wwPDB X-ray Structure Validation Summary Report (i)

Sep 22, 2026 – 02:14 PM EDT

PDB ID	:	2QJP / pdb_00002qjp
Title	:	Crystal structure of wild type rhodobacter sphaeroides with stigmatellin and antimycin inhibited
Authors	:	Esser, L.; Xia, D.
Deposited on	:	2007-07-08
Resolution	:	2.60 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:

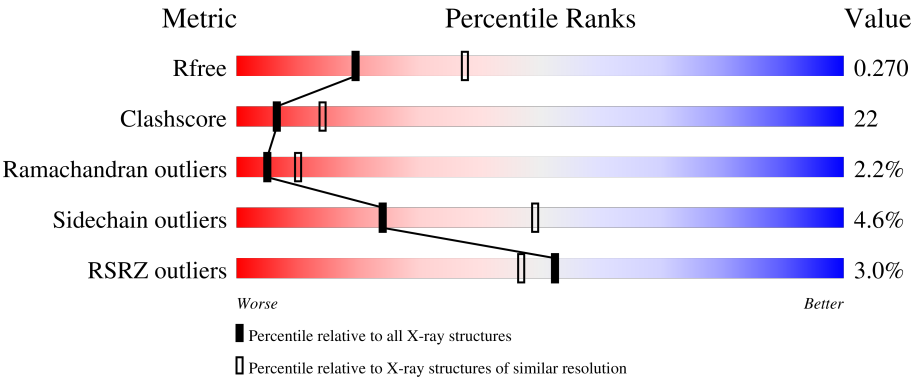
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	428	59% 36% 5%
1	D	428	2% 58% 37%
1	G	428	60% 36%
1	J	428	64% 31%
2	B	256	9% 57% 38% 5%

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Mol	Chain	Length	Quality of chain
2	E	256	6% 55% 39% 5%
2	H	256	5% 53% 41% 6%
2	K	256	6% 57% 37% 6%
3	C	179	2% 58% 36% 6%
3	F	179	2% 51% 42% 6%
3	I	179	3% 56% 38% 6%
3	L	179	4% 53% 39% 8%

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
10	HEC	B	301	X	-	-	-
10	HEC	E	301	X	-	-	-
10	HEC	H	301	X	-	-	-
10	HEC	K	301	X	-	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 28227 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 b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			
1	D	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			
1	G	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			
1	J	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			

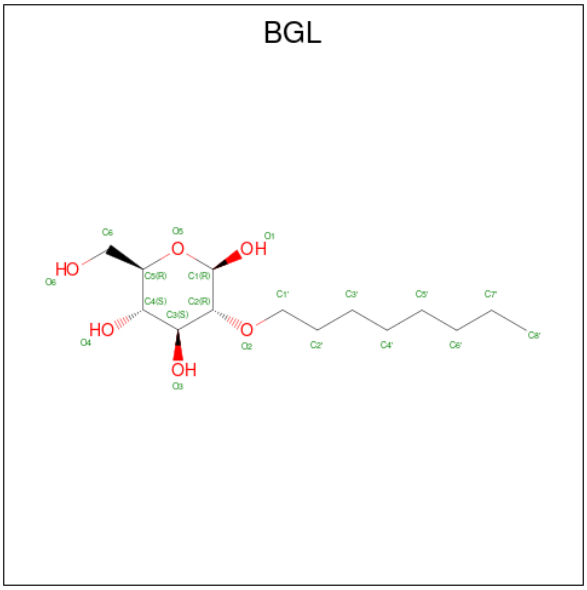
- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	E	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	H	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	K	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

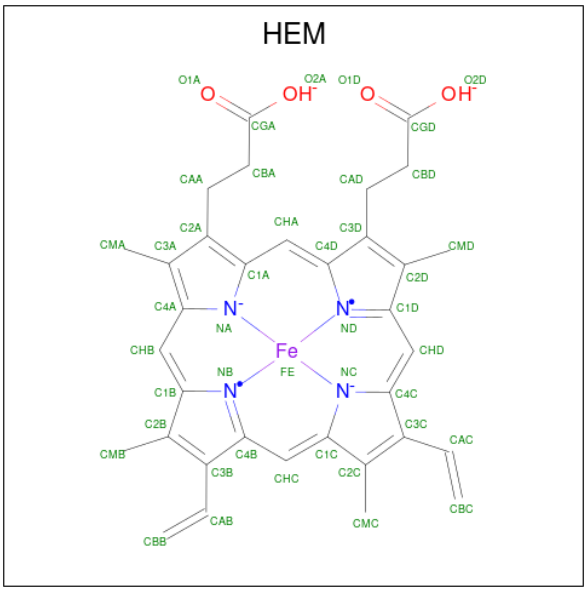
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			
3	F	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			
3	I	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			
3	L	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			

- Molecule 4 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: $C_{14}H_{28}O_6$).



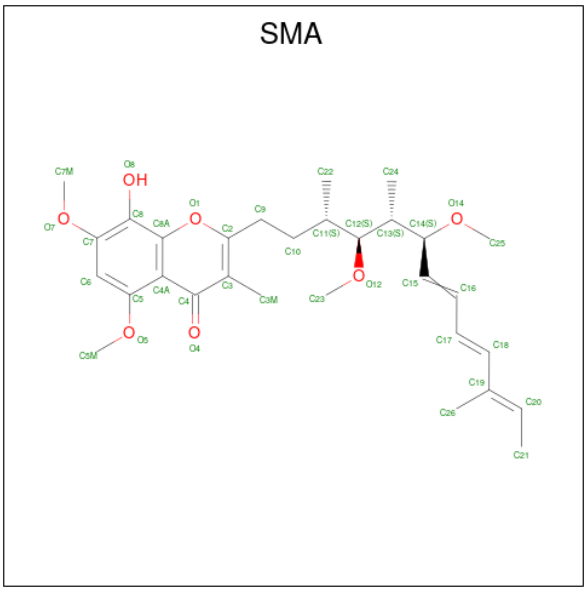
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0
4	G	1	Total C O 20 14 6	0	0
4	J	1	Total C O 20 14 6	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



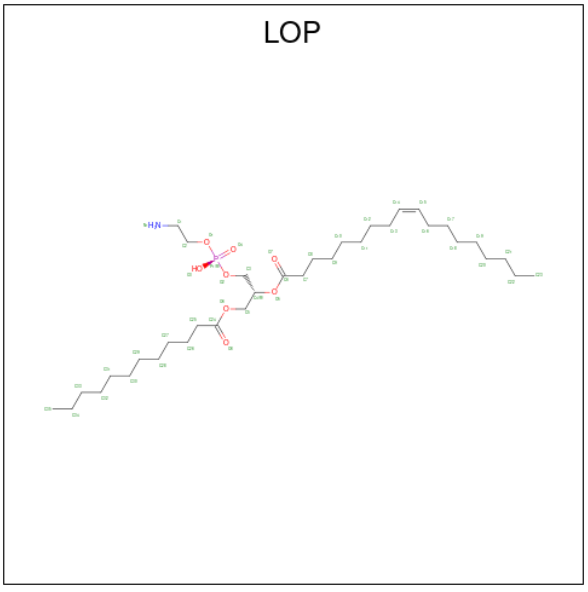
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



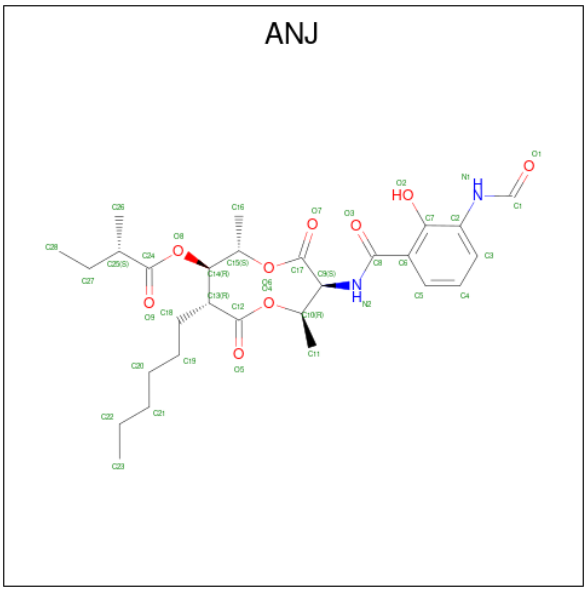
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 37 30 7	0	0
6	D	1	Total C O 37 30 7	0	0
6	G	1	Total C O 37 30 7	0	0
6	J	1	Total C O 37 30 7	0	0

- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: $C_{35}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 8 is (2R,3S,6S,7R,8R)-3-{[3-(FORMYLAMINO)-2-HYDROXYBENZOYL]AMINO}-8-HEXYL-2,6-DIMETHYL-4,9-DIOXO-1,5-DIOXONAN-7-YL (2S)-2-METHYLBUTANOATE (CCD ID: ANJ) (formula: $C_{28}H_{40}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			39	28	2	9		
8	D	1	Total	C	N	O	0	0
			39	28	2	9		
8	G	1	Total	C	N	O	0	0
			39	28	2	9		
8	J	1	Total	C	N	O	0	0
			39	28	2	9		

- Molecule 9 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

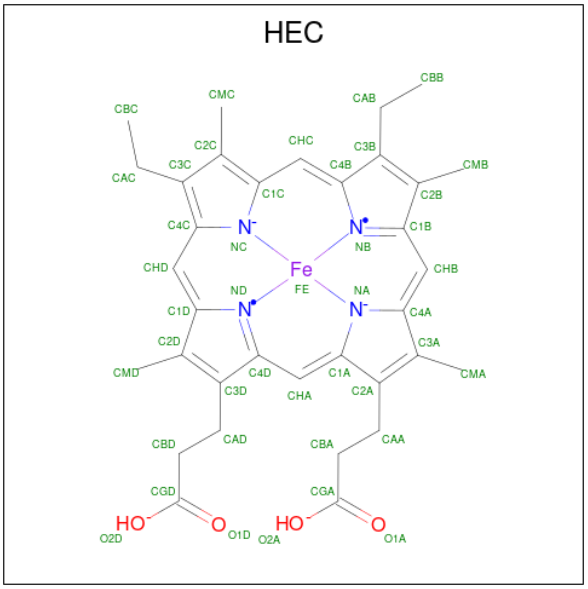
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Sr	0	0
			1	1		

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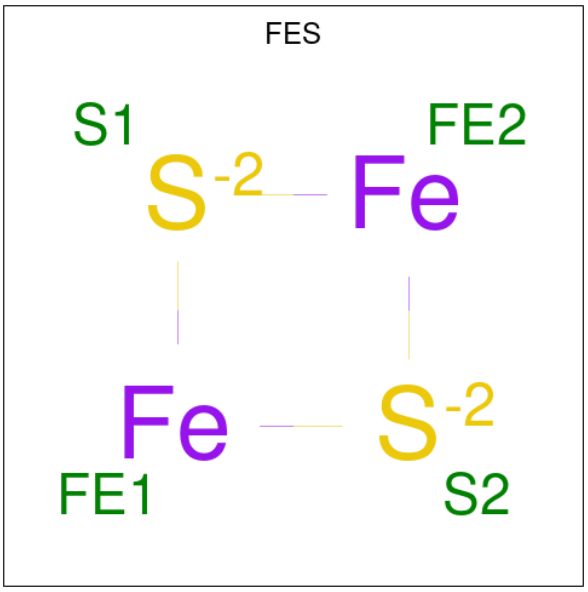
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total Sr 1 1	0	0
9	G	1	Total Sr 1 1	0	0
9	H	1	Total Sr 1 1	0	0
9	J	1	Total Sr 1 1	0	0
9	K	1	Total Sr 1 1	0	0

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C Fe N O 43 34 1 4 4	0	0
10	E	1	Total C Fe N O 43 34 1 4 4	0	0
10	H	1	Total C Fe N O 43 34 1 4 4	0	0
10	K	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total Fe S 4 2 2	0	0
11	F	1	Total Fe S 4 2 2	0	0
11	I	1	Total Fe S 4 2 2	0	0
11	L	1	Total Fe S 4 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	36	Total O 36 36	0	0
12	B	7	Total O 7 7	0	0
12	C	13	Total O 13 13	0	0
12	D	41	Total O 41 41	0	0
12	E	3	Total O 3 3	0	0
12	F	13	Total O 13 13	0	0
12	G	41	Total O 41 41	0	0
12	H	4	Total O 4 4	0	0

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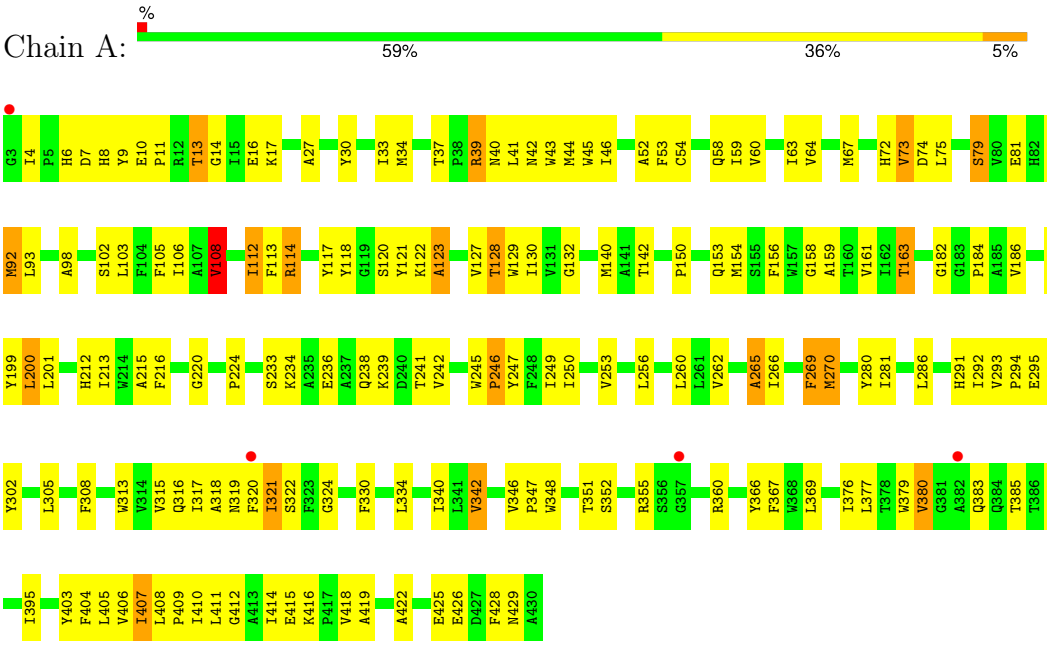
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	I	14	Total O 14 14	0	0
12	J	23	Total O 23 23	0	0
12	K	3	Total O 3 3	0	0
12	L	11	Total O 11 11	0	0

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 b

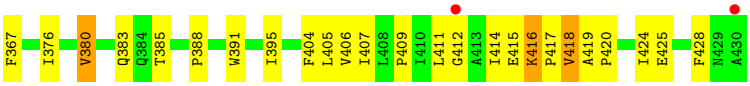
Chain A:



• Molecule 1: Cytochrome b

Chain D:

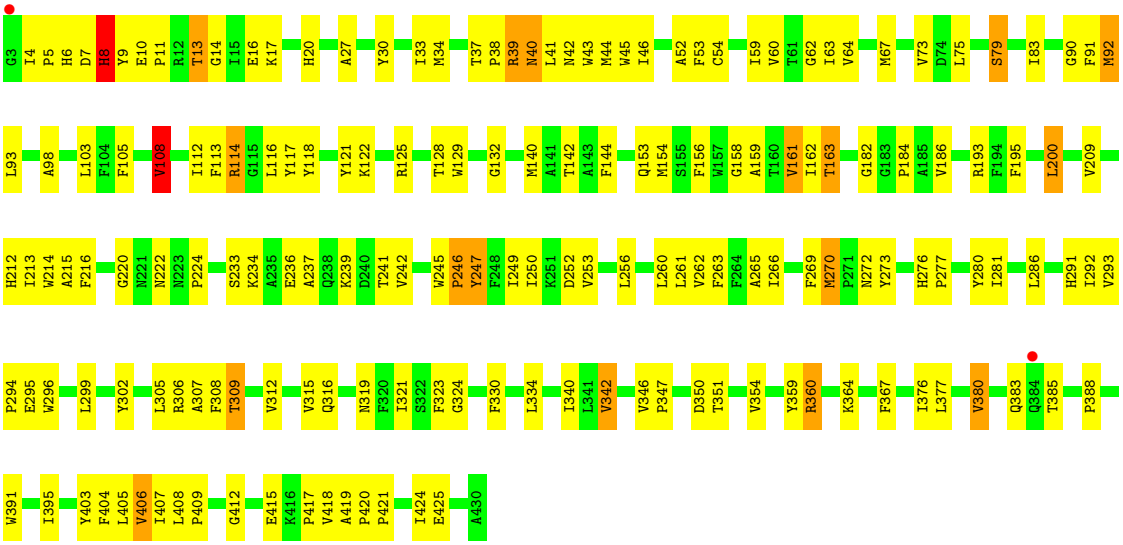




• Molecule 1: Cytochrome b

Chain G:

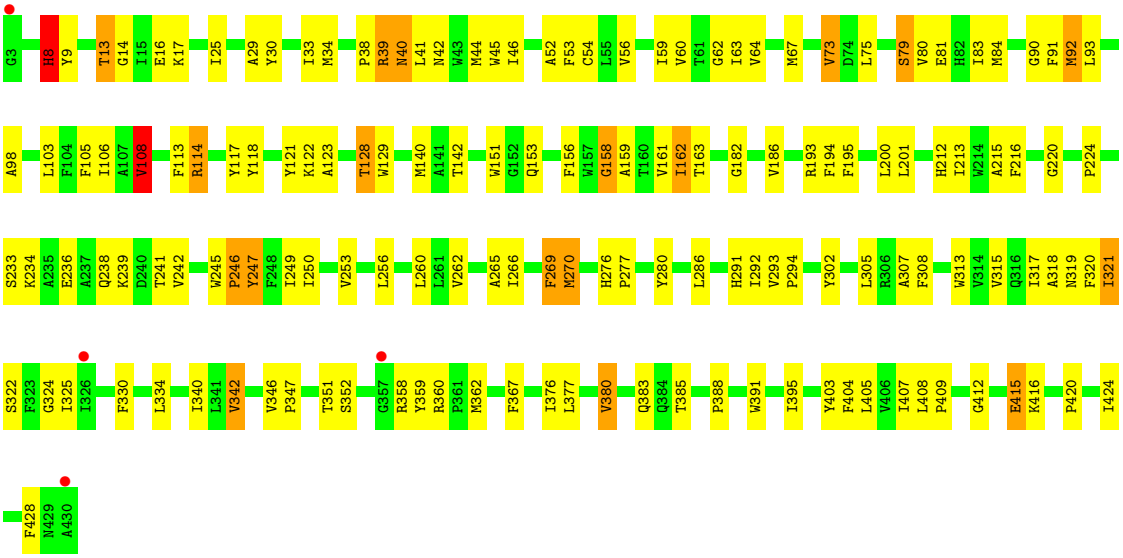




• Molecule 1: Cytochrome b

Chain J:

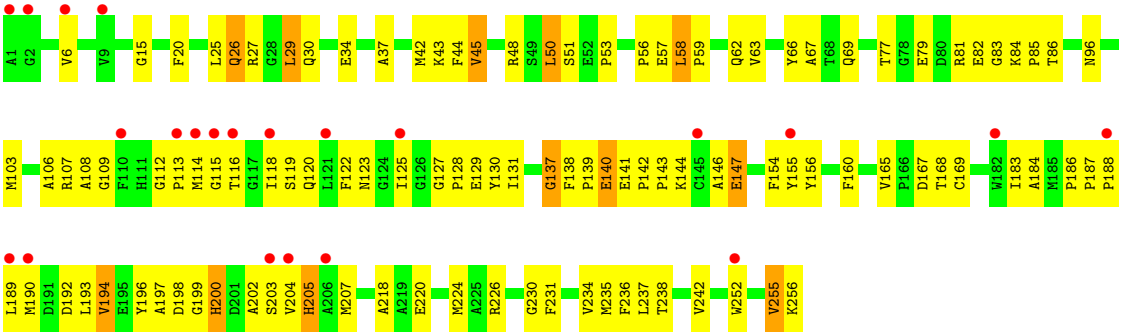




• Molecule 2: Cytochrome c1

Chain B:

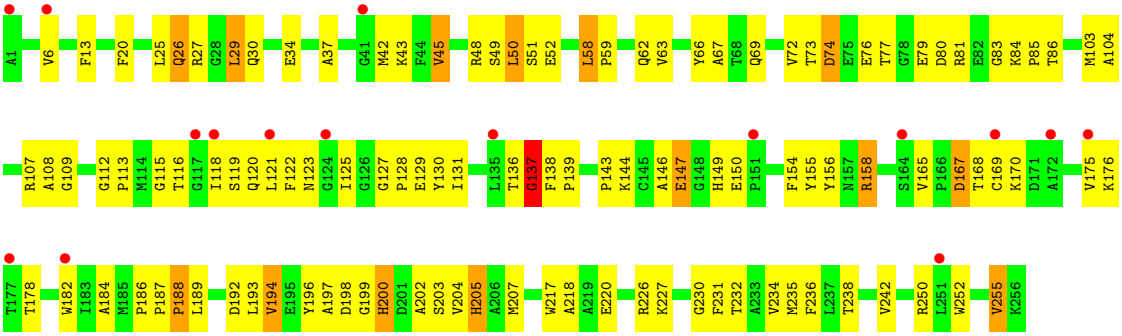




• Molecule 2: Cytochrome c1

Chain E:

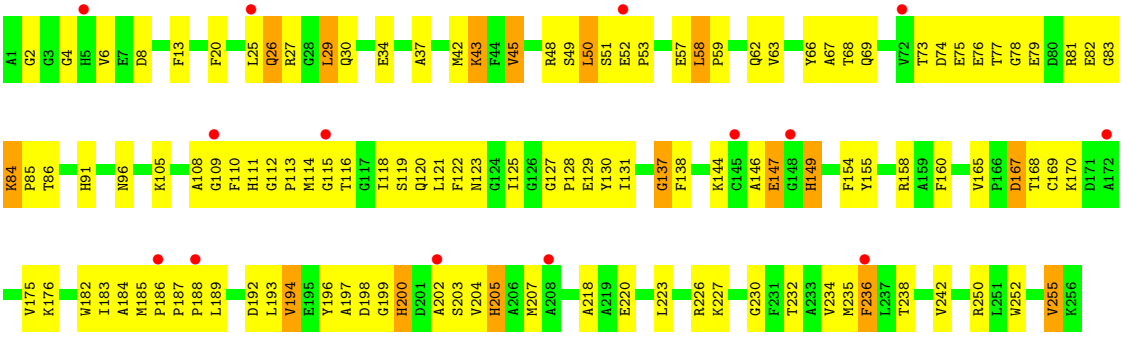




• Molecule 2: Cytochrome c1

Chain H:

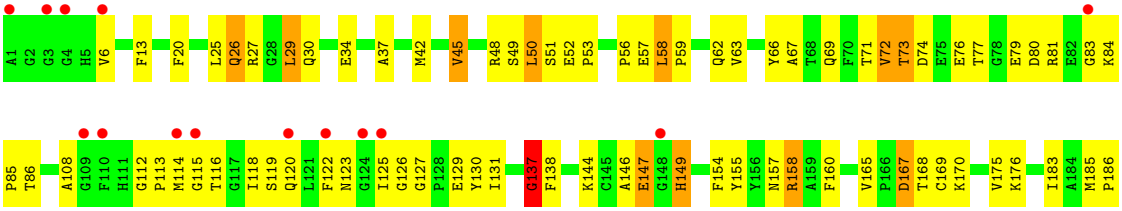




• Molecule 2: Cytochrome c1

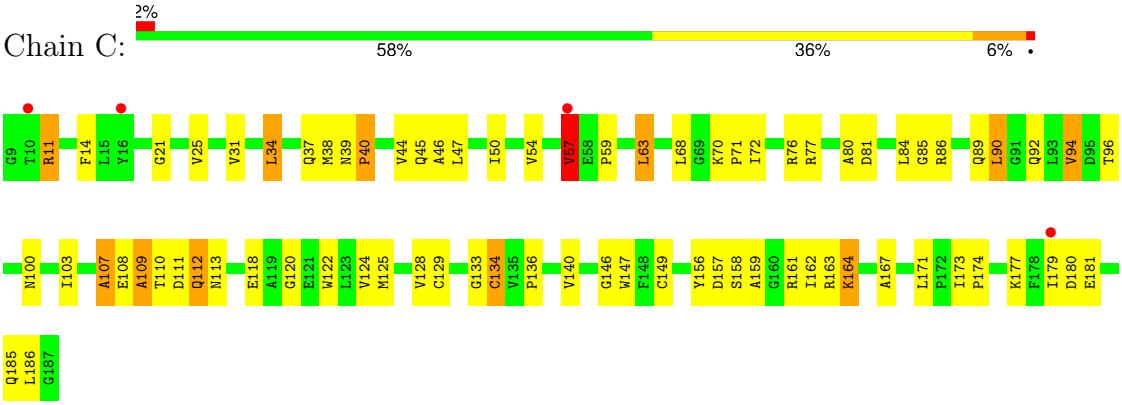
Chain K:



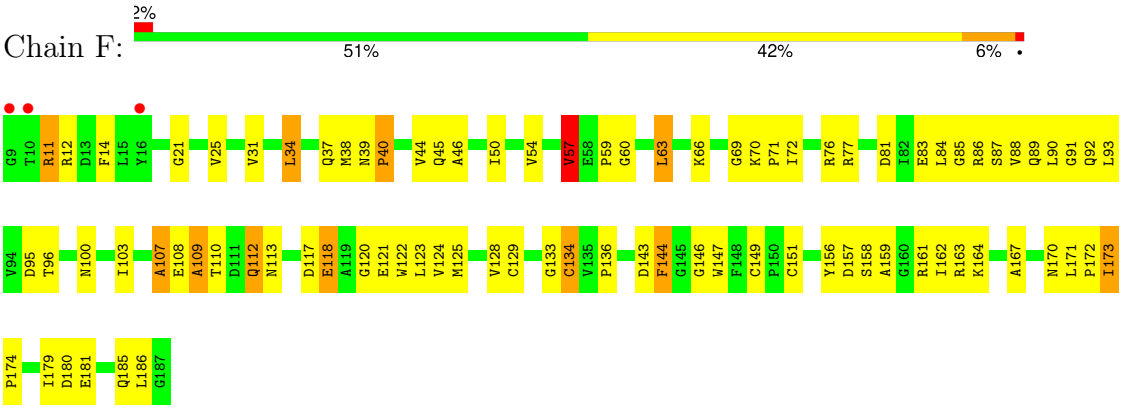




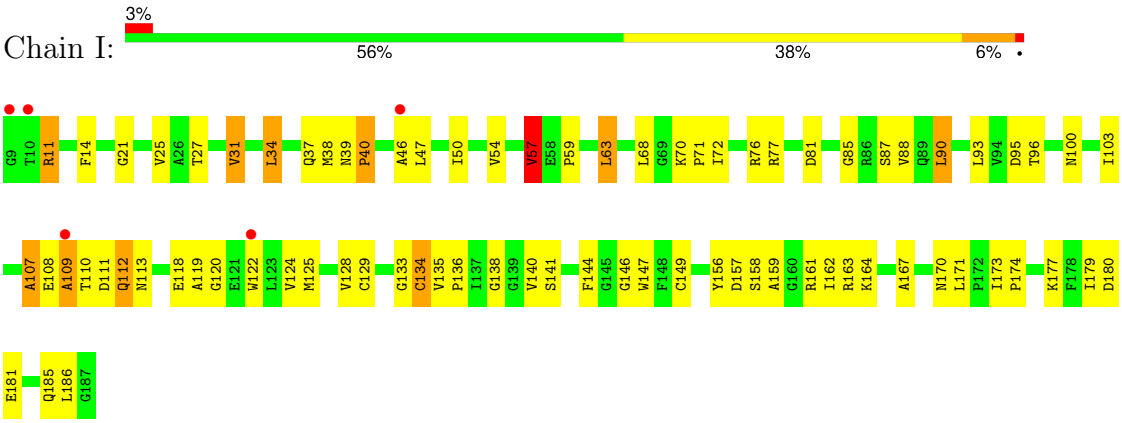
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

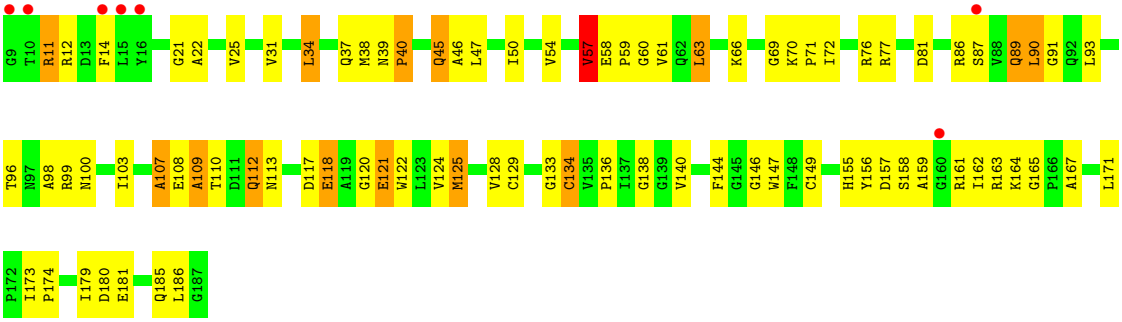


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit




G9 T10 R11 R12 D13 F14 L15 Y16 G21 A22 V25 V31 L34 Q37 M38 N39 P40 Q45 A46 L47 I50 V54 V57 E58 P59 G60 V61 Q62 L63 K66 G69 K70 P71 I72 R76 R77 D81 R86 S87 V88 Q89 L90 G91 Q92 L93
T96 N97 A98 R99 N100 I103 A107 E108 A109 T110 D111 Q112 N113 D117 E118 A119 G120 E121 W122 L123 V124 M126 V128 C129 G133 C134 V135 P136 I137 G138 G139 V140 F144 G145 G146 W147 F148 C149 H155 Y156 D157 S158 A159 G160 R161 I162 R163 K164 G165 P166 A167 L171
P172 I173 P174 I179 D180 E181 Q185 L186 G187

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.06Å 146.52Å 141.00Å 90.00° 110.21° 90.00°	Depositor
Resolution (Å)	17.98 – 2.60 17.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (17.98-2.60) 97.8 (17.98-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.277 0.254 , 0.270	Depositor DCC
R_{free} test set	5654 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28227	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3332e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: HEC, SR, LOP, FES, SMA, BGL, ANJ, 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	0.40	0/3565	1.04	30/4891 (0.6%)
1	D	0.40	0/3565	1.04	25/4891 (0.5%)
1	G	0.39	0/3565	1.02	25/4891 (0.5%)
1	J	0.40	0/3565	1.04	29/4891 (0.6%)
2	B	0.37	0/2010	1.00	5/2733 (0.2%)
2	E	0.36	0/2010	0.99	8/2733 (0.3%)
2	H	0.37	0/2010	1.00	6/2733 (0.2%)
2	K	0.36	0/2010	1.02	7/2733 (0.3%)
3	C	0.38	0/1371	1.05	6/1868 (0.3%)
3	F	0.37	0/1371	1.03	8/1868 (0.4%)
3	I	0.38	0/1371	1.04	6/1868 (0.3%)
3	L	0.36	0/1371	1.04	7/1868 (0.4%)
All	All	0.39	0/27784	1.03	162/37968 (0.4%)

There are no bond length outliers.

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	133	GLY	N-CA-C	9.93	125.41	113.79
3	L	133	GLY	N-CA-C	9.85	125.32	113.79
1	D	416	LYS	CA-C-N	9.82	129.77	119.85
1	D	416	LYS	C-N-CA	9.82	129.77	119.85
3	C	133	GLY	N-CA-C	9.69	125.13	113.79

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	3435	0	3420	145	0
1	D	3435	0	3420	161	0
1	G	3435	0	3420	140	0
1	J	3435	0	3420	126	0
2	B	1953	0	1848	92	0
2	E	1953	0	1848	120	0
2	H	1953	0	1848	114	0
2	K	1953	0	1848	95	0
3	C	1341	0	1307	54	0
3	F	1341	0	1307	76	0
3	I	1341	0	1307	65	0
3	L	1341	0	1307	73	0
4	A	20	0	28	3	0
4	E	20	0	28	2	0
4	G	20	0	28	1	0
4	J	20	0	28	1	0
5	A	86	0	60	9	0
5	D	86	0	60	11	0
5	G	86	0	60	7	0
5	J	86	0	60	5	0
6	A	37	0	42	2	0
6	D	37	0	42	3	0
6	G	37	0	42	2	0
6	J	37	0	42	3	0
7	A	45	0	67	3	0
7	D	45	0	67	5	0
7	G	45	0	67	5	0
7	J	45	0	67	5	0
8	A	39	0	39	9	0
8	D	39	0	39	12	0
8	G	39	0	39	6	0
8	J	39	0	39	10	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	1	0	0	0	0
10	B	43	0	30	7	0
10	E	43	0	30	5	0
10	H	43	0	30	4	0
10	K	43	0	30	1	0
11	C	4	0	0	0	0
11	F	4	0	0	0	0
11	I	4	0	0	0	0
11	L	4	0	0	0	0
12	A	36	0	0	2	0
12	B	7	0	0	3	0
12	C	13	0	0	0	0
12	D	41	0	0	4	0
12	E	3	0	0	0	0
12	F	13	0	0	2	0
12	G	41	0	0	3	0
12	H	4	0	0	0	0
12	I	14	0	0	0	0
12	J	23	0	0	1	0
12	K	3	0	0	1	0
12	L	11	0	0	1	0
All	All	28227	0	27364	1195	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 22.

The worst 5 of 1195 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:D:213:ILE:HD11	8:D:504:ANJ:H14	1.39	1.05
1:J:213:ILE:HD11	8:J:505:ANJ:H14	1.40	1.04
1:A:317:ILE:O	1:A:321:ILE:HG22	1.60	1.02
1:A:213:ILE:HD11	8:A:504:ANJ:H14	1.39	1.01
1:J:317:ILE:O	1:J:321:ILE:HG22	1.62	1.00

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	426/428 (100%)	398 (93%)	24 (6%)	4 (1%)	14	30
1	D	426/428 (100%)	402 (94%)	21 (5%)	3 (1%)	18	38
1	G	426/428 (100%)	400 (94%)	22 (5%)	4 (1%)	14	30
1	J	426/428 (100%)	397 (93%)	26 (6%)	3 (1%)	18	38
2	B	254/256 (99%)	227 (89%)	21 (8%)	6 (2%)	4	9
2	E	254/256 (99%)	229 (90%)	18 (7%)	7 (3%)	4	6
2	H	254/256 (99%)	225 (89%)	21 (8%)	8 (3%)	3	5
2	K	254/256 (99%)	229 (90%)	18 (7%)	7 (3%)	4	6
3	C	177/179 (99%)	143 (81%)	23 (13%)	11 (6%)	1	1
3	F	177/179 (99%)	144 (81%)	25 (14%)	8 (4%)	2	2
3	I	177/179 (99%)	144 (81%)	26 (15%)	7 (4%)	2	3
3	L	177/179 (99%)	142 (80%)	26 (15%)	9 (5%)	1	2
All	All	3428/3452 (99%)	3080 (90%)	271 (8%)	77 (2%)	5	10

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	137	GLY
2	B	147	GLU
2	B	200	HIS
3	C	109	ALA
2	E	137	GLY

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	353/353 (100%)	337 (96%)	16 (4%)	24	50
1	D	353/353 (100%)	338 (96%)	15 (4%)	26	52
1	G	353/353 (100%)	336 (95%)	17 (5%)	23	47
1	J	353/353 (100%)	339 (96%)	14 (4%)	28	55
2	B	203/203 (100%)	194 (96%)	9 (4%)	25	50
2	E	203/203 (100%)	194 (96%)	9 (4%)	25	50
2	H	203/203 (100%)	194 (96%)	9 (4%)	25	50
2	K	203/203 (100%)	192 (95%)	11 (5%)	20	42
3	C	138/138 (100%)	133 (96%)	5 (4%)	31	58
3	F	138/138 (100%)	132 (96%)	6 (4%)	26	51
3	I	138/138 (100%)	130 (94%)	8 (6%)	18	39
3	L	138/138 (100%)	128 (93%)	10 (7%)	13	30
All	All	2776/2776 (100%)	2647 (95%)	129 (5%)	24	49

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	167	ASP
3	L	11	ARG
2	E	76	GLU
2	E	58	LEU
3	L	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	383	GLN
2	K	22	GLN
3	L	45	GLN
2	E	69	GLN
2	E	62	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 for Mogul analysis.

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	$\#\|Z\| > 2$
4	BGL	G	431	-	20,20,20	0.87	1 (5%)	24,25,25	1.12	2 (8%)
6	SMA	A	1	-	38,38,38	2.26	10 (26%)	47,52,52	1.93	8 (17%)
6	SMA	J	503	-	38,38,38	2.14	8 (21%)	47,52,52	1.72	9 (19%)
10	HEC	H	301	2	50,50,50	1.13	2 (4%)	68,82,82	0.83	0
4	BGL	A	431	-	20,20,20	1.08	1 (5%)	24,25,25	0.71	0
7	LOP	A	503	-	44,44,44	0.59	0	47,49,49	1.33	8 (17%)
5	HEM	J	501	1	50,50,50	1.28	4 (8%)	67,82,82	1.07	3 (4%)
4	BGL	E	257	-	20,20,20	0.90	1 (5%)	24,25,25	1.16	2 (8%)
8	ANJ	J	505	-	40,40,40	1.88	11 (27%)	34,54,54	1.67	6 (17%)
5	HEM	G	502	1	50,50,50	1.23	4 (8%)	67,82,82	1.03	3 (4%)
5	HEM	D	501	1	50,50,50	1.28	4 (8%)	67,82,82	1.08	3 (4%)
11	FES	F	200	3	0,4,4	-	-	-		
7	LOP	J	504	-	44,44,44	0.57	0	47,49,49	1.39	8 (17%)
7	LOP	D	503	-	44,44,44	0.57	1 (2%)	47,49,49	1.29	7 (14%)
5	HEM	A	502	1	50,50,50	1.28	4 (8%)	67,82,82	1.04	3 (4%)
11	FES	I	200	3	0,4,4	-	-	-		
5	HEM	A	501	1	50,50,50	1.34	3 (6%)	67,82,82	1.05	3 (4%)
5	HEM	J	502	1	50,50,50	1.27	4 (8%)	67,82,82	1.07	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	HEM	G	501	1	50,50,50	1.31	4 (8%)	67,82,82	1.06	3 (4%)
10	HEC	K	301	2	50,50,50	1.07	2 (4%)	68,82,82	0.81	0
10	HEC	E	301	2	50,50,50	1.09	2 (4%)	68,82,82	0.81	0
11	FES	L	200	3	0,4,4	-	-	-		
6	SMA	G	503	-	38,38,38	2.32	9 (23%)	47,52,52	1.80	8 (17%)
5	HEM	D	502	1	50,50,50	1.27	3 (6%)	67,82,82	1.15	4 (5%)
7	LOP	G	504	-	44,44,44	0.61	0	47,49,49	1.30	5 (10%)
8	ANJ	D	504	-	40,40,40	1.87	11 (27%)	34,54,54	1.93	7 (20%)
8	ANJ	G	505	-	40,40,40	1.85	10 (25%)	34,54,54	1.76	6 (17%)
11	FES	C	200	3	0,4,4	-	-	-		
6	SMA	D	2	-	38,38,38	2.25	8 (21%)	47,52,52	1.73	11 (23%)
4	BGL	J	431	-	20,20,20	0.99	1 (5%)	24,25,25	0.78	0
10	HEC	B	301	2	50,50,50	1.08	2 (4%)	68,82,82	0.83	0
8	ANJ	A	504	-	40,40,40	1.86	9 (22%)	34,54,54	1.81	9 (26%)

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
4	BGL	G	431	-	-	0/11/31/31	0/1/1/1
6	SMA	A	1	-	-	4/34/34/34	0/2/2/2
10	HEC	H	301	2	1/1/3/7	9/14/54/54	-
6	SMA	J	503	-	-	5/34/34/34	0/2/2/2
4	BGL	A	431	-	-	0/11/31/31	0/1/1/1
7	LOP	A	503	-	-	12/48/48/48	-
5	HEM	J	501	1	-	5/14/54/54	-
4	BGL	E	257	-	-	0/11/31/31	0/1/1/1
8	ANJ	J	505	-	-	6/40/55/55	0/1/2/2
5	HEM	G	502	1	-	9/14/54/54	-
5	HEM	D	501	1	-	6/14/54/54	-
11	FES	F	200	3	-	-	0/1/1/1
7	LOP	J	504	-	-	7/48/48/48	-
7	LOP	D	503	-	-	11/48/48/48	-
5	HEM	A	502	1	-	6/14/54/54	-
11	FES	I	200	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	501	1	-	4/14/54/54	-
5	HEM	J	502	1	-	7/14/54/54	-
5	HEM	G	501	1	-	6/14/54/54	-
10	HEC	K	301	2	1/1/3/7	8/14/54/54	-
10	HEC	E	301	2	1/1/3/7	10/14/54/54	-
11	FES	L	200	3	-	-	0/1/1/1
6	SMA	G	503	-	-	5/34/34/34	0/2/2/2
5	HEM	D	502	1	-	6/14/54/54	-
7	LOP	G	504	-	-	9/48/48/48	-
8	ANJ	D	504	-	-	6/40/55/55	0/1/2/2
8	ANJ	G	505	-	-	4/40/55/55	0/1/2/2
11	FES	C	200	3	-	-	0/1/1/1
6	SMA	D	2	-	-	5/34/34/34	0/2/2/2
4	BGL	J	431	-	-	0/11/31/31	0/1/1/1
10	HEC	B	301	2	1/1/3/7	7/14/54/54	-
8	ANJ	A	504	-	-	2/40/55/55	0/1/2/2

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	503	SMA	O5-C5	7.42	1.49	1.37
6	A	1	SMA	O5-C5	7.39	1.49	1.37
6	G	503	SMA	O7-C7	7.29	1.49	1.37
6	D	2	SMA	O5-C5	7.26	1.48	1.37
6	A	1	SMA	O7-C7	7.05	1.48	1.37

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1	SMA	O7-C7-C8	7.20	122.06	114.53
8	G	505	ANJ	O6-C17-C9	-5.49	101.65	110.28
8	A	504	ANJ	O6-C17-C9	-5.45	101.70	110.28
8	D	504	ANJ	C19-C18-C13	-5.44	104.68	114.28
8	D	504	ANJ	O6-C17-C9	-5.09	102.27	110.28

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	301	HEC	NA

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Mol	Chain	Res	Type	Atom
10	E	301	HEC	NA
10	H	301	HEC	NA
10	K	301	HEC	NA

5 of 159 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	HEM	C2C-C3C-CAC-CBC
5	A	501	HEM	C4C-C3C-CAC-CBC
5	A	502	HEM	C2B-C3B-CAB-CBB
5	A	502	HEM	C4B-C3B-CAB-CBB
5	D	501	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

28 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	431	BGL	1	0
6	A	1	SMA	2	0
6	J	503	SMA	3	0
10	H	301	HEC	4	0
4	A	431	BGL	3	0
7	A	503	LOP	3	0
5	J	501	HEM	2	0
4	E	257	BGL	2	0
8	J	505	ANJ	10	0
5	G	502	HEM	3	0
5	D	501	HEM	6	0
7	J	504	LOP	5	0
7	D	503	LOP	5	0
5	A	502	HEM	5	0
5	A	501	HEM	4	0
5	J	502	HEM	3	0
5	G	501	HEM	4	0
10	K	301	HEC	1	0
10	E	301	HEC	5	0
6	G	503	SMA	2	0
5	D	502	HEM	5	0
7	G	504	LOP	5	0
8	D	504	ANJ	12	0
8	G	505	ANJ	6	0
6	D	2	SMA	3	0

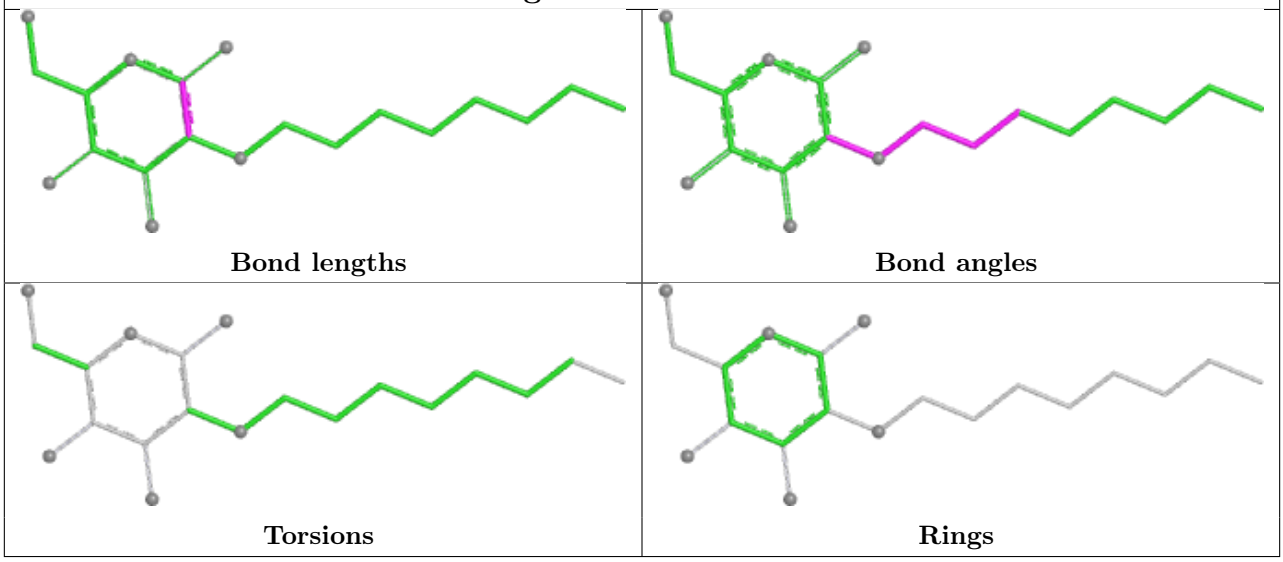
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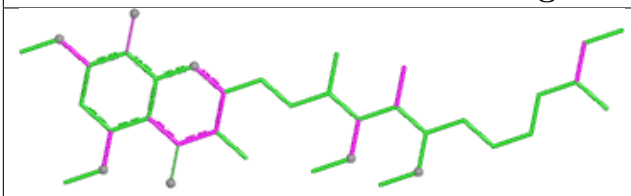
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	431	BGL	1	0
10	B	301	HEC	7	0
8	A	504	ANJ	9	0

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.

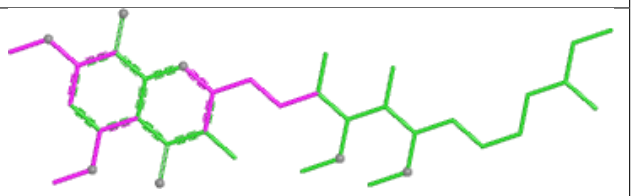
Ligand BGL G 431



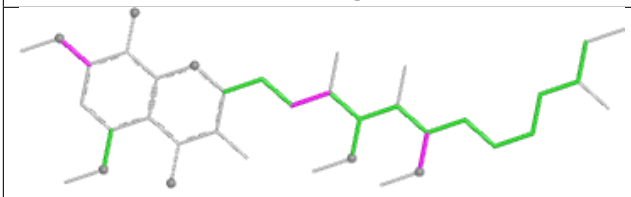
Ligand SMA A 1



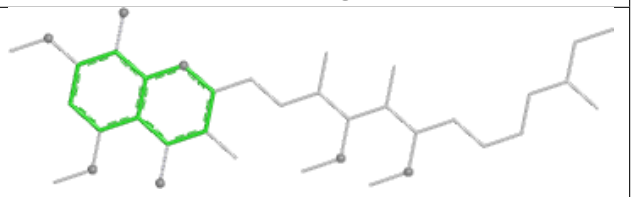
Bond lengths



Bond angles

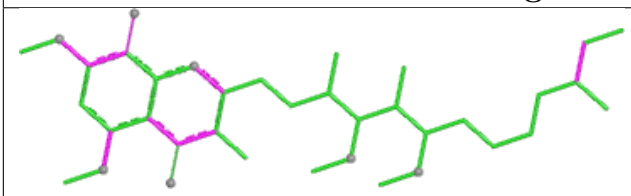


Torsions

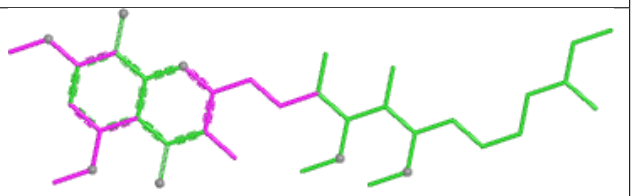


Rings

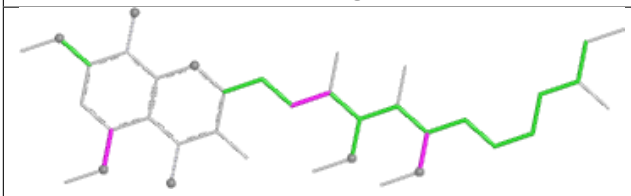
Ligand SMA J 503



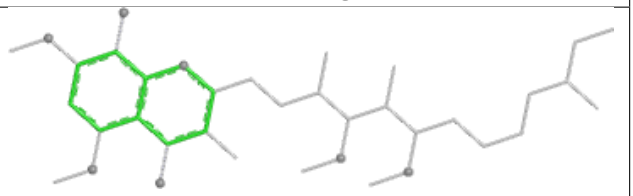
Bond lengths



Bond angles

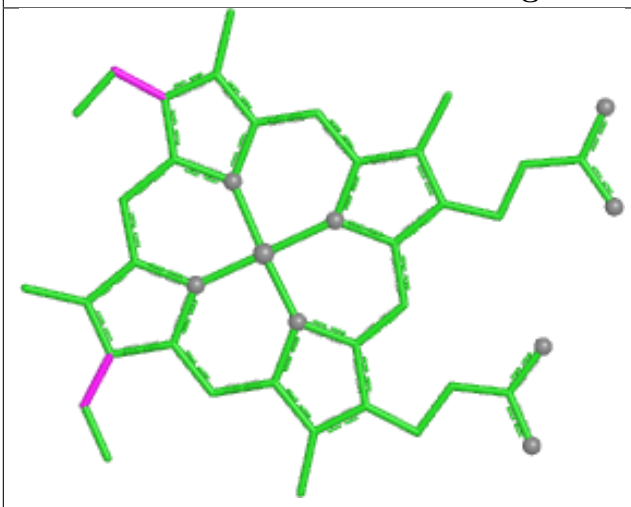


Torsions

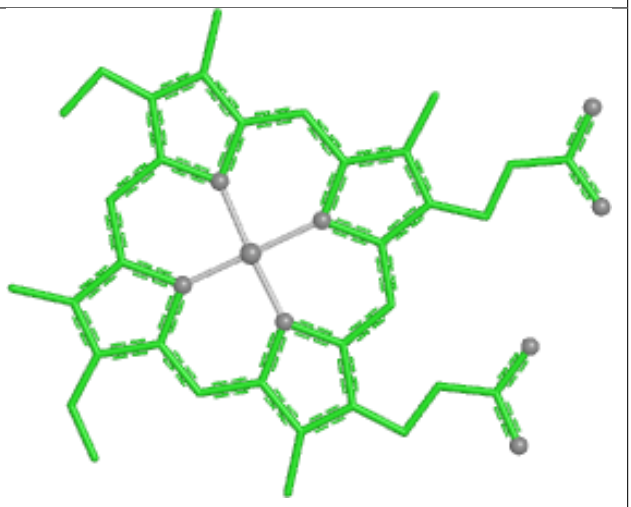


Rings

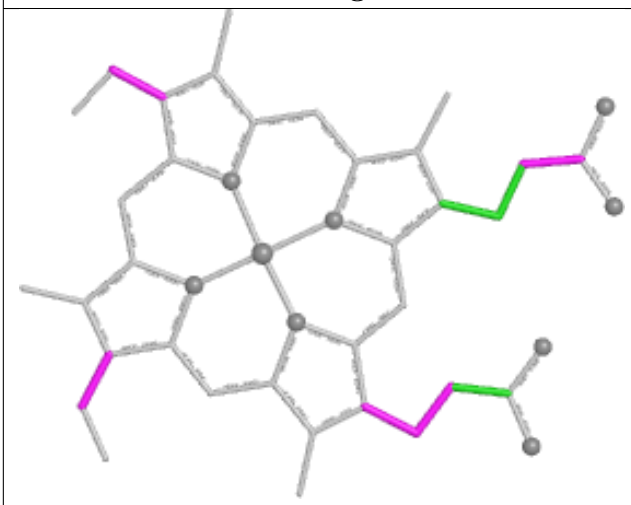
Ligand HEC H 301



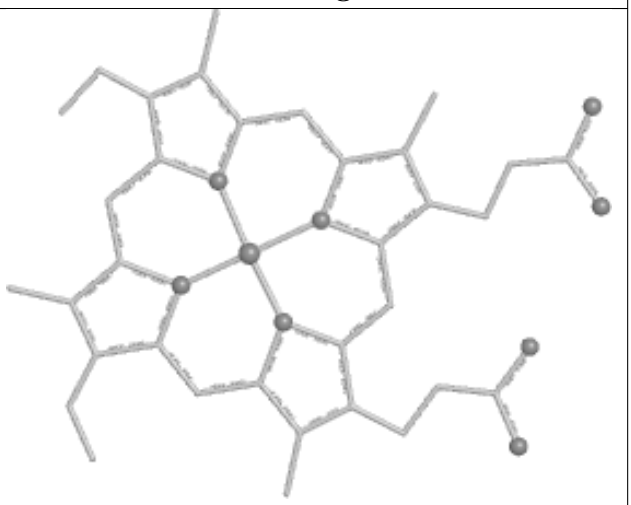
Bond lengths



Bond angles

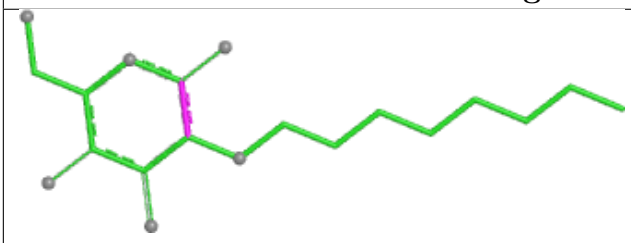


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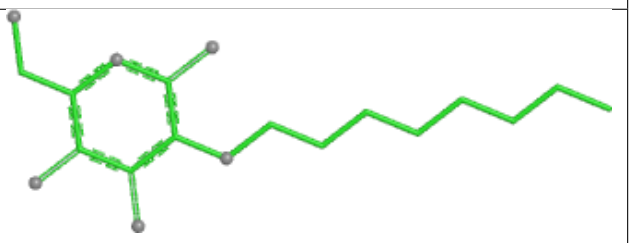


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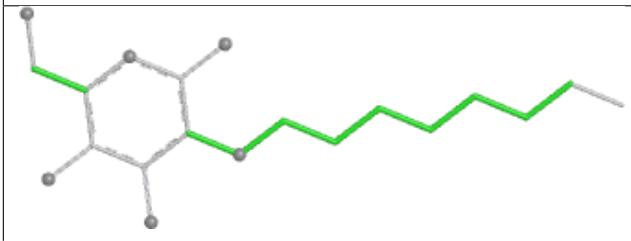
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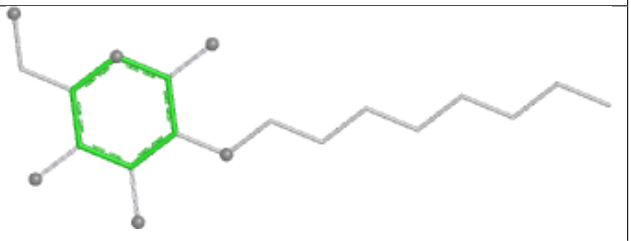
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Bond angles

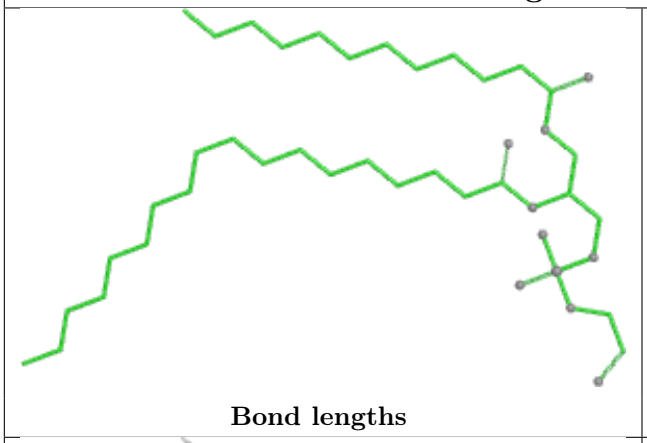


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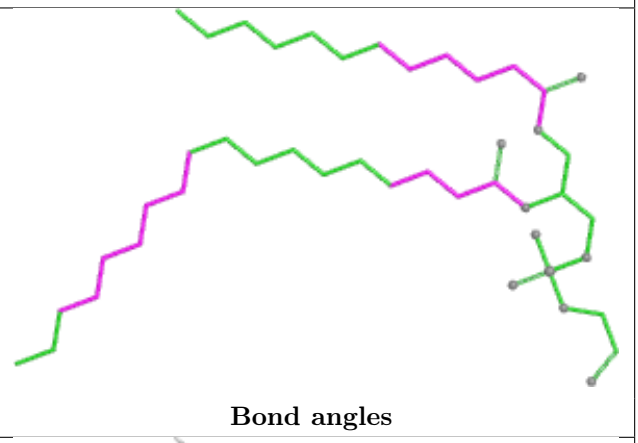


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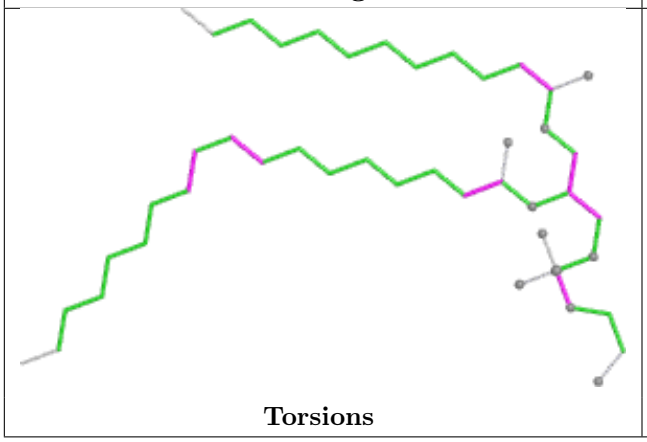
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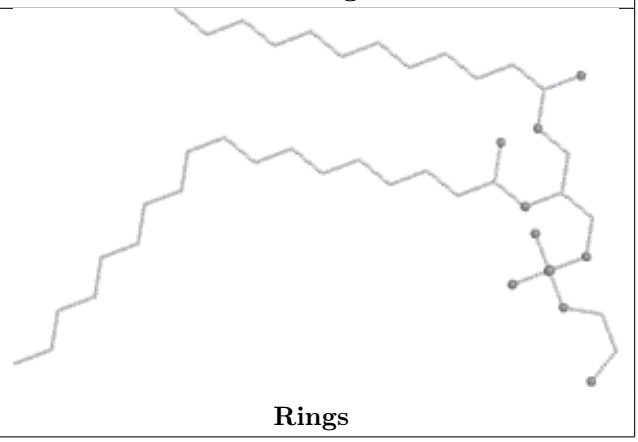
Bond lengths



Bond angles

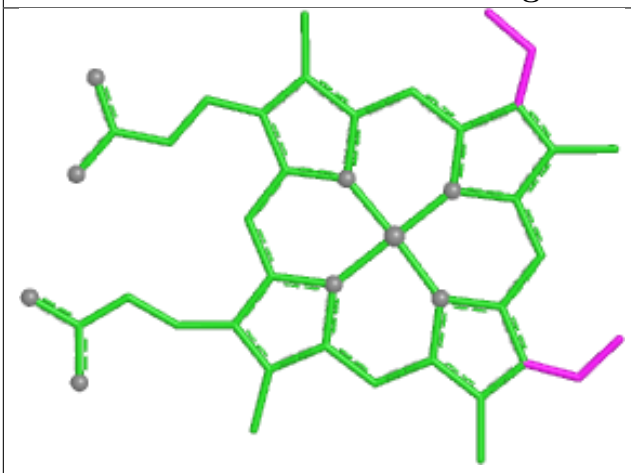


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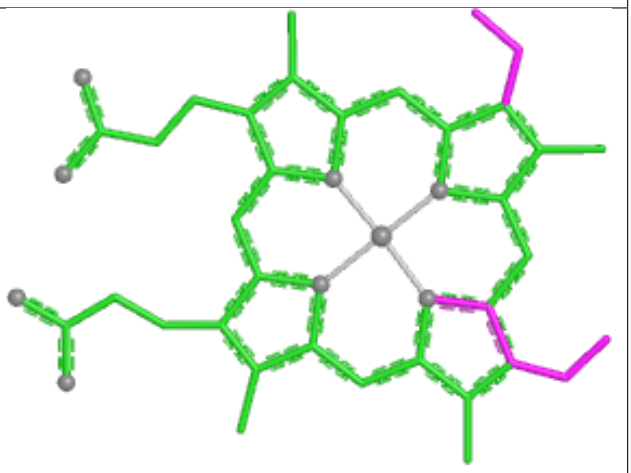


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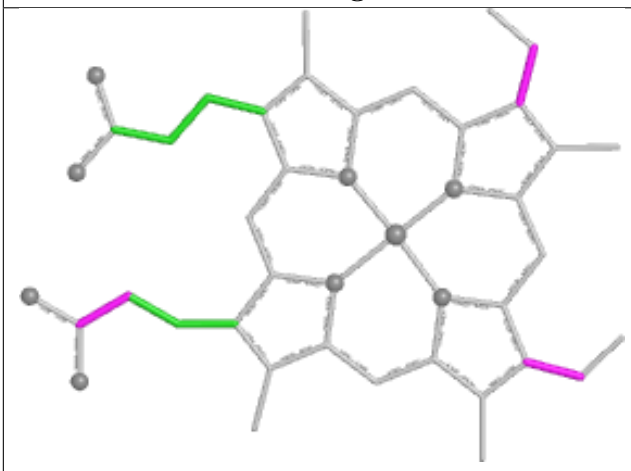
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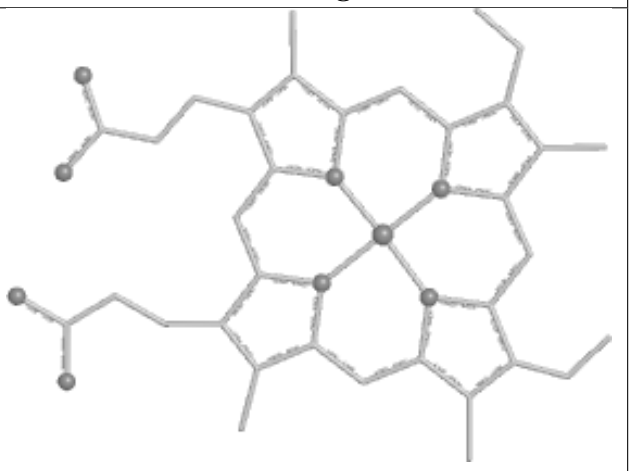
Bond lengths



Bond angles

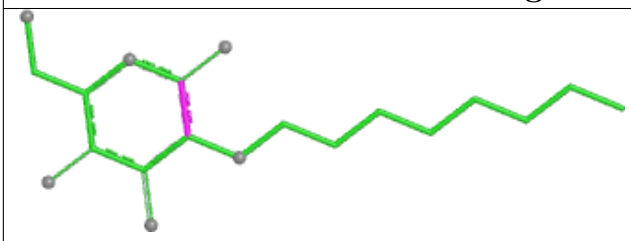


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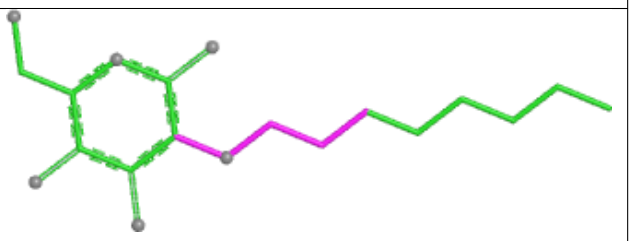


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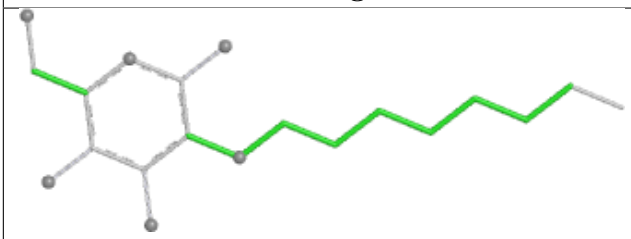
Ligand BGL E 257



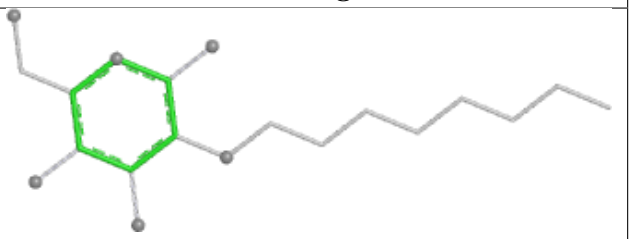
Bond lengths



Bond angles

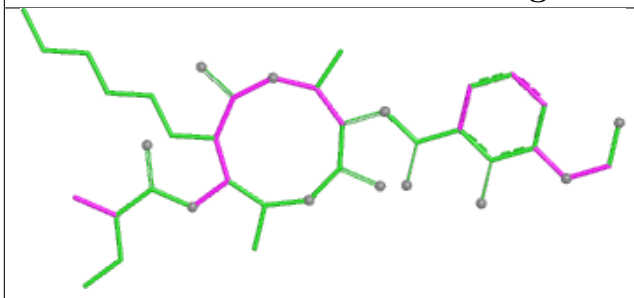


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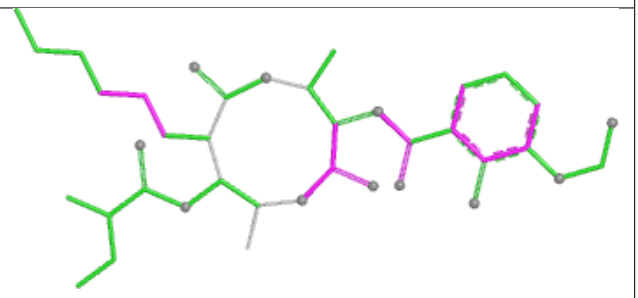


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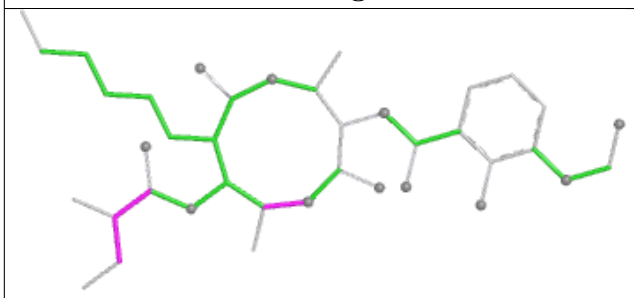
Ligand ANJ J 505



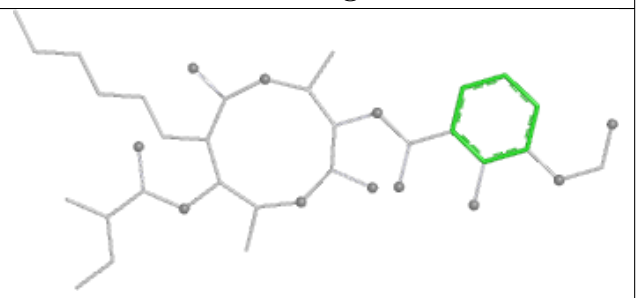
Bond lengths



Bond angles

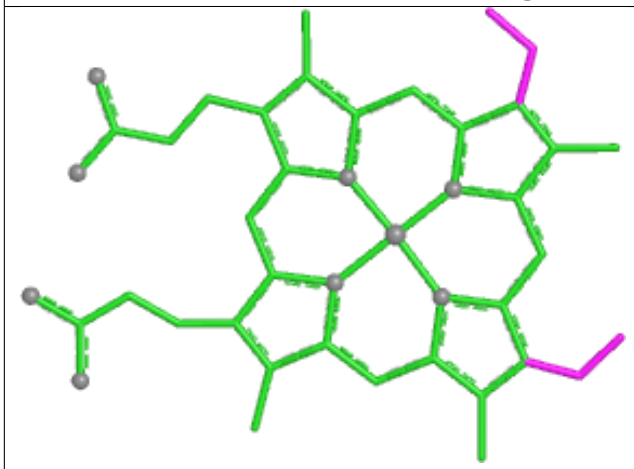


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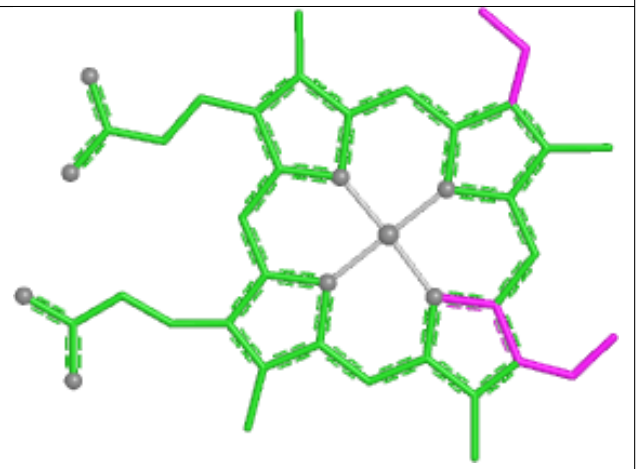


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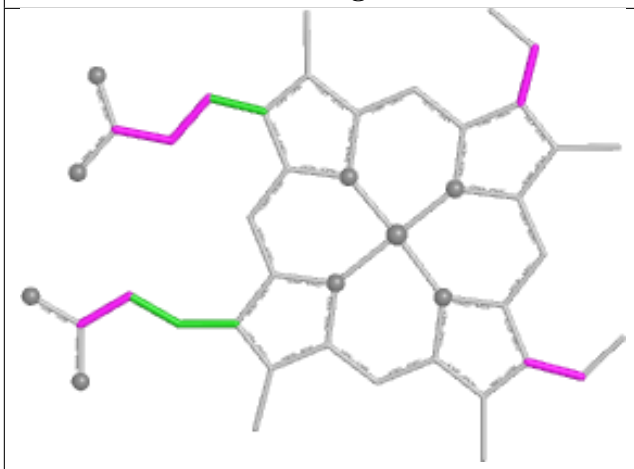
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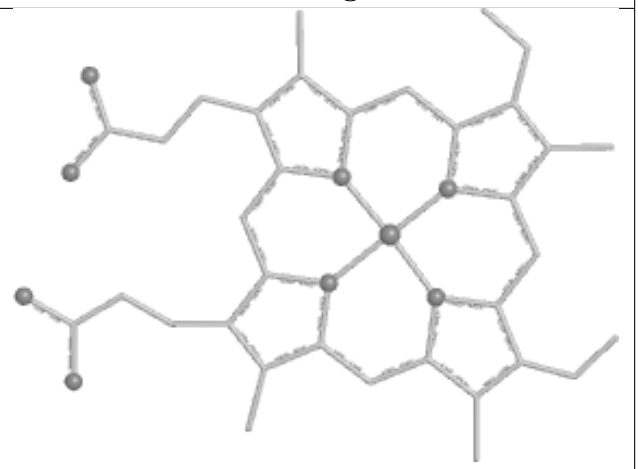
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Bond angles

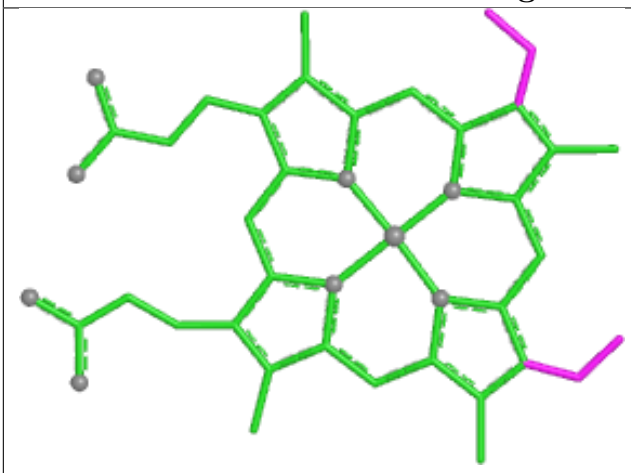


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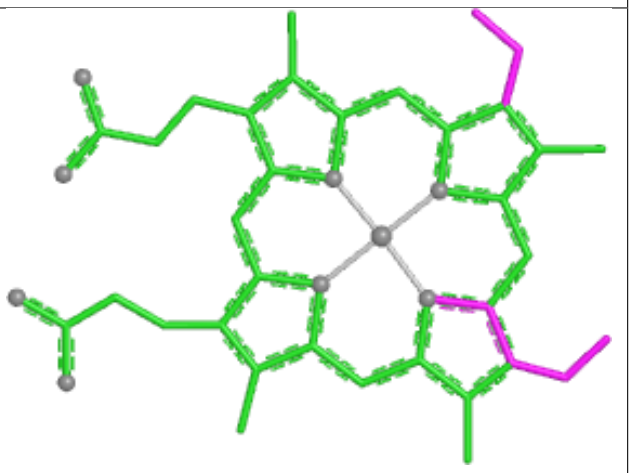


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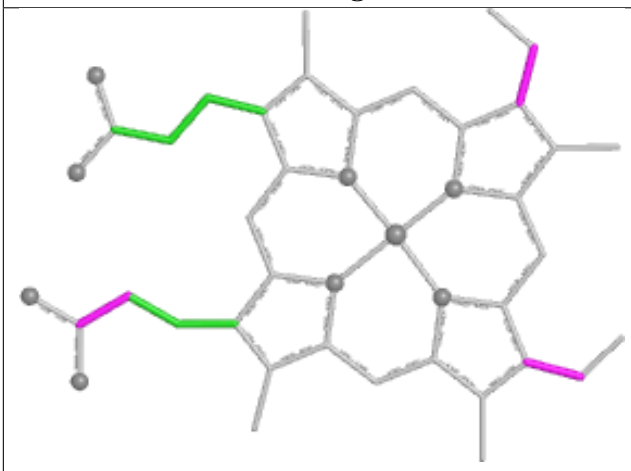
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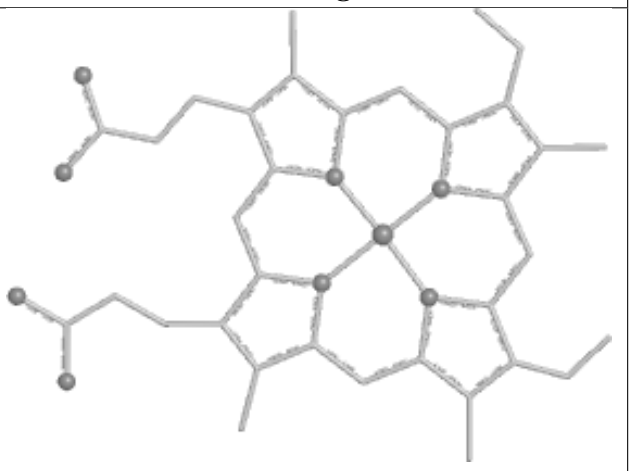
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Bond angles

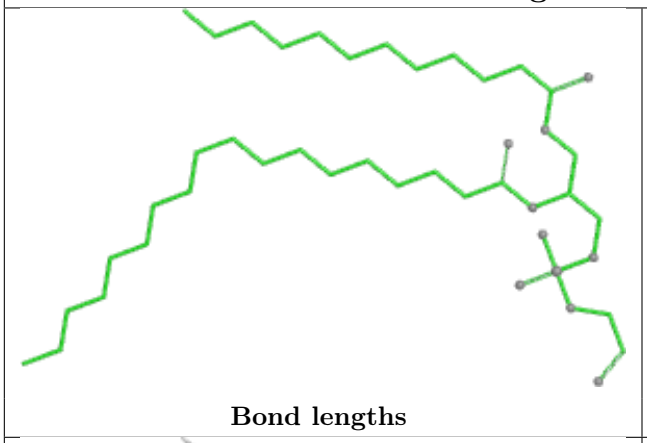


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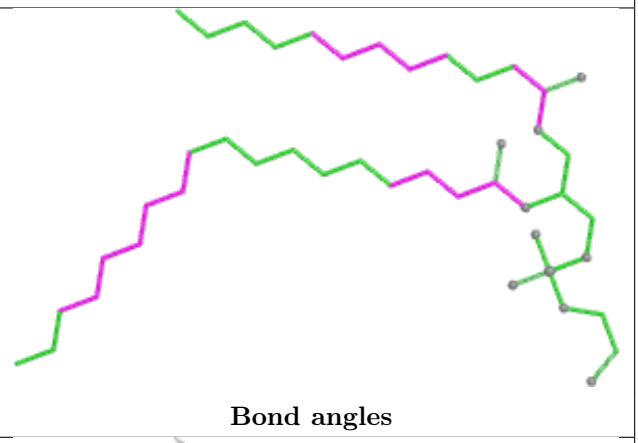


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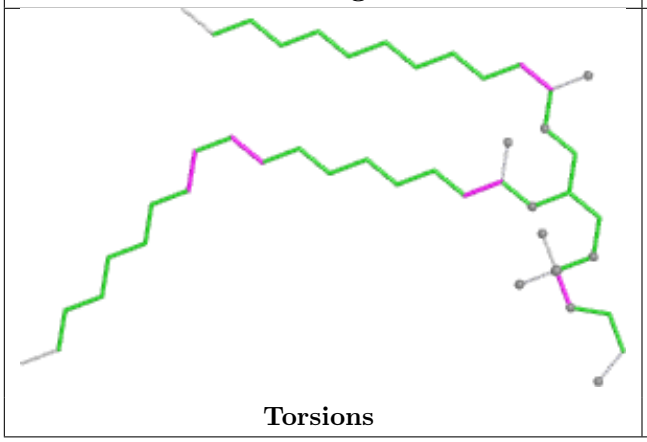
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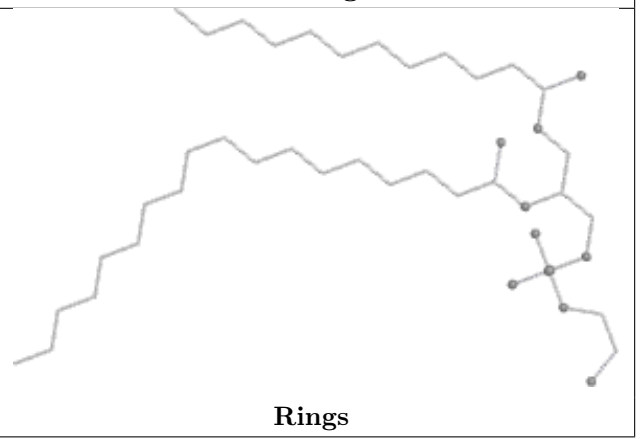
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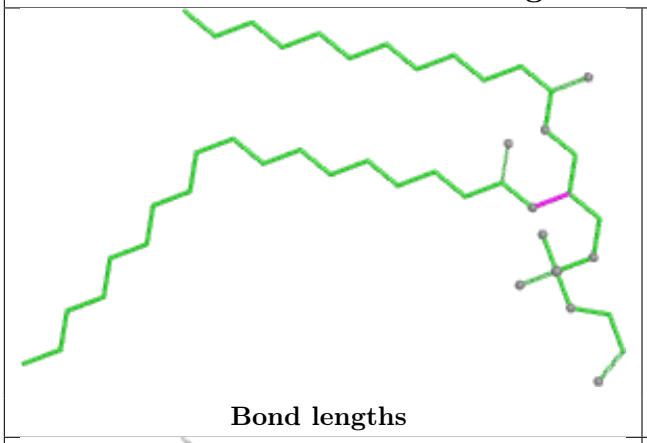


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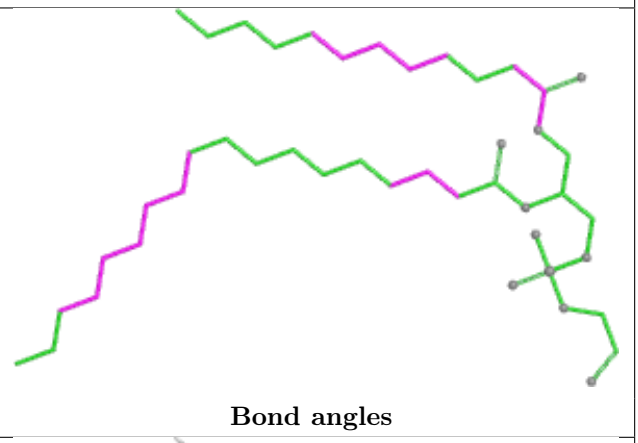


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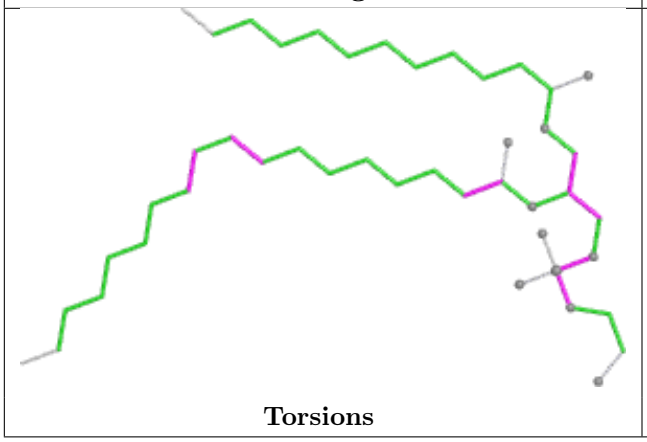
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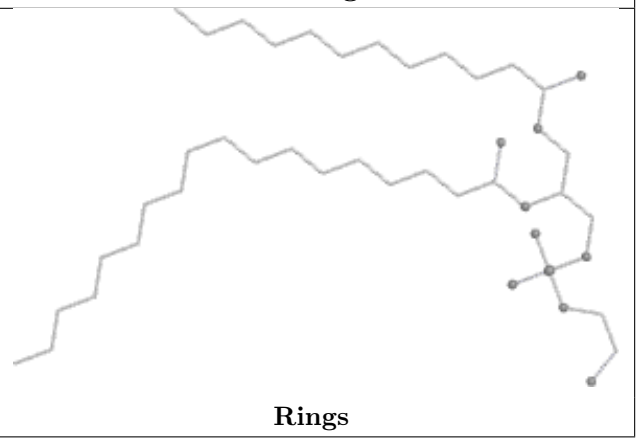
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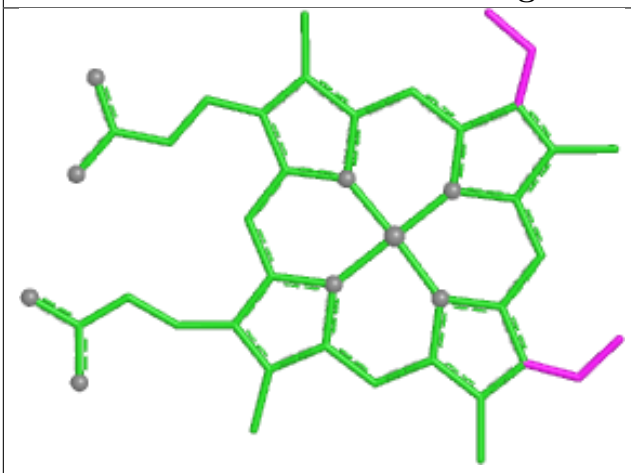


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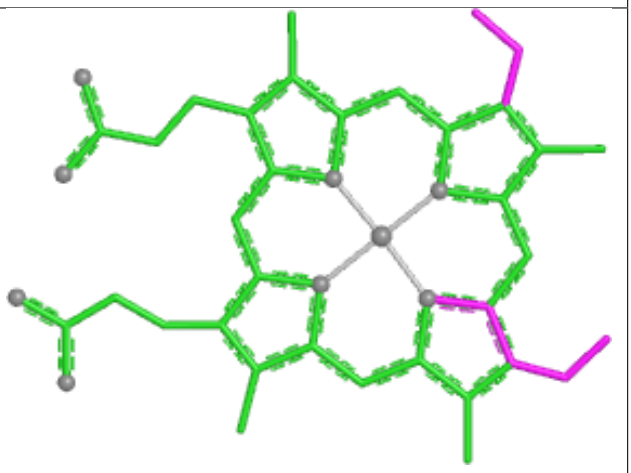


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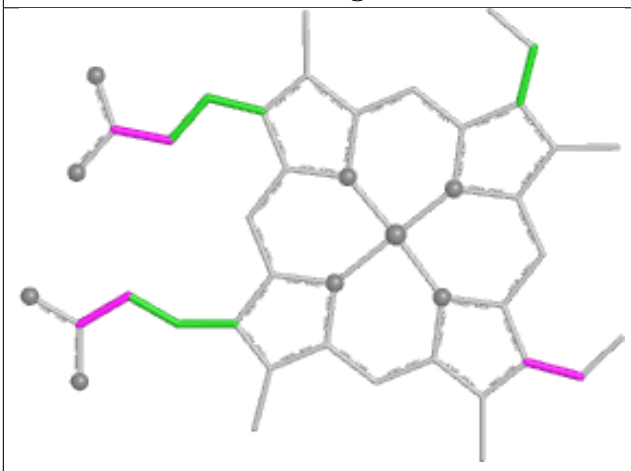
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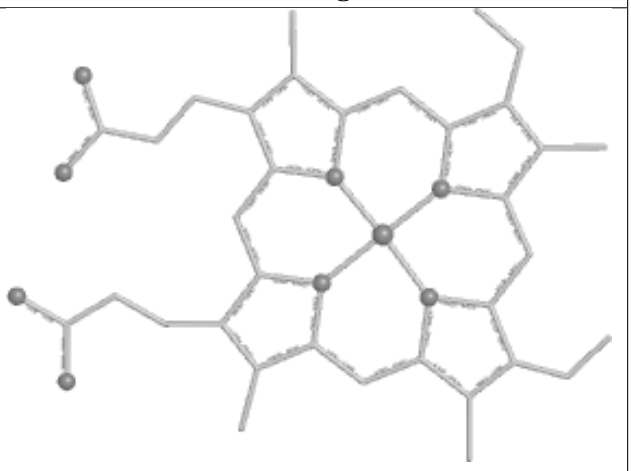
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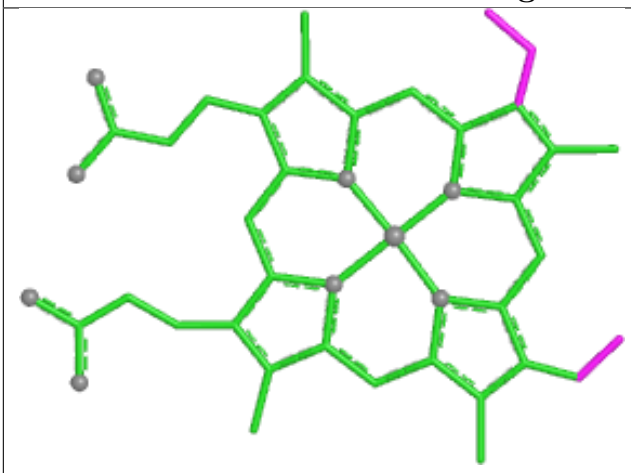


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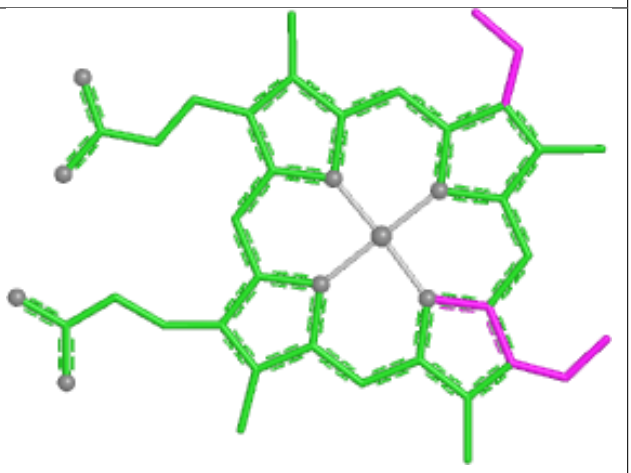


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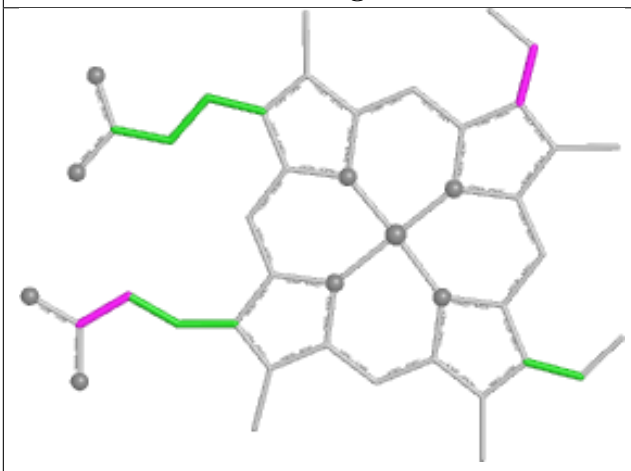
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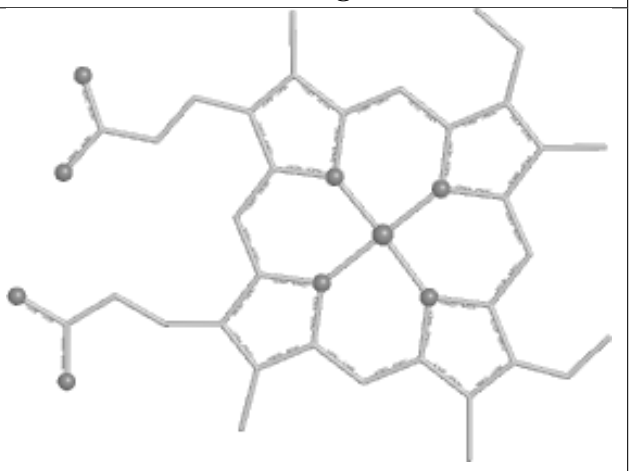
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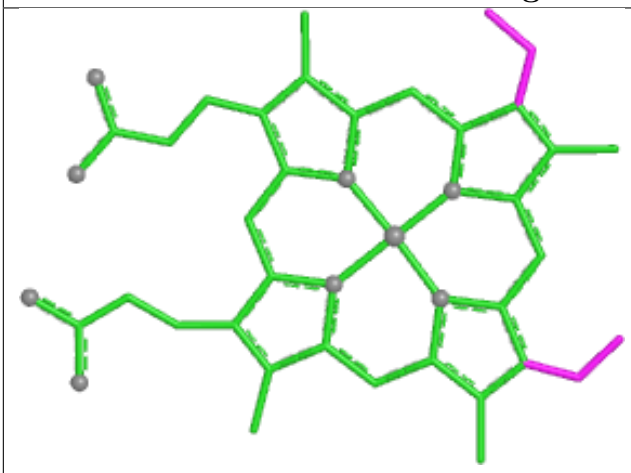


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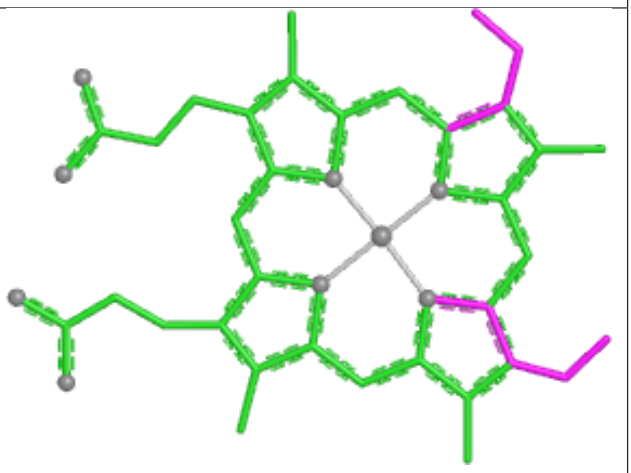


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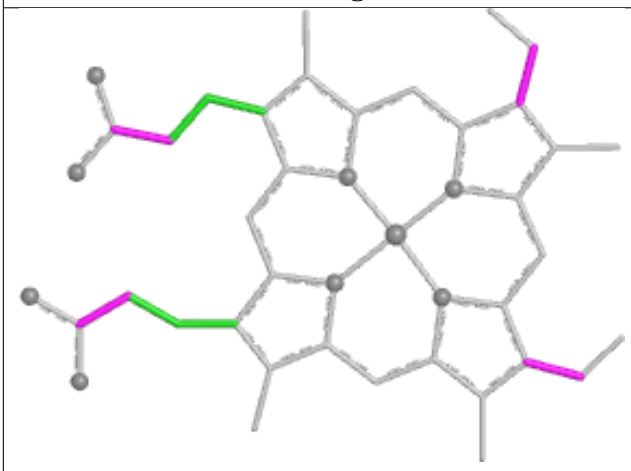
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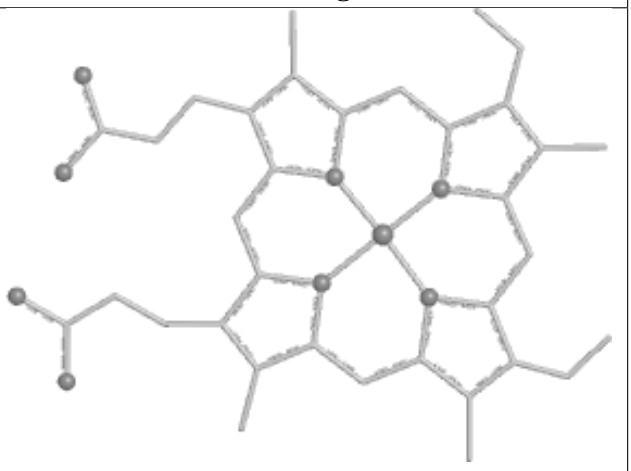
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Bond angles

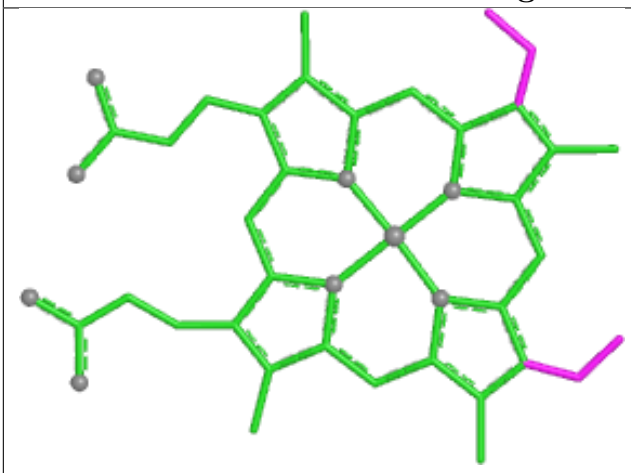


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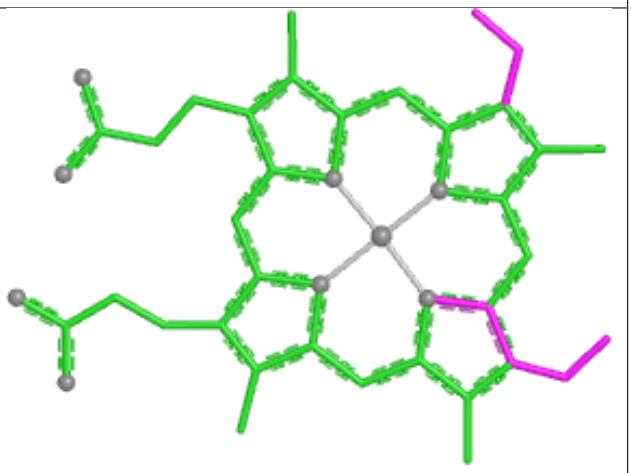


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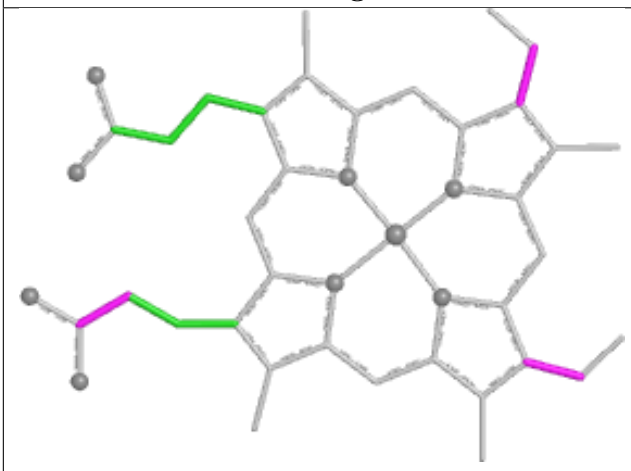
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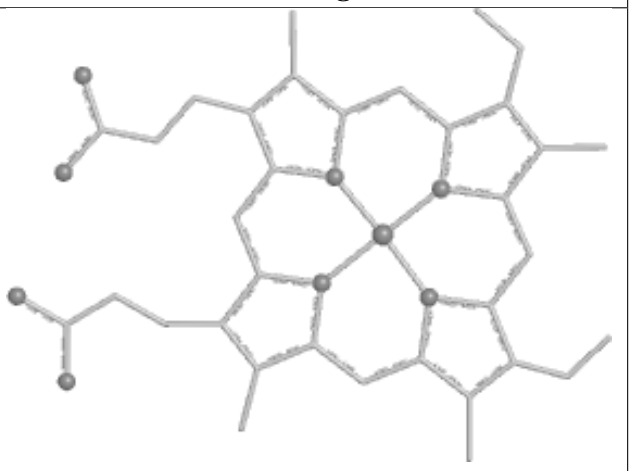
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Bond angles

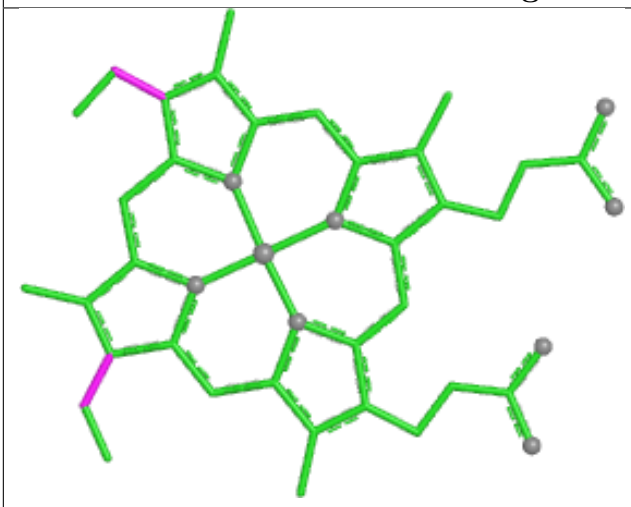


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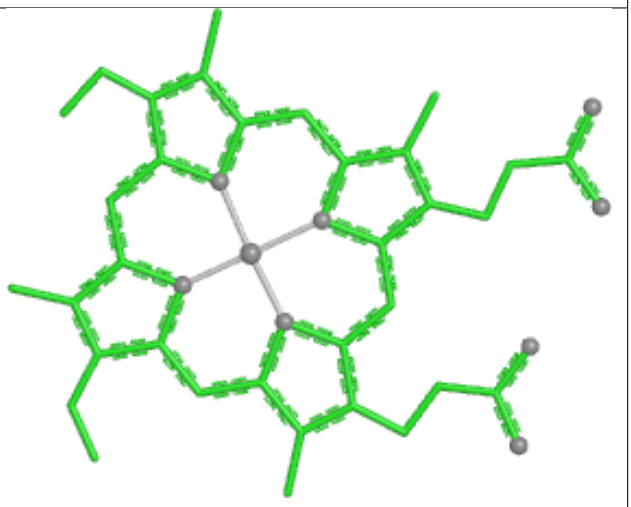


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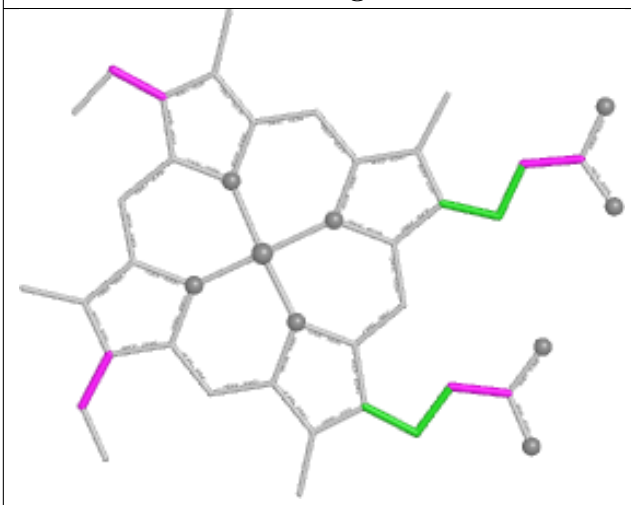
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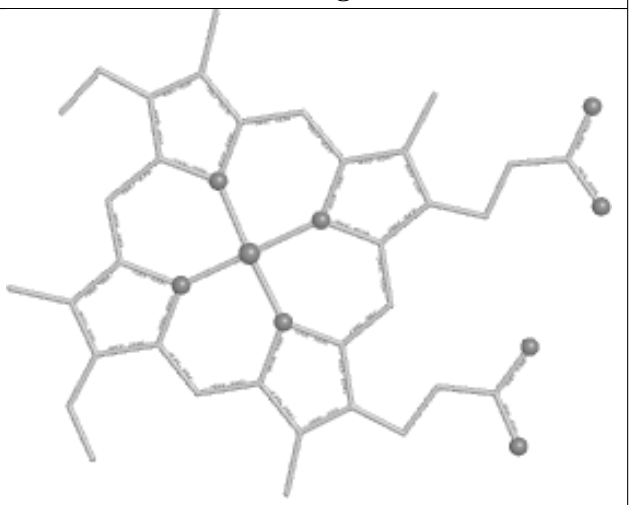
Bond lengths



Bond angles

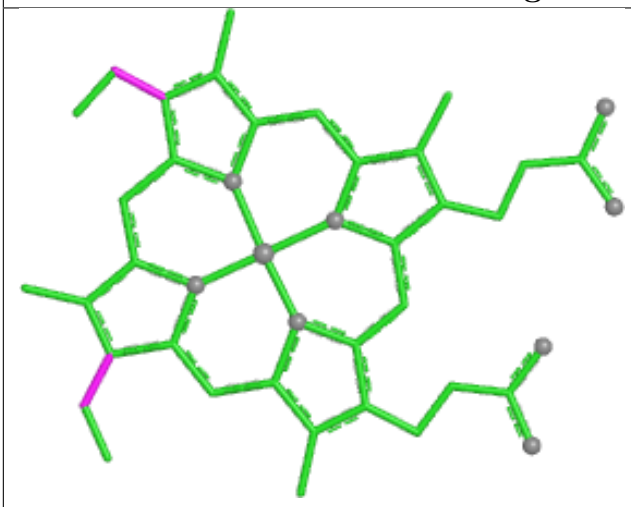


Torsions

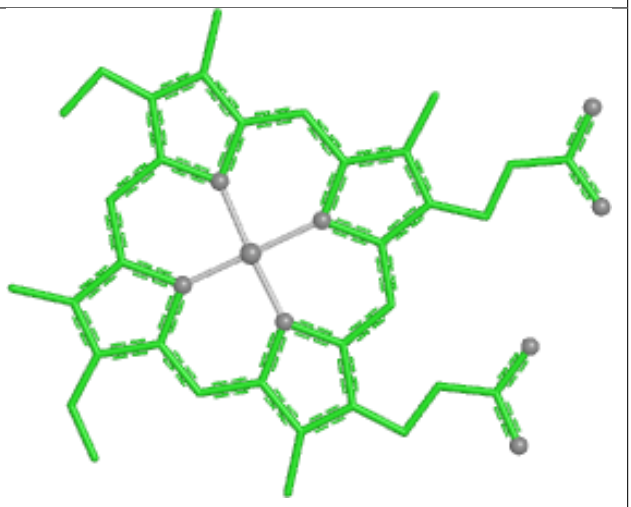


Rings

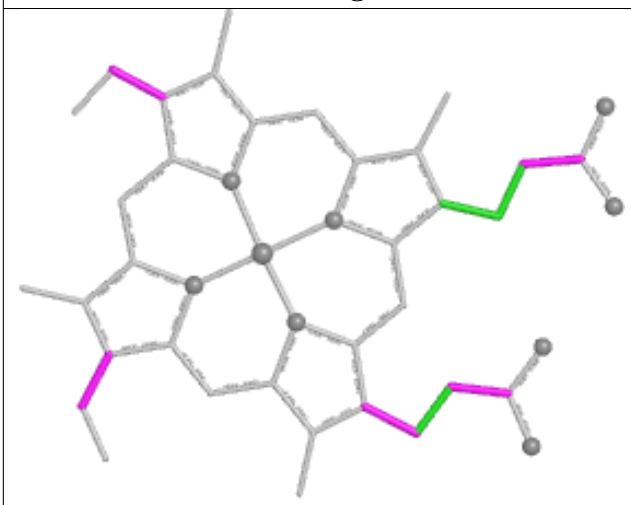
Ligand HEC E 301



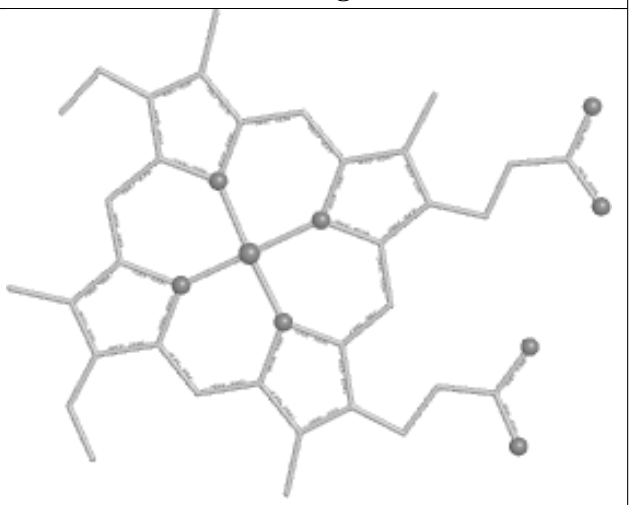
Bond lengths



Bond angles

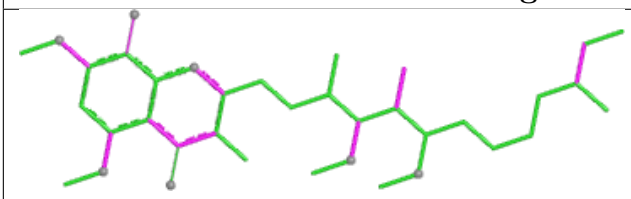


Torsions

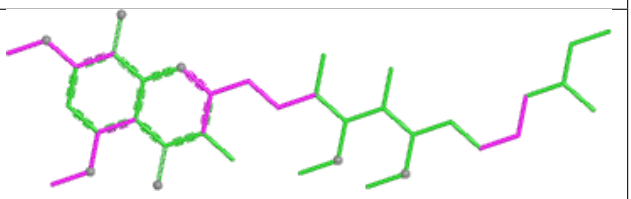


Rings

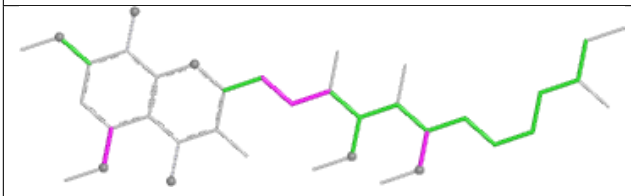
Ligand SMA G 503



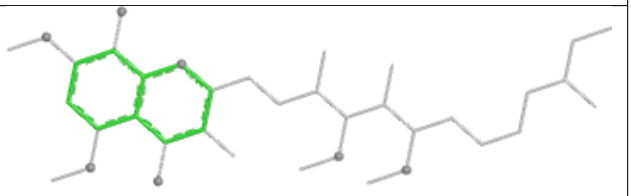
Bond lengths



Bond angles

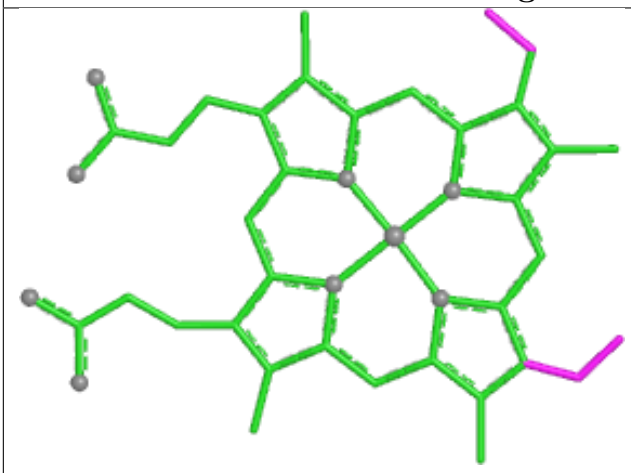


Torsions

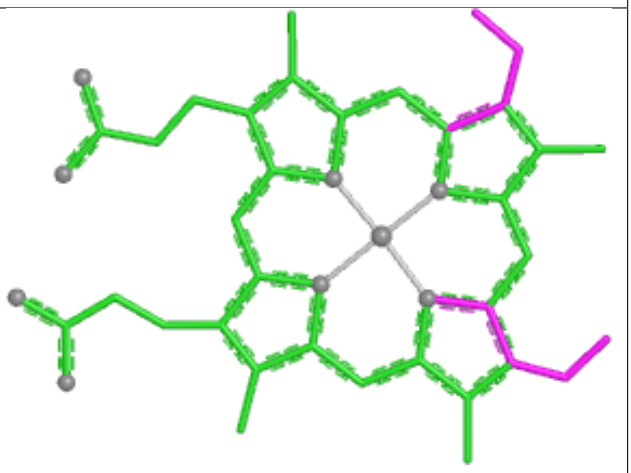


Rings

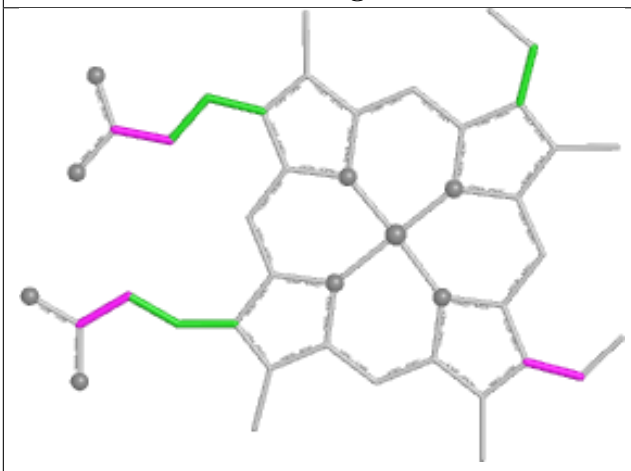
Ligand HEM D 502



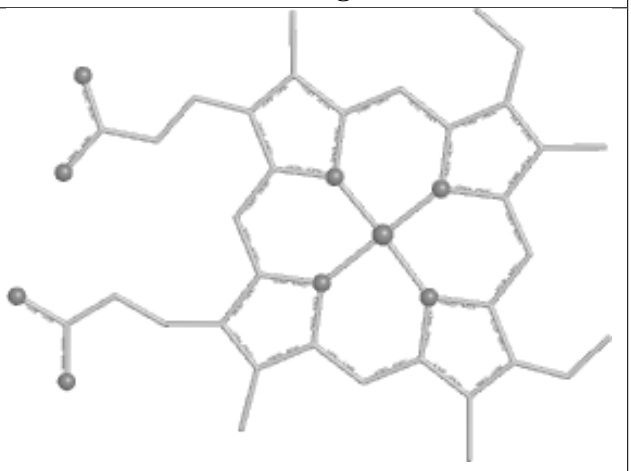
Bond lengths



Bond angles

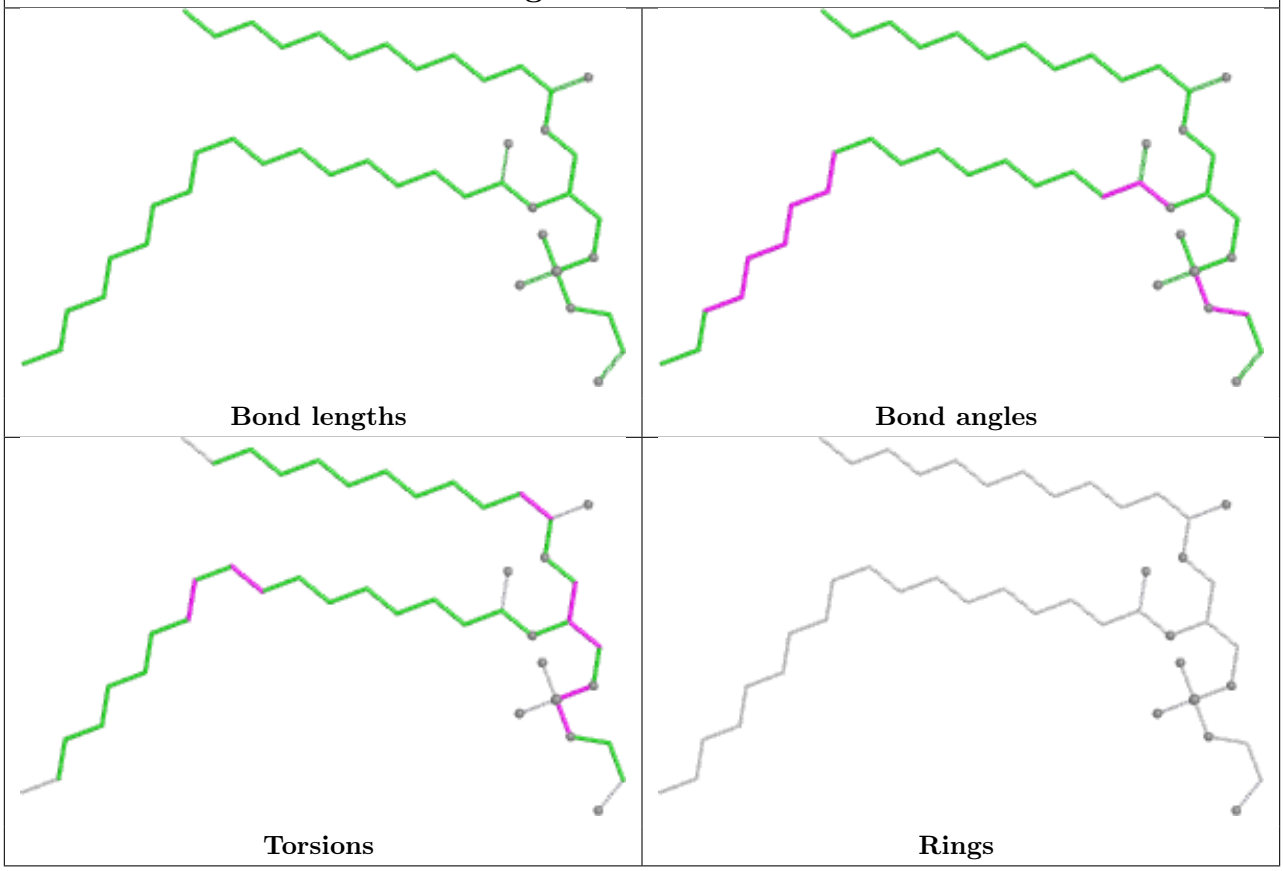


Torsions

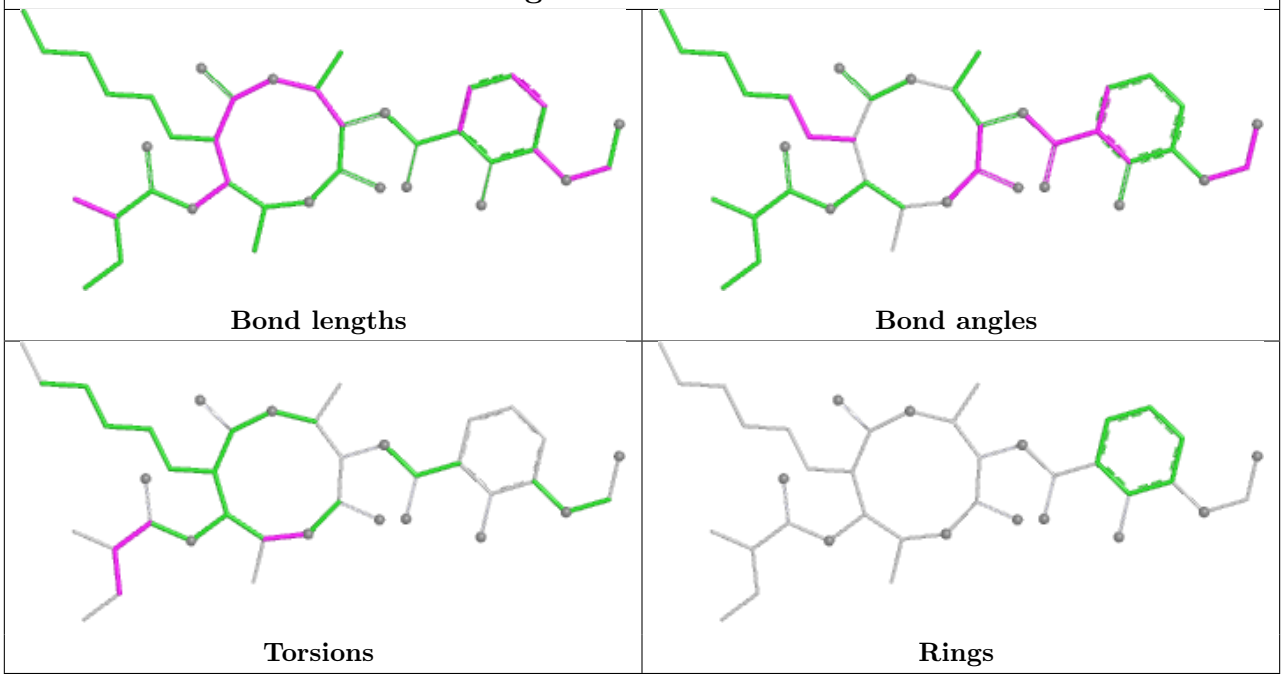


Rings

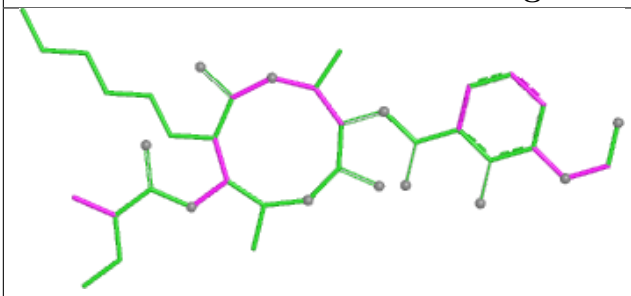
Ligand LOP G 504



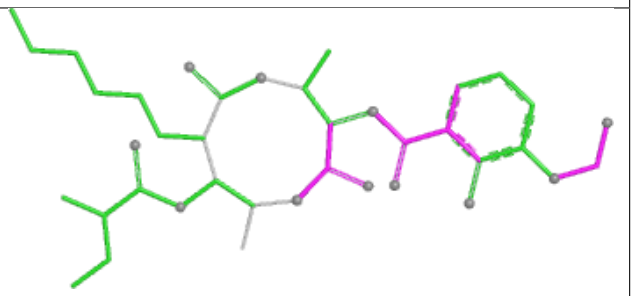
Ligand ANJ D 504



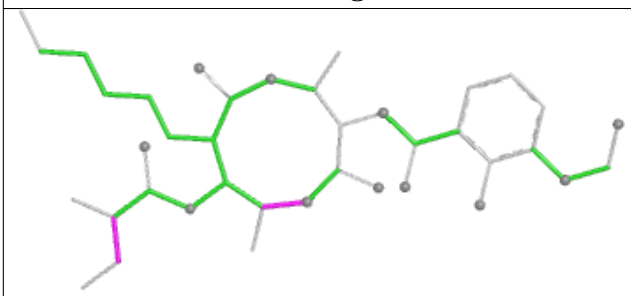
Ligand ANJ G 505



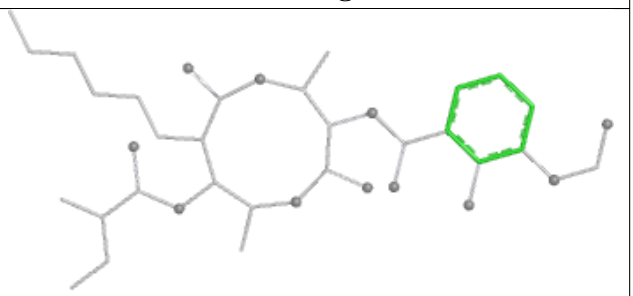
Bond lengths



Bond angles

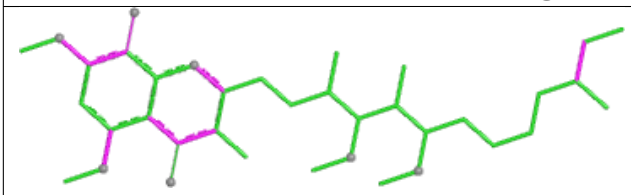


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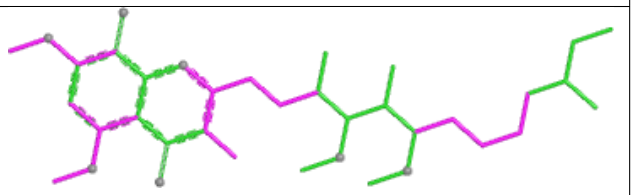


Rings

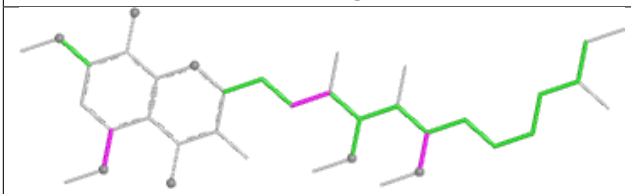
Ligand SMA D 2



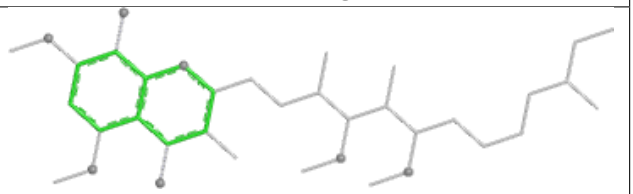
Bond lengths



Bond angles

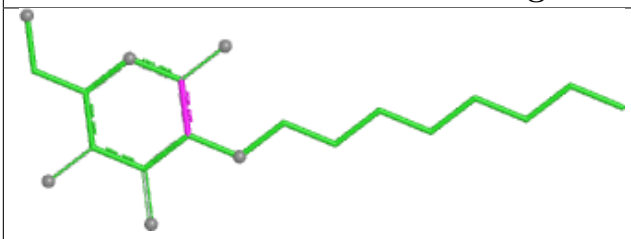


Torsions

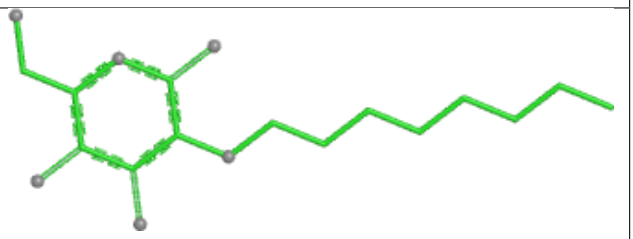


Rings

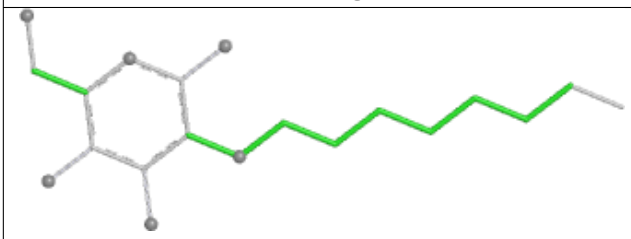
Ligand BGL J 431



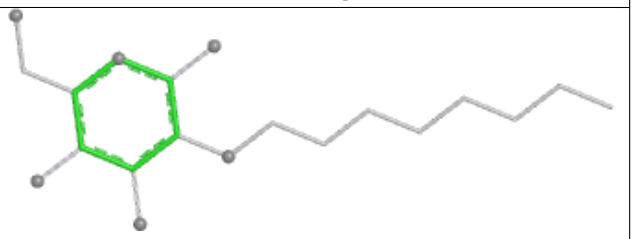
Bond lengths



Bond angles

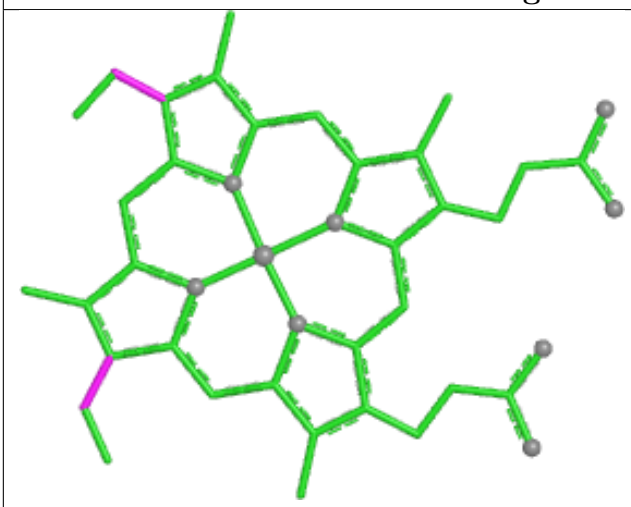


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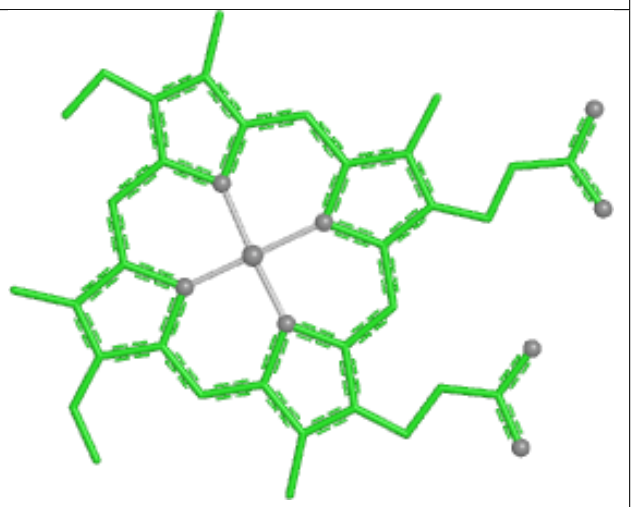


Rings

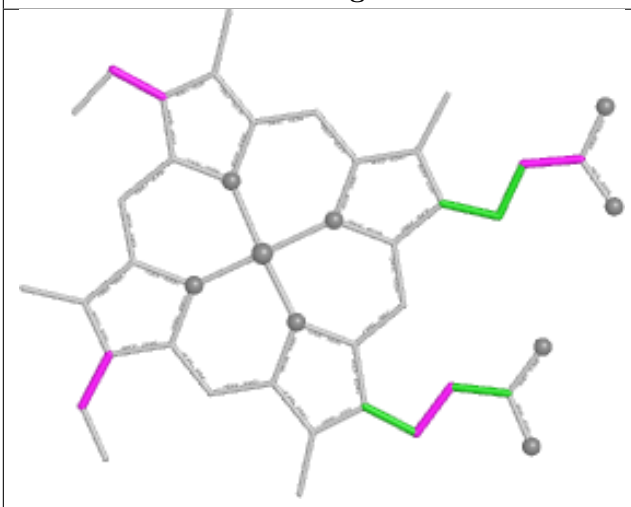
Ligand HEC B 301



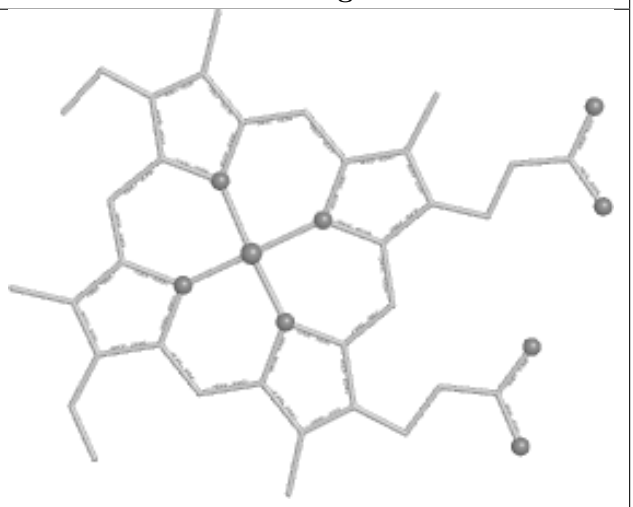
Bond lengths



Bond angles

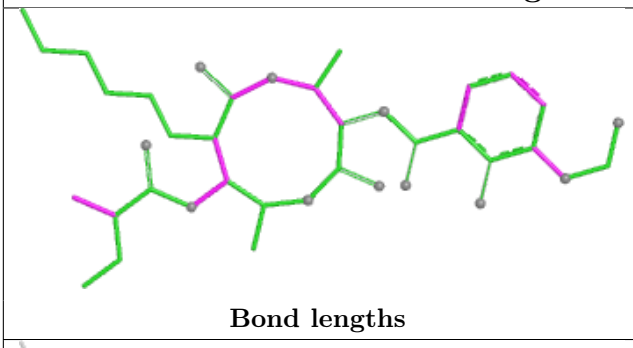


Torsions

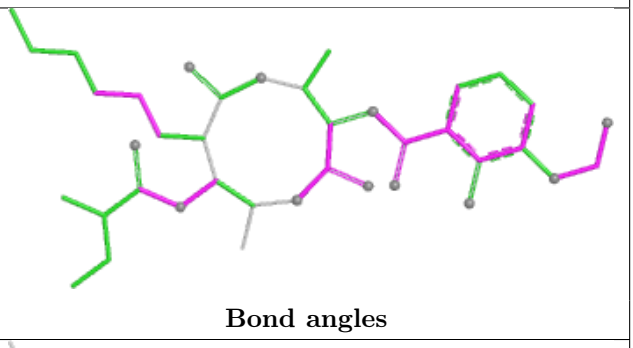


Rings

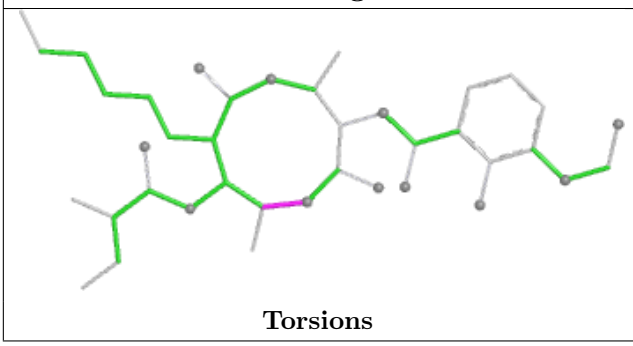
Ligand ANJ A 504



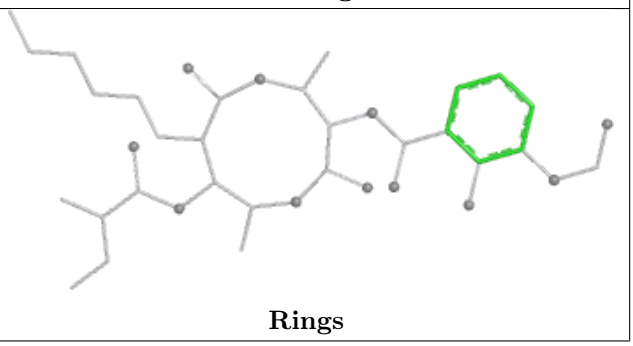
Bond lengths



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	428/428 (100%)	0.15	4 (0%)	81	78	42, 63, 104, 129	0
1	D	428/428 (100%)	0.20	7 (1%)	70	66	43, 62, 100, 128	0
1	G	428/428 (100%)	0.23	2 (0%)	87	85	43, 64, 104, 128	0
1	J	428/428 (100%)	0.17	4 (0%)	81	78	43, 62, 100, 126	0
2	B	256/256 (100%)	0.75	22 (8%)	16	12	55, 89, 125, 149	0
2	E	256/256 (100%)	0.67	16 (6%)	26	20	65, 93, 128, 148	0
2	H	256/256 (100%)	0.71	14 (5%)	30	25	57, 90, 126, 151	0
2	K	256/256 (100%)	0.56	15 (5%)	28	23	62, 91, 127, 150	0
3	C	179/179 (100%)	0.56	4 (2%)	62	57	49, 82, 123, 155	0
3	F	179/179 (100%)	0.45	3 (1%)	69	64	49, 84, 124, 155	0
3	I	179/179 (100%)	0.58	5 (2%)	55	49	50, 83, 125, 156	0
3	L	179/179 (100%)	0.58	7 (3%)	43	38	52, 85, 124, 156	0
All	All	3452/3452 (100%)	0.41	103 (2%)	52	47	42, 75, 122, 156	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	10	THR	6.2
2	K	124	GLY	4.4
3	F	9	GLY	4.3
2	B	206	ALA	4.1
2	B	116	THR	4.0

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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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	BGL	J	431	20/20	0.71	0.22	95,96,100,101	0
7	LOP	G	504	45/45	0.74	0.15	70,87,96,98	0
4	BGL	G	431	20/20	0.77	0.21	97,99,102,102	0
4	BGL	A	431	20/20	0.78	0.14	89,92,93,93	0
4	BGL	E	257	20/20	0.79	0.16	101,101,102,102	0
7	LOP	J	504	45/45	0.81	0.15	81,84,95,97	0
7	LOP	A	503	45/45	0.84	0.13	79,99,105,107	0
7	LOP	D	503	45/45	0.85	0.14	75,88,94,94	0
8	ANJ	A	504	39/39	0.87	0.12	70,74,77,78	0
8	ANJ	G	505	39/39	0.87	0.13	69,72,79,81	0
8	ANJ	J	505	39/39	0.88	0.11	51,67,82,85	0
8	ANJ	D	504	39/39	0.89	0.11	49,66,79,82	0
6	SMA	J	503	37/37	0.91	0.11	45,50,56,56	0
6	SMA	D	2	37/37	0.91	0.11	47,53,62,64	0
6	SMA	G	503	37/37	0.91	0.10	51,58,60,62	0
9	SR	G	432	1/1	0.92	0.07	135,135,135,135	0
9	SR	J	432	1/1	0.92	0.12	114,114,114,114	0
9	SR	H	257	1/1	0.93	0.06	117,117,117,117	0
6	SMA	A	1	37/37	0.93	0.09	46,55,58,58	0
9	SR	K	257	1/1	0.93	0.05	144,144,144,144	0
9	SR	E	258	1/1	0.94	0.06	126,126,126,126	0
5	HEM	G	502	43/43	0.95	0.11	47,52,54,54	0
5	HEM	A	502	43/43	0.95	0.10	43,47,51,52	0
5	HEM	A	501	43/43	0.96	0.09	61,64,70,73	0
5	HEM	J	501	43/43	0.96	0.09	55,56,57,58	0
5	HEM	J	502	43/43	0.96	0.09	36,43,47,48	0
5	HEM	D	501	43/43	0.96	0.10	60,61,62,64	0
5	HEM	D	502	43/43	0.96	0.10	34,42,45,46	0
10	HEC	B	301	43/43	0.96	0.11	61,65,67,69	0
10	HEC	E	301	43/43	0.96	0.10	74,80,81,81	0
10	HEC	H	301	43/43	0.96	0.10	66,70,71,72	0
11	FES	C	200	4/4	0.96	0.07	54,54,54,54	0

Continued on next page...

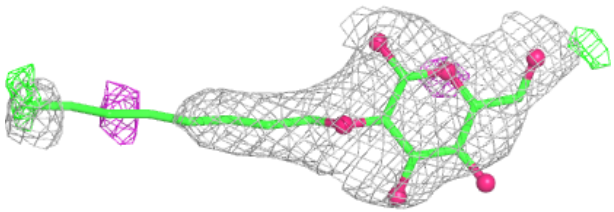
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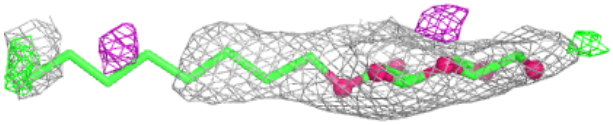
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SR	B	257	1/1	0.97	0.04	126,126,126,126	0
10	HEC	K	301	43/43	0.97	0.10	73,79,80,81	0
5	HEM	G	501	43/43	0.97	0.09	55,59,63,65	0
11	FES	I	200	4/4	0.98	0.05	53,53,54,54	0
11	FES	L	200	4/4	0.98	0.07	56,57,57,57	0
11	FES	F	200	4/4	0.99	0.04	55,55,55,55	0

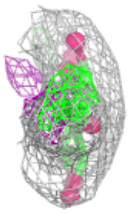
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BGL J 431:

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

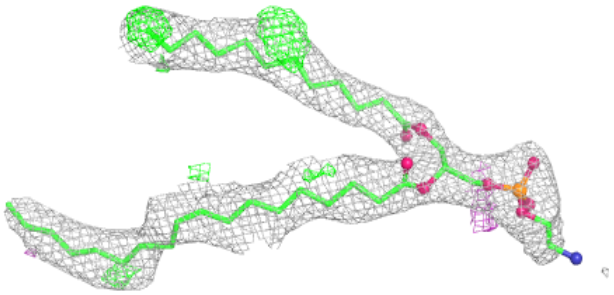


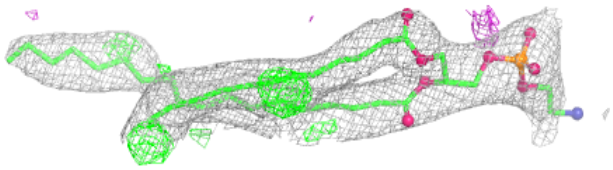


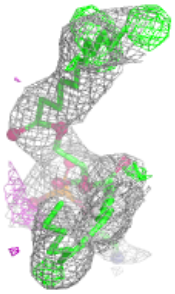


Electron density around LOP G 504:

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

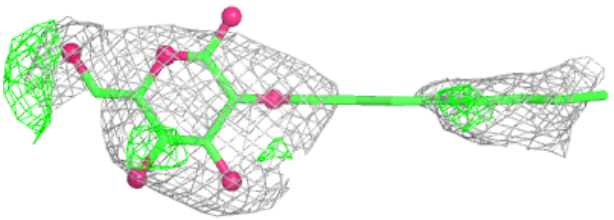


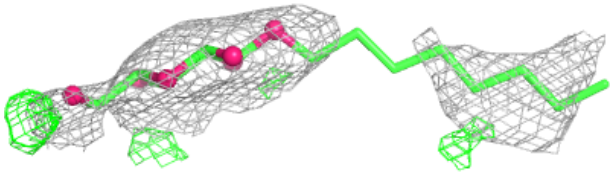


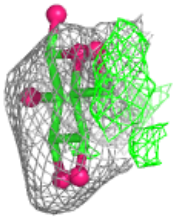


Electron density around BGL G 431:

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

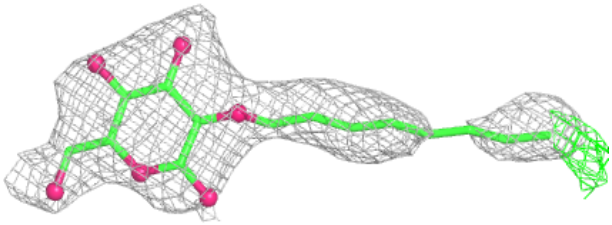


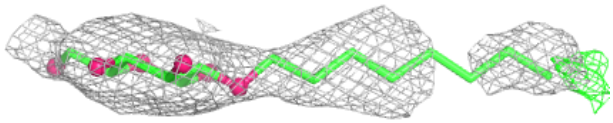


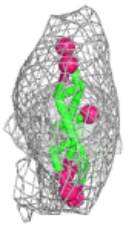


Electron density around BGL A 431:

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

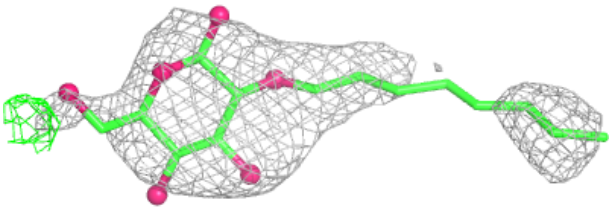


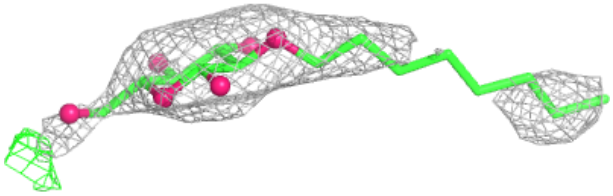


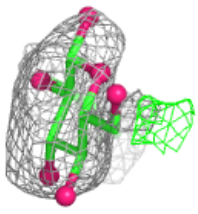


Electron density around BGL E 257:

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

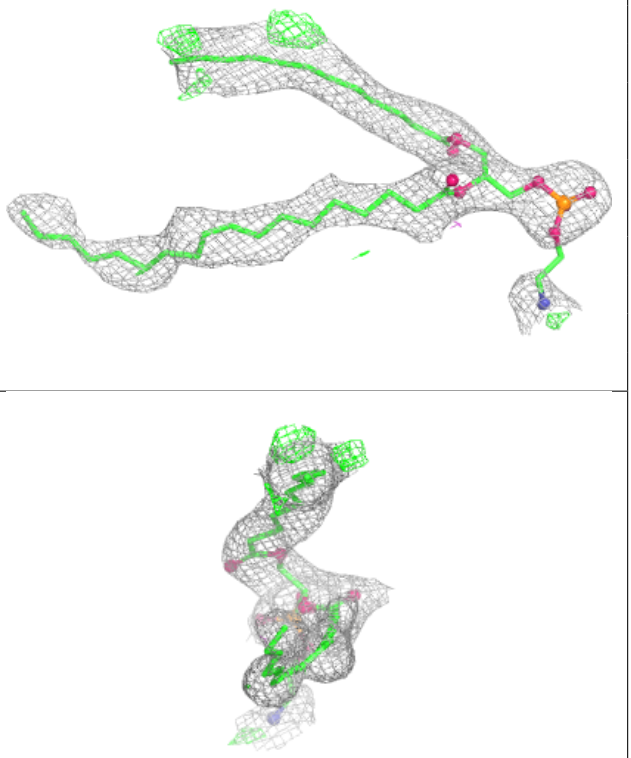


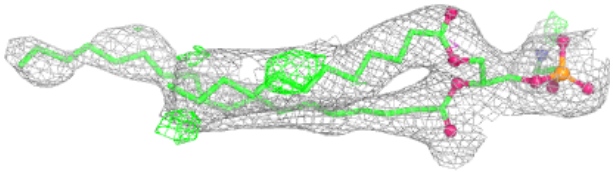




Electron density around LOP J 504:

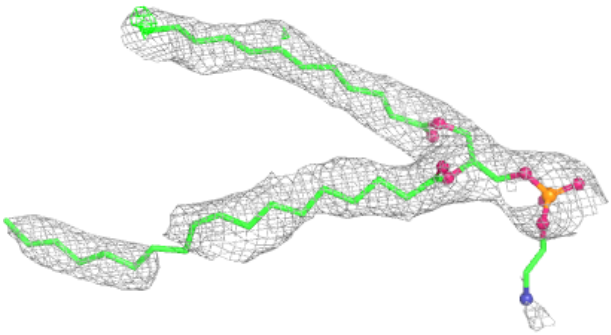
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

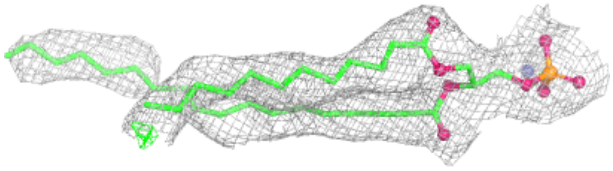


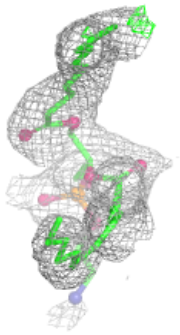


Electron density around LOP A 503:

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

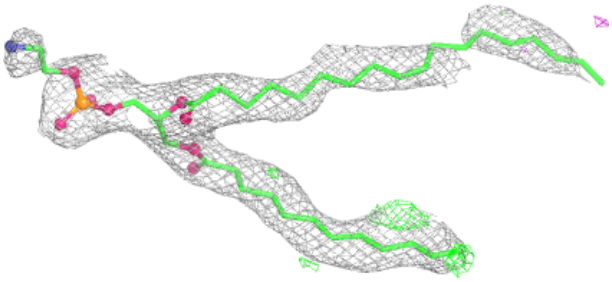


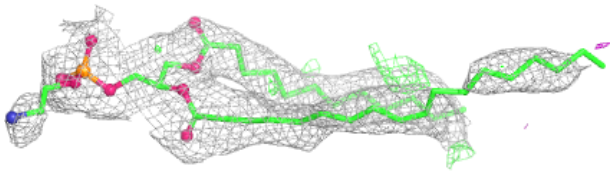


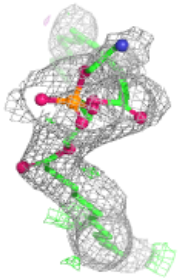


Electron density around LOP D 503:

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

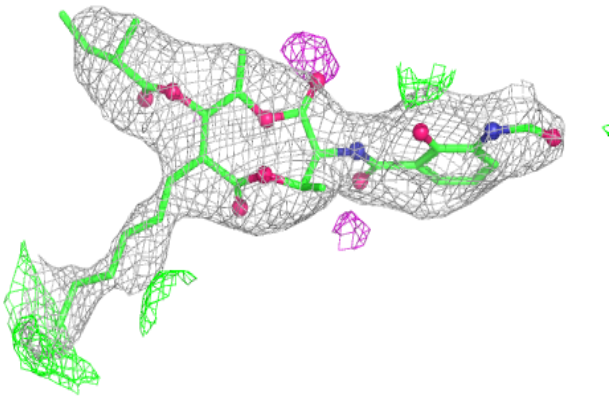


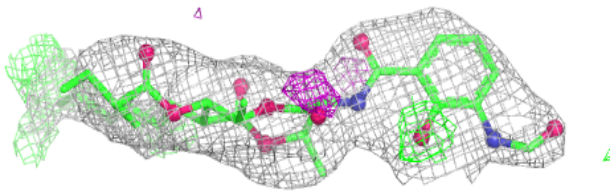


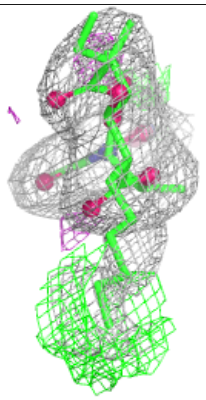


Electron density around ANJ A 504:

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

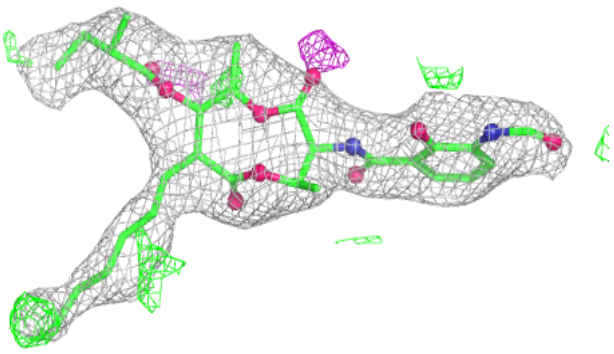


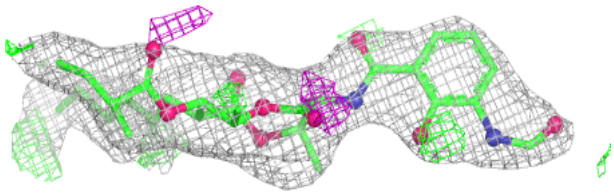


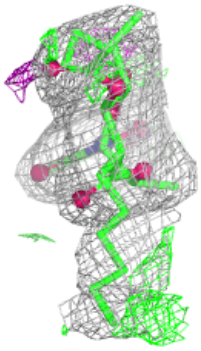


Electron density around ANJ G 505:

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

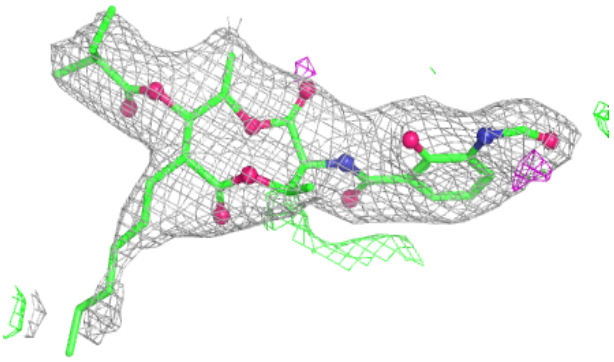


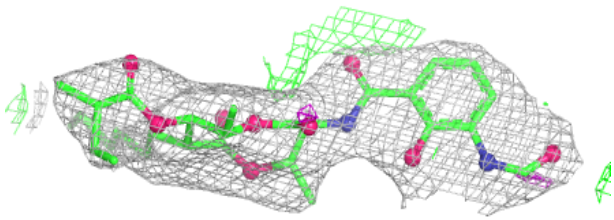


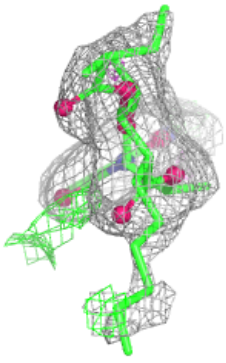


Electron density around ANJ J 505:

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

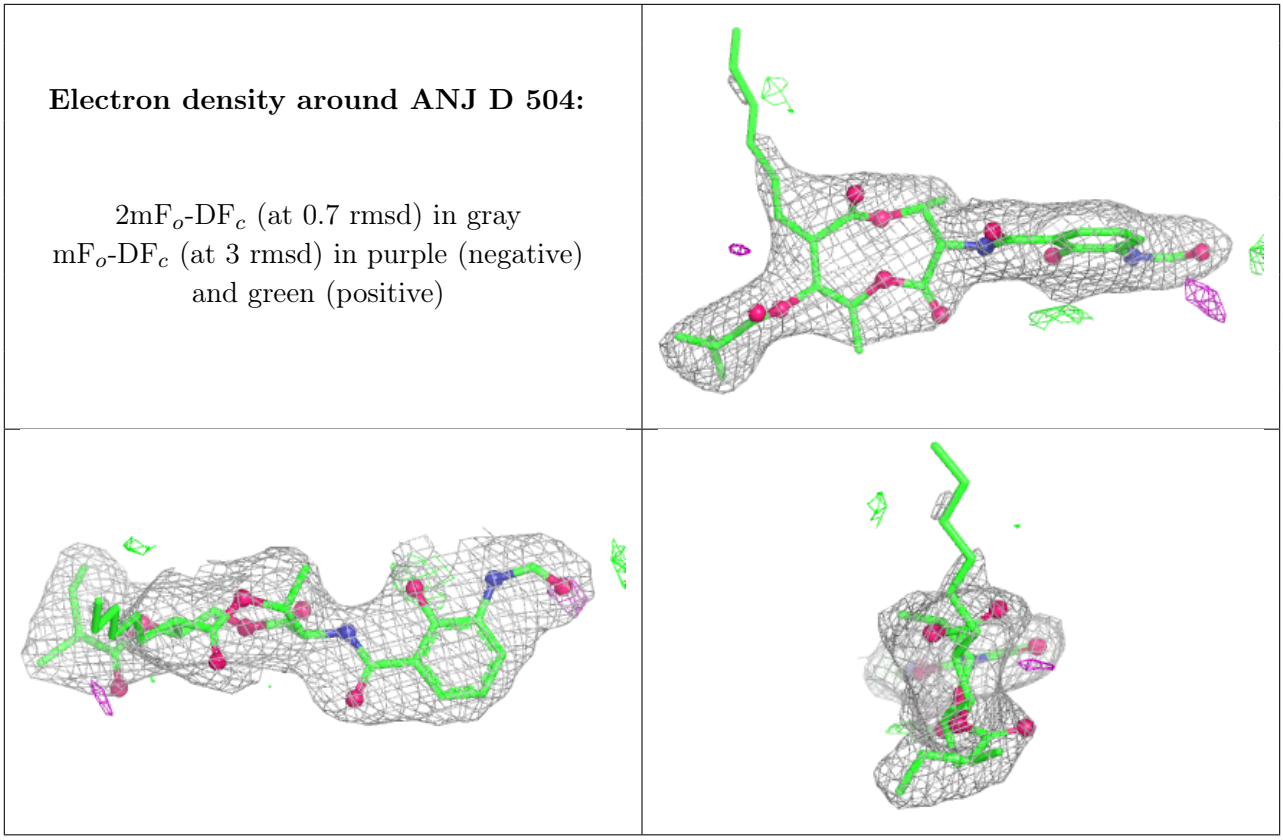






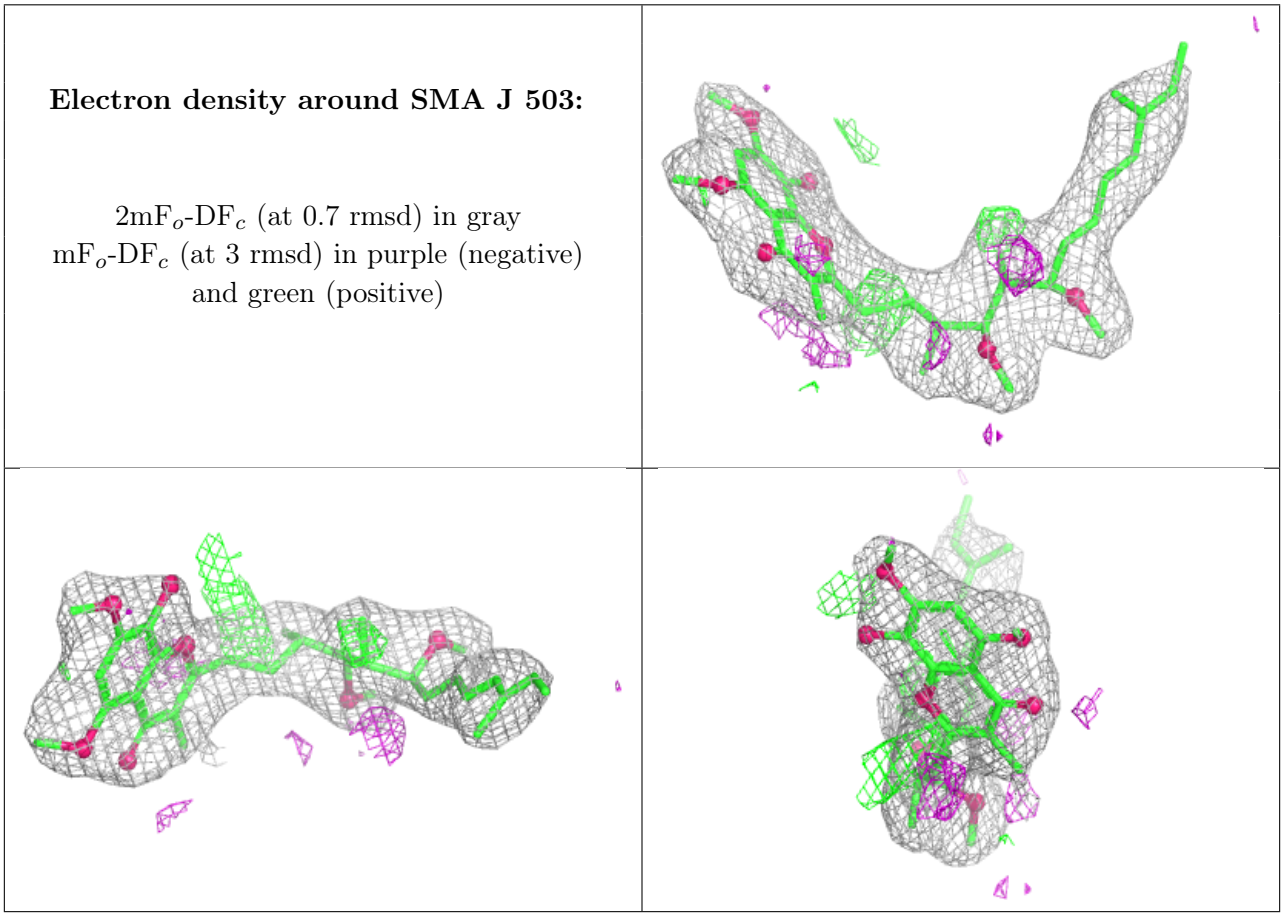
Electron density around ANJ D 504:

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



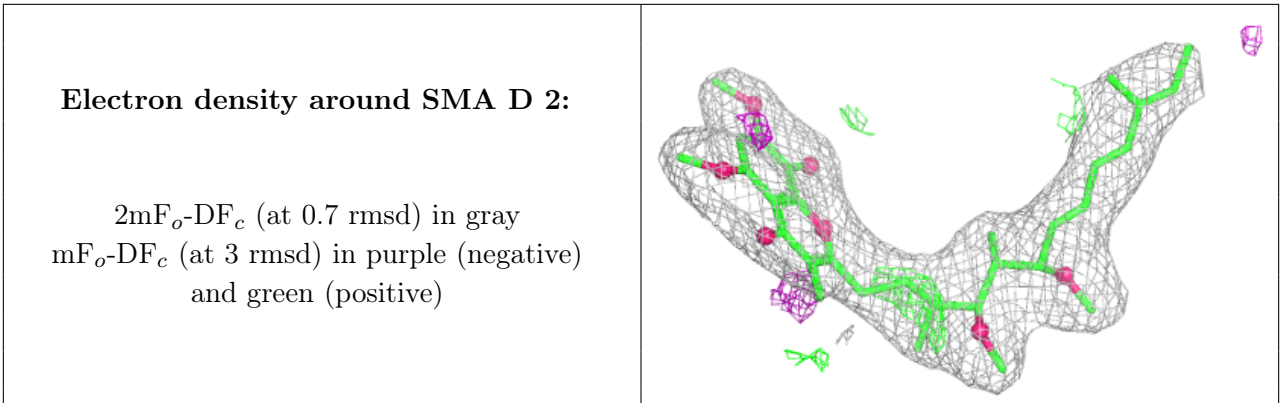
Electron density around SMA J 503:

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



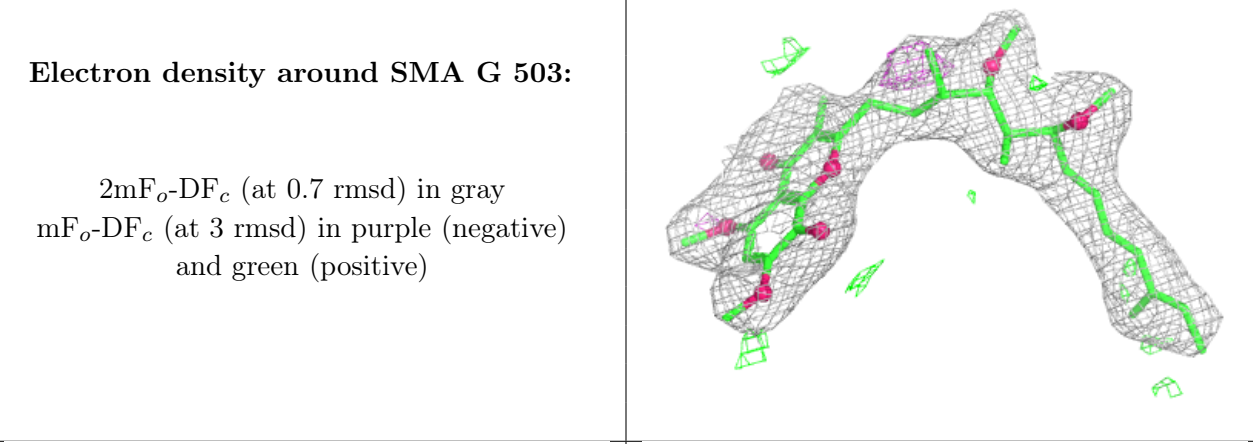
Electron density around SMA D 2:

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



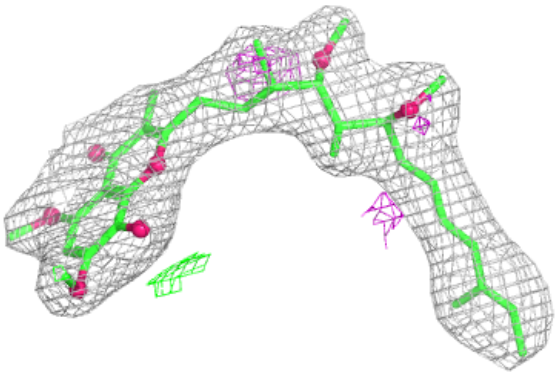
Electron density around SMA G 503:

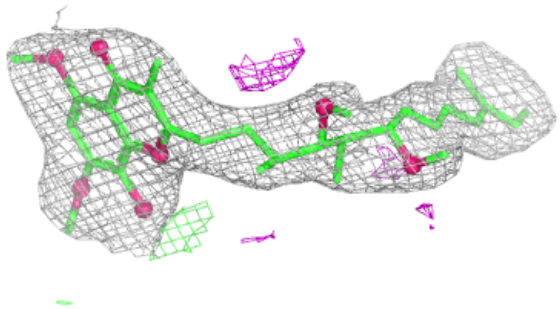
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

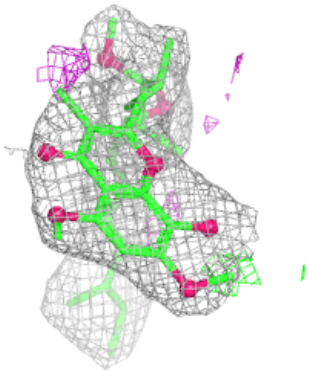


Electron density around SMA A 1:

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

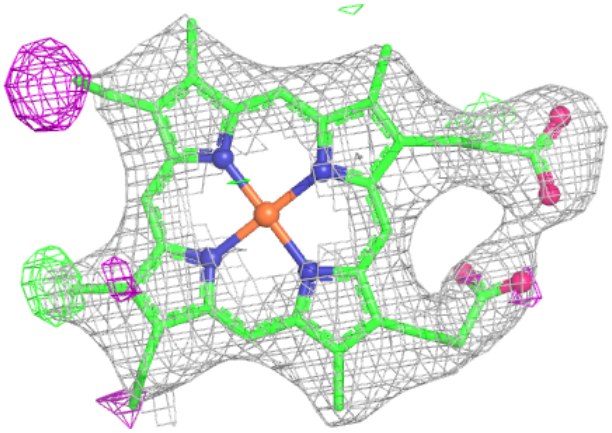


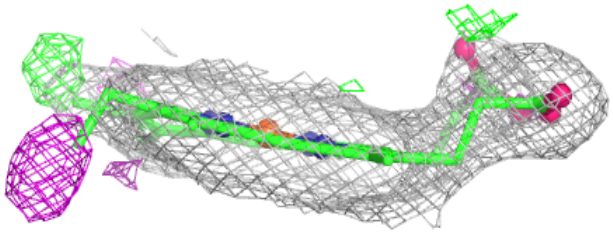


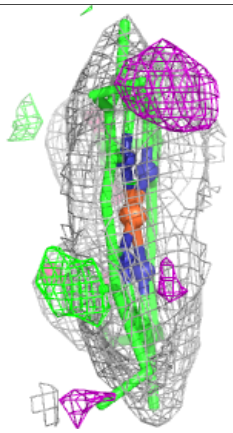


Electron density around HEM G 502:

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

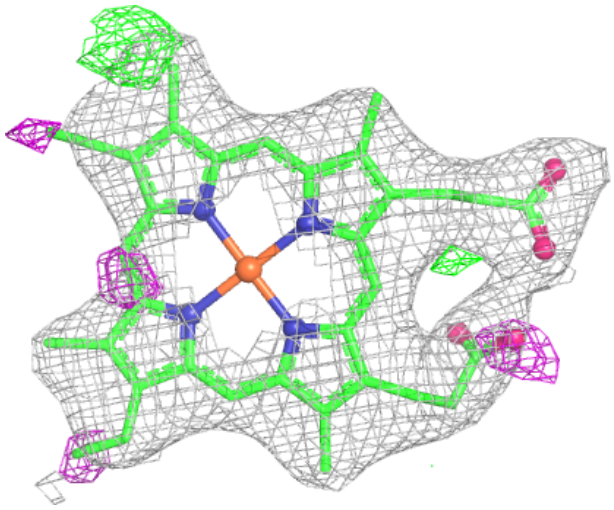


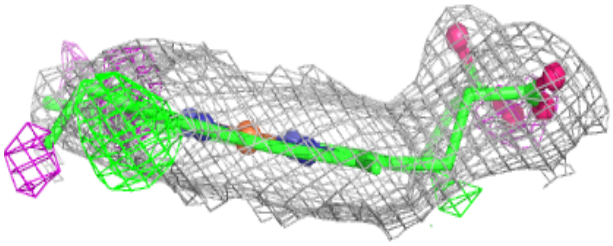


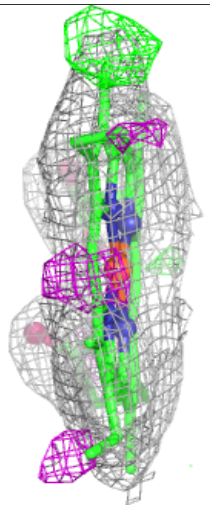


Electron density around HEM A 502:

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

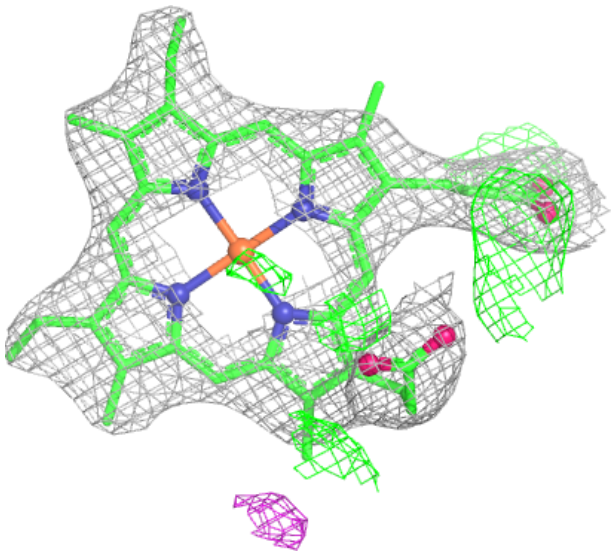


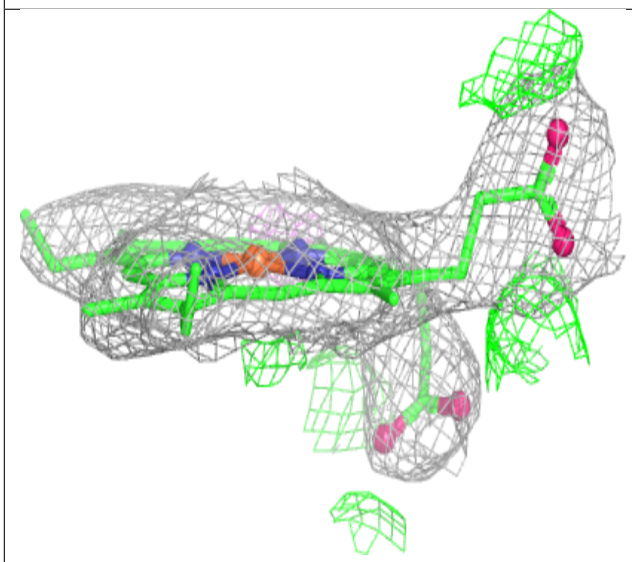


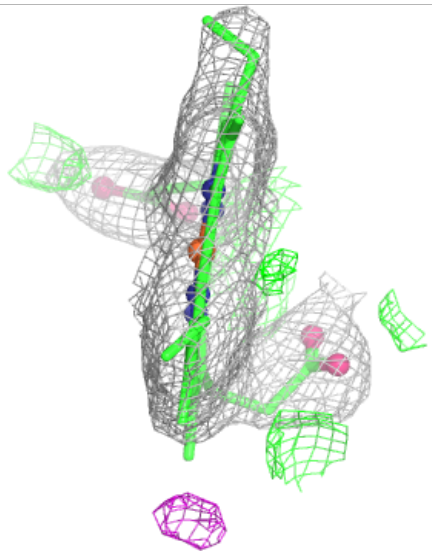


Electron density around HEM A 501:

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

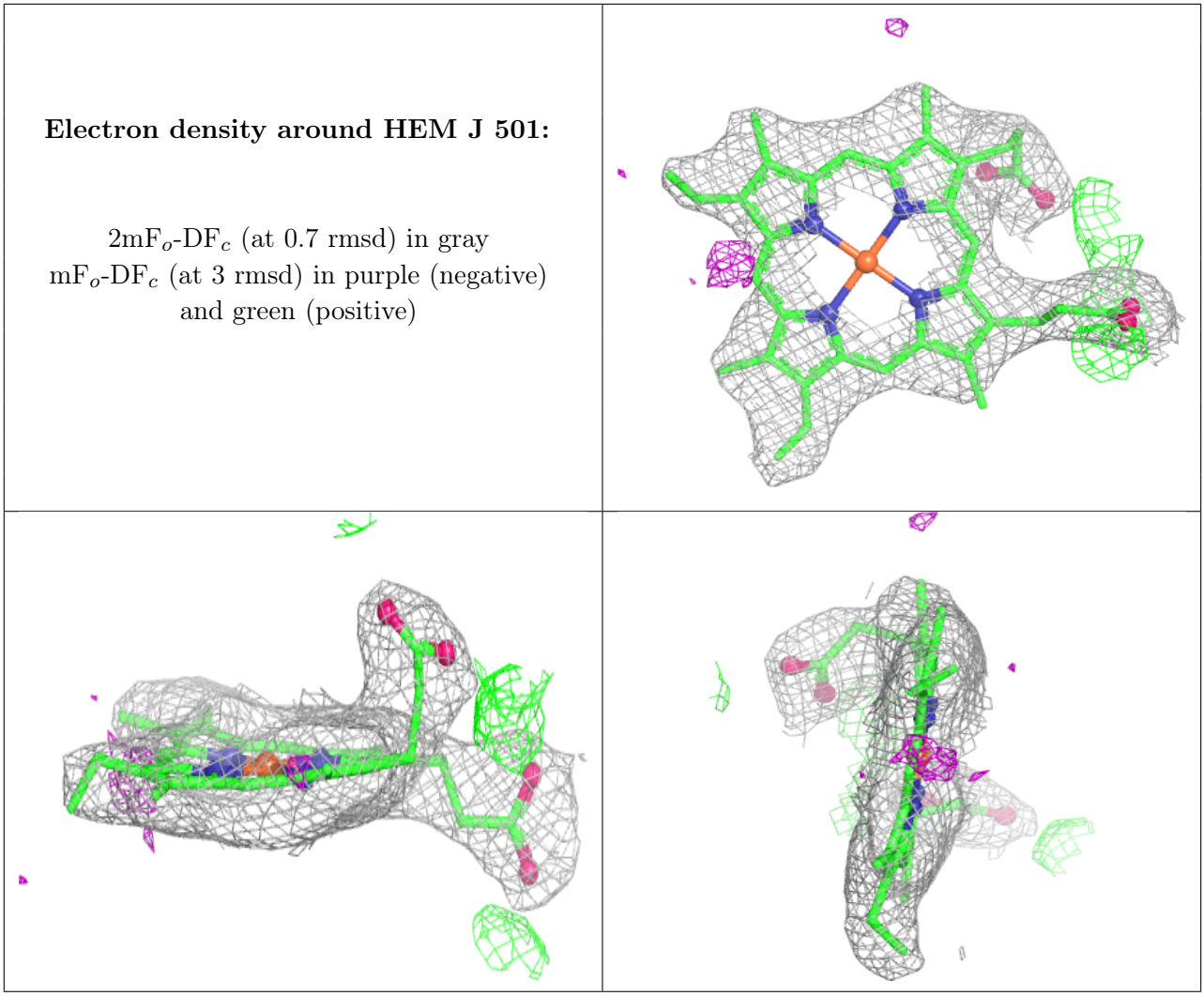






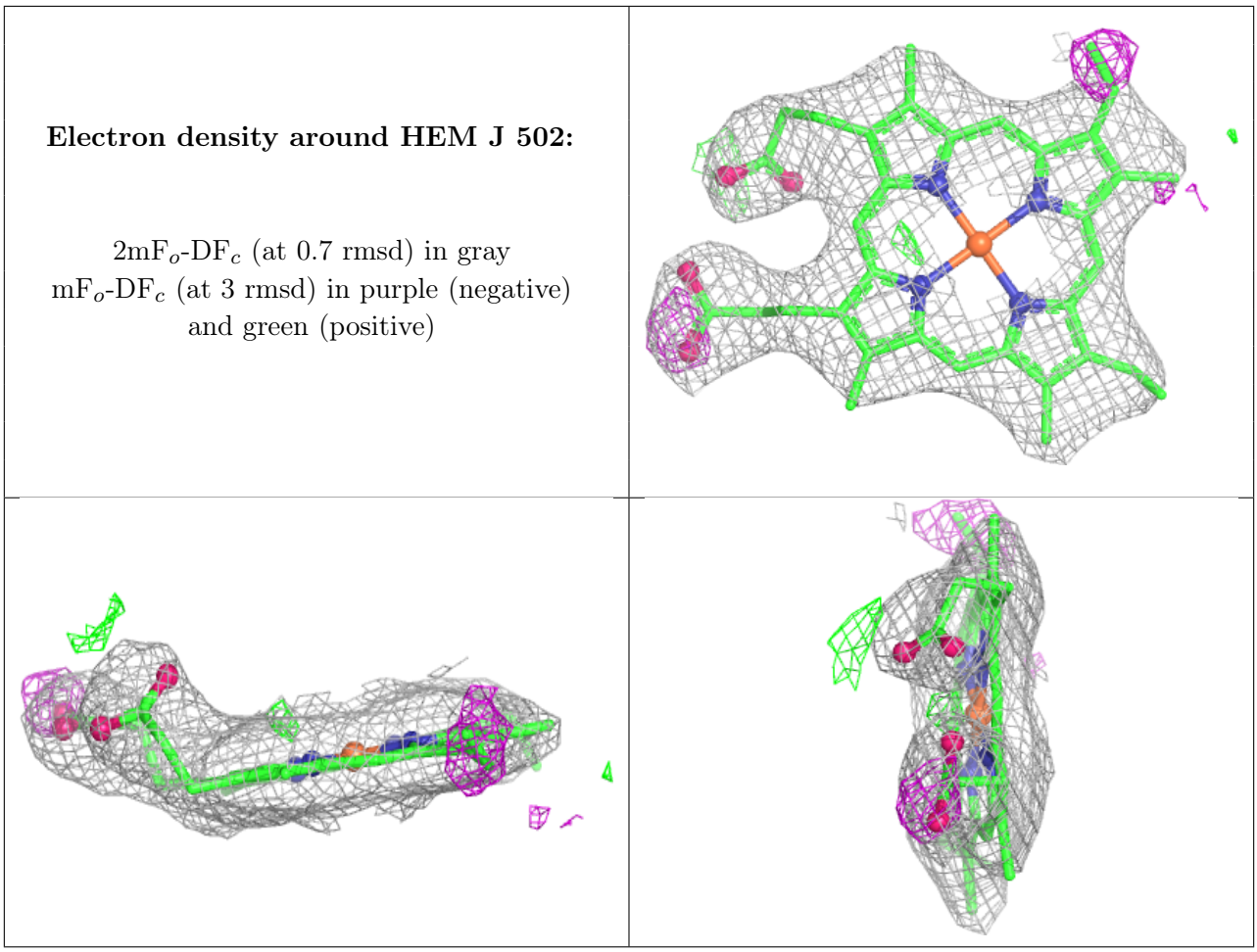
Electron density around HEM J 501:

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



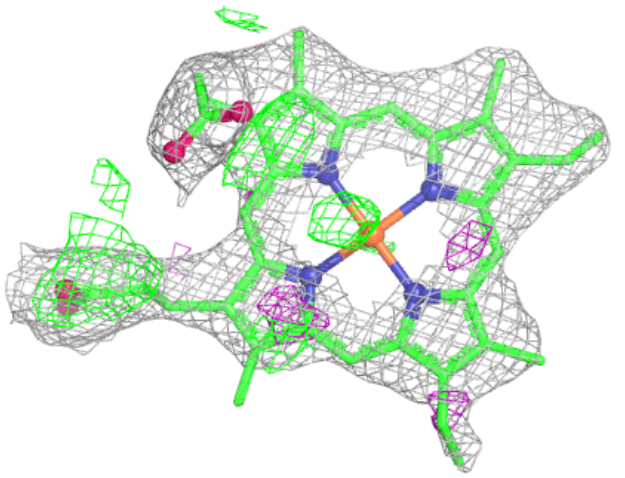
Electron density around HEM J 502:

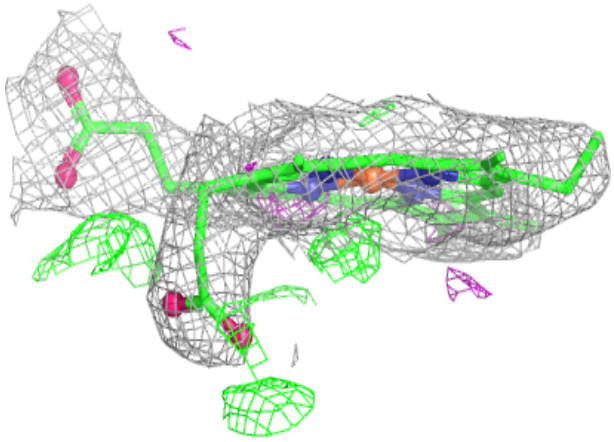
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

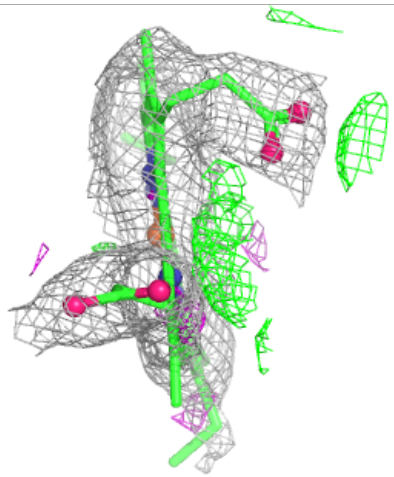


Electron density around HEM D 501:

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

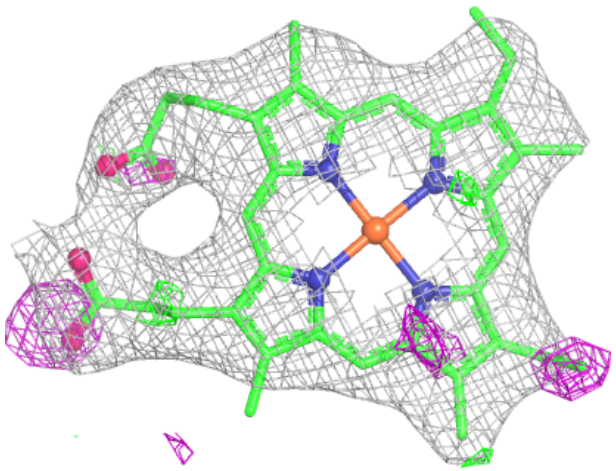


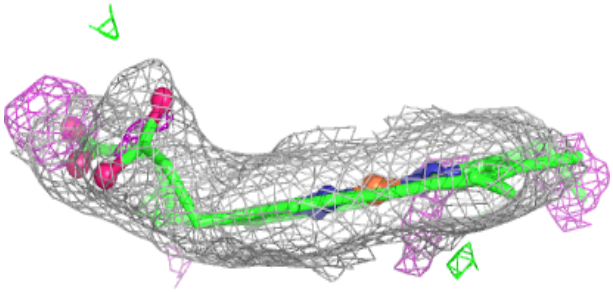


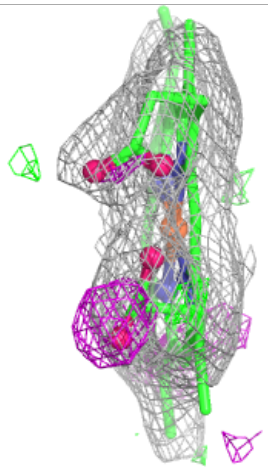


Electron density around HEM D 502:

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

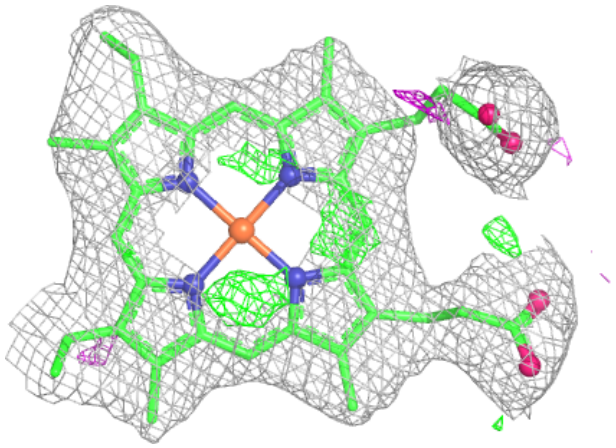


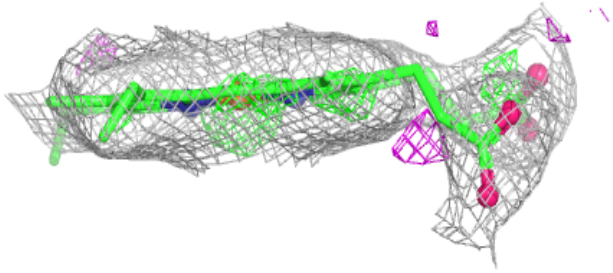


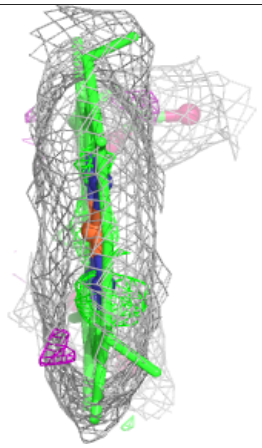


Electron density around HEC B 301:

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

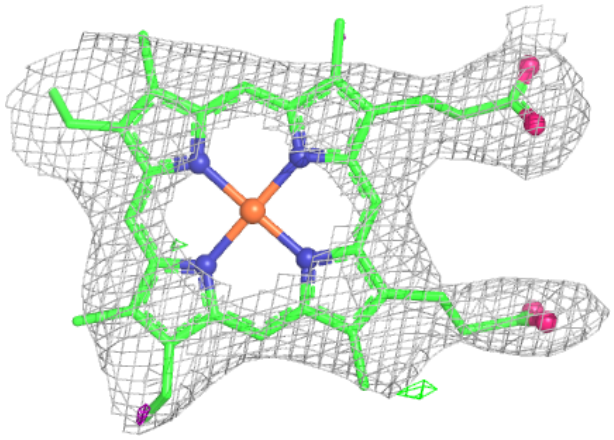


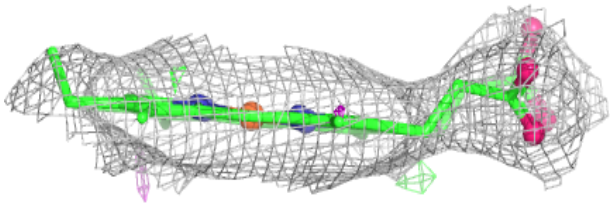


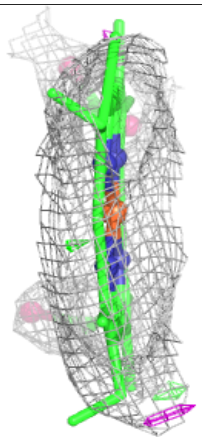


Electron density around HEC E 301:

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

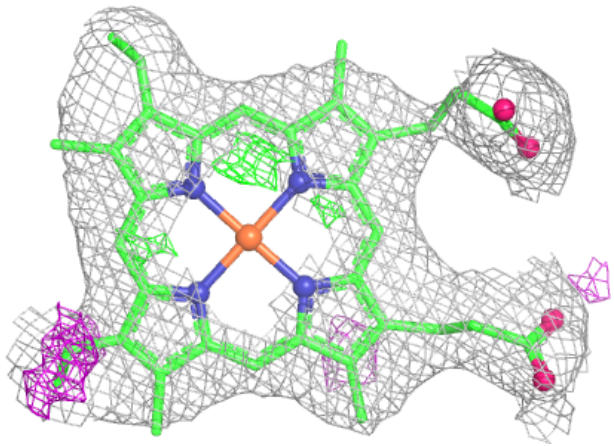


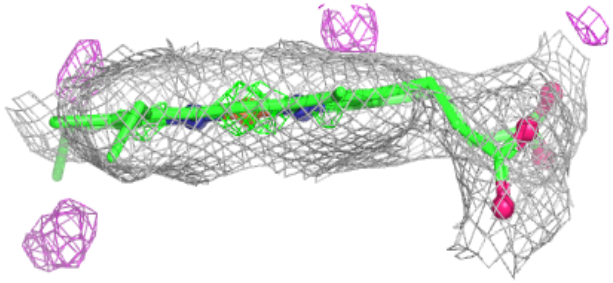


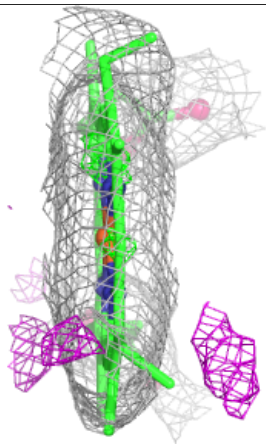


Electron density around HEC H 301:

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

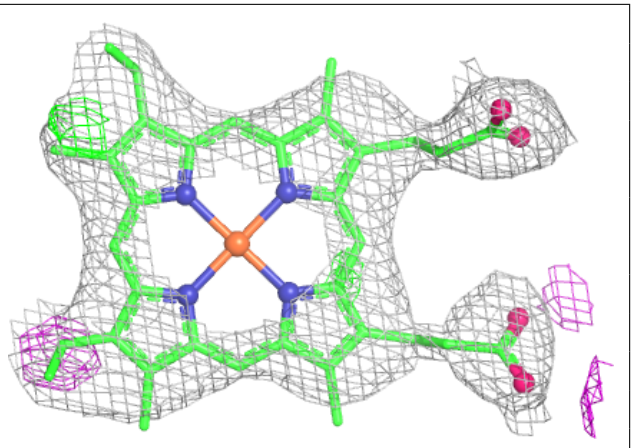


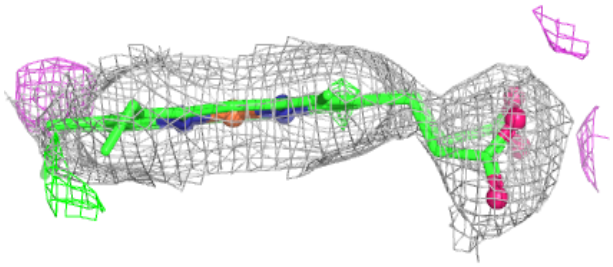


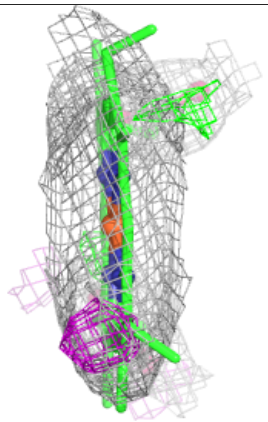


Electron density around HEC K 301:

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

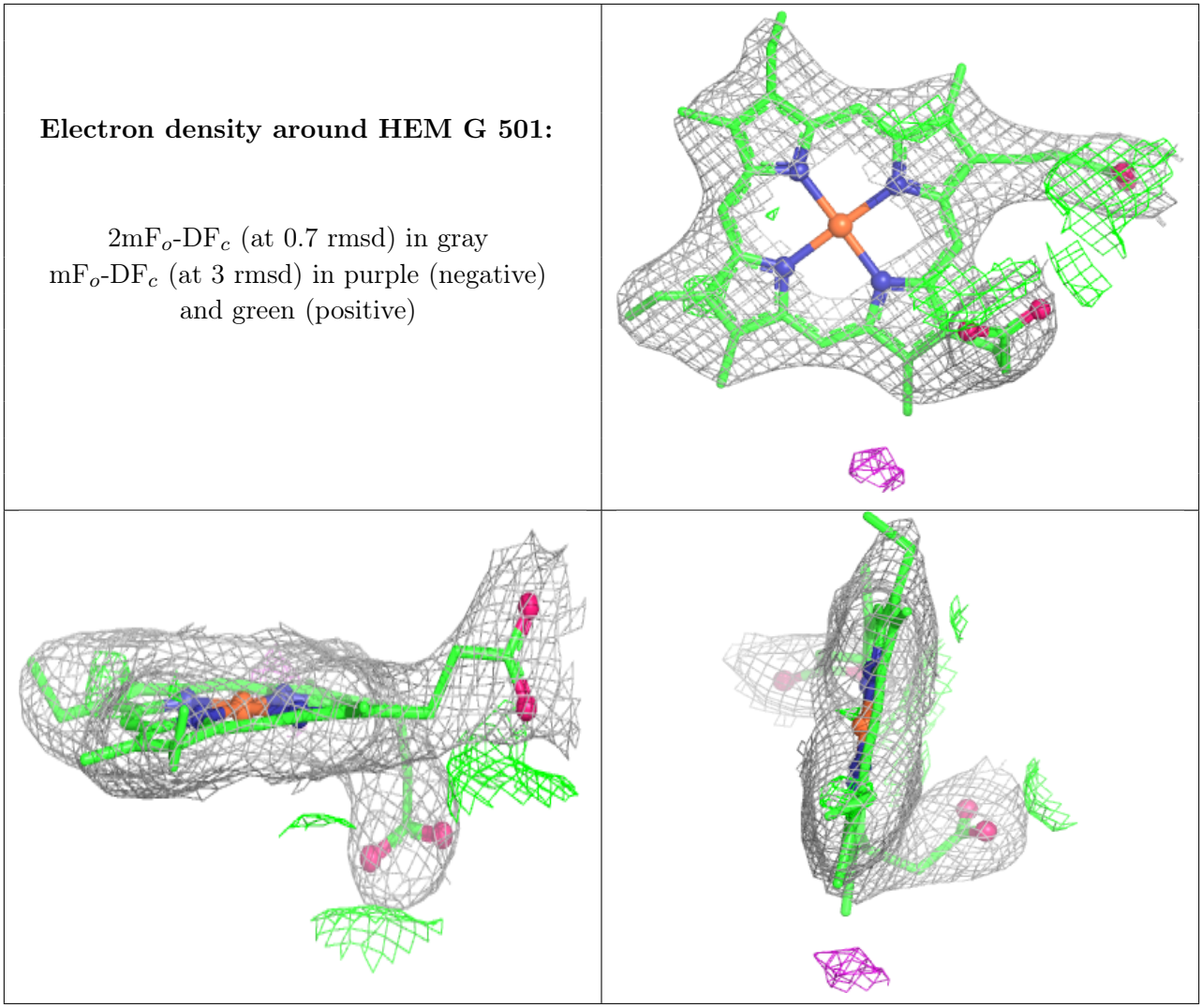






Electron density around HEM G 501:

$2mF_o$-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.