wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 04:54 AM EDT

PDB ID	:	3CWB
Title	:	Chicken Cytochrome BC1 Complex inhibited by an iodinated analogue of the polyketide Crocacin-D
Authors	:	Huang, L.; Cromartie, T.; Viner, R.; Crowley, P.J.; Berry, E.A.
Deposited on	:	2008-04-21
Resolution	:	3.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

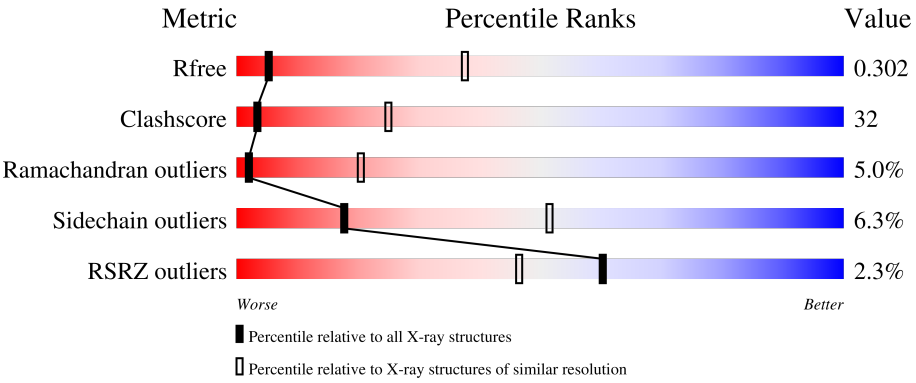
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.51 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	446	48% 44% 7%
1	N	446	46% 46% 7%
2	B	441	40% 49% 6% 5%
2	O	441	39% 50% 6%
3	C	380	43% 50% 7%

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Mol	Chain	Length	Quality of chain
3	P	380	2% 44% 48% 7%
4	D	241	51% 46%
4	Q	241	% 49% 47%
5	E	196	8% 39% 54% 7%
5	R	196	4% 41% 49% 10%
6	F	110	54% 35% 9%
6	S	110	% 55% 34% 9%
7	G	81	% 57% 36% 7%
7	T	81	9% 53% 36% 9%
8	H	77	44% 42% 5% 9%
8	U	77	30% 48% 9% 13%
9	I	52	12% 54% 37% 8%
9	V	52	17% 44% 44% 6% 6%
10	J	61	3% 67% 30%
10	W	61	3% 54% 34% 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
11	PEE	A	2008	-	-	-	X
11	PEE	C	2005	-	-	-	X
11	PEE	P	3008	-	X	-	X
11	PEE	W	3005	-	-	-	X
12	BOG	D	2091	-	-	-	X
12	BOG	P	2010	-	-	-	X
12	BOG	Q	3091	-	-	-	X
18	CDL	P	3003	-	-	-	X

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 32696 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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1508	948	262	292	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			
6	S	100	Total	C	N	O	S	0	0	0
			881	565	158	155	3			

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

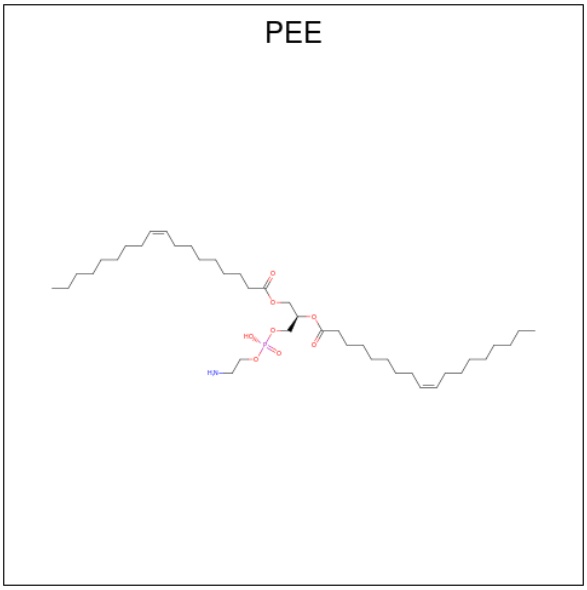
- Molecule 9 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	51	Total	C	N	O	S	0	0	2
			302	181	61	58	2			
9	V	49	Total	C	N	O	S	0	0	3
			292	176	59	55	2			

- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

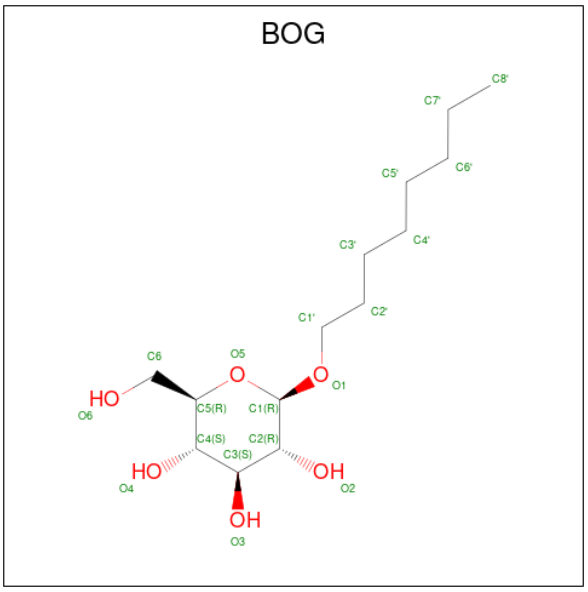
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	61	Total C N O 497 321 87 89	0	0	0
10	W	59	Total C N O 478 311 85 82	0	0	0

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



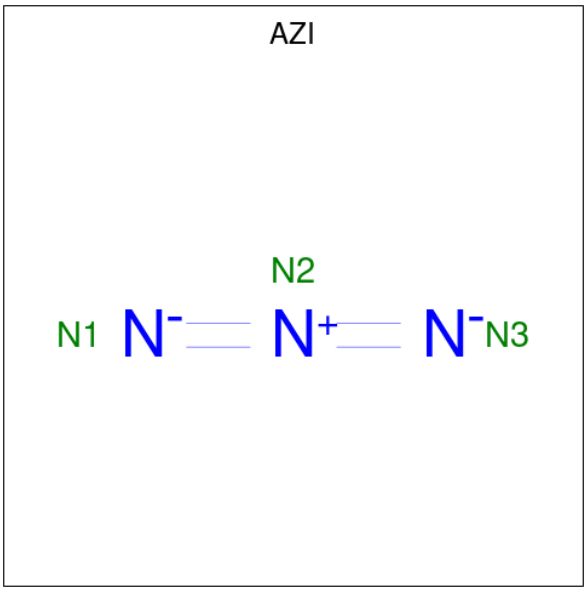
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O P 21 12 8 1	0	0
11	C	1	Total C N O P 50 40 1 8 1	0	0
11	C	1	Total C N O P 49 39 1 8 1	0	0
11	P	1	Total C N O P 49 39 1 8 1	0	0
11	P	1	Total O P 5 4 1	0	0
11	W	1	Total C N O P 50 40 1 8 1	0	0

- Molecule 12 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



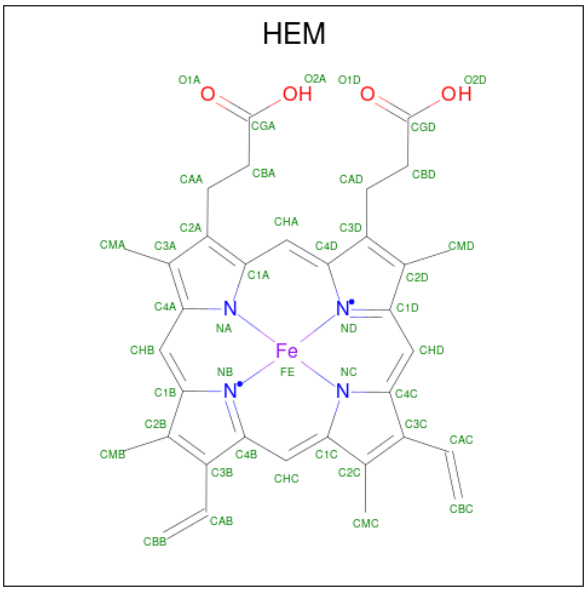
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C O 12 10 2	0	0
12	D	1	Total C O 20 14 6	0	0
12	E	1	Total C O 20 14 6	0	0
12	P	1	Total C O 19 13 6	0	0
12	Q	1	Total C O 20 14 6	0	0
12	Q	1	Total C O 20 14 6	0	0

- Molecule 13 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total N 3 3	0	0
13	P	1	Total N 3 3	0	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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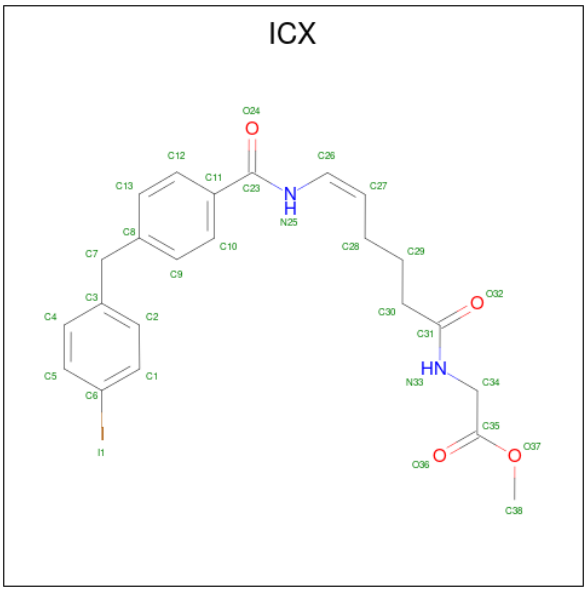
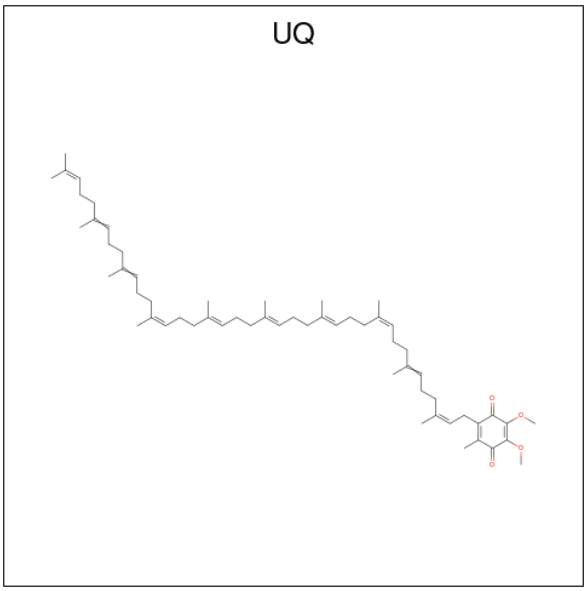
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
14	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 15 is methyl N-[(5Z)-6-({[4-(4-iodobenzyl)phenyl]carbonyl}amino)hex-5-enoyl]glycinate (three-letter code: ICX) (formula: $C_{23}H_{25}IN_2O_4$).



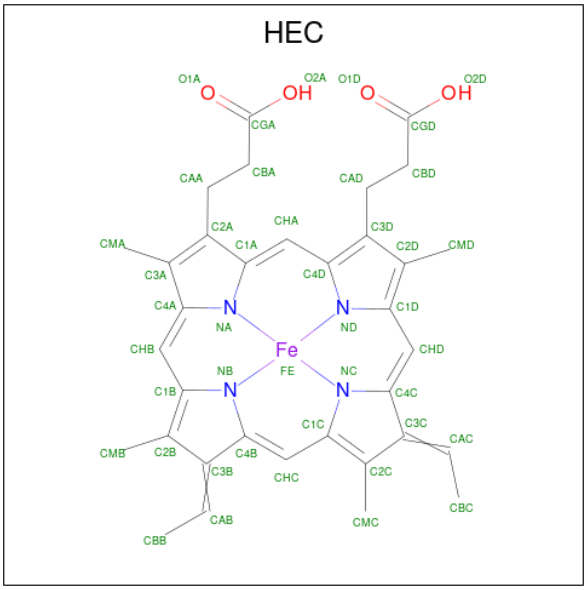
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	I	N	O	0	0
			30	23	1	2	4		
15	P	1	Total	C	I	N	O	0	0
			30	23	1	2	4		

- Molecule 16 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



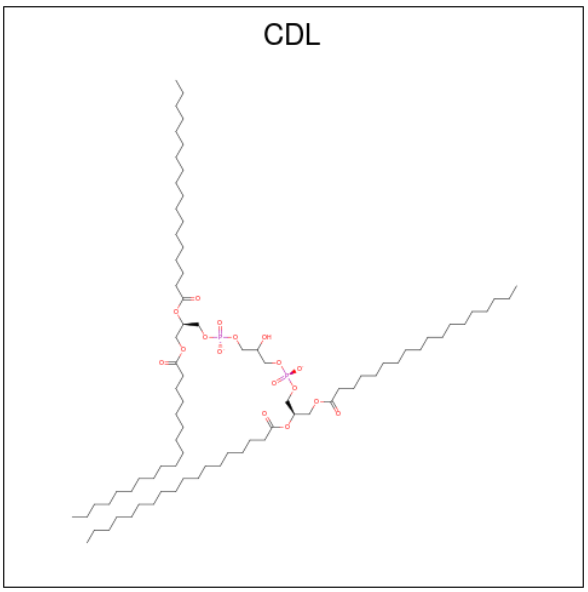
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 19 15 4	0	0
16	P	1	Total C O 19 15 4	0	0

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



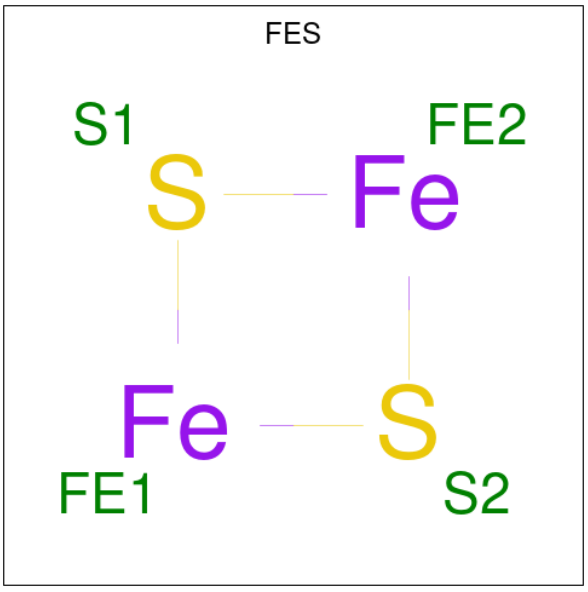
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total C Fe N O 43 34 1 4 4	0	0
17	Q	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			42	23	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		
18	P	1	Total	C	O	P	0	0
			42	23	17	2		
18	P	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	E	1	Total Fe S 4 2 2	0	0
19	R	1	Total Fe S 4 2 2	0	0

- Molecule 20 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	E	1	Total O 2 2	0	0
20	P	2	Total O 2 2	0	0
20	Q	1	Total O 1 1	0	0

- Molecule 21 is water.

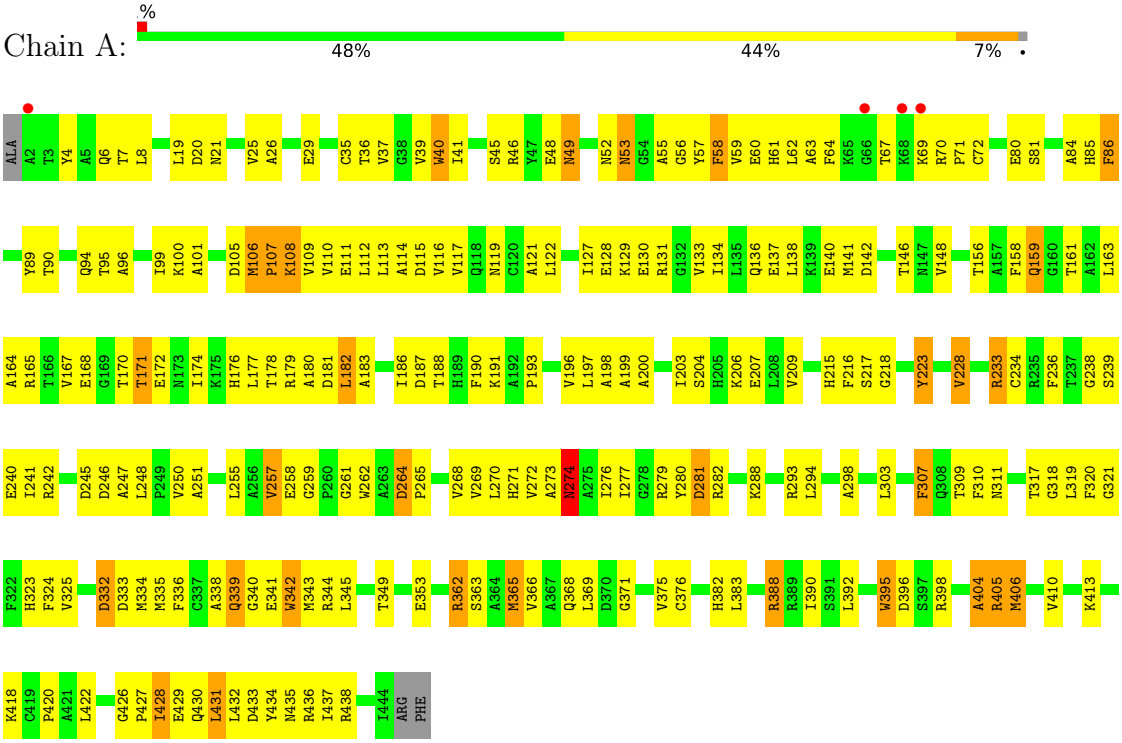
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	C	8	Total O 8 8	0	0
21	P	7	Total O 7 7	0	0
21	U	1	Total O 1 1	0	0

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.

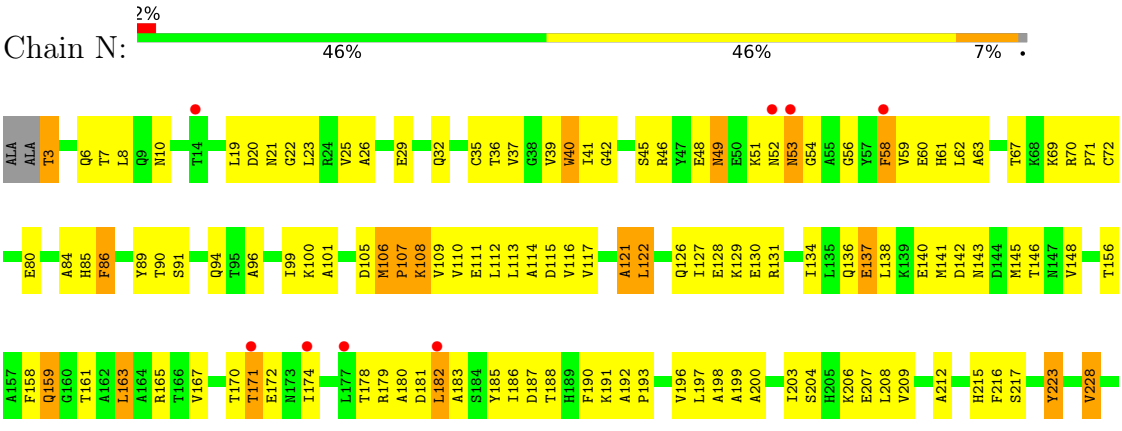
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

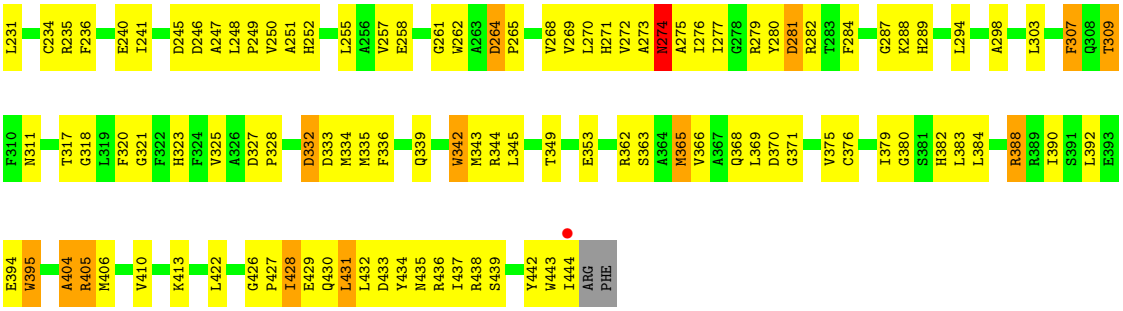
Chain A:



• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

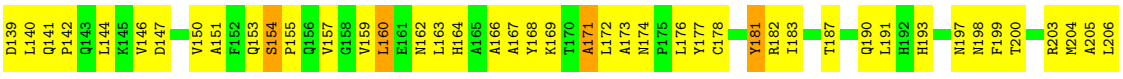
Chain N:

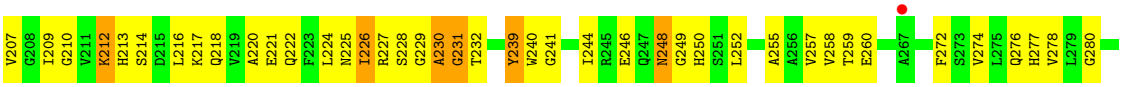


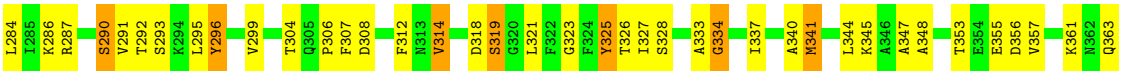


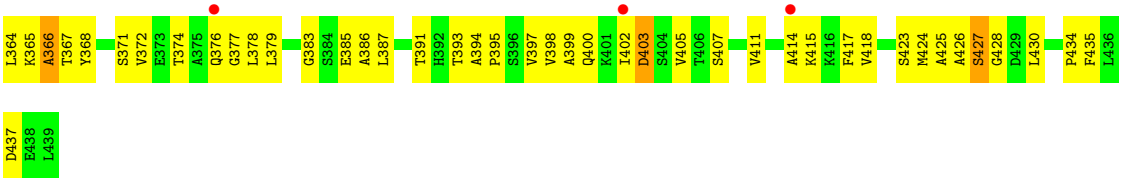
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



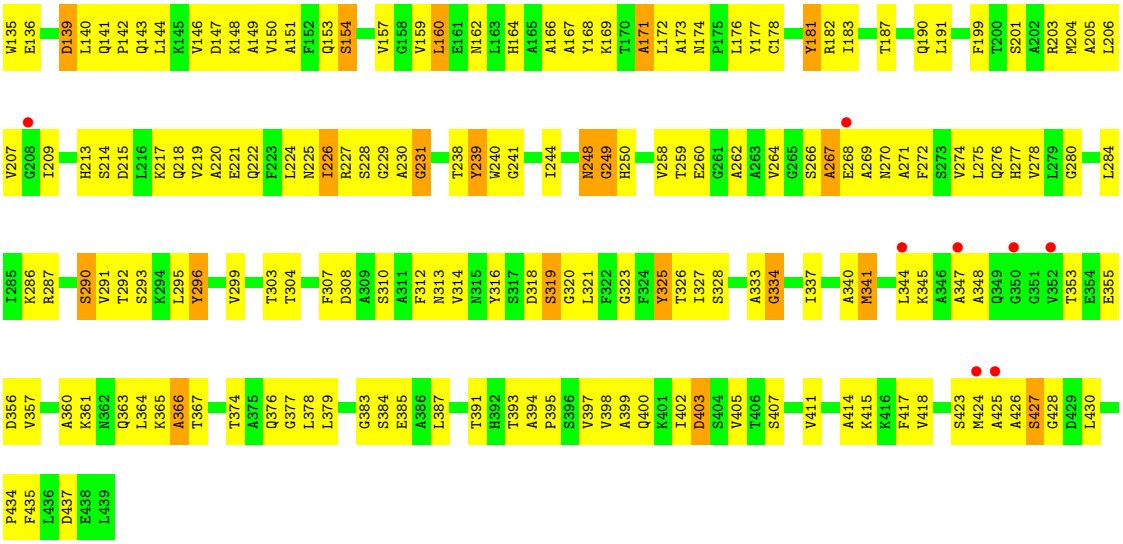






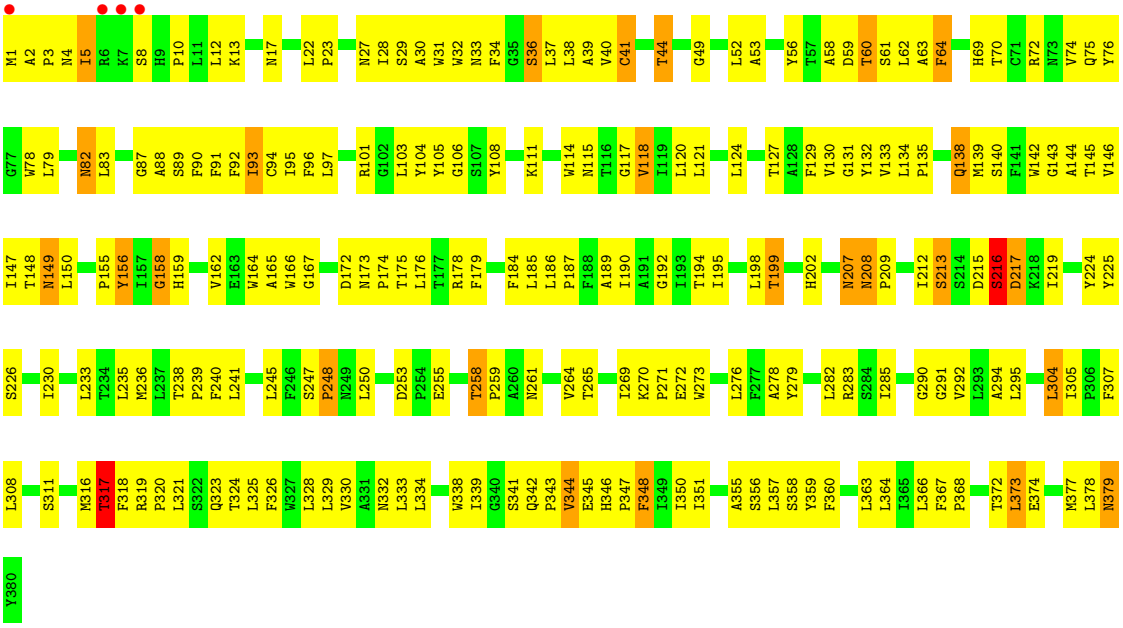
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain O:



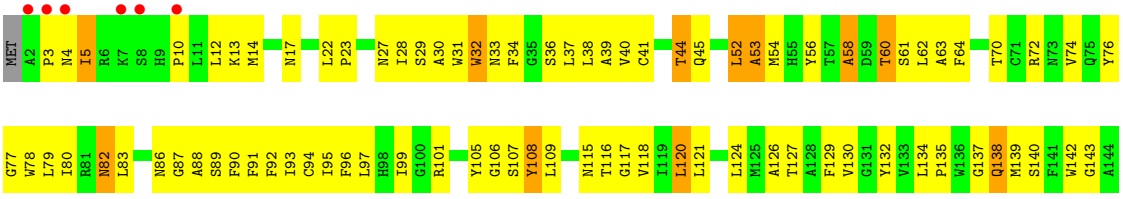
• Molecule 3: Cytochrome b

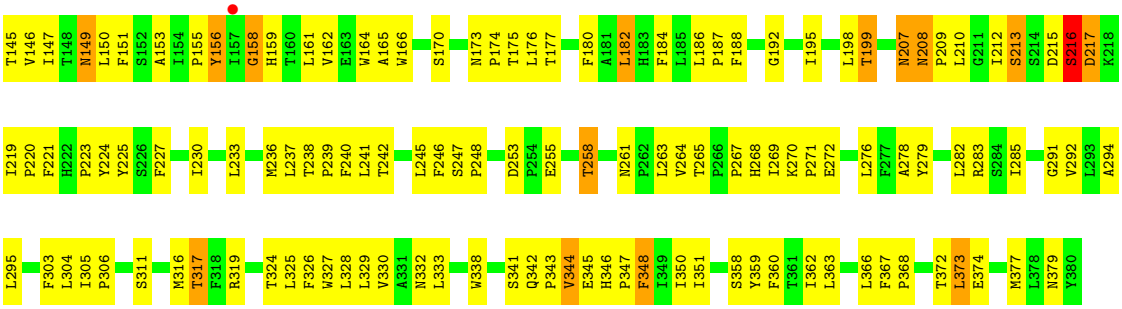
Chain C:



• Molecule 3: Cytochrome b

Chain P:



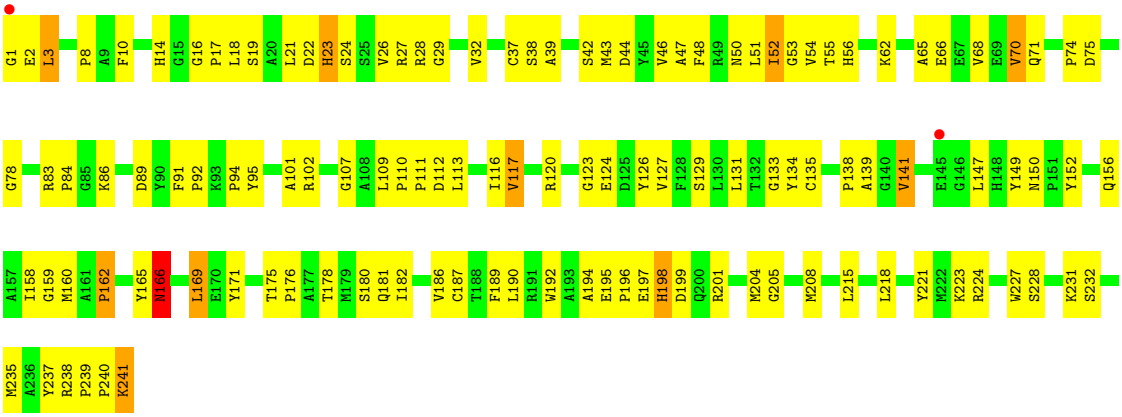


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:

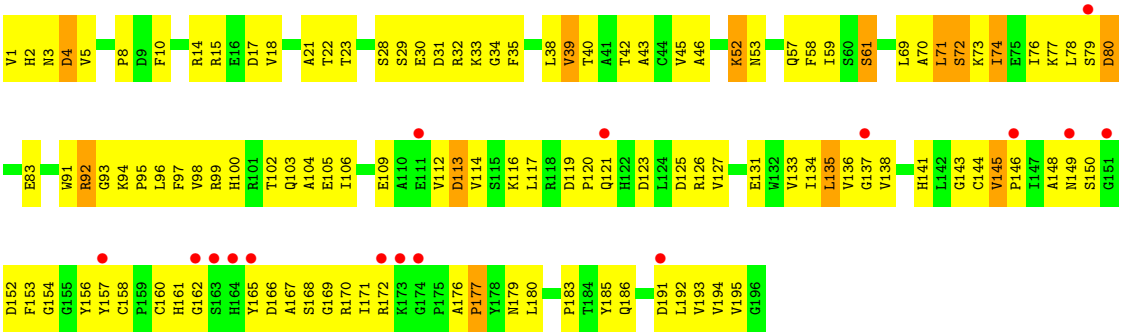
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q:

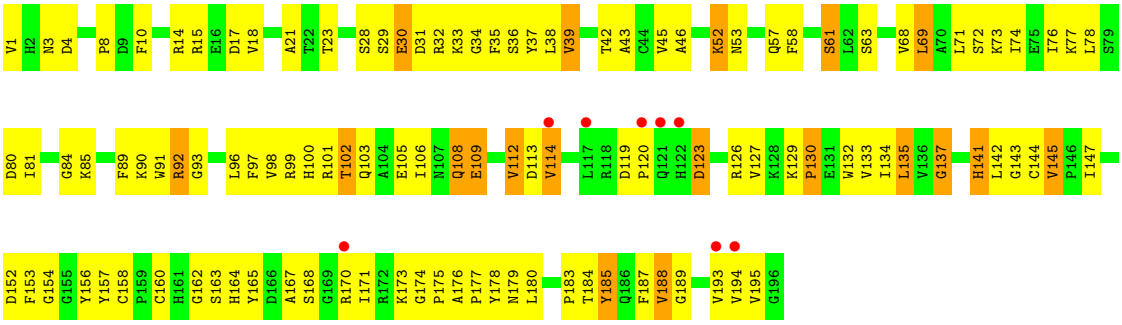


• Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN

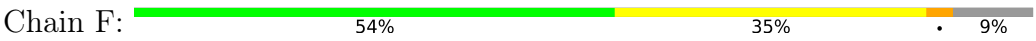
Chain E:

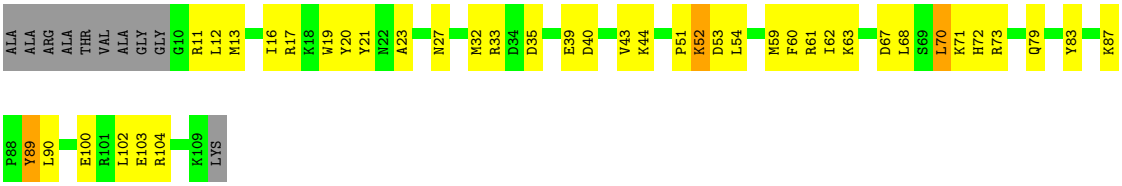


• Molecule 5: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR PROTEIN



• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

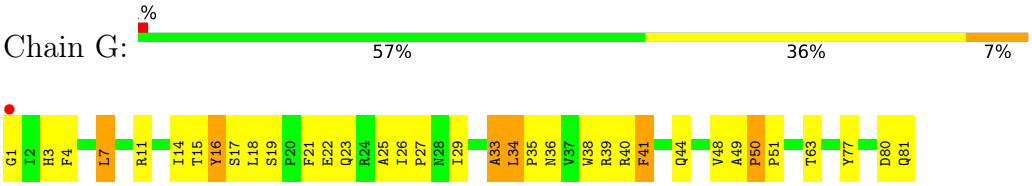




• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

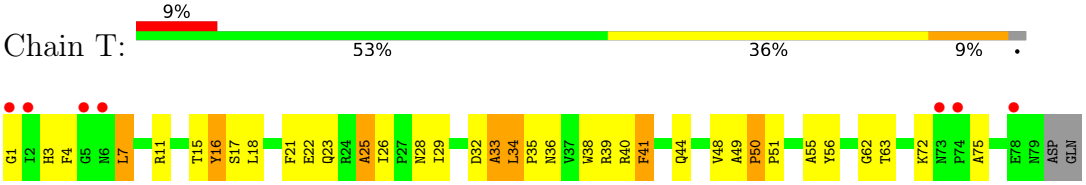
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G:



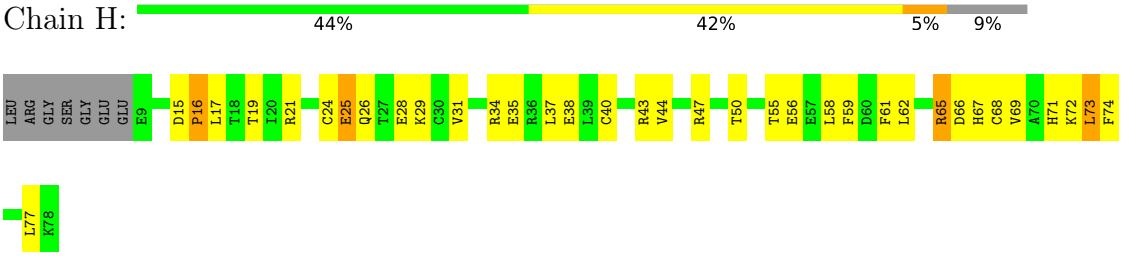
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T:



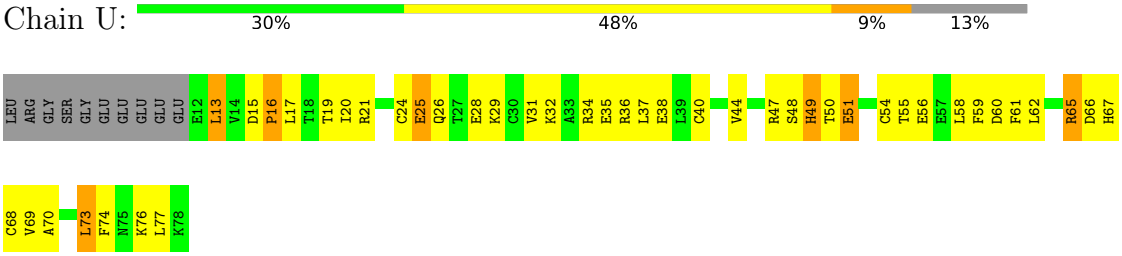
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H:



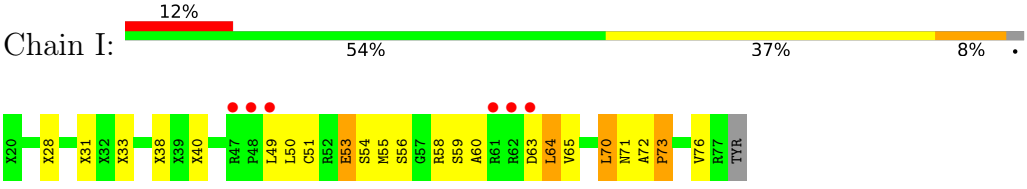
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:



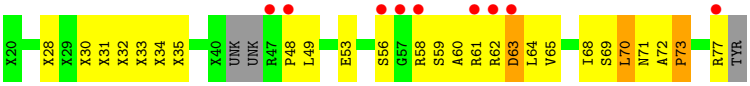
• Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence

Chain I:



• Molecule 9: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, leader sequence

Chain V:

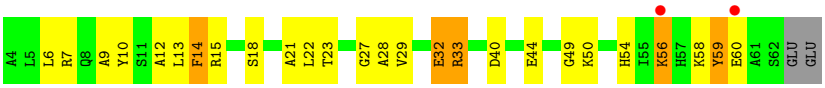


• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:

• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	174.78Å 182.66Å 242.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.98 – 3.51 44.88 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.8 (21.98-3.51) 98.9 (44.88-3.51)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.285 , 0.319 0.263 , 0.302	Depositor DCC
R_{free} test set	4918 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	86.3	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	32696	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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, CDL, UQ, BOG, AZI, HEC, ICX, UNL, FES, PEE

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	0.52	0/3511	0.72	0/4757
1	N	0.53	0/3508	0.72	0/4753
2	B	0.47	0/3196	0.66	0/4334
2	O	0.48	0/3202	0.67	0/4343
3	C	0.63	0/3122	0.76	0/4273
3	P	0.53	0/3114	0.72	0/4263
4	D	0.58	0/1956	0.72	0/2658
4	Q	0.47	0/1956	0.67	0/2658
5	E	0.42	0/1547	0.69	1/2103 (0.0%)
5	R	0.47	0/1542	0.73	1/2097 (0.0%)
6	F	0.66	0/901	0.72	0/1207
6	S	0.50	0/901	0.64	0/1207
7	G	0.58	0/698	0.70	0/946
7	T	0.49	0/680	0.65	0/923
8	H	0.53	0/582	0.67	0/779
8	U	0.37	0/561	0.68	1/751 (0.1%)
9	I	0.47	0/218	0.71	0/293
9	V	0.46	0/218	0.69	0/293
10	J	0.52	0/508	0.65	0/682
10	W	0.47	0/489	0.61	0/658
All	All	0.52	0/32410	0.70	3/43978 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	143	GLY	N-CA-C	7.12	130.89	113.10
5	E	143	GLY	N-CA-C	6.33	128.92	113.10
8	U	49	HIS	N-CA-C	-5.70	95.61	111.00

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	3440	0	3353	227	0
1	N	3437	0	3349	220	0
2	B	3141	0	3142	275	0
2	O	3147	0	3146	259	0
3	C	3020	0	3070	211	0
3	P	3012	0	3058	216	0
4	D	1898	0	1846	123	0
4	Q	1898	0	1846	135	0
5	E	1513	0	1478	128	0
5	R	1508	0	1466	131	0
6	F	881	0	887	42	0
6	S	881	0	887	48	0
7	G	676	0	659	42	0
7	T	658	0	647	48	0
8	H	574	0	548	37	0
8	U	553	0	535	40	0
9	I	302	0	251	36	0
9	V	292	0	251	29	0
10	J	497	0	490	19	0
10	W	478	0	478	29	0
11	A	21	0	13	0	0
11	C	99	0	149	5	0
11	P	54	0	72	2	0
11	W	50	0	77	1	0
12	C	12	0	18	0	0
12	D	20	0	28	5	0
12	E	20	0	28	1	0
12	P	19	0	24	1	0
12	Q	40	0	56	0	0
13	C	3	0	0	0	0
13	P	3	0	0	0	0
14	C	86	0	60	19	0
14	P	86	0	60	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	30	0	25	2	0
15	P	30	0	25	2	0
16	C	19	0	17	5	0
16	P	19	0	17	6	0
17	D	43	0	30	3	0
17	Q	43	0	30	3	0
18	D	42	0	28	3	0
18	G	40	0	24	1	0
18	P	82	0	52	5	0
19	E	4	0	0	1	0
19	R	4	0	0	0	0
20	E	2	0	0	0	0
20	P	2	0	0	0	0
20	Q	1	0	0	0	0
21	C	8	0	0	2	0
21	P	7	0	0	2	0
21	U	1	0	0	0	0
All	All	32696	0	32220	2098	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 32.

The worst 5 of 2098 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)
3:C:17:ASN:HD21	7:G:1:GLY:HA3	1.15	1.08
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.37	1.04
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.42	1.01
5:E:73:LYS:O	5:E:74:ILE:HG13	1.60	1.00
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.06	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	441/446 (99%)	345 (78%)	75 (17%)	21 (5%)	2	21
1	N	440/446 (99%)	344 (78%)	75 (17%)	21 (5%)	2	21
2	B	419/441 (95%)	342 (82%)	62 (15%)	15 (4%)	3	28
2	O	420/441 (95%)	333 (79%)	67 (16%)	20 (5%)	2	21
3	C	378/380 (100%)	300 (79%)	62 (16%)	16 (4%)	3	24
3	P	377/380 (99%)	302 (80%)	60 (16%)	15 (4%)	3	25
4	D	239/241 (99%)	195 (82%)	35 (15%)	9 (4%)	3	27
4	Q	239/241 (99%)	190 (80%)	36 (15%)	13 (5%)	2	19
5	E	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	1	15
5	R	194/196 (99%)	146 (75%)	31 (16%)	17 (9%)	1	9
6	F	98/110 (89%)	73 (74%)	22 (22%)	3 (3%)	4	32
6	S	98/110 (89%)	74 (76%)	22 (22%)	2 (2%)	7	41
7	G	79/81 (98%)	61 (77%)	14 (18%)	4 (5%)	2	20
7	T	77/81 (95%)	61 (79%)	11 (14%)	5 (6%)	1	15
8	H	68/77 (88%)	49 (72%)	16 (24%)	3 (4%)	2	23
8	U	65/77 (84%)	42 (65%)	17 (26%)	6 (9%)	1	8
9	I	29/52 (56%)	14 (48%)	10 (34%)	5 (17%)	0	2
9	V	29/52 (56%)	18 (62%)	8 (28%)	3 (10%)	0	7
10	J	59/61 (97%)	42 (71%)	15 (25%)	2 (3%)	3	30
10	W	57/61 (93%)	42 (74%)	9 (16%)	6 (10%)	0	7
All	All	4000/4170 (96%)	3120 (78%)	681 (17%)	199 (5%)	2	20

5 of 199 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	CYS
1	A	159	GLN
2	B	26	ILE
2	B	38	LEU
2	B	171	ALA

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	365/368 (99%)	338 (93%)	27 (7%)	13	45
1	N	365/368 (99%)	336 (92%)	29 (8%)	12	42
2	B	332/347 (96%)	313 (94%)	19 (6%)	20	54
2	O	333/347 (96%)	314 (94%)	19 (6%)	20	54
3	C	329/329 (100%)	306 (93%)	23 (7%)	15	47
3	P	328/329 (100%)	307 (94%)	21 (6%)	17	51
4	D	200/200 (100%)	190 (95%)	10 (5%)	24	58
4	Q	200/200 (100%)	190 (95%)	10 (5%)	24	58
5	E	166/166 (100%)	156 (94%)	10 (6%)	19	53
5	R	165/166 (99%)	153 (93%)	12 (7%)	14	45
6	F	92/96 (96%)	89 (97%)	3 (3%)	38	68
6	S	92/96 (96%)	89 (97%)	3 (3%)	38	68
7	G	71/71 (100%)	64 (90%)	7 (10%)	8	34
7	T	69/71 (97%)	63 (91%)	6 (9%)	10	39
8	H	65/71 (92%)	62 (95%)	3 (5%)	27	61
8	U	63/71 (89%)	59 (94%)	4 (6%)	18	51
9	I	23/26 (88%)	22 (96%)	1 (4%)	29	62
9	V	23/26 (88%)	22 (96%)	1 (4%)	29	62
10	J	49/49 (100%)	47 (96%)	2 (4%)	30	64
10	W	47/49 (96%)	45 (96%)	2 (4%)	29	62
All	All	3377/3446 (98%)	3165 (94%)	212 (6%)	18	51

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	171	THR
2	O	239	TYR
7	T	4	PHE

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Mol	Chain	Res	Type
1	N	228	VAL
1	N	395	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	313	GLN
6	S	108	ASN
4	Q	31	GLN
5	R	57	GLN
8	U	75	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 4 are unknown - leaving 30 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	$\#\|Z\| > 2$
15	ICX	P	3001	-	31,31,31	1.38	6 (19%)	36,39,39	0.91	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	HEC	Q	501	4	32,50,50	2.33	3 (9%)	24,82,82	1.82	3 (12%)
18	CDL	P	3003	-	41,41,99	1.18	2 (4%)	47,53,111	1.07	2 (4%)
12	BOG	E	2009	-	20,20,20	1.15	2 (10%)	25,25,25	0.92	1 (4%)
11	PEE	W	3005	-	49,49,50	1.54	10 (20%)	52,54,55	0.87	3 (5%)
12	BOG	C	3010	-	11,11,20	1.03	2 (18%)	10,11,25	0.91	1 (10%)
16	UQ	P	3002	-	19,19,63	2.57	10 (52%)	23,26,79	1.27	2 (8%)
15	ICX	C	2001	-	31,31,31	1.32	4 (12%)	36,39,39	1.04	2 (5%)
17	HEC	D	501	4	32,50,50	2.50	7 (21%)	24,82,82	1.91	6 (25%)
18	CDL	G	2004	-	39,39,99	1.29	5 (12%)	45,51,111	1.08	3 (6%)
11	PEE	P	3008	-	4,4,50	3.44	4 (100%)	6,6,55	0.57	0
14	HEM	P	502	3	41,50,50	1.61	8 (19%)	45,82,82	1.42	5 (11%)
11	PEE	C	2007	-	48,48,50	1.37	7 (14%)	51,53,55	0.82	3 (5%)
13	AZI	C	2011	-	0,2,2	-	-	0,1,1	-	-
11	PEE	P	3007	-	48,48,50	1.39	6 (12%)	51,53,55	0.82	2 (3%)
11	PEE	C	2005	-	49,49,50	1.48	10 (20%)	52,54,55	0.87	3 (5%)
19	FES	E	501	5	0,4,4	-	-	-		
19	FES	R	501	5	0,4,4	-	-	-		
12	BOG	D	2091	-	20,20,20	1.12	2 (10%)	25,25,25	0.97	1 (4%)
16	UQ	C	2002	-	19,19,63	2.49	9 (47%)	23,26,79	1.25	2 (8%)
14	HEM	C	502	3	41,50,50	2.08	9 (21%)	45,82,82	1.84	10 (22%)
12	BOG	Q	3009	-	20,20,20	1.21	3 (15%)	25,25,25	1.14	1 (4%)
11	PEE	A	2008	-	20,20,50	1.80	5 (25%)	23,25,55	0.74	1 (4%)
13	AZI	P	3011	-	0,2,2	-	-	0,1,1	-	-
12	BOG	P	2010	-	18,18,20	1.11	3 (16%)	22,22,25	0.55	0
18	CDL	D	2003	-	41,41,99	1.18	1 (2%)	47,53,111	1.05	2 (4%)
14	HEM	C	501	3	41,50,50	2.10	11 (26%)	45,82,82	2.44	14 (31%)
18	CDL	P	3004	-	39,39,99	1.25	3 (7%)	45,51,111	1.07	3 (6%)
14	HEM	P	501	3	41,50,50	1.94	10 (24%)	45,82,82	2.37	19 (42%)
12	BOG	Q	3091	-	20,20,20	1.16	3 (15%)	25,25,25	0.95	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ICX	P	3001	-	-	2/24/24/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEC	Q	501	4	-	6/10/54/54	-
18	CDL	P	3003	-	-	24/51/51/110	-
12	BOG	E	2009	-	-	6/11/31/31	0/1/1/1
11	PEE	W	3005	-	-	27/53/53/54	-
12	BOG	C	3010	-	-	4/9/9/31	-
16	UQ	P	3002	-	-	2/11/35/87	0/1/1/1
15	ICX	C	2001	-	-	2/24/24/24	0/2/2/2
17	HEC	D	501	4	-	4/10/54/54	-
18	CDL	G	2004	-	-	21/49/49/110	-
14	HEM	P	502	3	-	6/12/54/54	-
11	PEE	C	2007	-	-	24/52/52/54	-
11	PEE	P	3007	-	-	25/52/52/54	-
11	PEE	C	2005	-	-	26/53/53/54	-
19	FES	E	501	5	-	-	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
12	BOG	D	2091	-	-	4/11/31/31	0/1/1/1
16	UQ	C	2002	-	-	2/11/35/87	0/1/1/1
14	HEM	C	502	3	-	6/12/54/54	-
12	BOG	Q	3009	-	-	4/11/31/31	0/1/1/1
11	PEE	A	2008	-	-	12/24/24/54	-
12	BOG	P	2010	-	-	2/6/26/31	0/1/1/1
18	CDL	D	2003	-	-	23/51/51/110	-
14	HEM	C	501	3	-	6/12/54/54	-
18	CDL	P	3004	-	-	21/49/49/110	-
14	HEM	P	501	3	-	4/12/54/54	-
12	BOG	Q	3091	-	-	6/11/31/31	0/1/1/1

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C2B-C3B	-11.00	1.29	1.40
17	D	501	HEC	C2B-C3B	-10.50	1.29	1.40
14	C	502	HEM	C3C-C2C	-6.24	1.31	1.40
16	P	3002	UQ	C7-C6	5.96	1.61	1.51
17	D	501	HEC	C3C-C2C	-5.95	1.34	1.40

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	501	HEM	CBA-CAA-C2A	-7.08	100.53	112.62
14	C	501	HEM	CBA-CAA-C2A	-6.74	101.11	112.62
14	P	501	HEM	CMB-C2B-C1B	6.09	134.31	125.04
17	D	501	HEC	CBA-CAA-C2A	5.74	122.28	112.60
14	C	501	HEM	CMB-C2B-C1B	5.69	133.71	125.04

There are no chirality outliers.

5 of 269 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	C1-O3P-P-O2P
11	A	2008	PEE	C1-O3P-P-O1P
11	C	2005	PEE	C11-C10-O2-C2
11	C	2005	PEE	C1-O3P-P-O2P
11	C	2005	PEE	C1-O3P-P-O1P

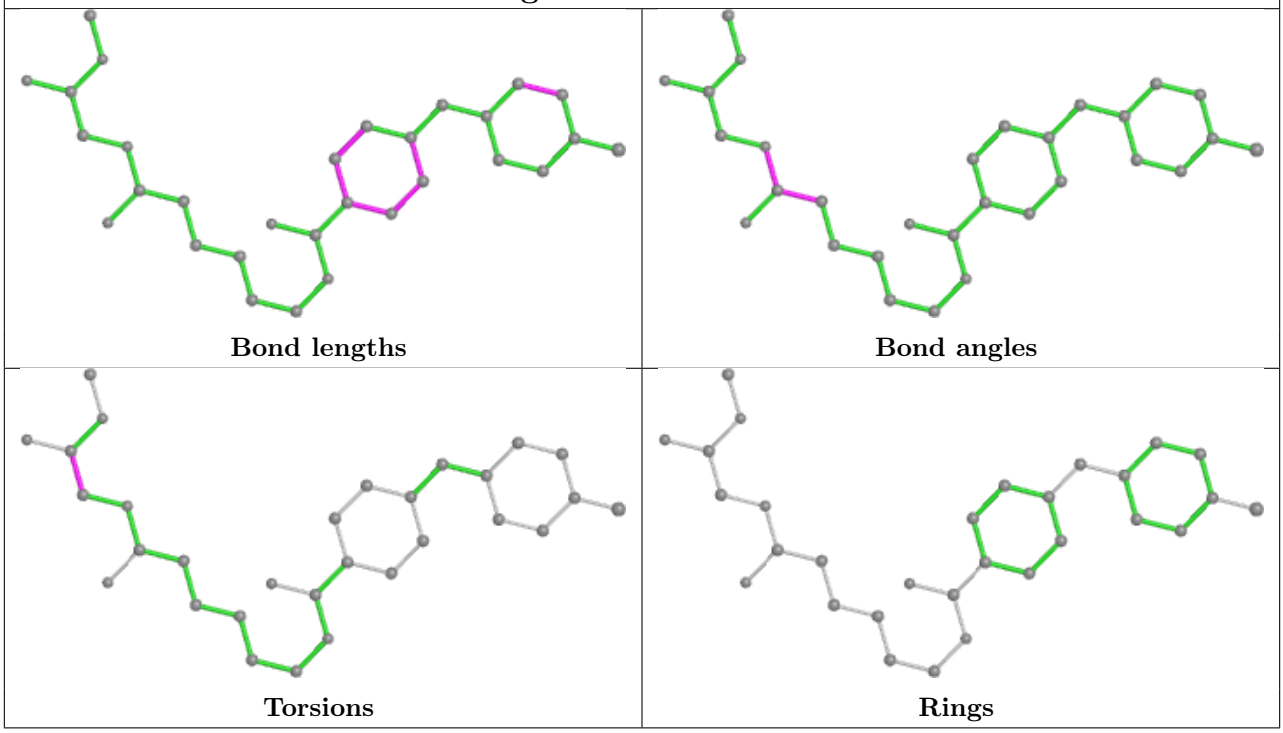
There are no ring outliers.

22 monomers are involved in 83 short contacts:

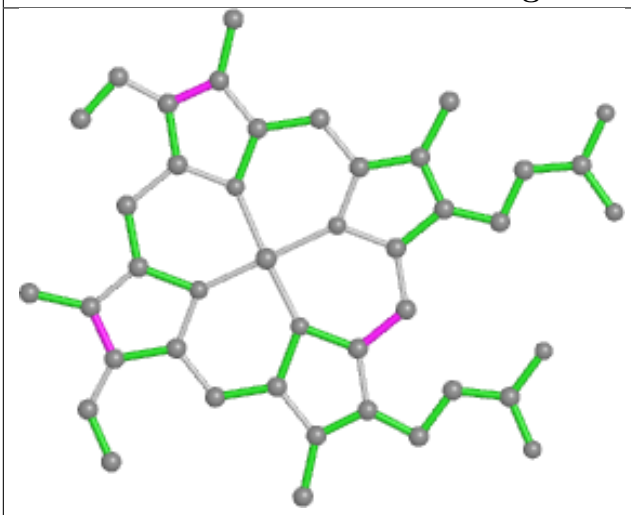
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	P	3001	ICX	2	0
17	Q	501	HEC	3	0
18	P	3003	CDL	3	0
12	E	2009	BOG	1	0
11	W	3005	PEE	1	0
16	P	3002	UQ	6	0
15	C	2001	ICX	2	0
17	D	501	HEC	3	0
18	G	2004	CDL	1	0
14	P	502	HEM	11	0
11	C	2007	PEE	3	0
11	P	3007	PEE	2	0
11	C	2005	PEE	2	0
19	E	501	FES	1	0
12	D	2091	BOG	5	0
16	C	2002	UQ	5	0
14	C	502	HEM	10	0
12	P	2010	BOG	1	0
18	D	2003	CDL	3	0
14	C	501	HEM	9	0
18	P	3004	CDL	2	0
14	P	501	HEM	8	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.

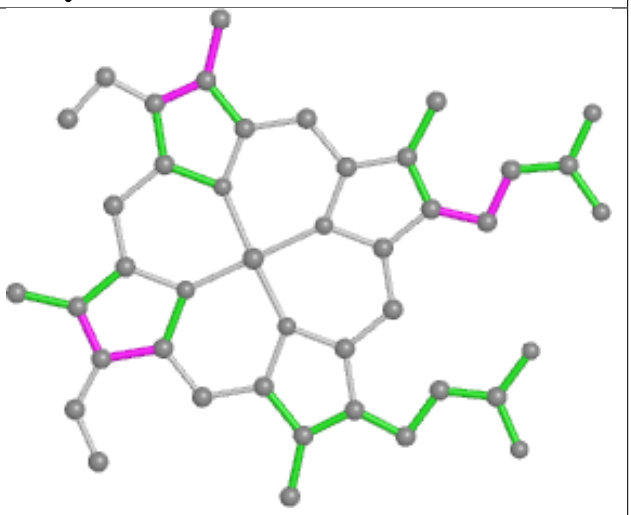
Ligand ICX P 3001



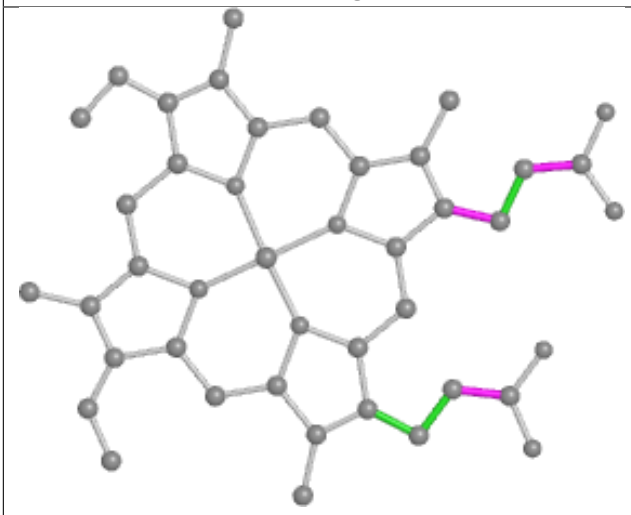
Ligand HEC Q 501



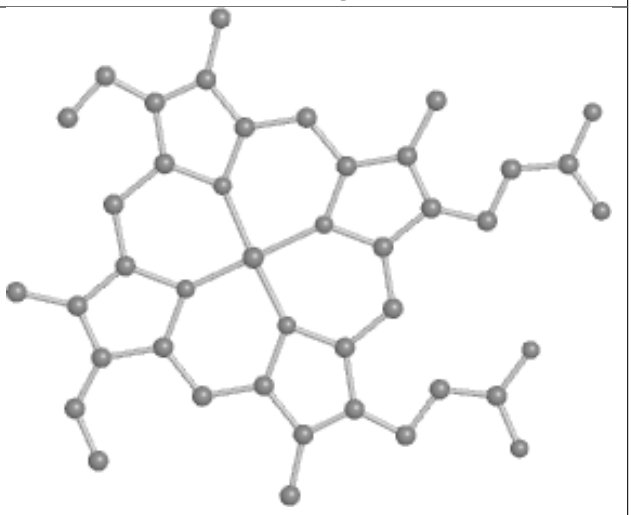
Bond lengths



Bond angles

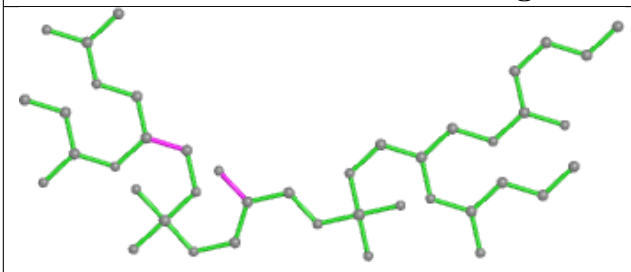


Torsions

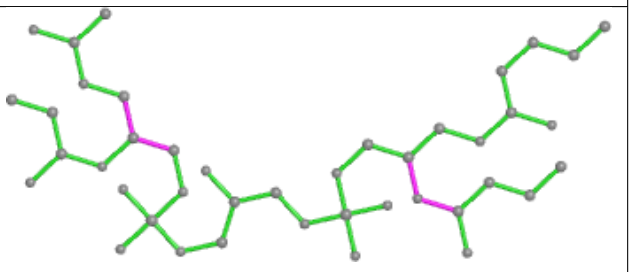


Rings

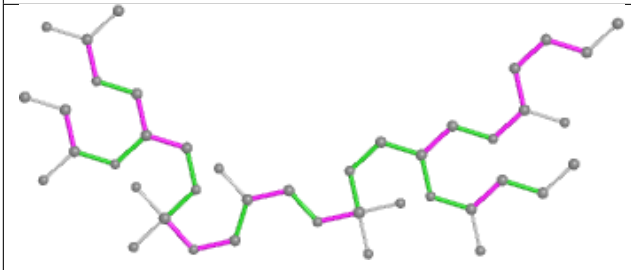
Ligand CDL P 3003



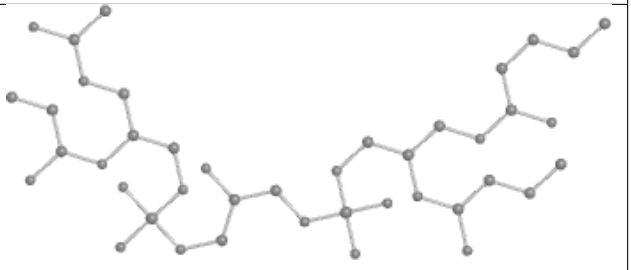
Bond lengths



Bond angles

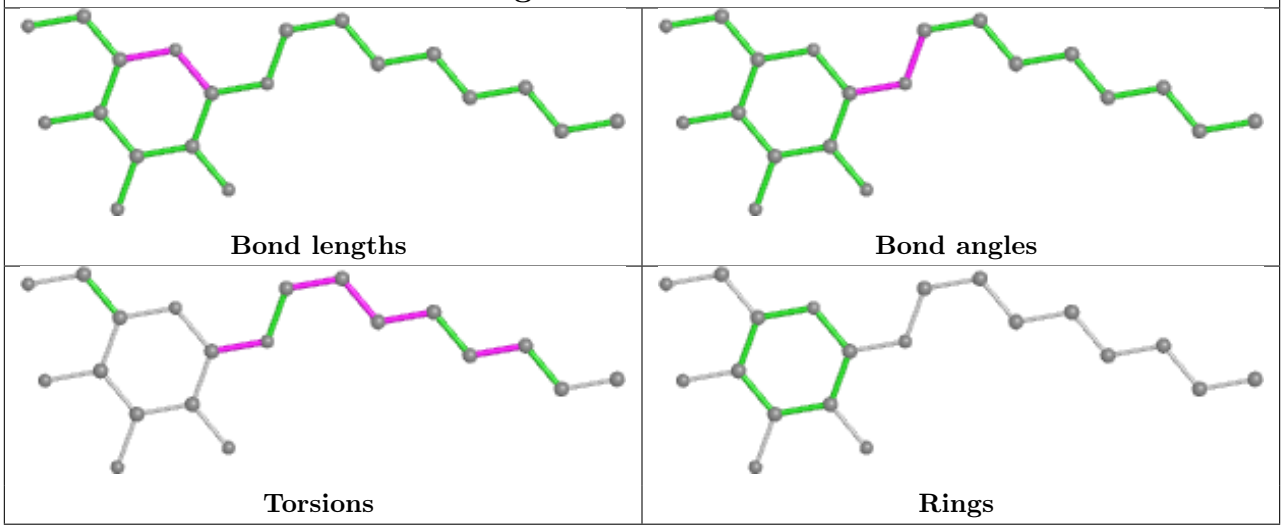


Torsions

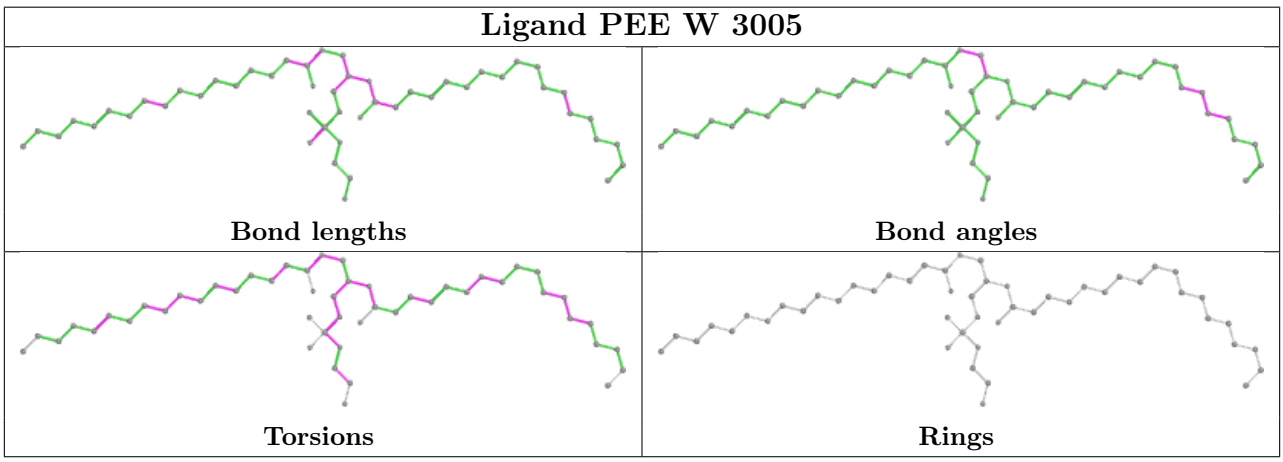


Rings

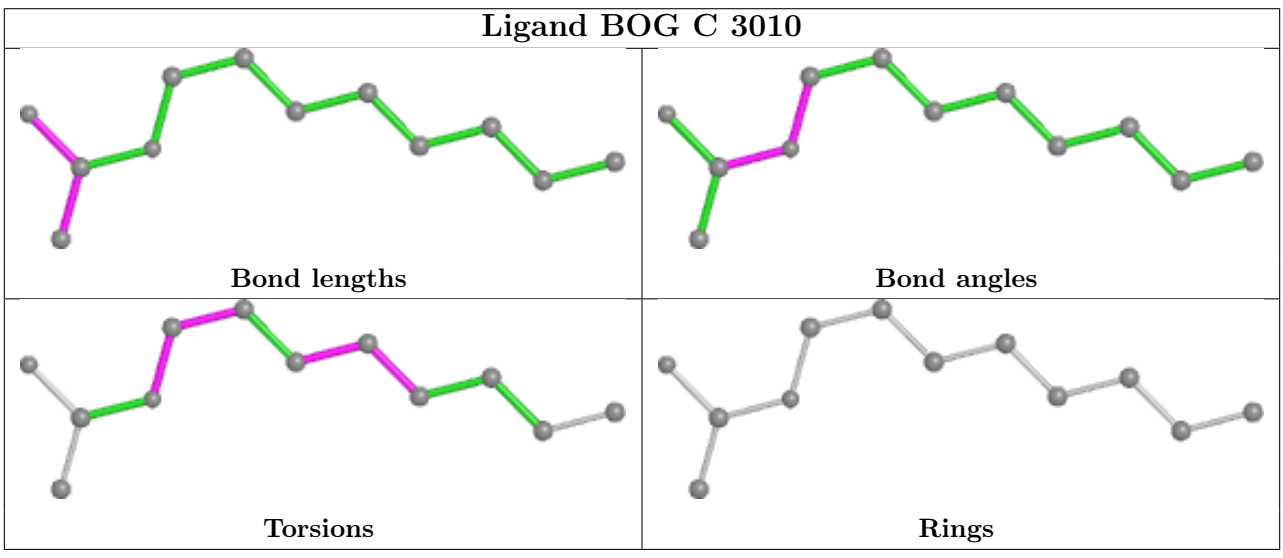
Ligand BOG E 2009



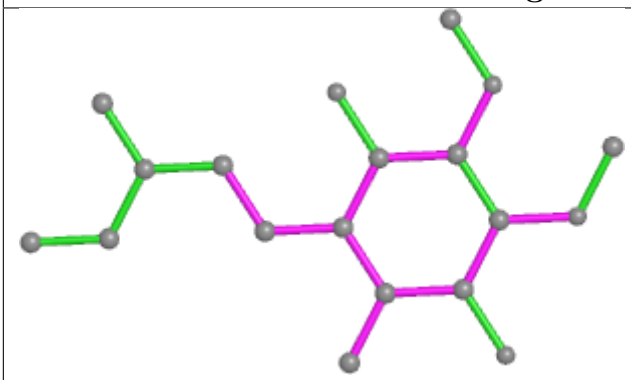
Ligand PEE W 3005



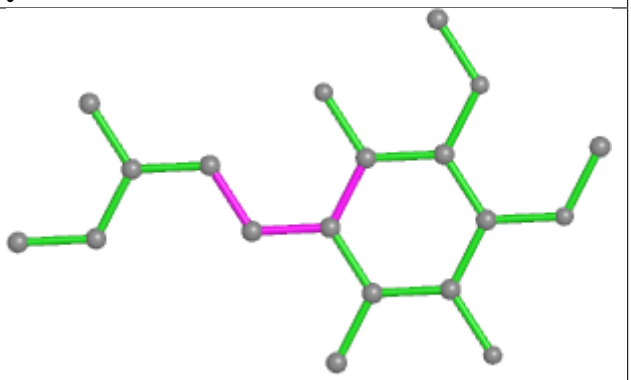
Ligand BOG C 3010



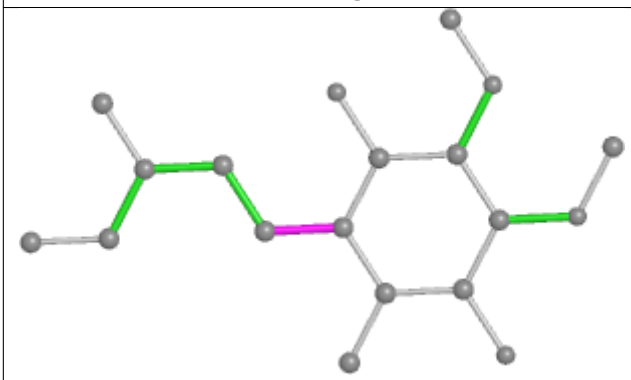
Ligand UQ P 3002



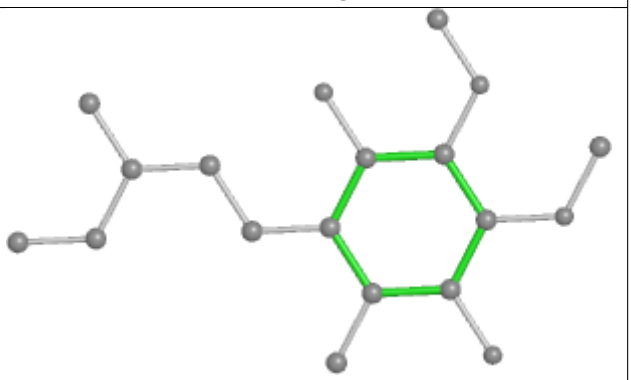
Bond lengths



Bond angles

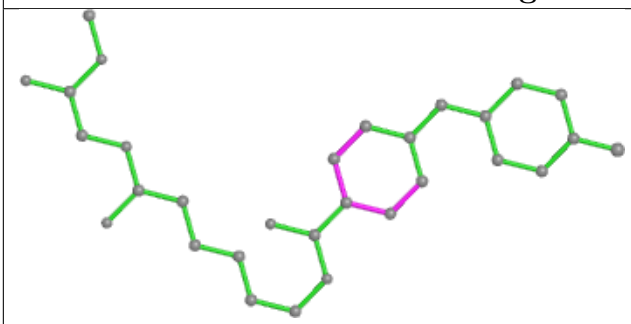


Torsions



Rings

Ligand ICX C 2001



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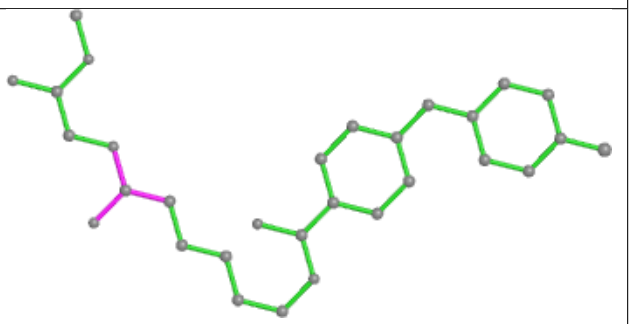
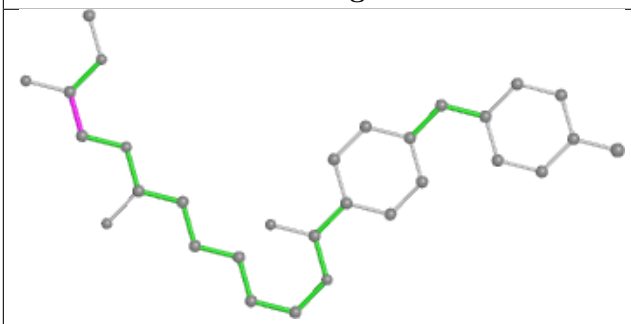


Bond angles



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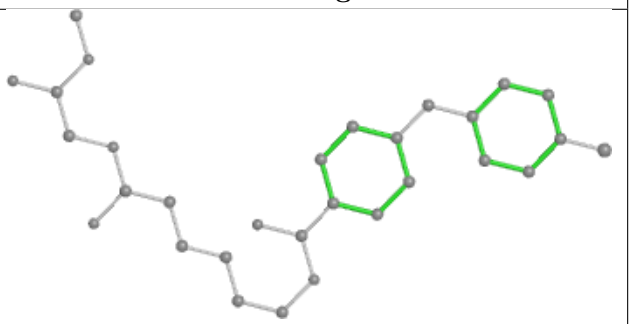
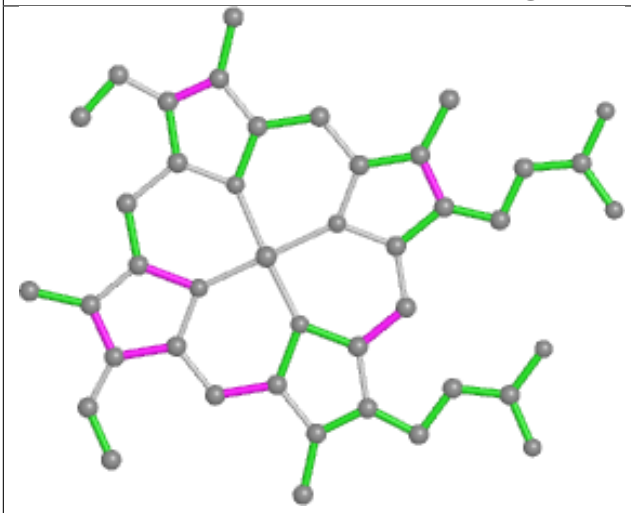


Rings

Ligand HEC D 501



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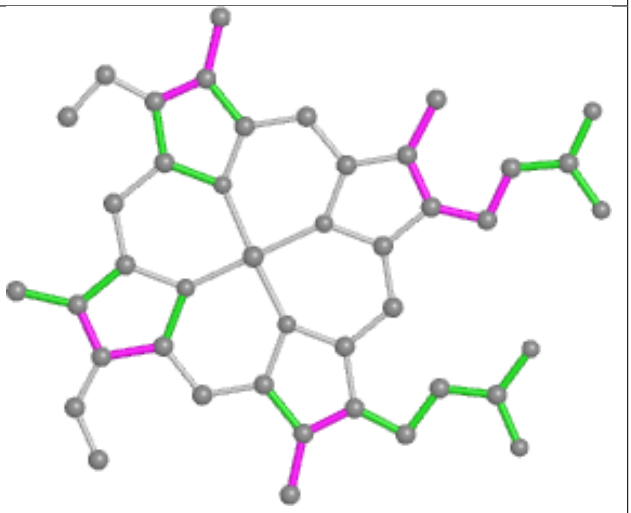
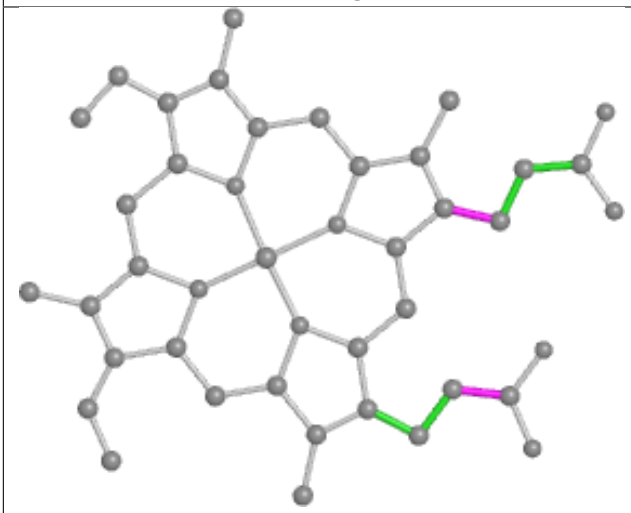
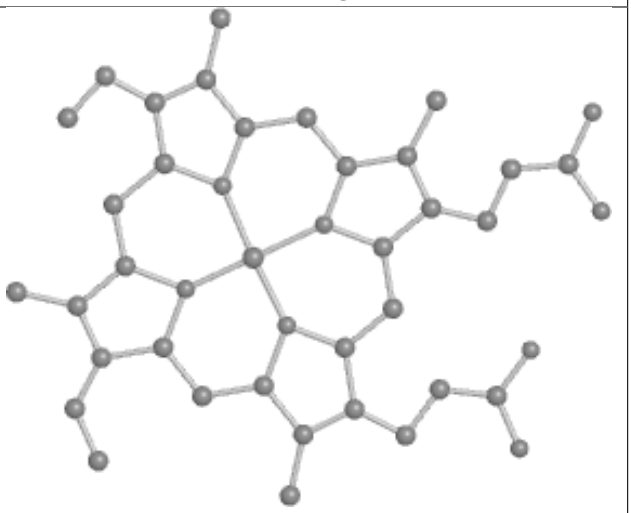


Bond angles

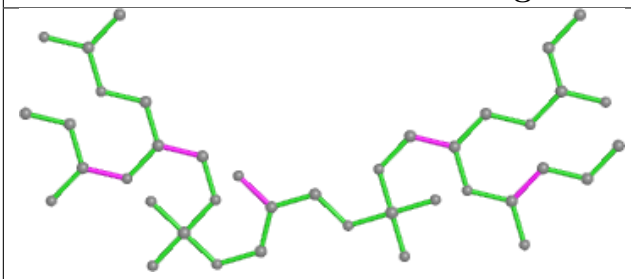


Torsions

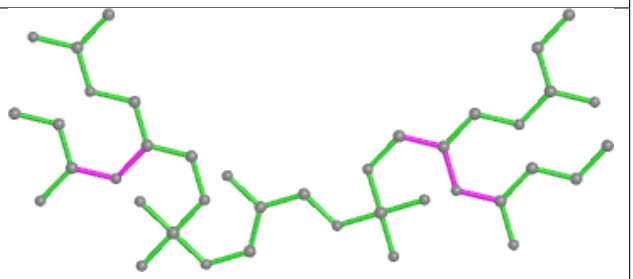


Rings

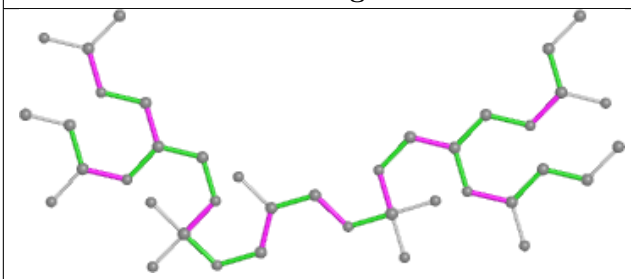
Ligand CDL G 2004



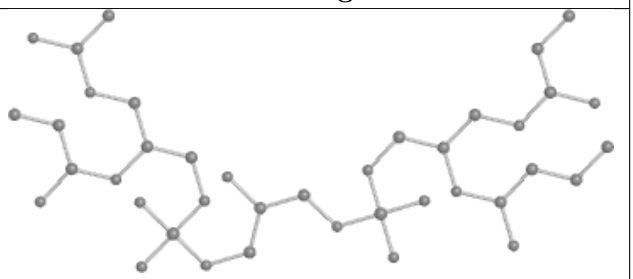
Bond lengths



Bond angles

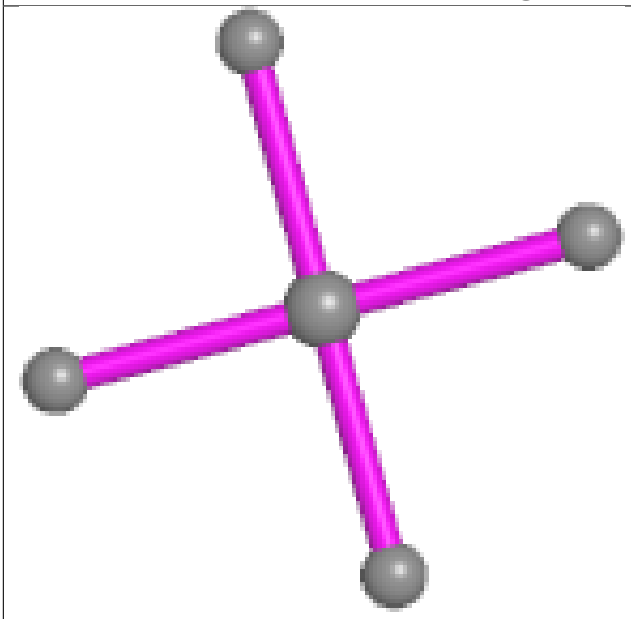


Torsions



Rings

Ligand PEE P 3008



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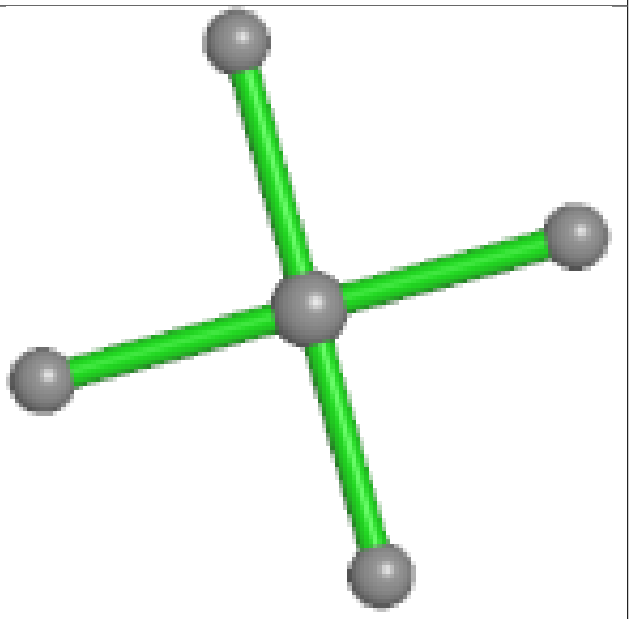
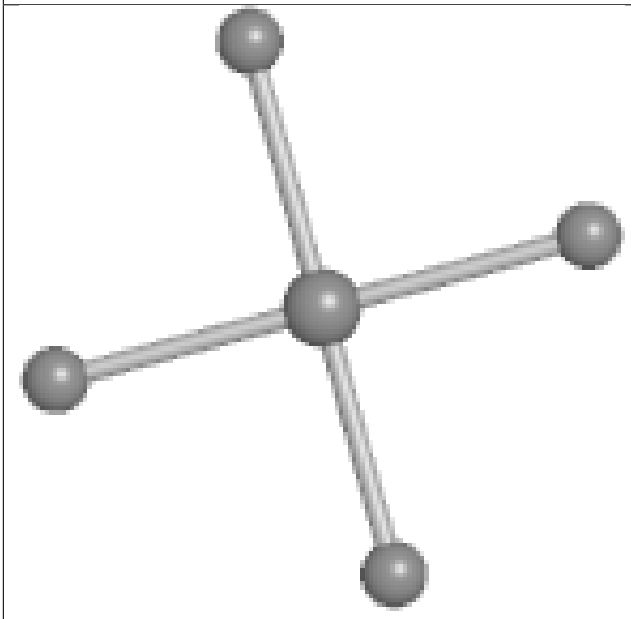
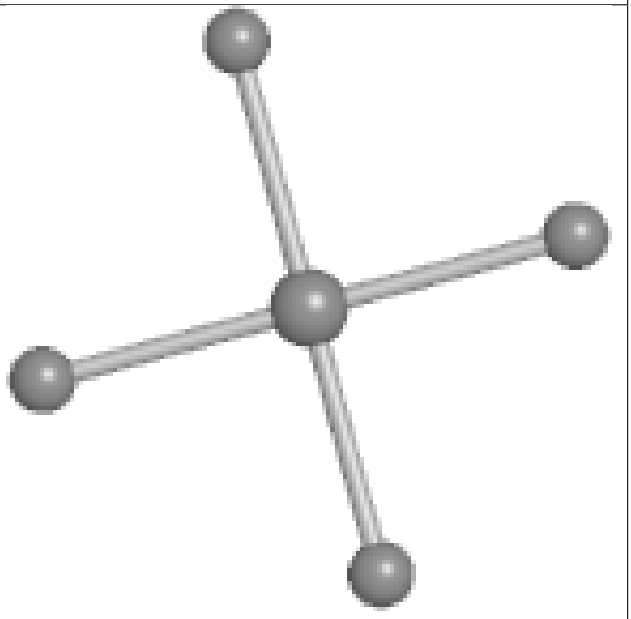


Bond angles

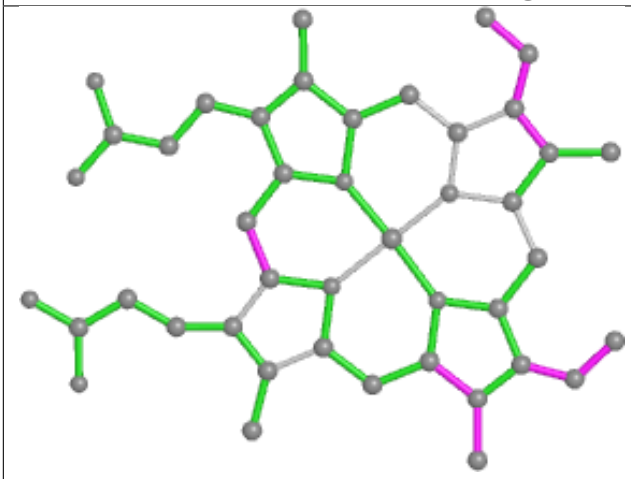


Torsions

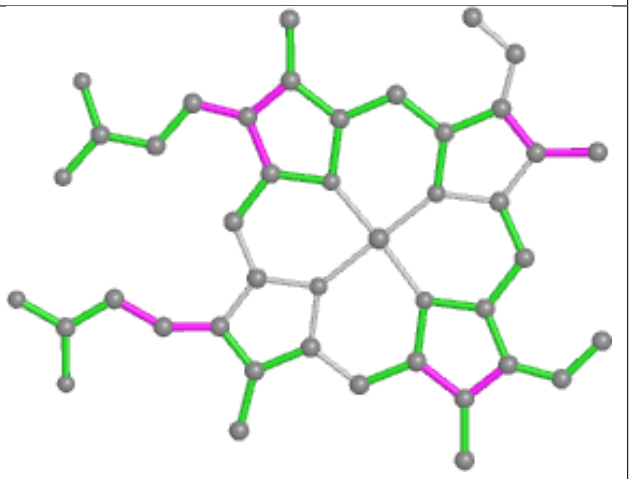


Rings

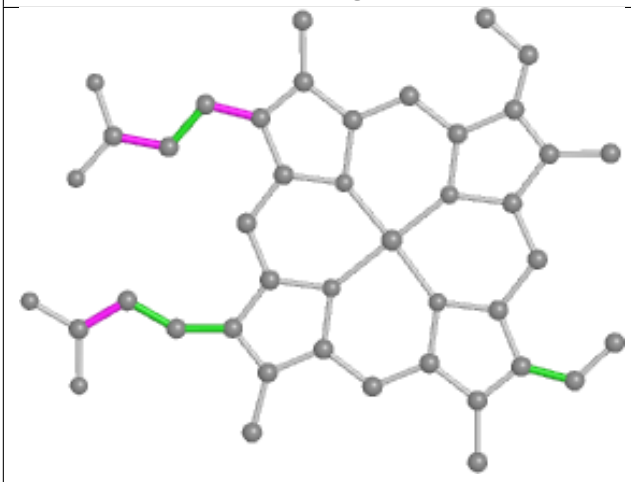
Ligand HEM P 502



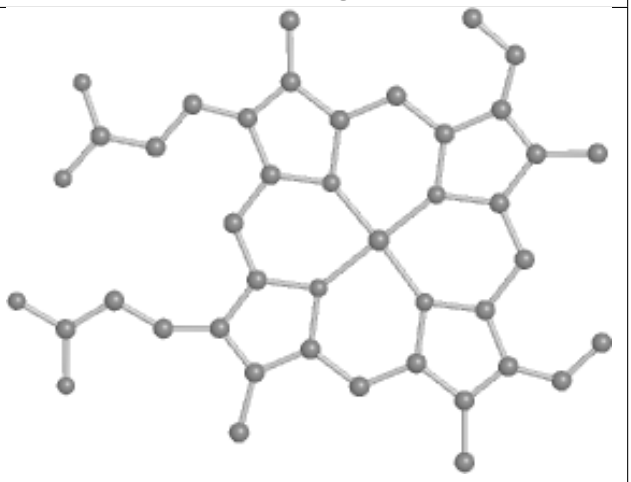
Bond lengths



Bond angles

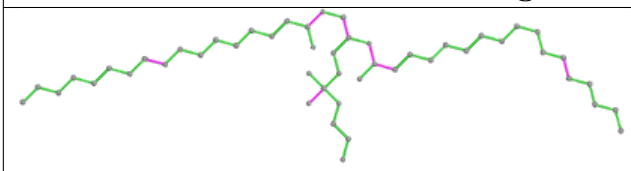


Torsions



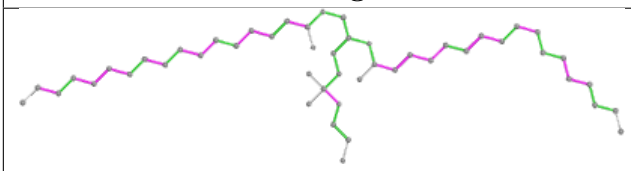
Rings

Ligand PEE C 2007

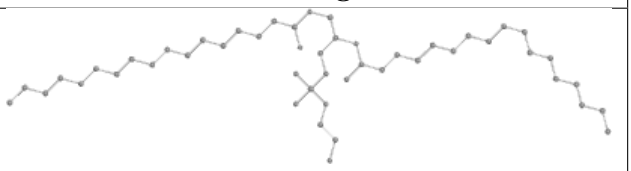


Bond lengths

Bond angles

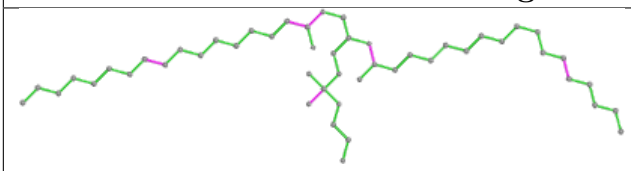


Torsions

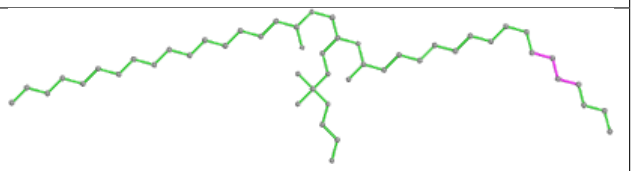


Rings

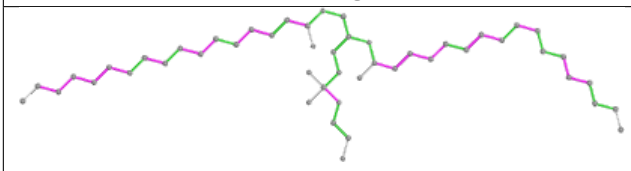
Ligand PEE P 3007



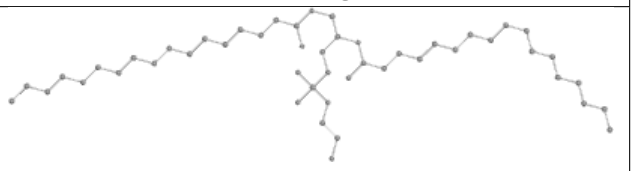
Bond lengths



Bond angles

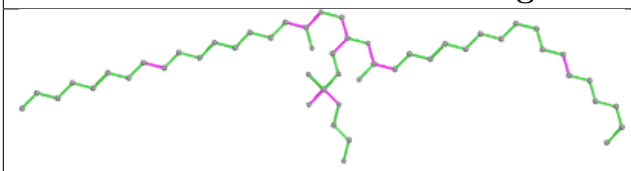


Torsions

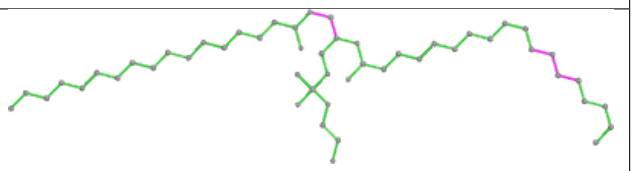


Rings

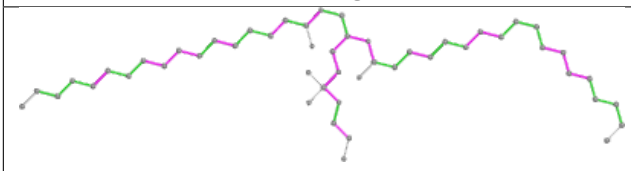
Ligand PEE C 2005



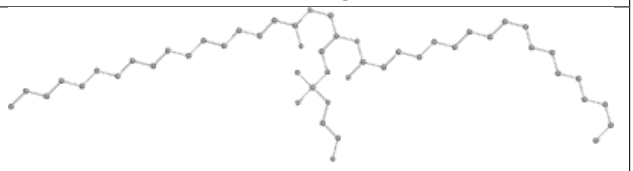
Bond lengths



Bond angles

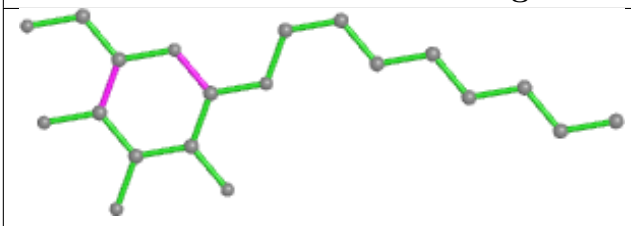


Torsions

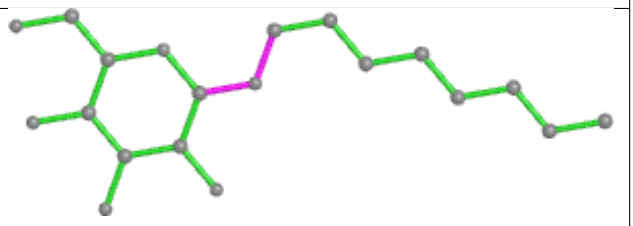


Rings

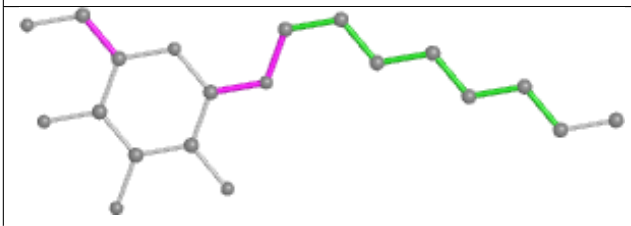
Ligand BOG D 2091



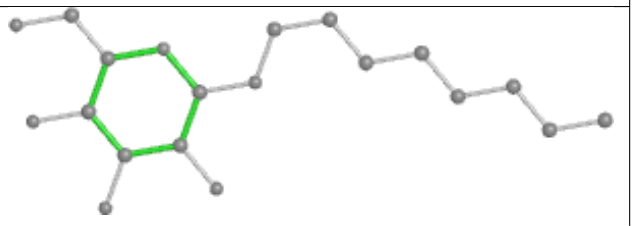
Bond lengths



Bond angles

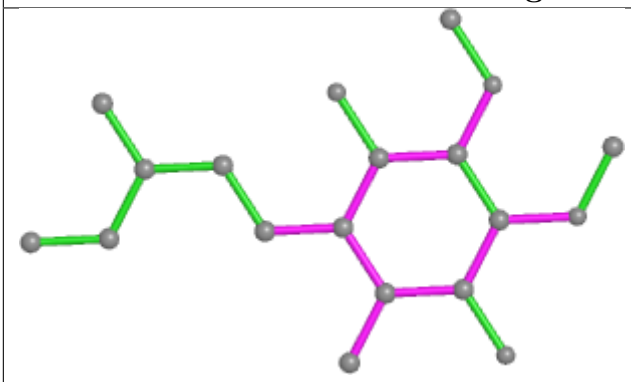


Torsions

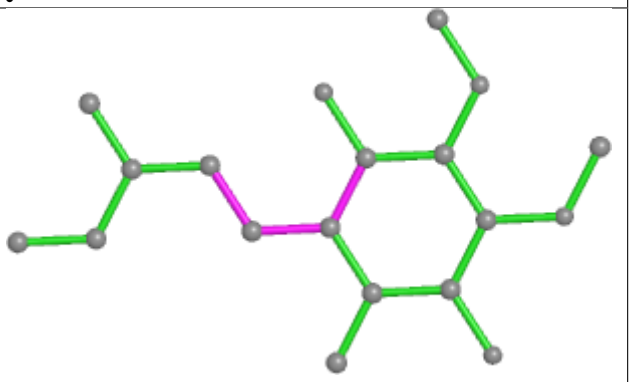


Rings

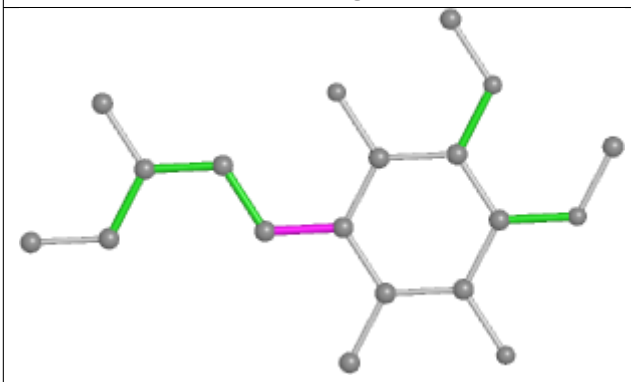
Ligand UQ C 2002



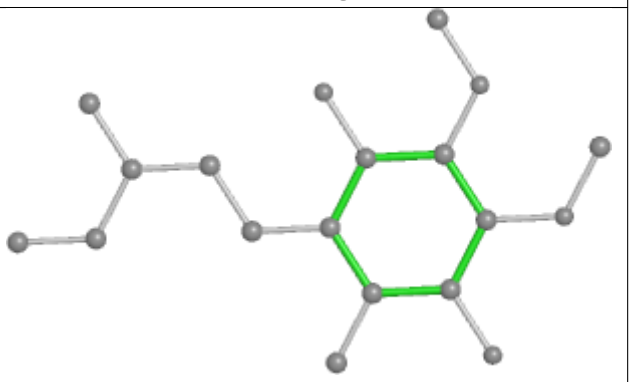
Bond lengths



Bond angles

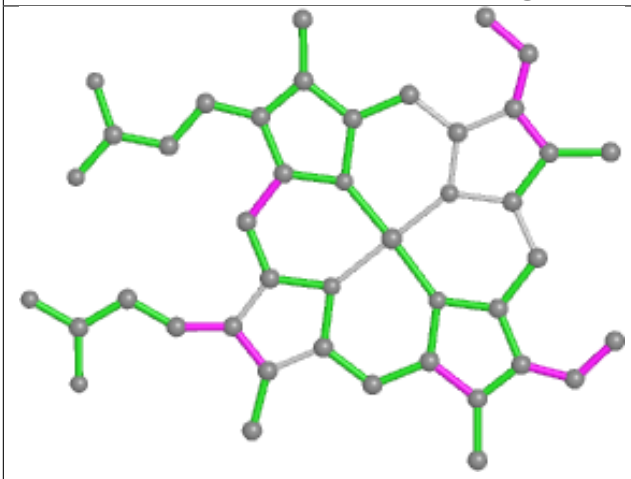


Torsions

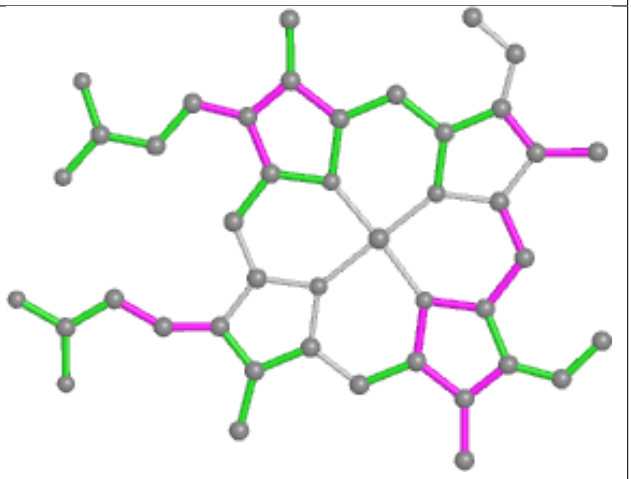


Rings

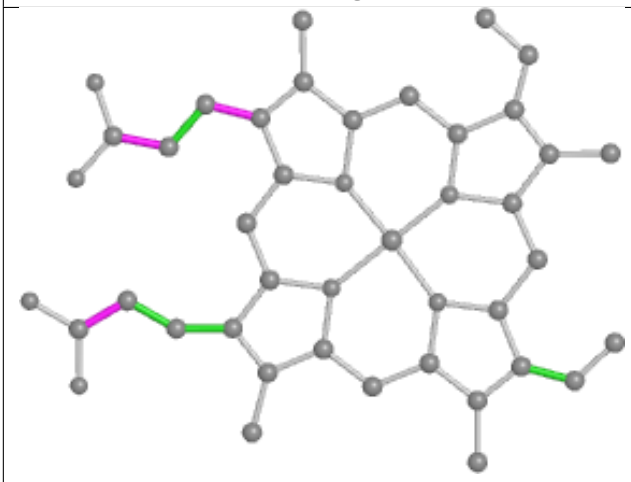
Ligand HEM C 502



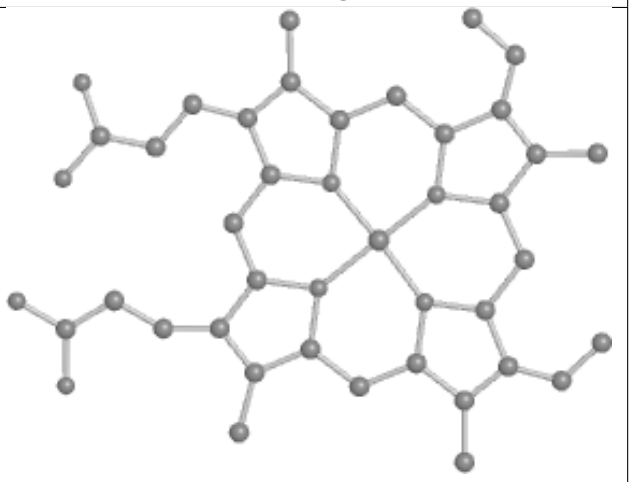
Bond lengths



Bond angles

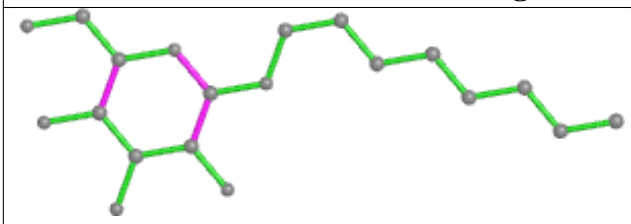


Torsions

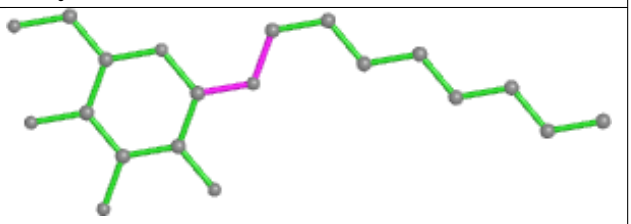


Rings

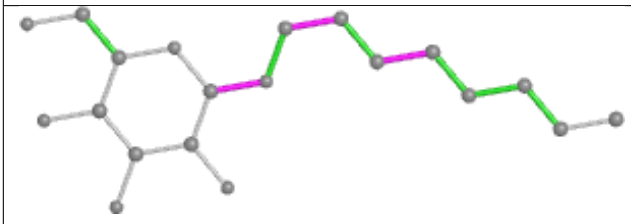
Ligand BOG Q 3009



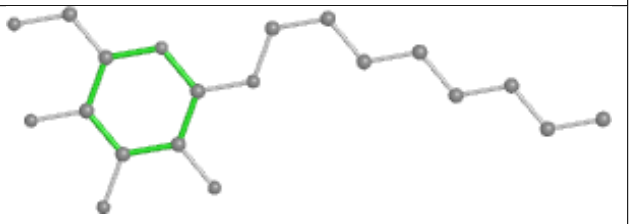
Bond lengths



Bond angles

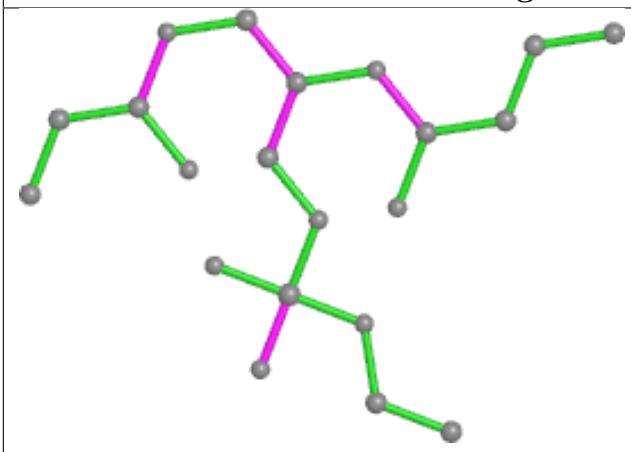


Torsions

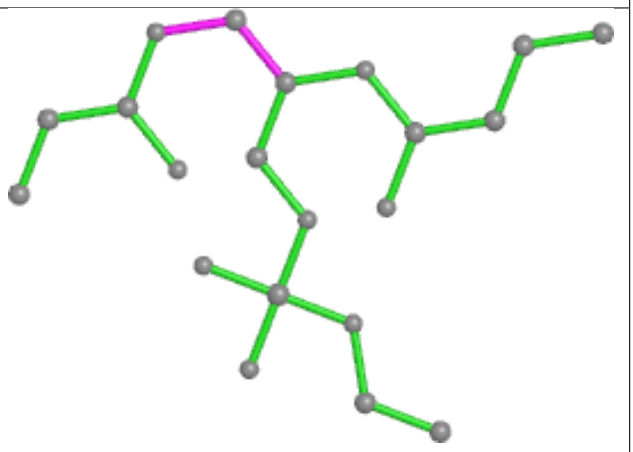


Rings

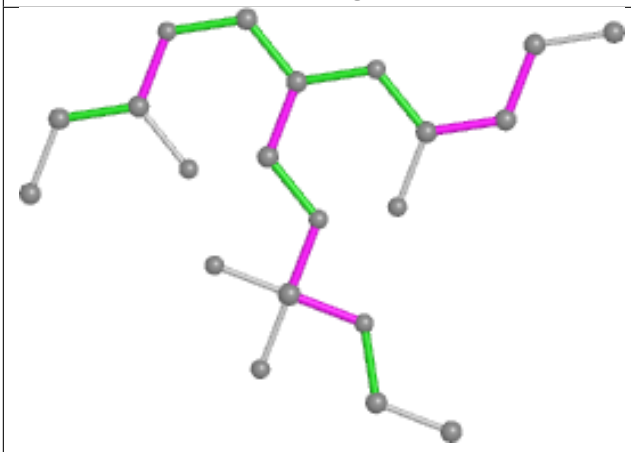
Ligand PEE A 2008



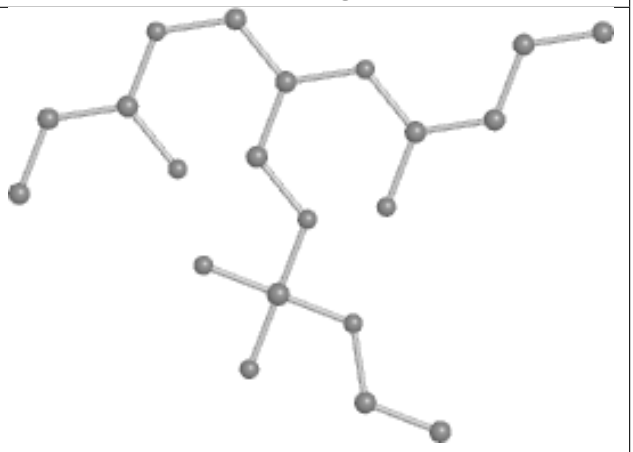
Bond lengths



Bond angles

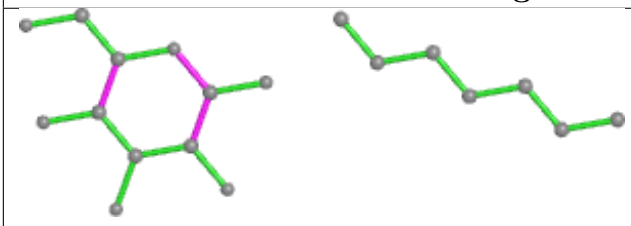


Torsions

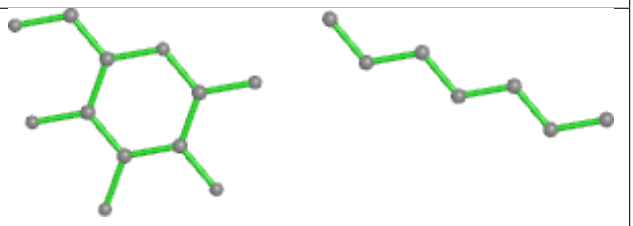


Rings

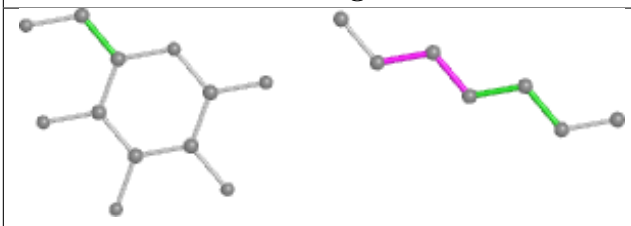
Ligand BOG P 2010



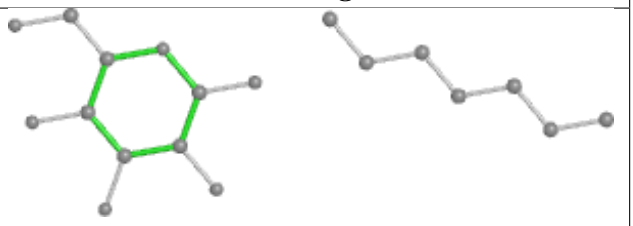
Bond lengths



Bond angles

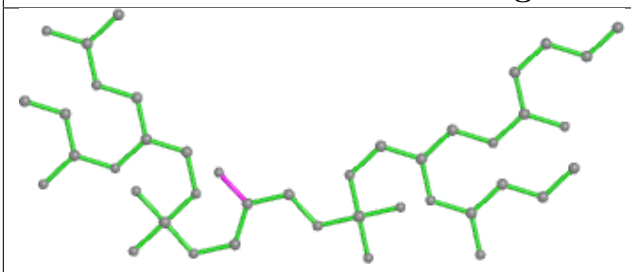


Torsions

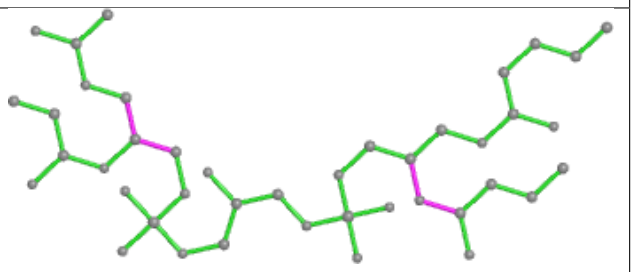


Rings

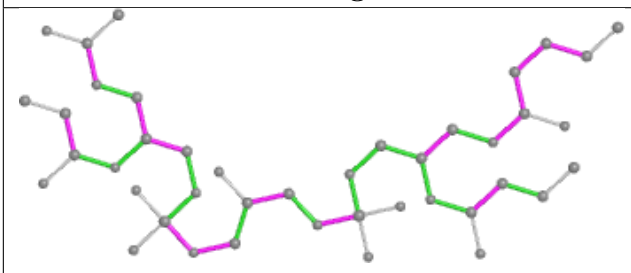
Ligand CDL D 2003



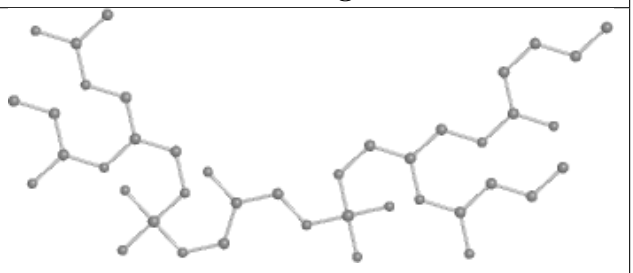
Bond lengths



Bond angles

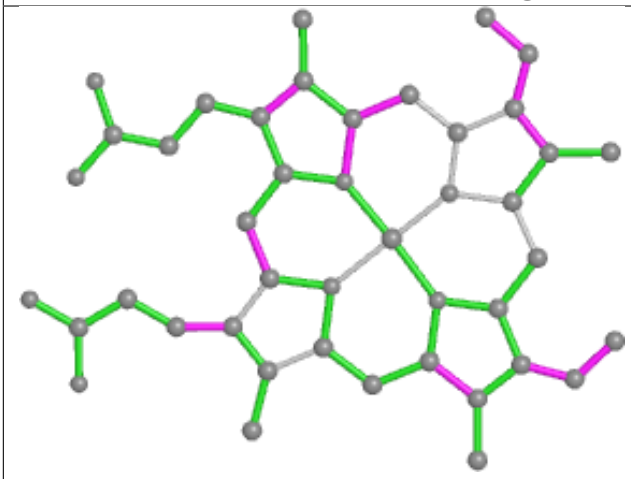


Torsions

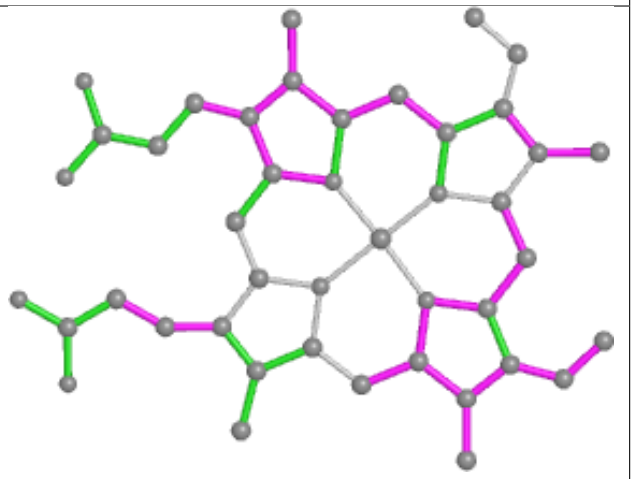


Rings

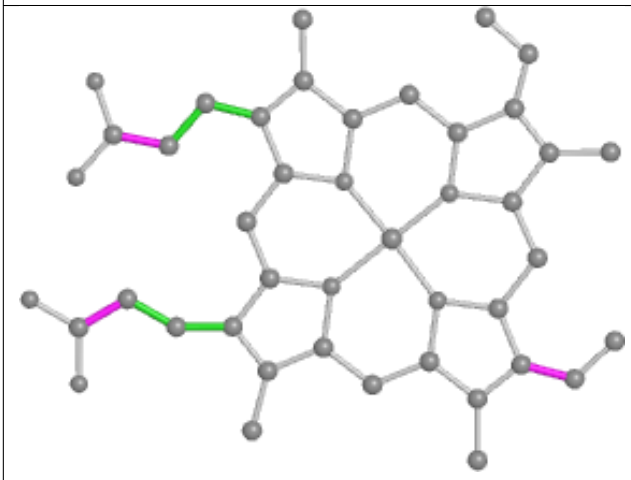
Ligand HEM C 501



Bond lengths



Bond angles



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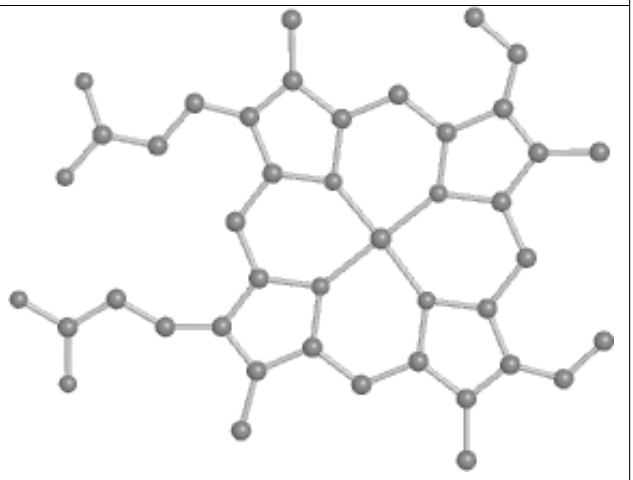
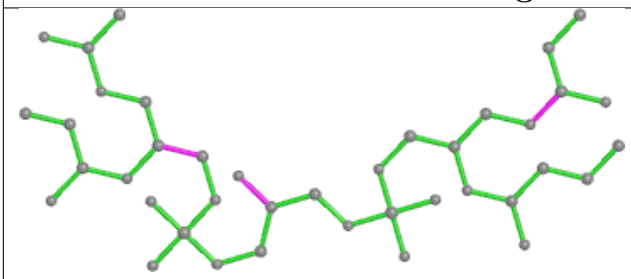
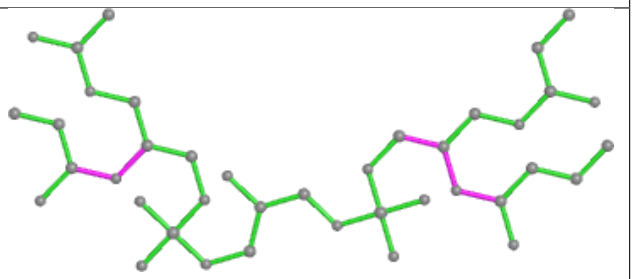


Rings

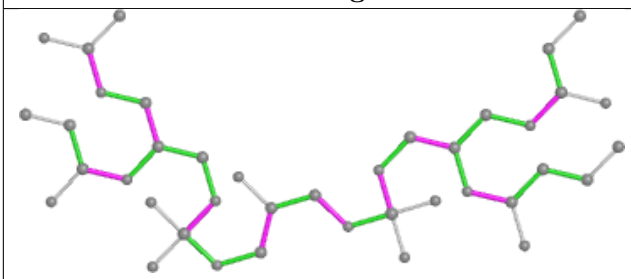
Ligand CDL P 3004



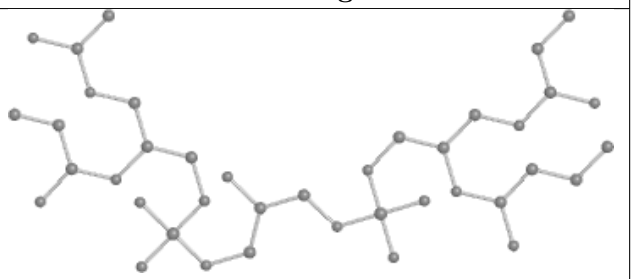
Bond lengths



Bond angles

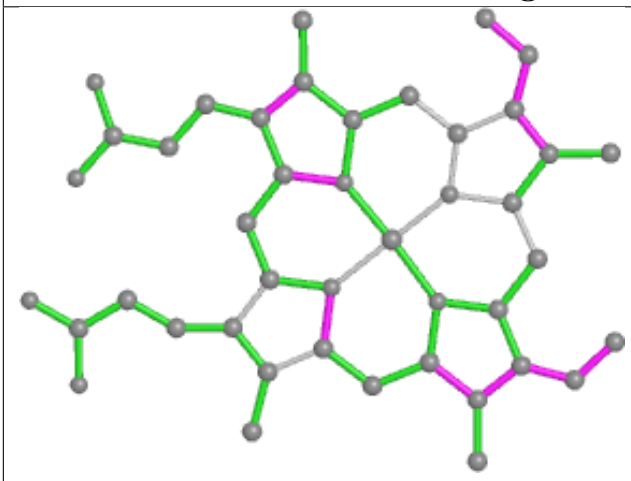


Torsions

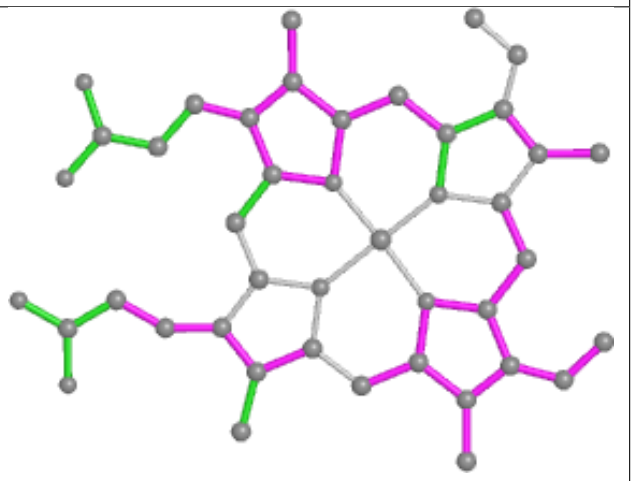


Rings

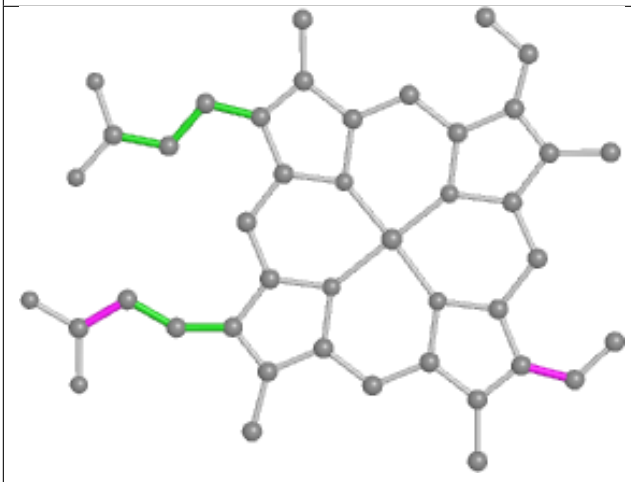
Ligand HEM P 501



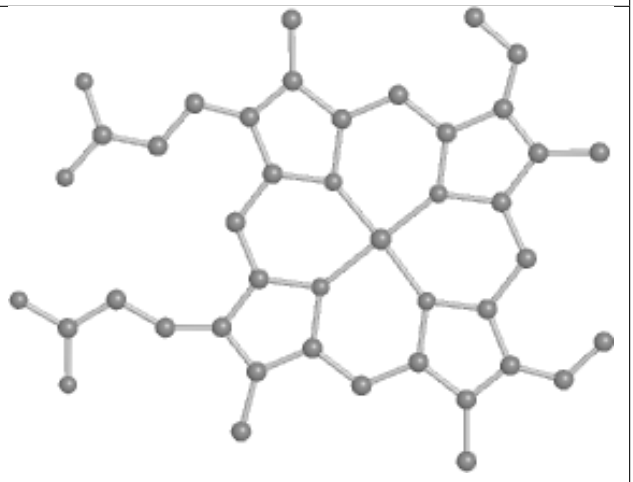
Bond lengths



Bond angles

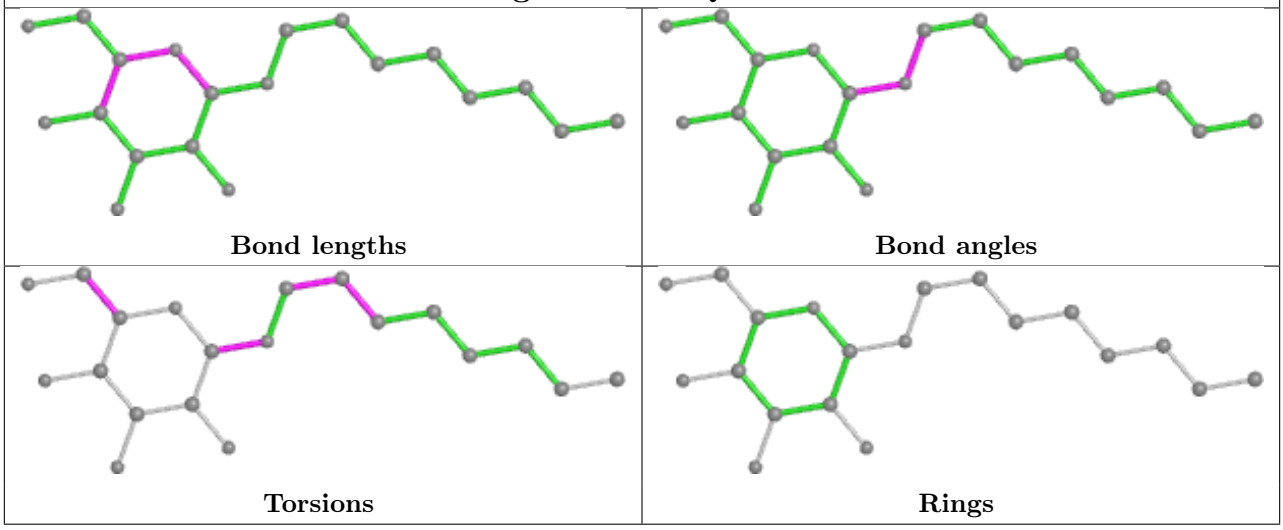


Torsions



Rings

Ligand BOG Q 3091



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	443/446 (99%)	-0.31	4 (0%) 84 73	36, 89, 137, 150	0
1	N	442/446 (99%)	-0.28	9 (2%) 65 52	54, 91, 136, 153	0
2	B	421/441 (95%)	-0.16	4 (0%) 82 71	60, 113, 170, 193	0
2	O	422/441 (95%)	-0.13	9 (2%) 63 50	51, 100, 146, 172	0
3	C	380/380 (100%)	-0.66	4 (1%) 80 69	19, 50, 104, 192	0
3	P	379/380 (99%)	-0.45	7 (1%) 68 55	29, 89, 132, 186	0
4	D	241/241 (100%)	-0.50	1 (0%) 92 87	30, 58, 109, 133	0
4	Q	241/241 (100%)	-0.33	2 (0%) 86 75	65, 105, 150, 165	0
5	E	196/196 (100%)	0.32	16 (8%) 11 10	45, 137, 184, 198	127 (64%)
5	R	196/196 (100%)	0.02	8 (4%) 37 27	53, 101, 166, 184	0
6	F	100/110 (90%)	-0.74	0 100 100	31, 61, 87, 102	0
6	S	100/110 (90%)	-0.12	1 (1%) 82 71	77, 117, 167, 188	0
7	G	81/81 (100%)	-0.32	1 (1%) 79 67	43, 77, 128, 156	0
7	T	79/81 (97%)	0.10	7 (8%) 9 8	71, 137, 202, 211	0
8	H	70/77 (90%)	-0.38	0 100 100	51, 94, 117, 153	0
8	U	67/77 (87%)	-0.06	0 100 100	141, 175, 213, 219	0
9	I	31/52 (59%)	1.11	6 (19%) 1 1	109, 158, 223, 229	0
9	V	31/52 (59%)	1.21	9 (29%) 0 0	109, 157, 222, 224	0
10	J	61/61 (100%)	-0.38	2 (3%) 46 35	65, 82, 144, 187	0
10	W	59/61 (96%)	0.01	2 (3%) 45 34	75, 107, 139, 154	0
All	All	4040/4170 (96%)	-0.25	92 (2%) 60 46	19, 93, 168, 229	127 (3%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	163	SER	10.8
7	T	1	GLY	6.8
3	P	8	SER	6.2
5	E	162	GLY	5.5
9	V	61	ARG	5.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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
12	BOG	Q	3091	20/20	0.31	0.90	242,249,250,251	0
12	BOG	P	2010	19/20	0.55	0.41	102,248,249,249	0
11	PEE	A	2008	21/51	0.57	0.56	225,229,230,230	0
11	PEE	W	3005	50/51	0.66	0.51	129,146,150,152	0
18	CDL	P	3003	42/100	0.67	0.46	203,214,224,225	0
11	PEE	P	3008	5/51	0.68	0.82	213,213,214,214	0
18	CDL	P	3004	40/100	0.69	0.39	164,168,173,174	0
12	BOG	C	3010	12/20	0.74	0.39	168,168,170,170	0
12	BOG	D	2091	20/20	0.74	0.46	178,180,180,180	0
18	CDL	D	2003	42/100	0.77	0.38	144,158,180,181	0
11	PEE	C	2005	50/51	0.78	0.41	122,134,139,141	0
16	UQ	P	3002	19/63	0.80	0.36	163,166,168,168	0
20	UNL	P	3014	1/-	0.80	0.32	33,33,33,33	0
13	AZI	C	2011	3/3	0.83	0.33	46,46,47,49	0
11	PEE	P	3007	49/51	0.83	0.39	107,122,143,144	0
16	UQ	C	2002	19/63	0.88	0.41	123,126,128,129	0
13	AZI	P	3011	3/3	0.88	0.37	54,54,55,56	0
20	UNL	E	2012	2/-	0.89	0.20	36,36,36,38	0
11	PEE	C	2007	49/51	0.90	0.28	63,76,100,101	0

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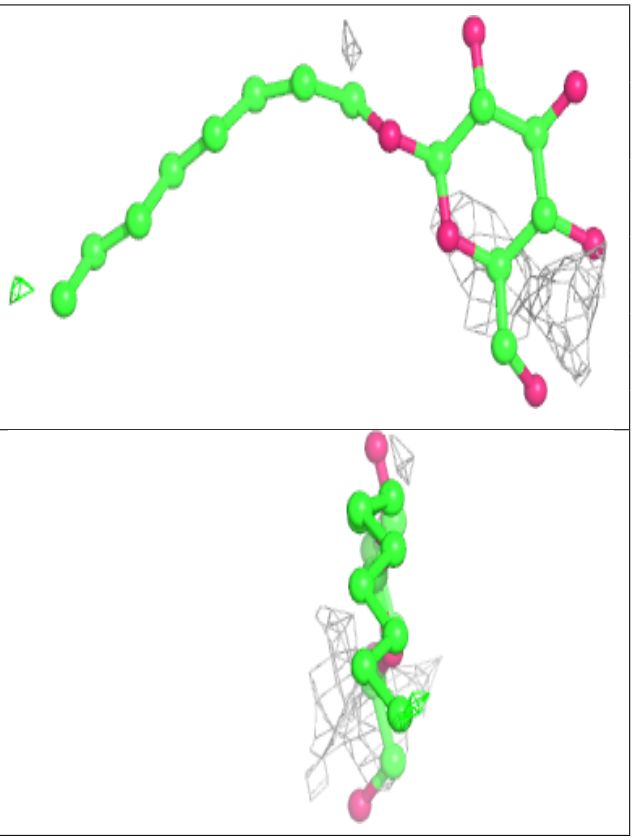
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	UNL	Q	3012	1/-	0.90	0.20	8,8,8,8	0
18	CDL	G	2004	40/100	0.91	0.23	92,97,116,117	0
12	BOG	Q	3009	20/20	0.92	0.28	87,110,112,112	0
15	ICX	P	3001	30/30	0.93	0.30	101,117,133,136	0
12	BOG	E	2009	20/20	0.93	0.25	71,73,77,77	0
17	HEC	Q	501	43/43	0.95	0.19	76,84,88,90	0
20	UNL	P	3013	1/-	0.95	0.49	40,40,40,40	0
14	HEM	P	501	43/43	0.96	0.22	53,59,72,77	0
14	HEM	C	501	43/43	0.97	0.22	30,35,50,57	0
14	HEM	P	502	43/43	0.97	0.21	58,62,69,70	0
17	HEC	D	501	43/43	0.98	0.17	25,36,45,53	0
15	ICX	C	2001	30/30	0.98	0.19	43,56,65,66	0
14	HEM	C	502	43/43	0.98	0.18	25,30,40,43	0
19	FES	E	501	4/4	0.98	0.12	105,105,107,107	4
19	FES	R	501	4/4	0.99	0.08	60,61,62,63	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.

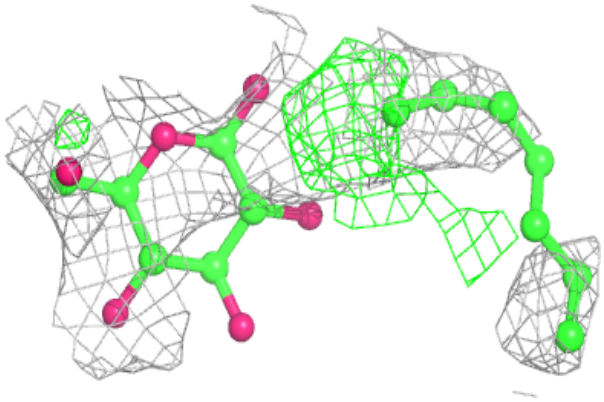
Electron density around BOG Q 3091:

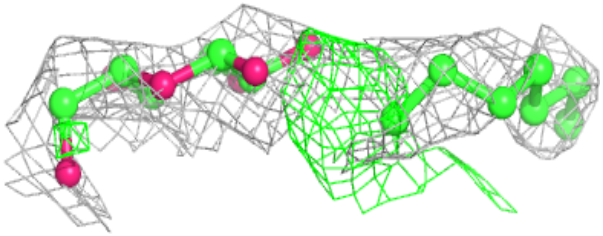
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

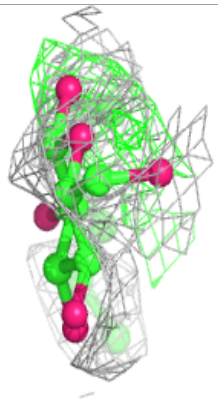


Electron density around BOG P 2010:

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

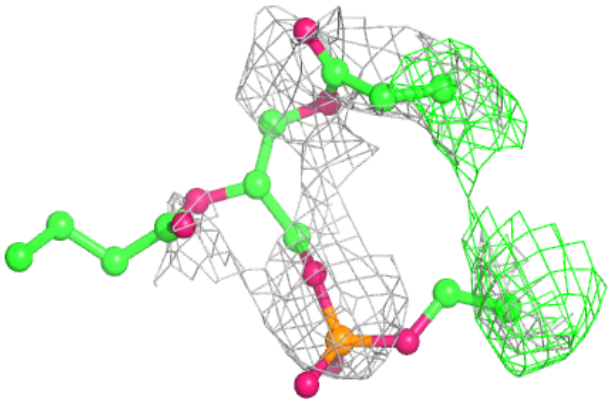


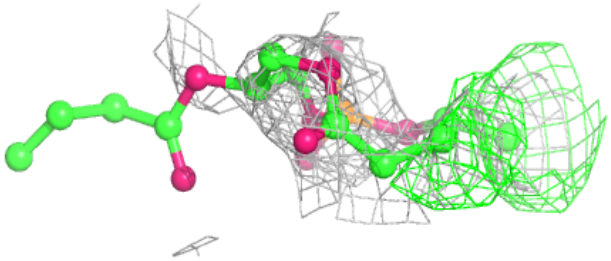


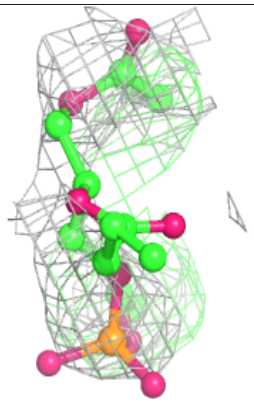


Electron density around PEE A 2008:

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

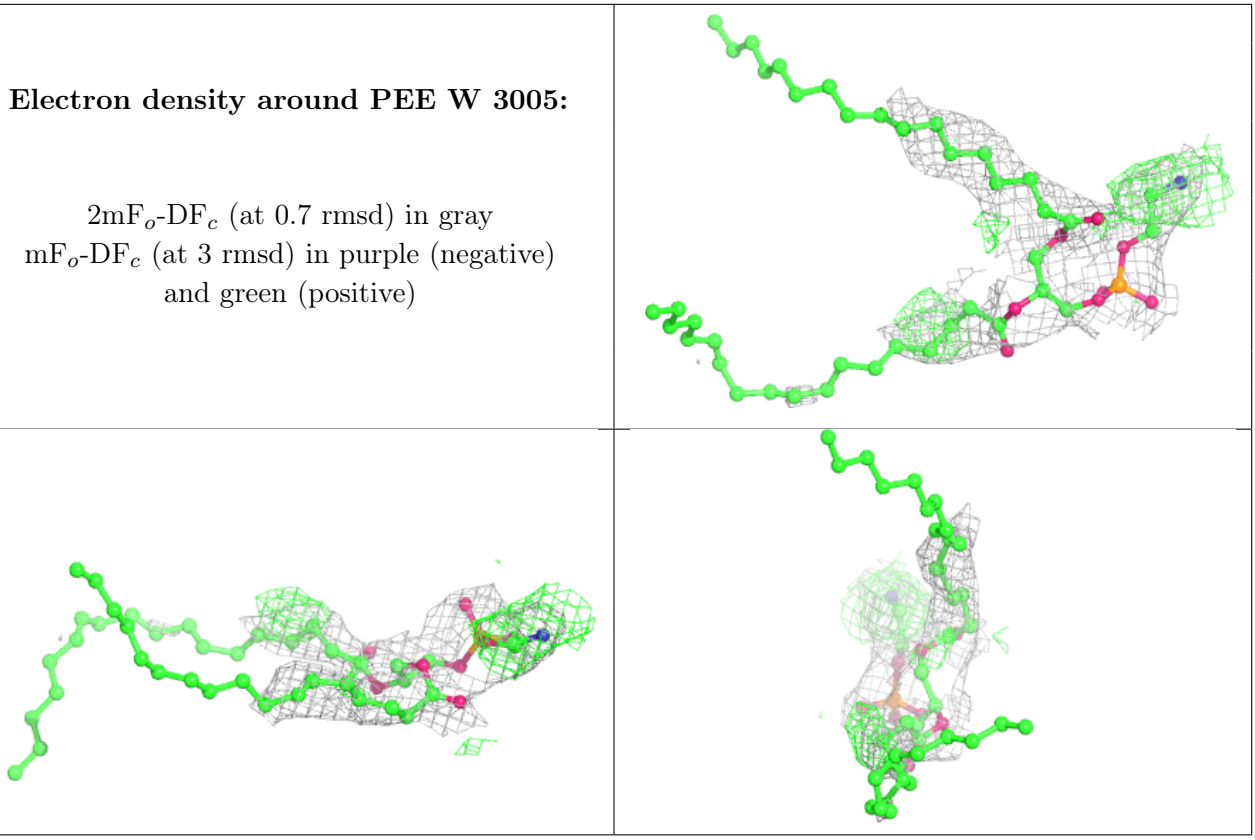






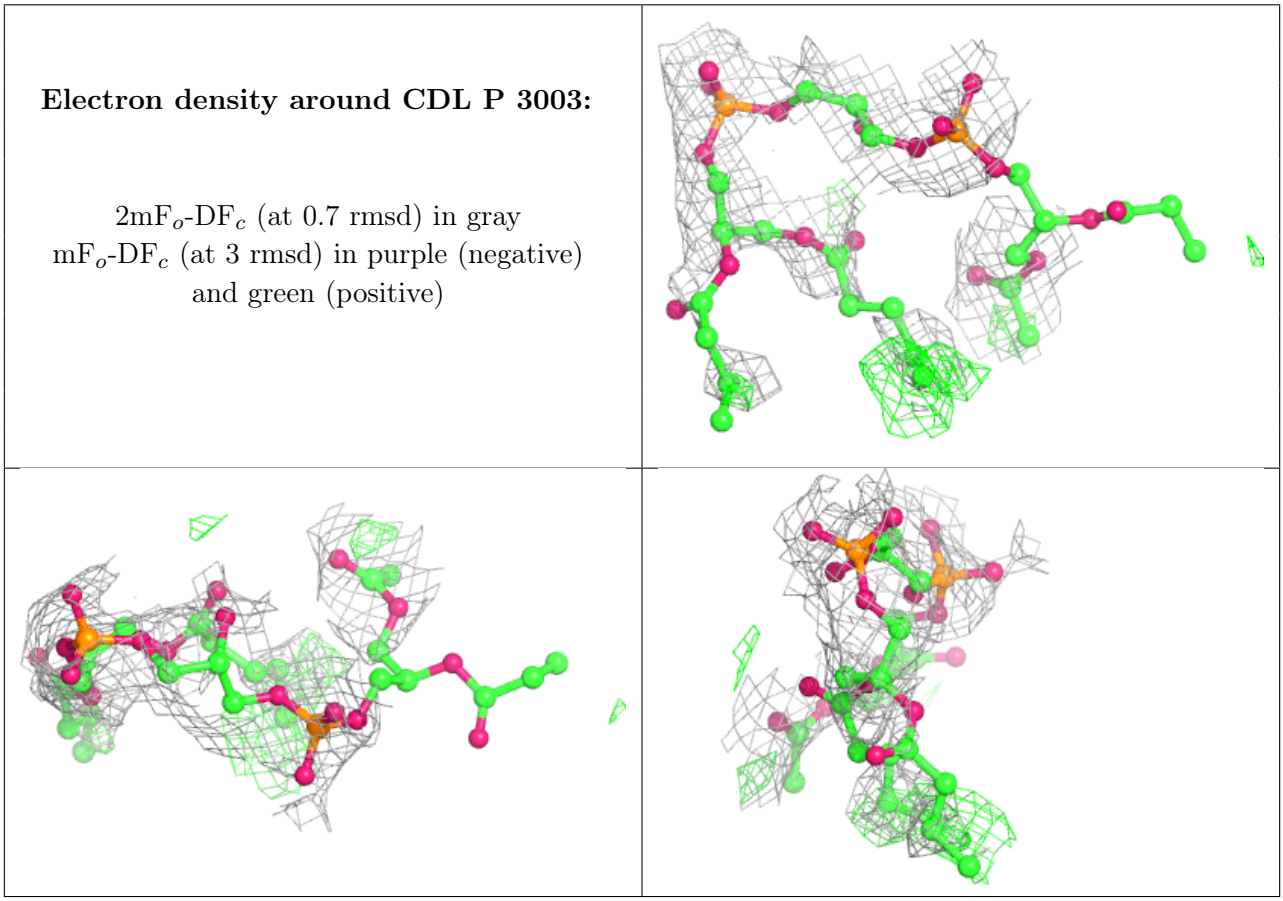
Electron density around PEE W 3005:

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



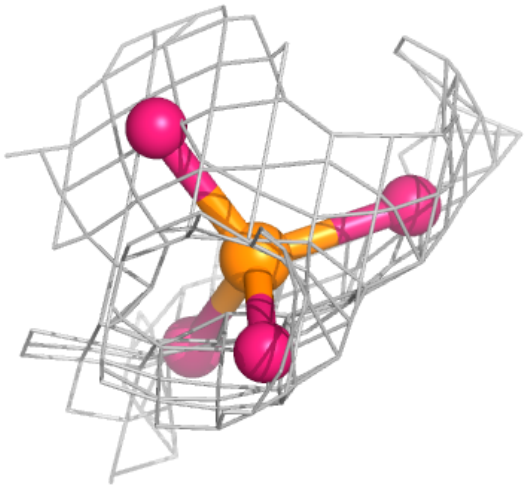
Electron density around CDL P 3003:

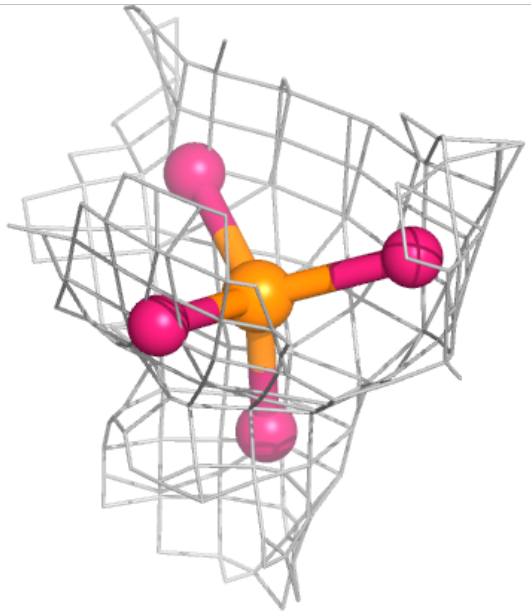
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

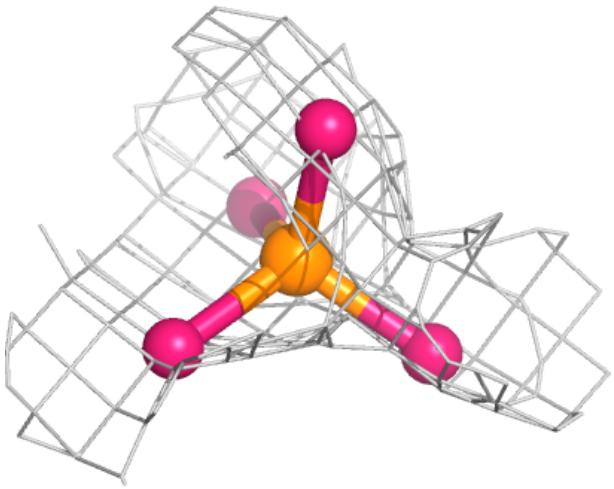


Electron density around PEE P 3008:

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

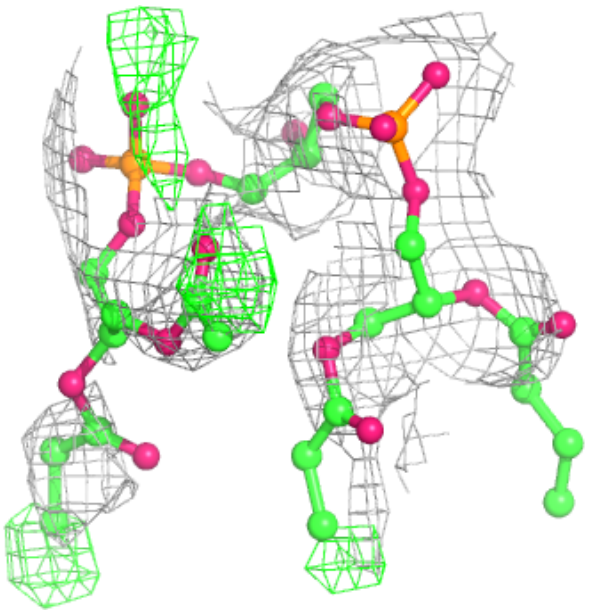


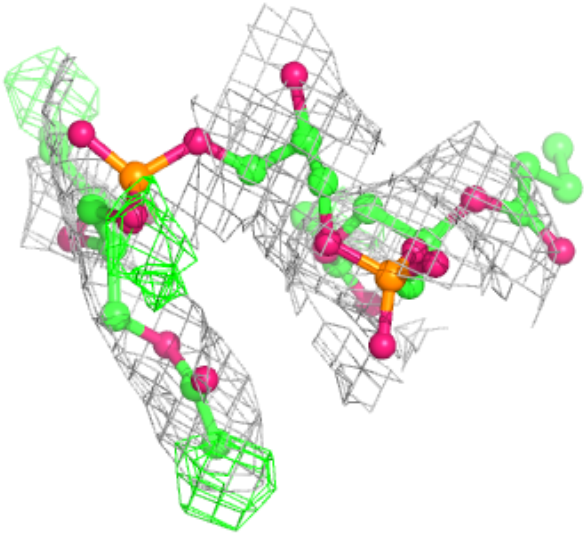


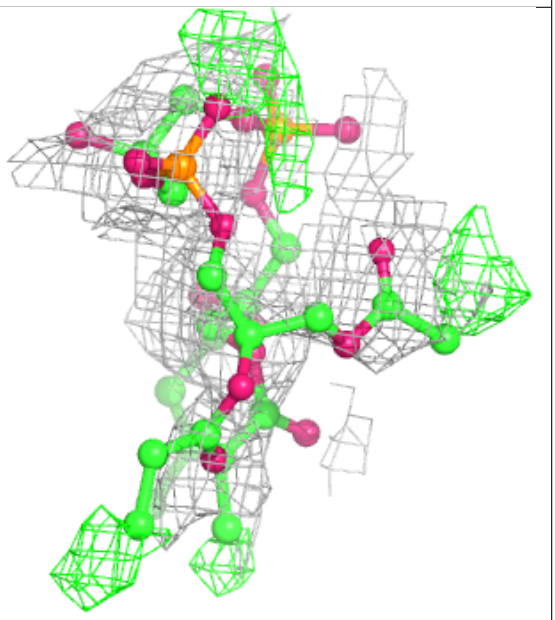


Electron density around CDL P 3004:

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

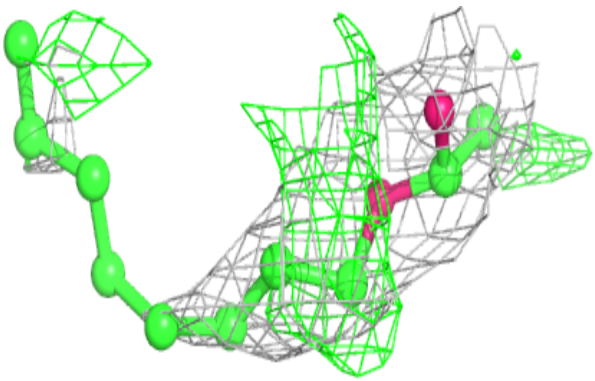


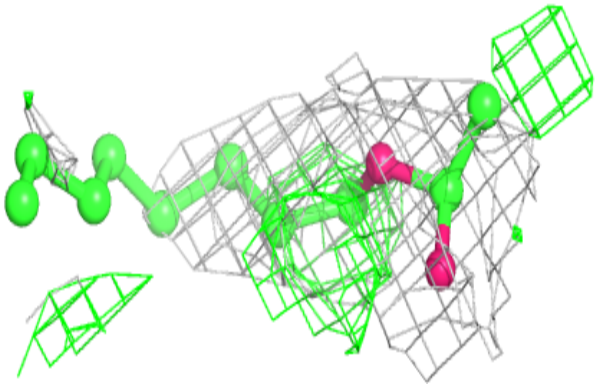


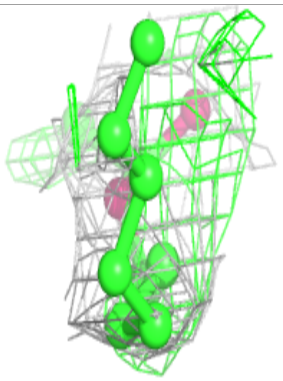


Electron density around BOG C 3010:

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

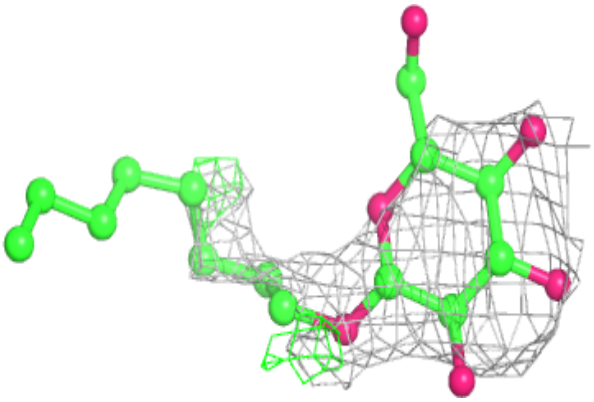


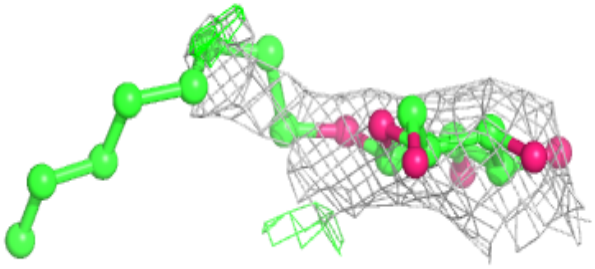


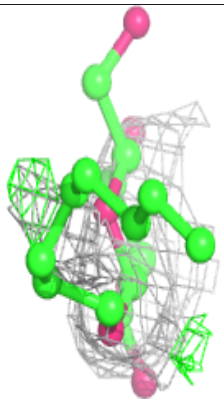


Electron density around BOG D 2091:

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

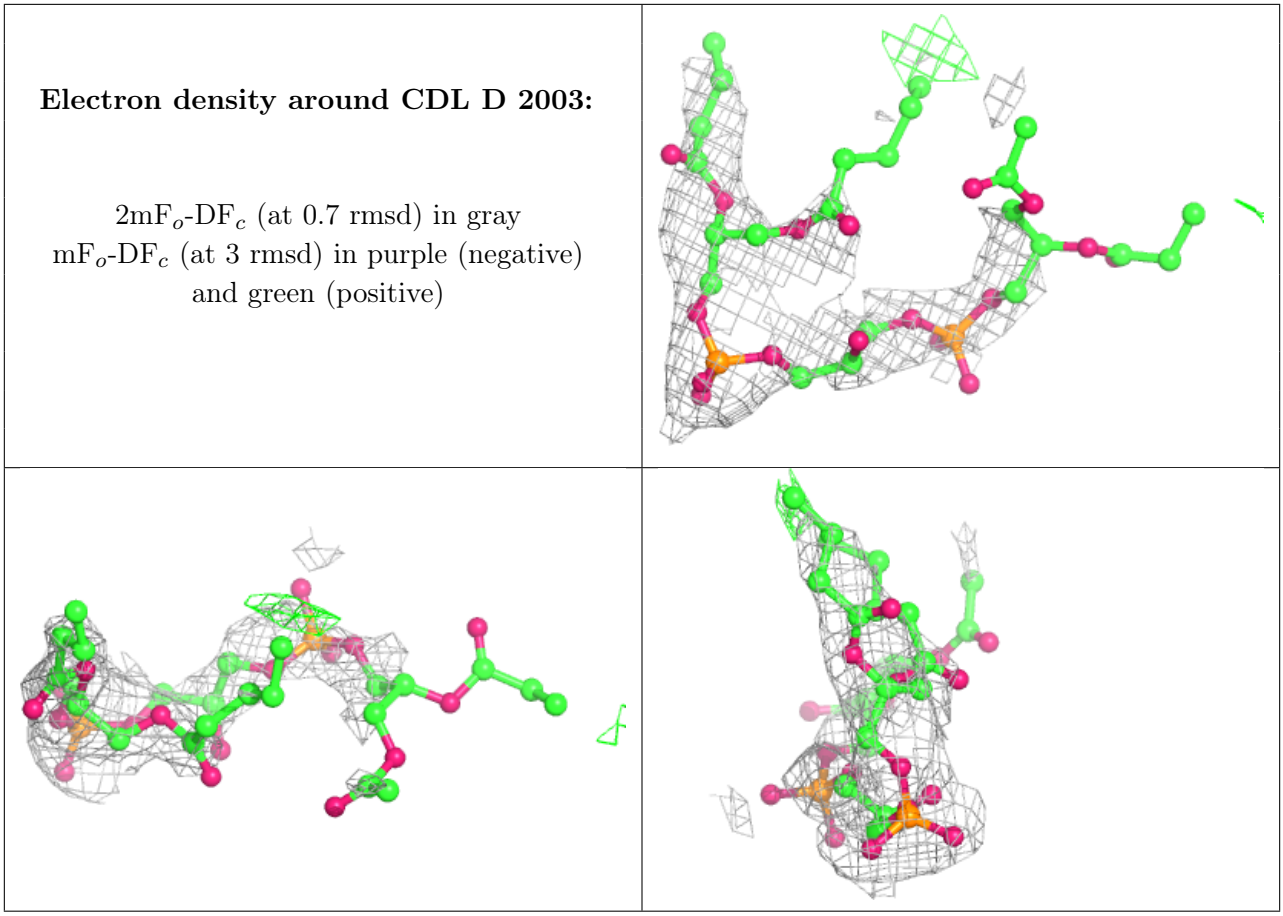






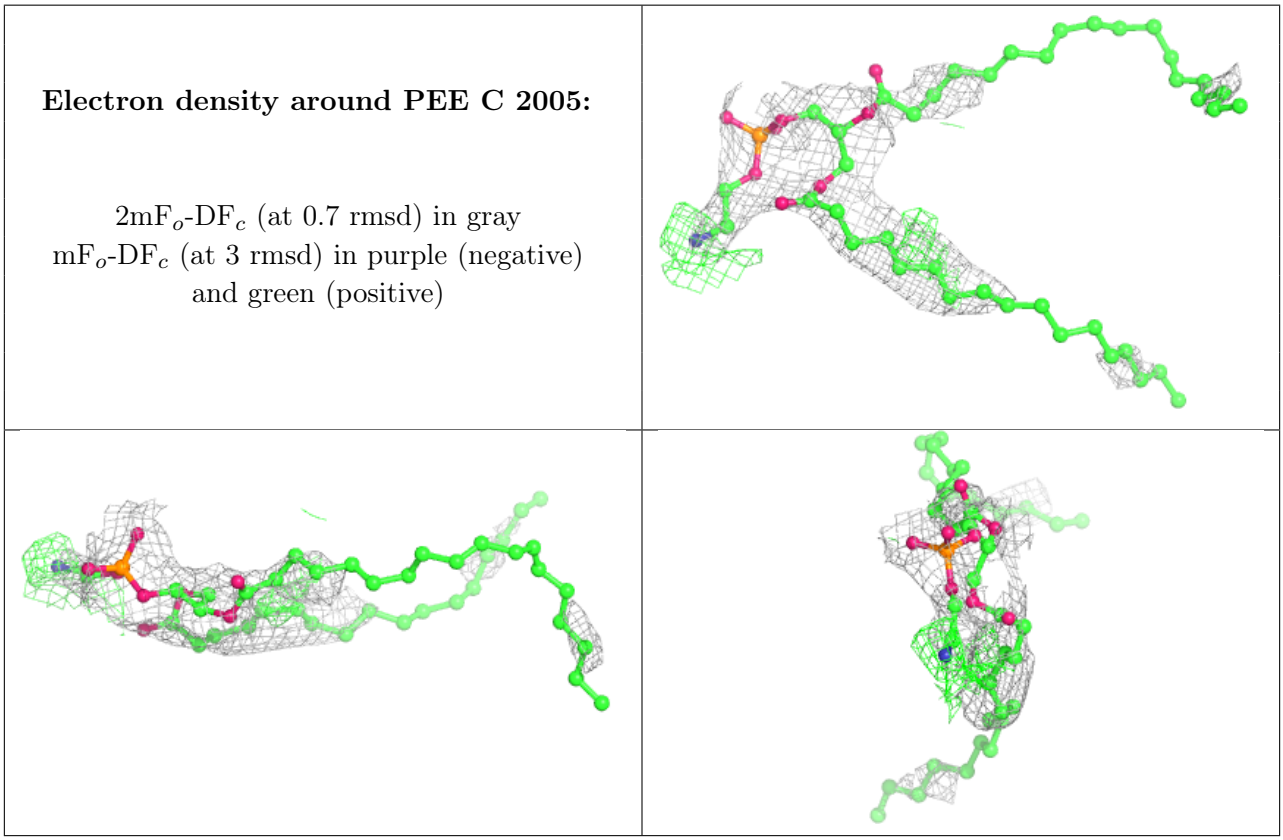
Electron density around CDL D 2003:

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



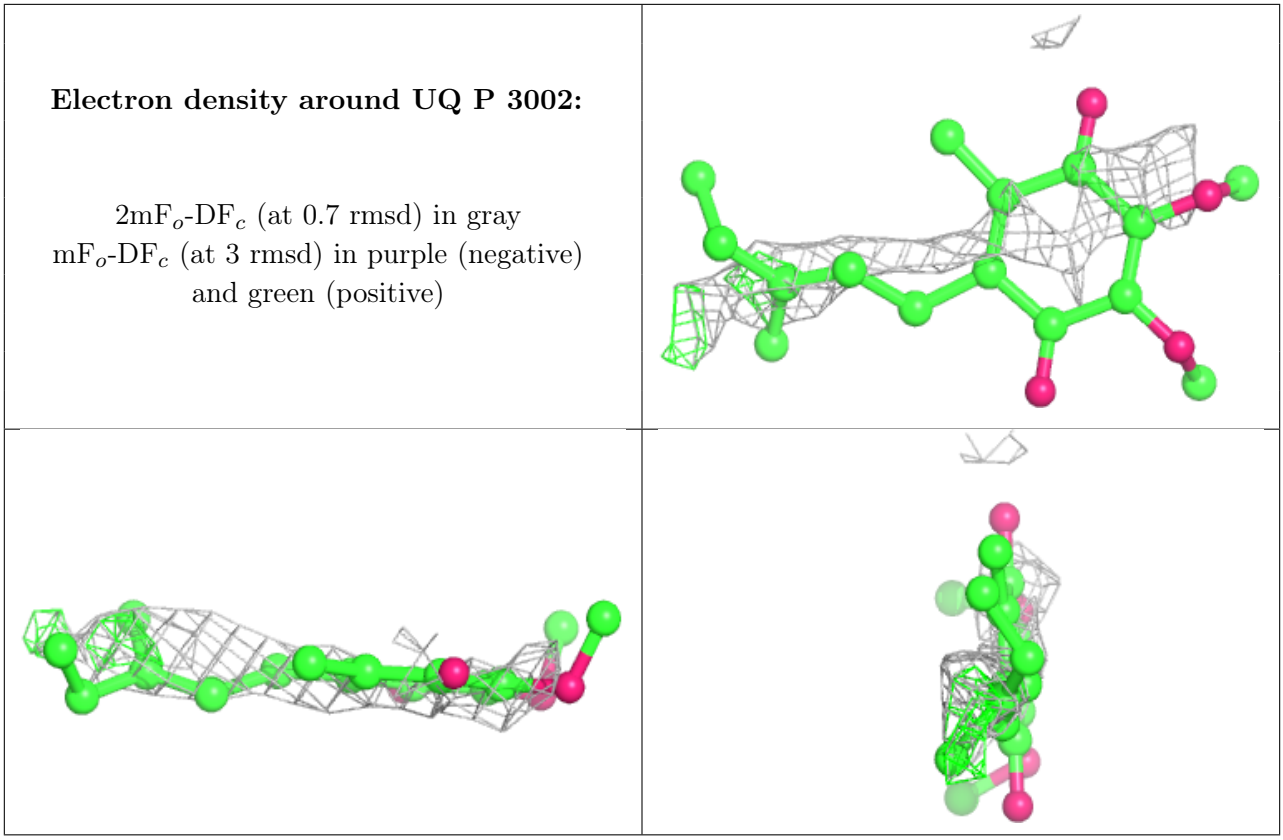
Electron density around PEE C 2005:

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



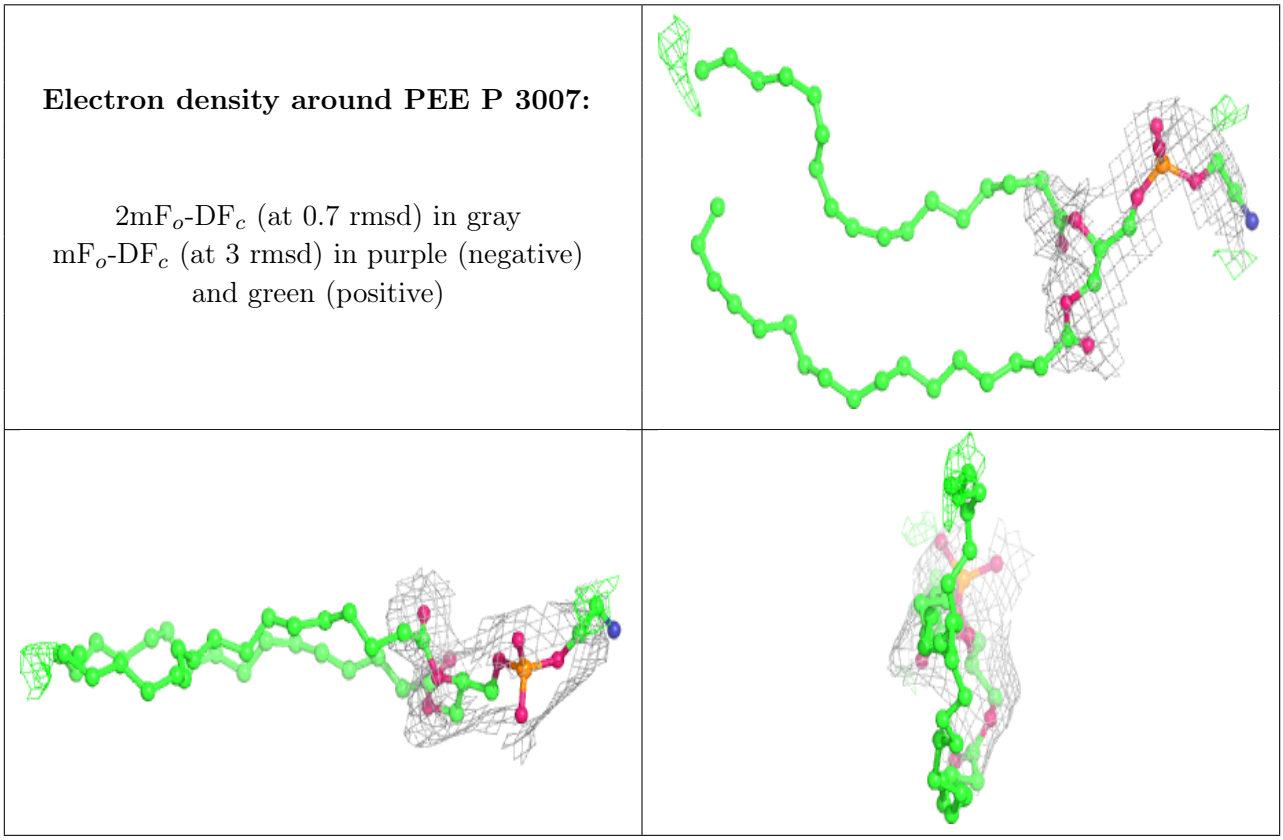
Electron density around UQ P 3002:

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



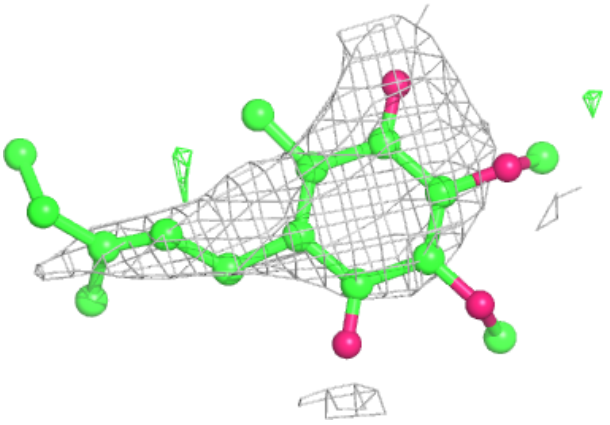
Electron density around PEE P 3007:

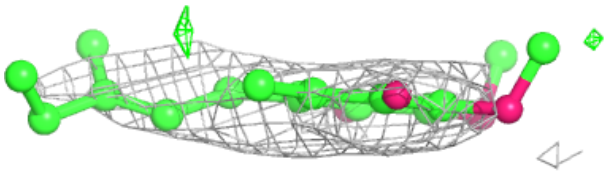
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

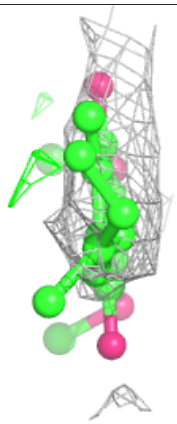


Electron density around UQ C 2002:

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

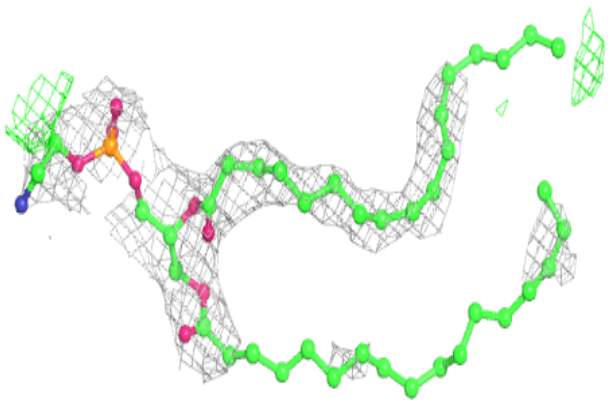


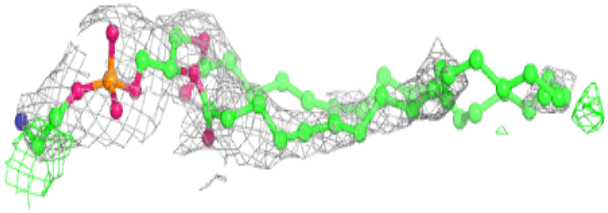




Electron density around PEE C 2007:

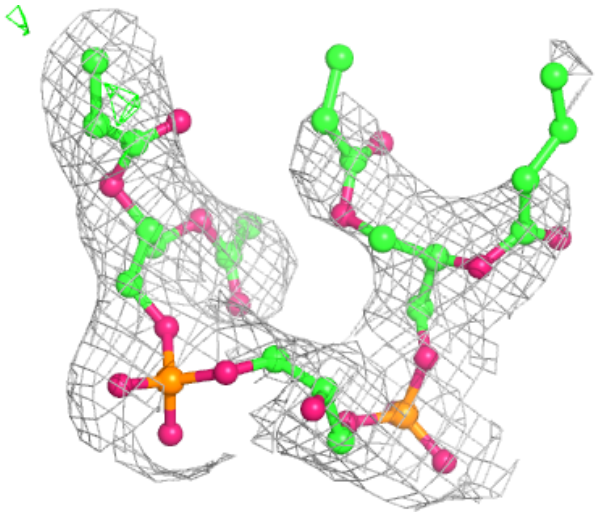
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

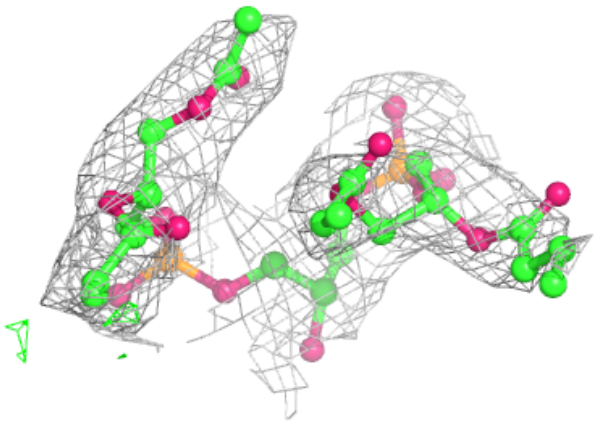


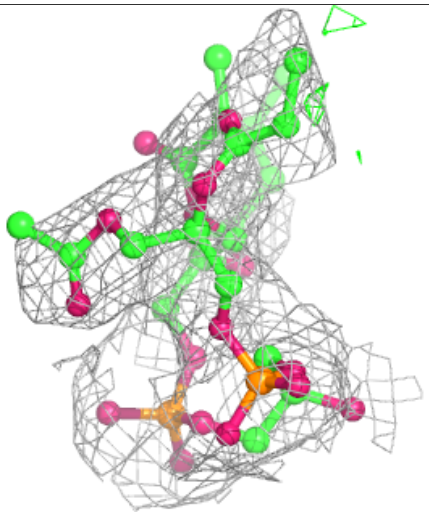


Electron density around CDL G 2004:

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

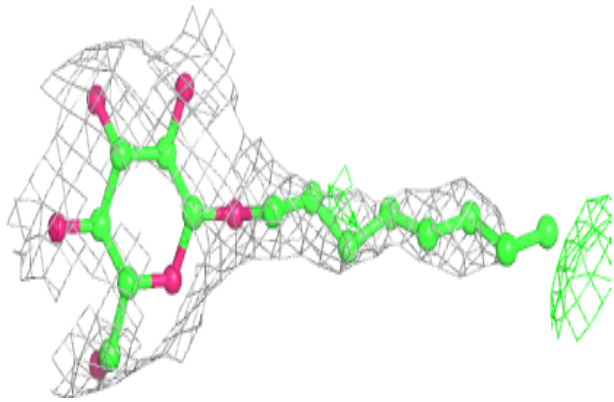


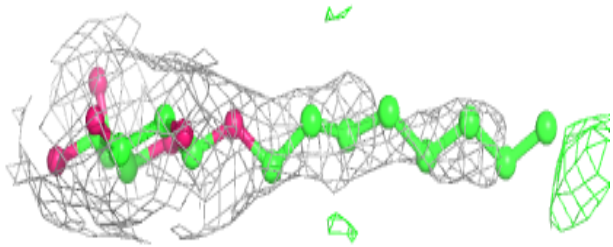


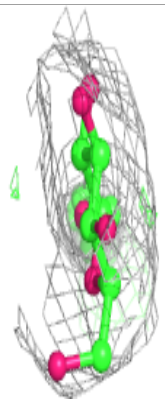


Electron density around BOG Q 3009:

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

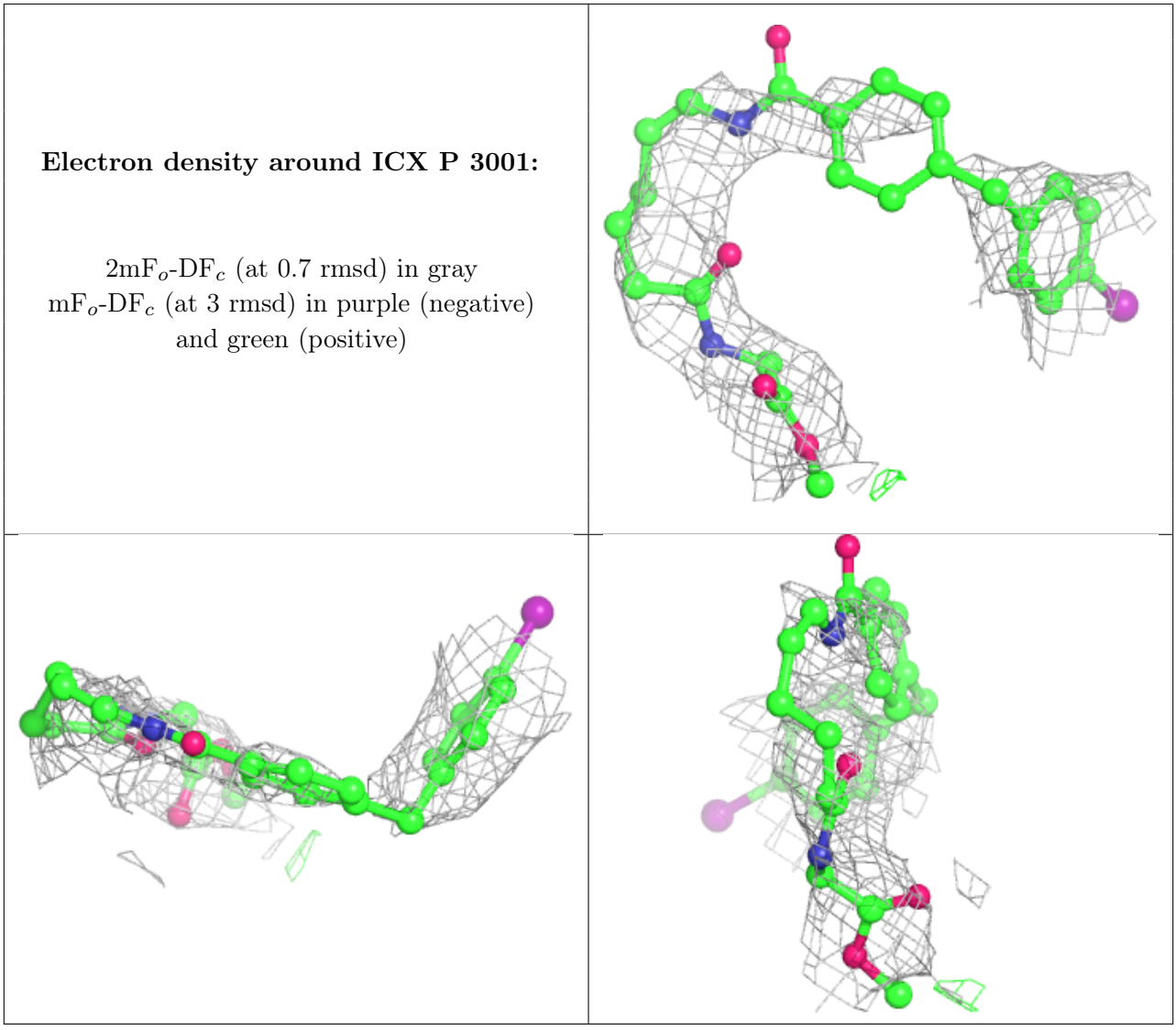






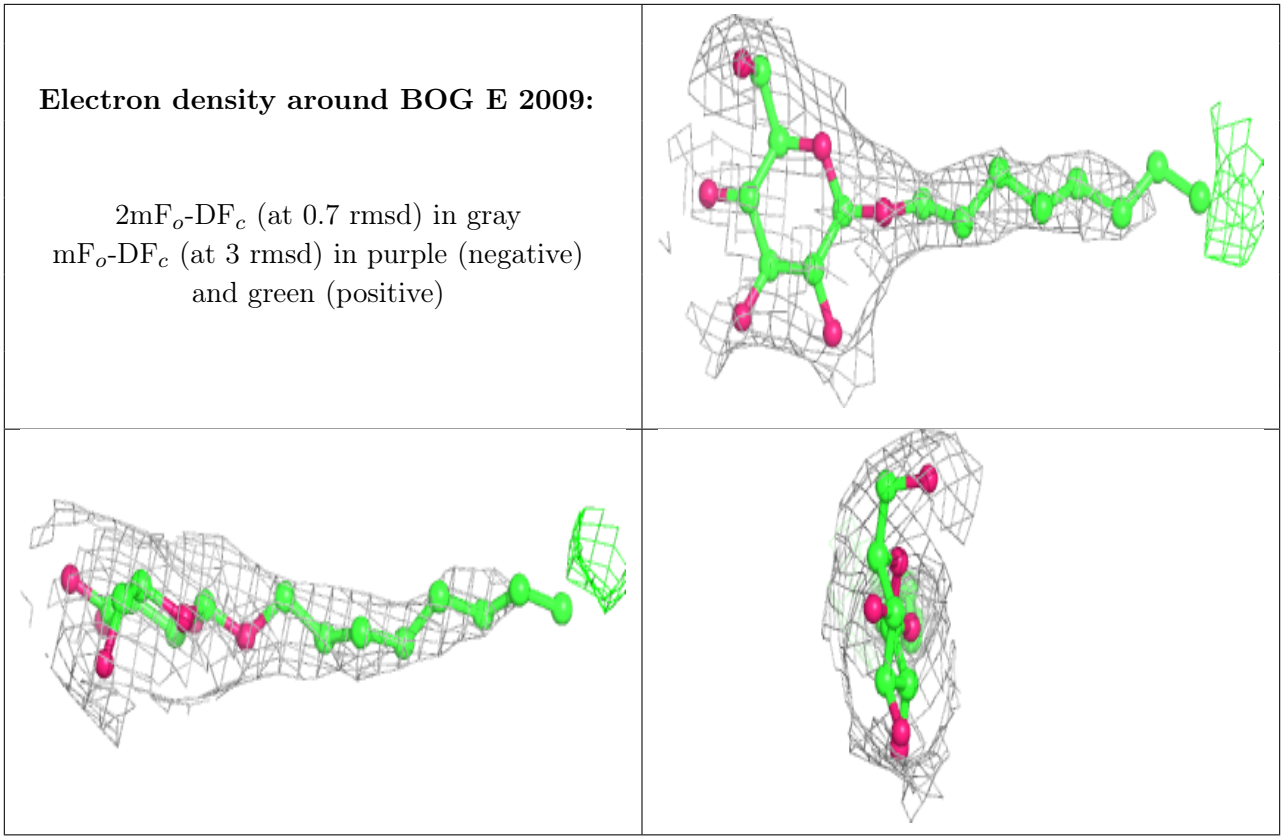
Electron density around ICX P 3001:

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



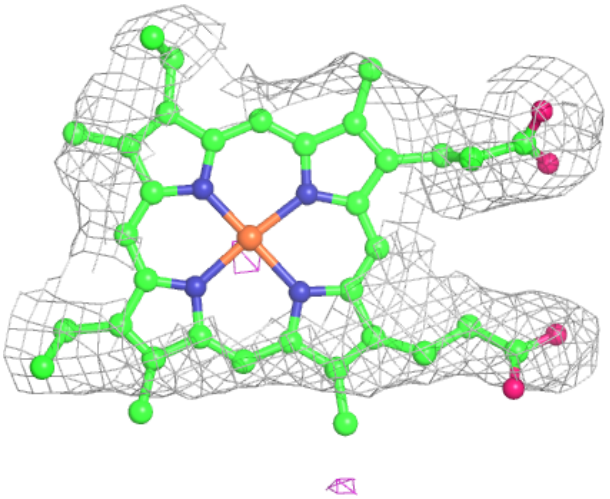
Electron density around BOG E 2009:

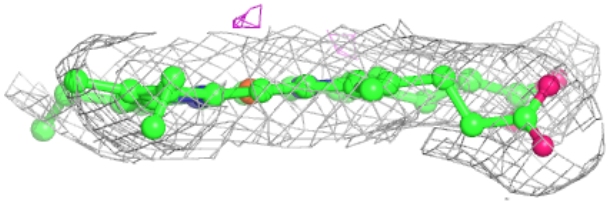
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

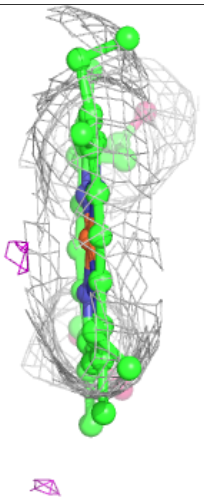


Electron density around HEC Q 501:

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

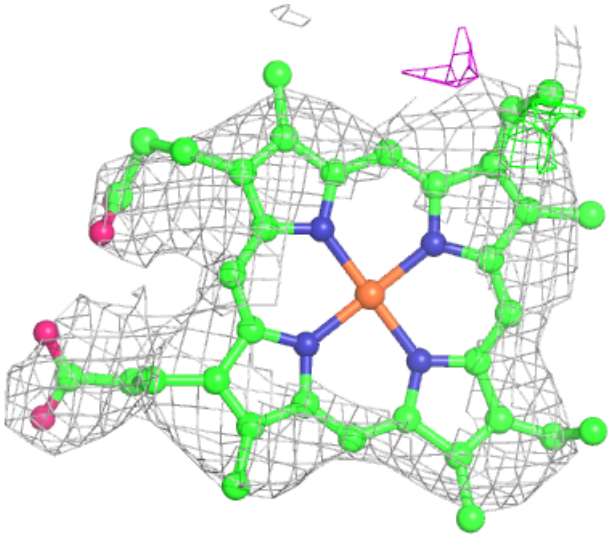


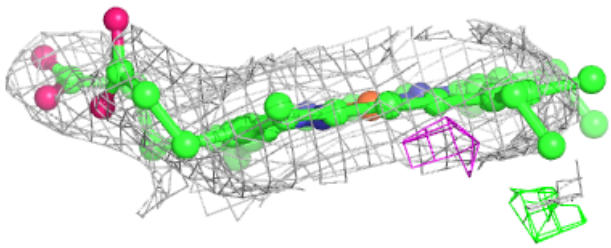


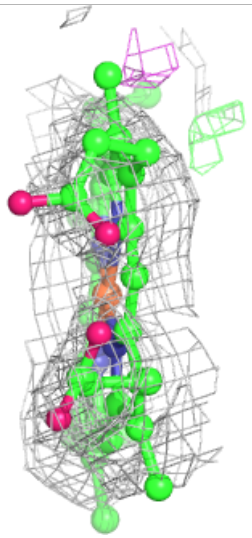


Electron density around HEM P 501:

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

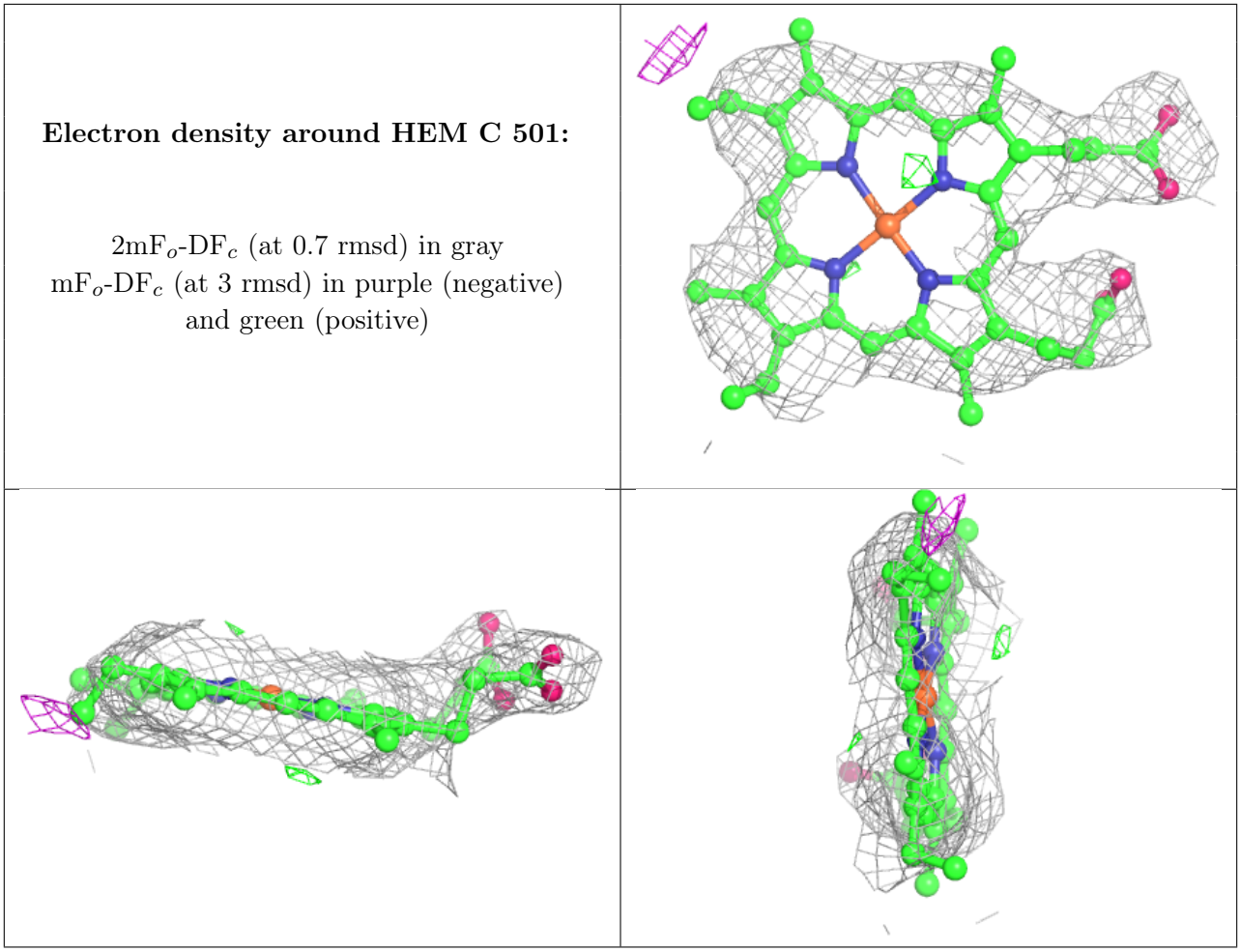






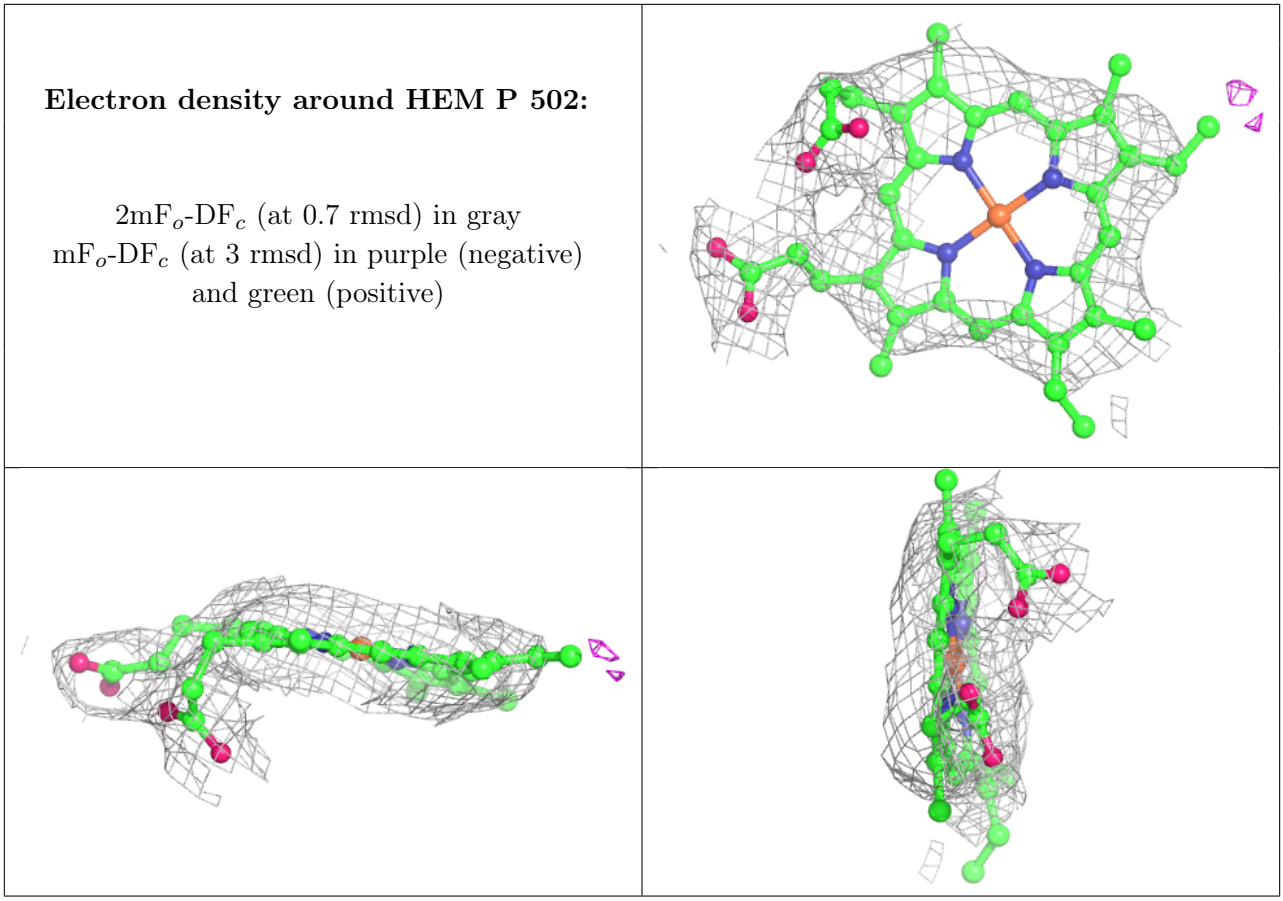
Electron density around HEM C 501:

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



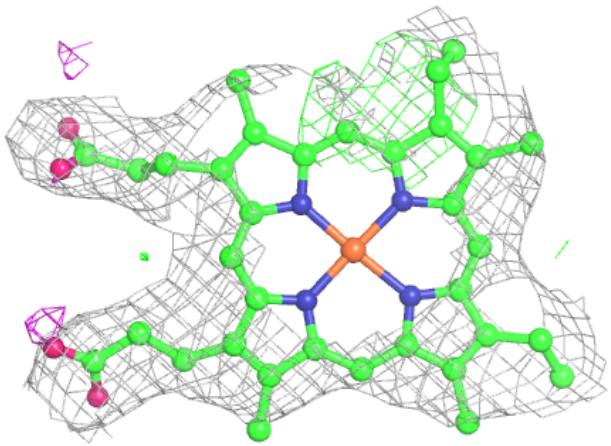
Electron density around HEM P 502:

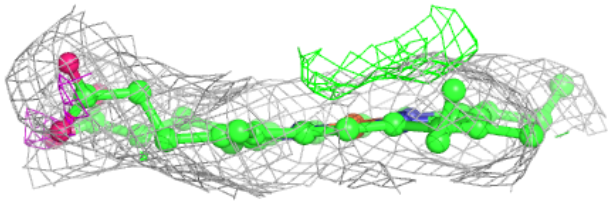
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

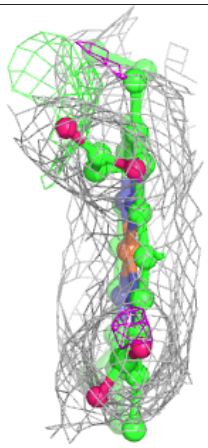


Electron density around HEC D 501:

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

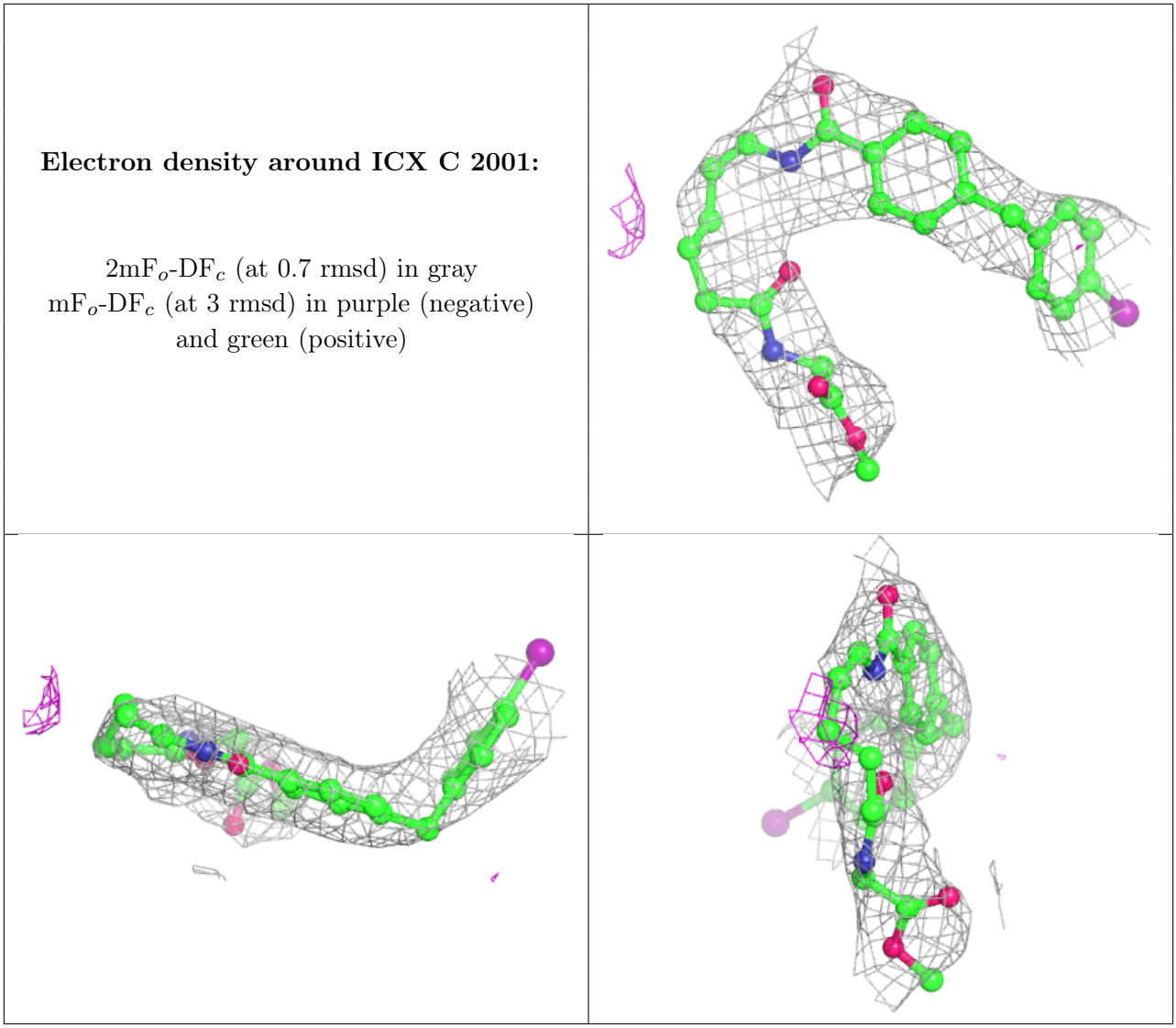






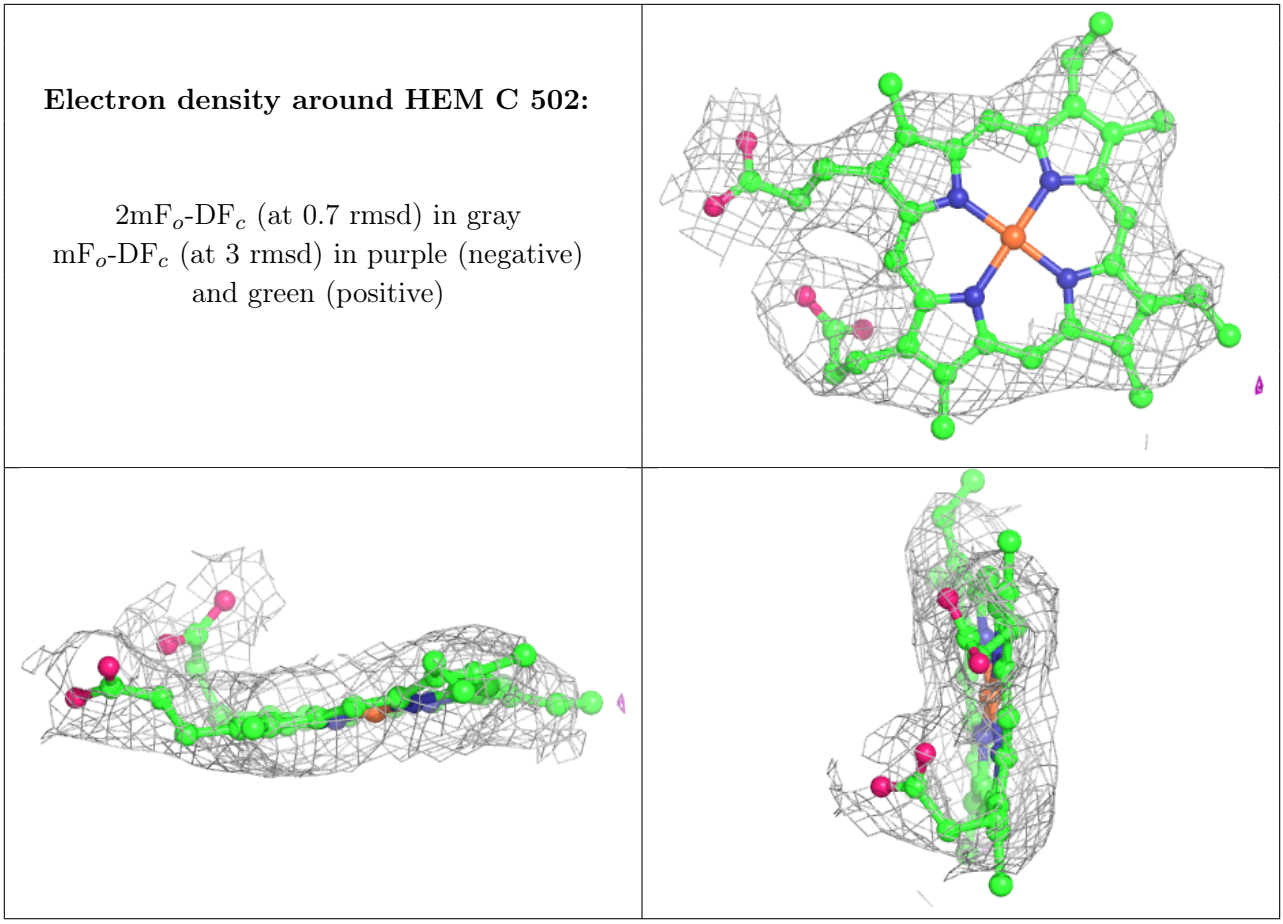
Electron density around ICX C 2001:

$2mF_o$-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 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.