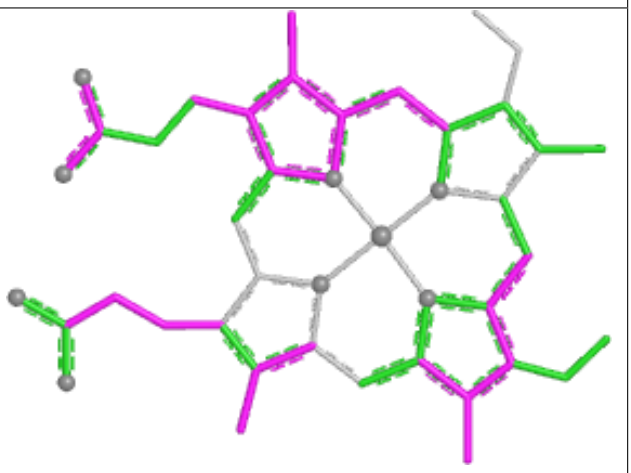


Rings

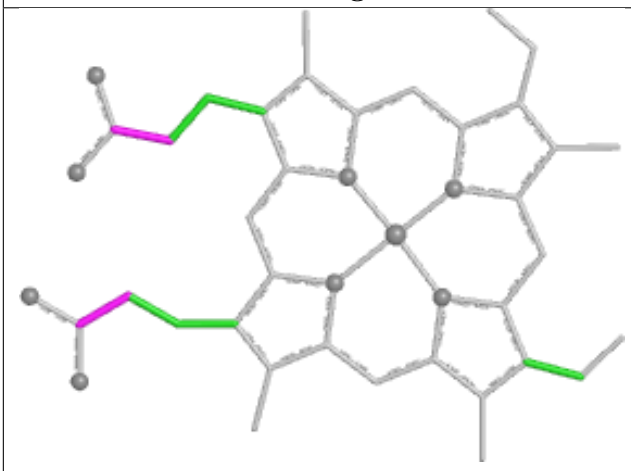
Ligand HEM B 500



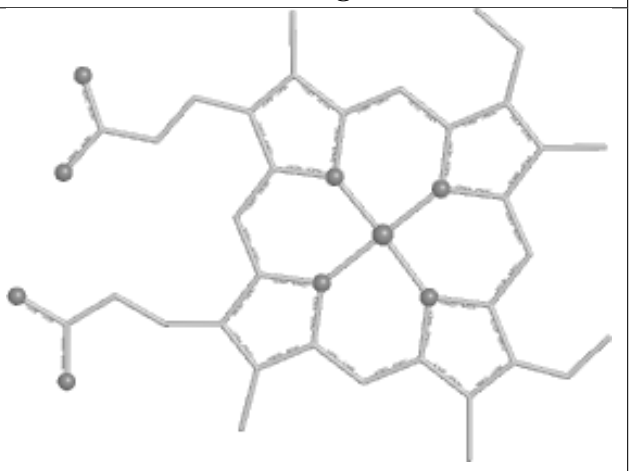
Bond lengths



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	462/476 (97%)	-1.73	0	100	100	26, 51, 74, 82	0
1	B	459/476 (96%)	-1.73	0	100	100	28, 51, 74, 82	0
1	C	462/476 (97%)	-1.73	0	100	100	24, 50, 74, 79	0
1	D	458/476 (96%)	-1.73	0	100	100	24, 51, 74, 82	0
1	E	459/476 (96%)	-1.75	0	100	100	26, 51, 74, 87	0
1	F	453/476 (95%)	-1.62	0	100	100	24, 51, 74, 79	0
All	All	2753/2856 (96%)	-1.72	0	100	100	24, 51, 74, 87	0

There are no RSRZ outliers to report.

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
4	CM5	B	608	34/34	0.98	0.05	46,84,100,100	0

Continued on next page...

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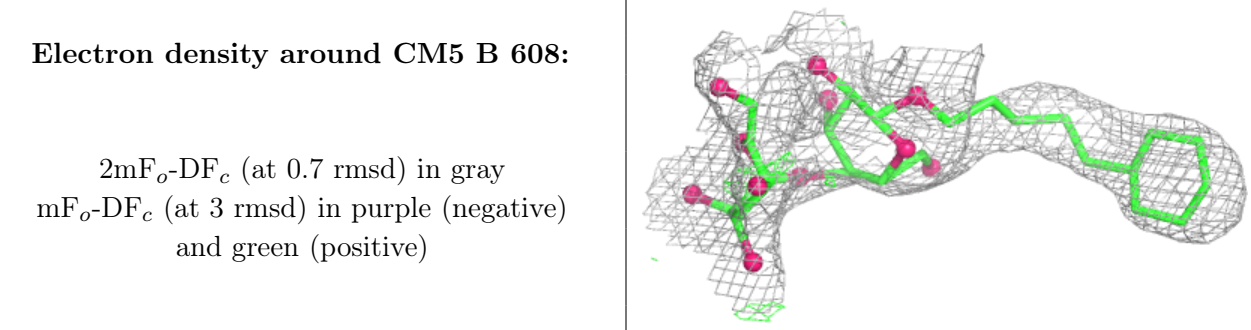
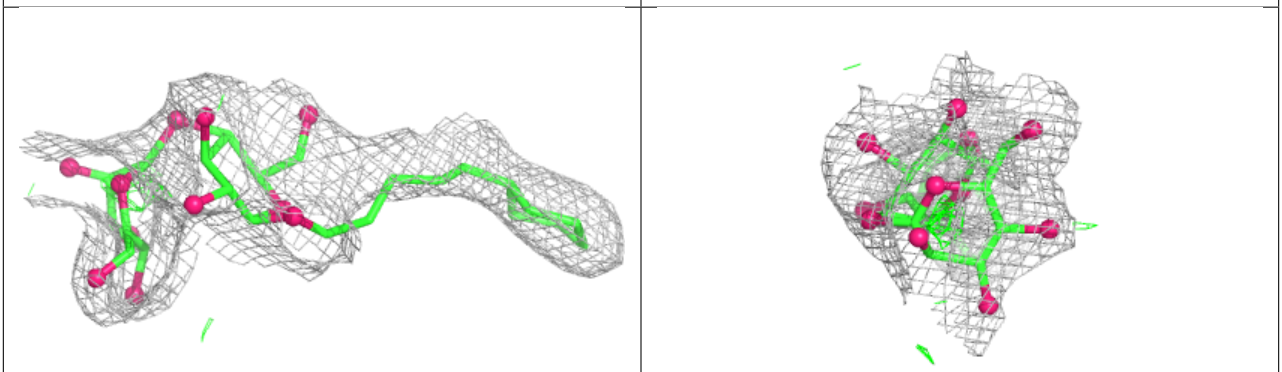
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CM5	D	607	34/34	0.98	0.07	72,97,101,103	0
4	CM5	E	605	34/34	0.98	0.04	66,73,91,92	0
3	3QU	C	501	7/16	0.99	0.06	47,50,51,52	0
3	3QU	E	501	13/16	0.99	0.04	55,57,60,63	0
4	CM5	A	601	34/34	0.99	0.04	53,60,73,74	0
4	CM5	B	602	34/34	0.99	0.04	61,72,84,85	0
2	HEM	F	500	43/43	0.99	0.04	53,65,66,67	0
4	CM5	C	603	34/34	0.99	0.05	54,63,70,71	0
4	CM5	D	604	34/34	0.99	0.04	58,67,77,79	0
3	3QU	A	501	7/16	0.99	0.05	47,50,51,52	0
3	3QU	B	501	16/16	0.99	0.04	47,51,60,66	0
4	CM5	F	606	34/34	0.99	0.06	45,62,74,76	0
2	HEM	C	500	43/43	1.00	0.03	21,27,36,46	0
2	HEM	D	500	43/43	1.00	0.03	23,33,38,39	0
3	3QU	D	501	13/16	1.00	0.04	47,49,54,54	0
2	HEM	E	500	43/43	1.00	0.02	17,28,36,40	0
2	HEM	A	500	43/43	1.00	0.03	25,31,39,43	0
2	HEM	B	500	43/43	1.00	0.02	15,20,29,31	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 CM5 B 608:

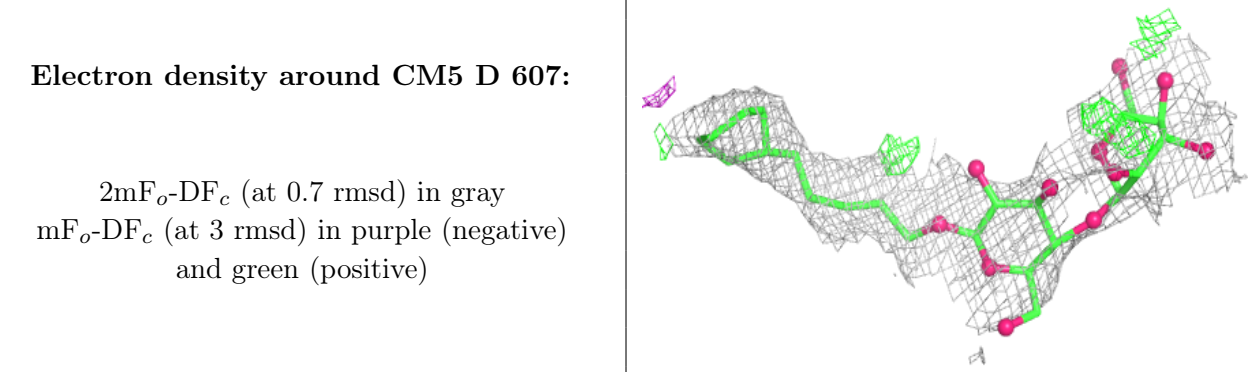
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

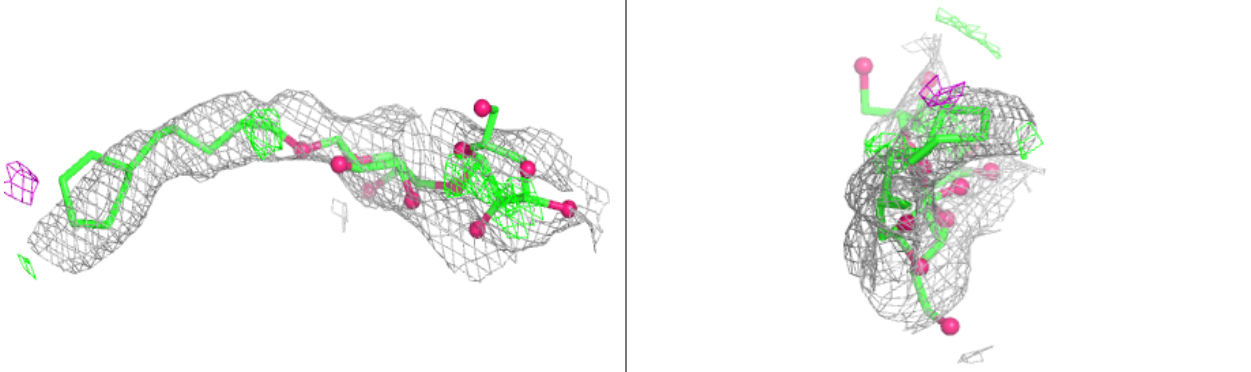




Electron density around CM5 D 607:

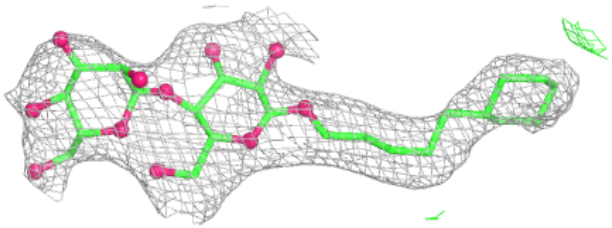
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

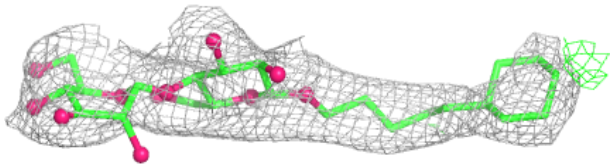


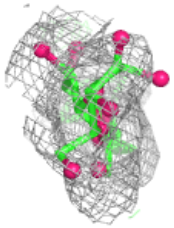


Electron density around CM5 E 605:

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

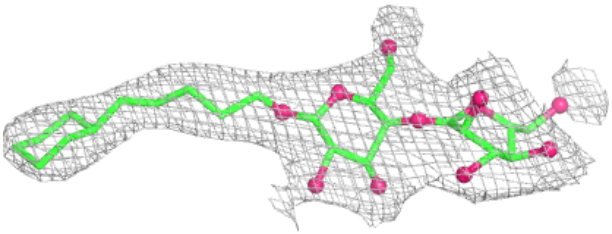


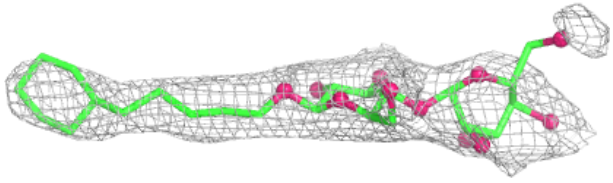


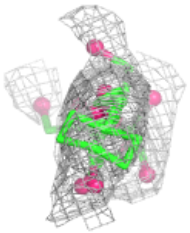


Electron density around CM5 A 601:

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

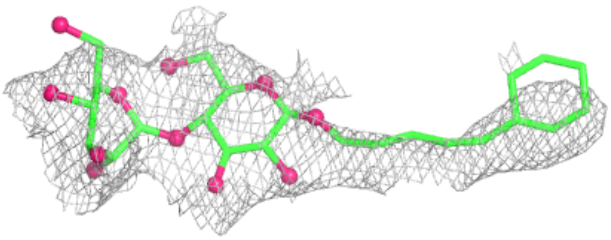


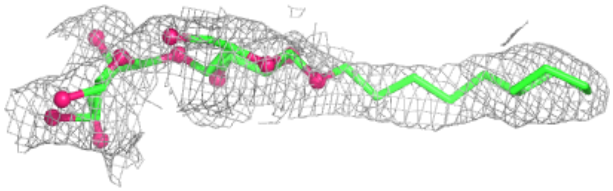


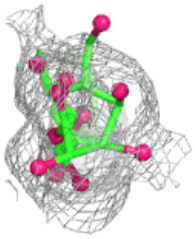


Electron density around CM5 B 602:

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

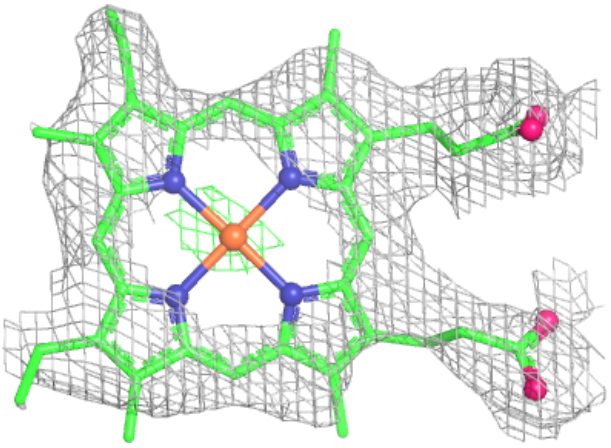


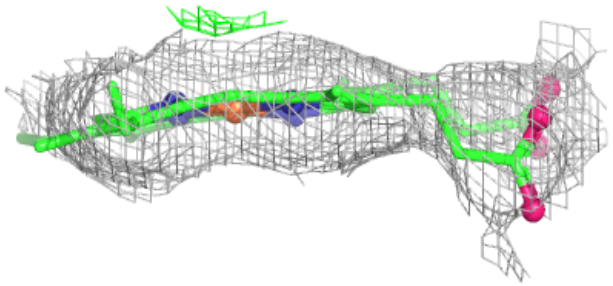


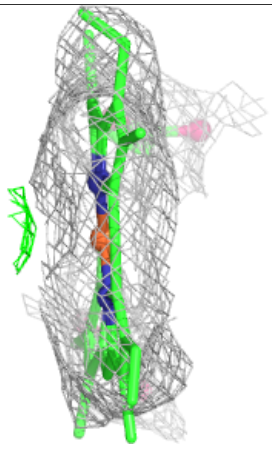


Electron density around HEM F 500:

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

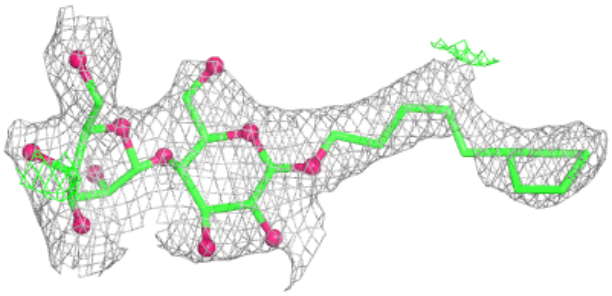


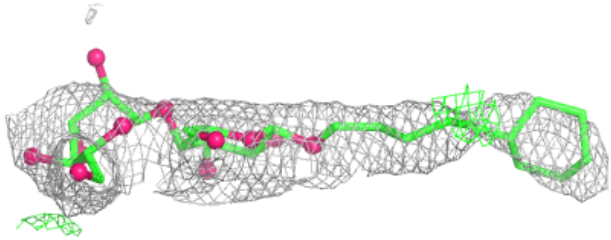


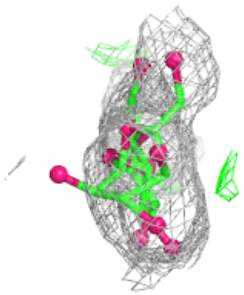


Electron density around CM5 C 603:

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

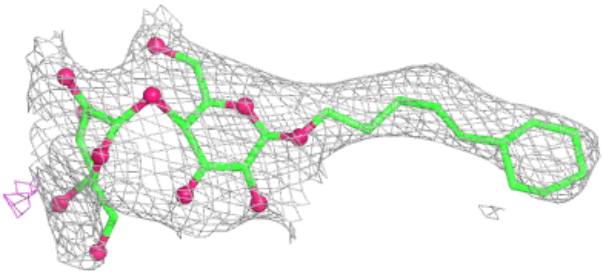


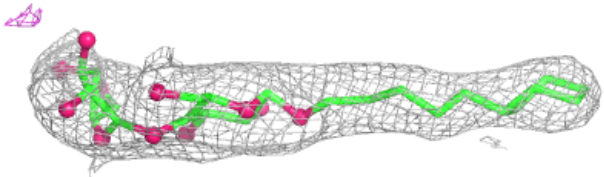


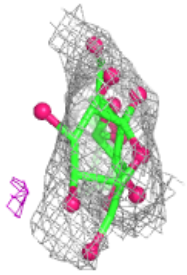


Electron density around CM5 D 604:

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

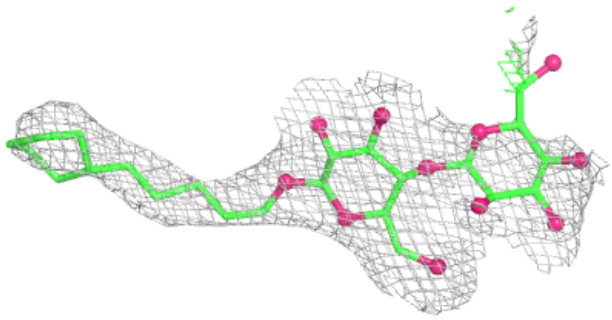


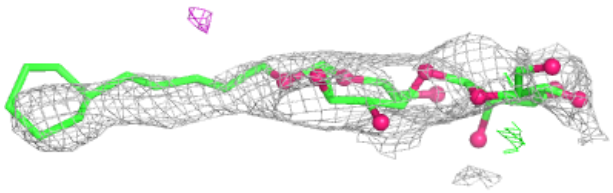


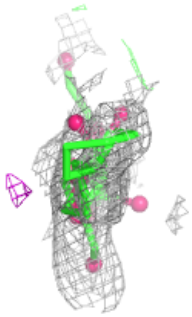


Electron density around CM5 F 606:

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

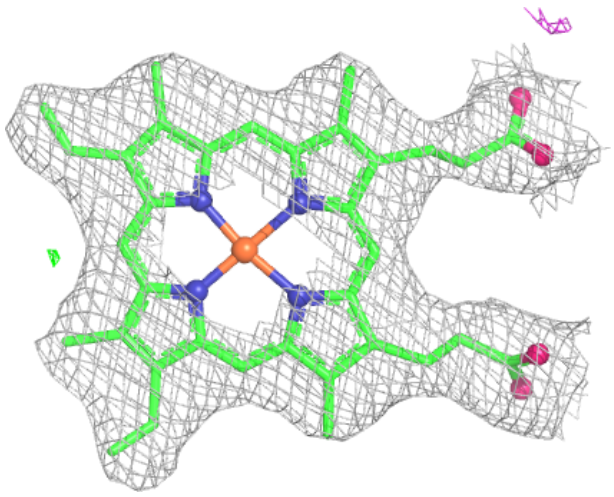


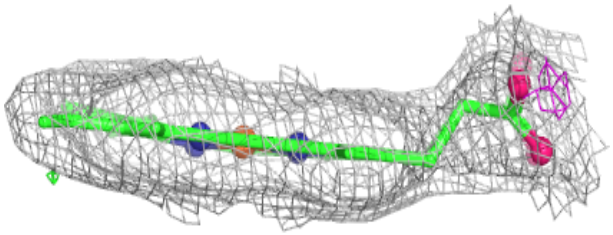


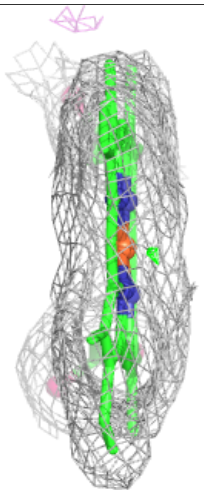


Electron density around HEM C 500:

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

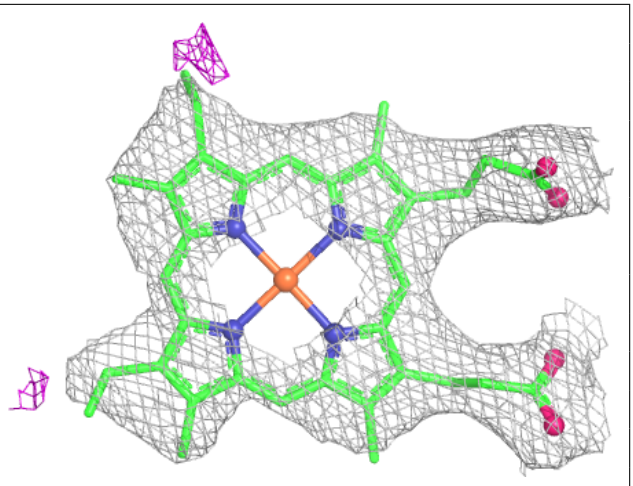


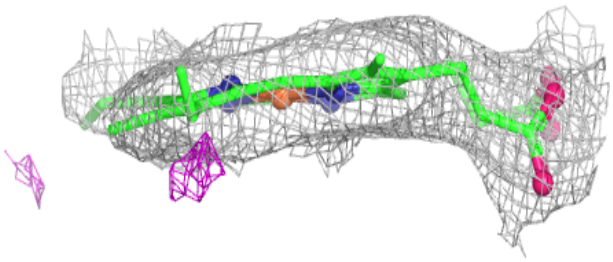


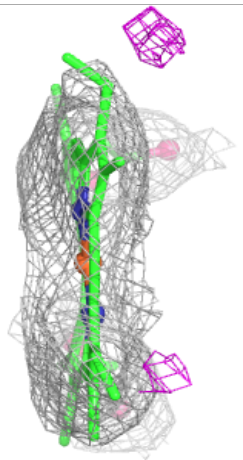


Electron density around HEM D 500:

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

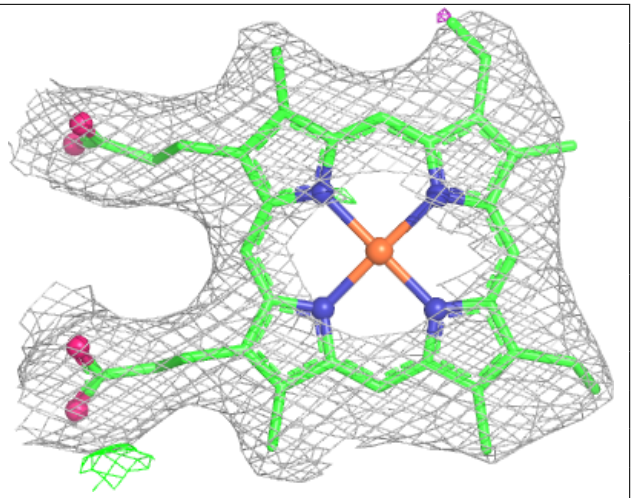


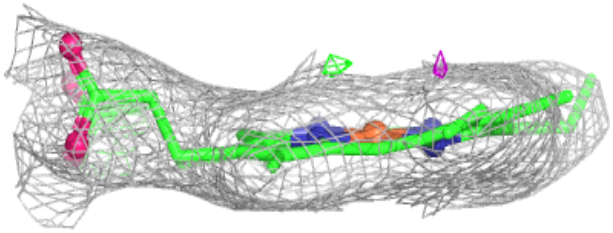


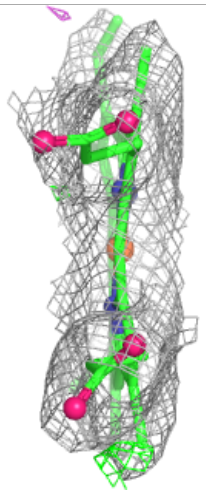


Electron density around HEM E 500:

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

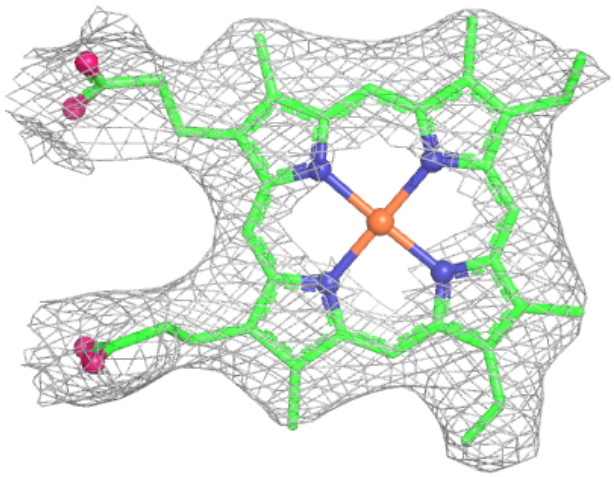


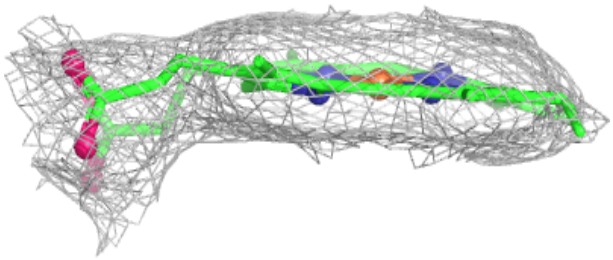


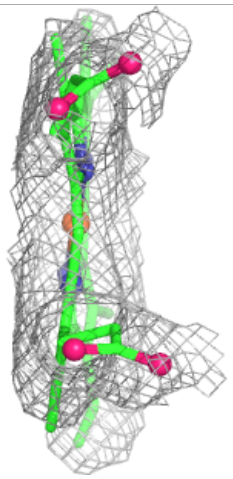


Electron density around HEM A 500:

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

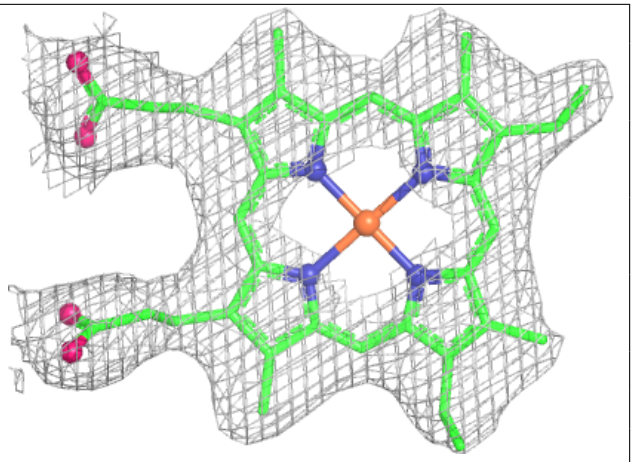


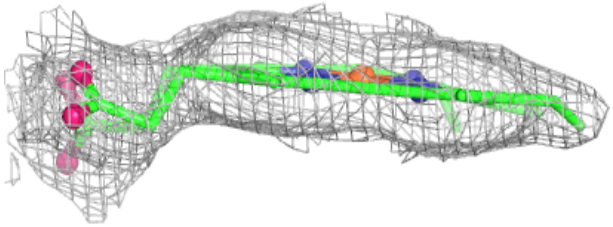


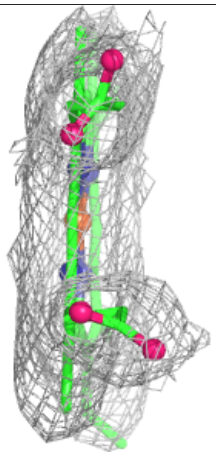


Electron density around HEM B 500:

$2mF_o$-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

There are no such residues in this entry.