wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 02:56 PM EDT

PDB ID	:	3H1K / pdb_00003h1k
Title	:	Chicken cytochrome BC1 complex with ZN++ and an iodinated derivative of kresoxim-methyl bound
Authors	:	Berry, E.A.; Zhang, Z.; Bellamy, H.D.; Huang, L.S.
Deposited on	:	2009-04-12
Resolution	:	3.48 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:

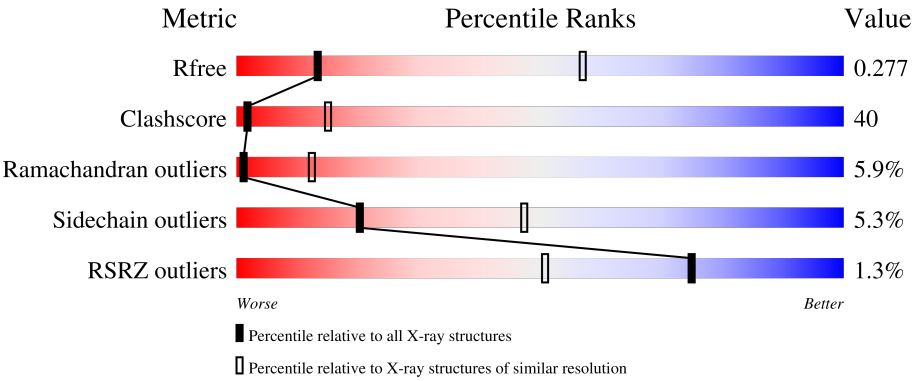
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	39% 53% 7%
1	N	446	36% 55% 7%
2	B	441	% 32% 54% 10%
2	O	441	30% 54% 12%
3	C	380	37% 54% 8%

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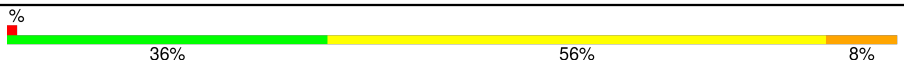
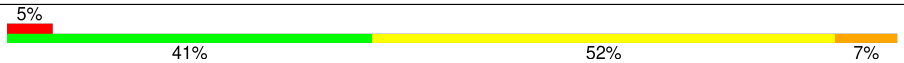
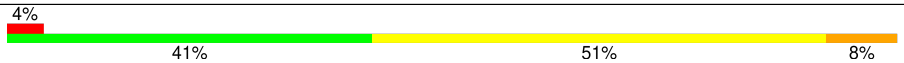
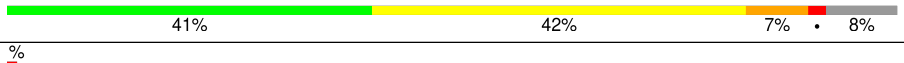
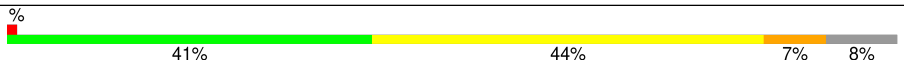
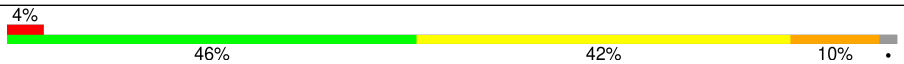
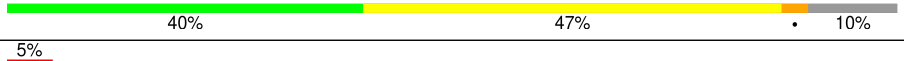
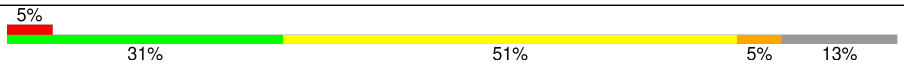
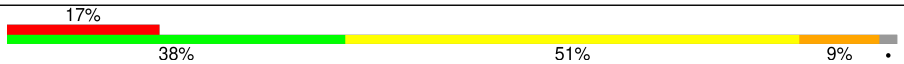
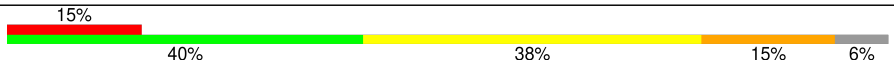
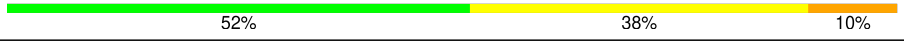
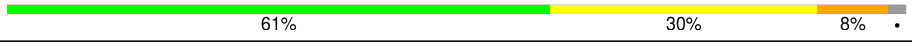
Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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	P	3008	-	X	-	-
19	HEC	D	501	X	-	-	-
19	HEC	Q	501	X	-	-	-
21	FES	E	501	-	-	X	-
21	FES	R	501	-	-	X	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 32673 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	0
			3442	2157	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	426	Total	C	N	O	S	0	0	0
			3164	1987	551	616	10			
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 Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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
			1513	952	263	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	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	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	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

- 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	69	Total	C	N	O	S	0	0	0
			571	348	105	113	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

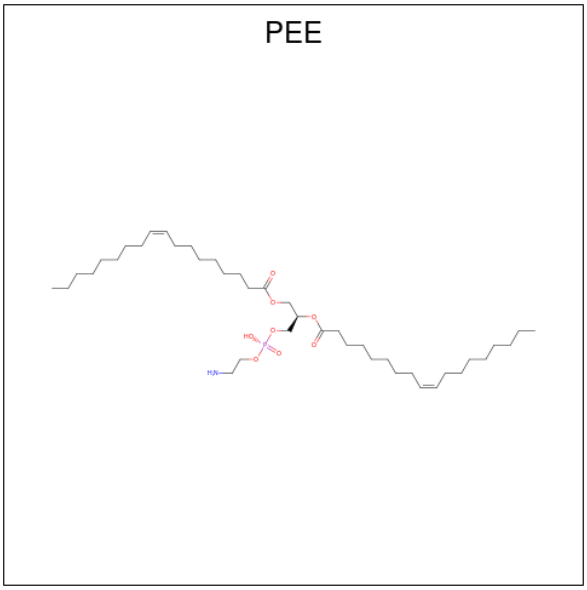
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	53	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	60	Total C N O 479 311 86 82	0	0	1

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O P 18 9 8 1	0	0
11	C	1	Total C N O P 49 39 1 8 1	0	0
11	E	1	Total C N O P 50 40 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	R	1	Total C N O P 50 40 1 8 1	0	0

- Molecule 12 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	2	Total O 2 2	0	0

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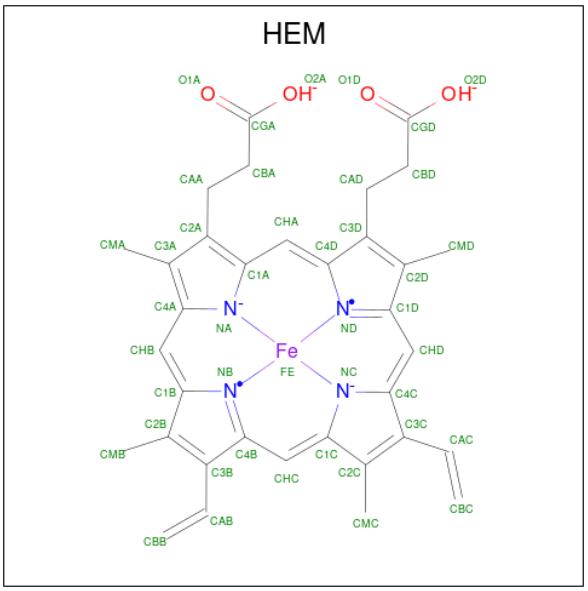
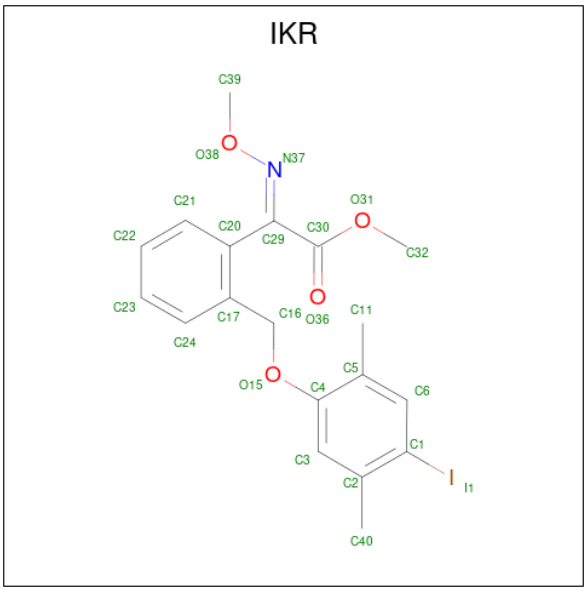
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total O 1 1	0	0
12	N	1	Total O 1 1	0	0
12	P	1	Total O 1 1	0	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



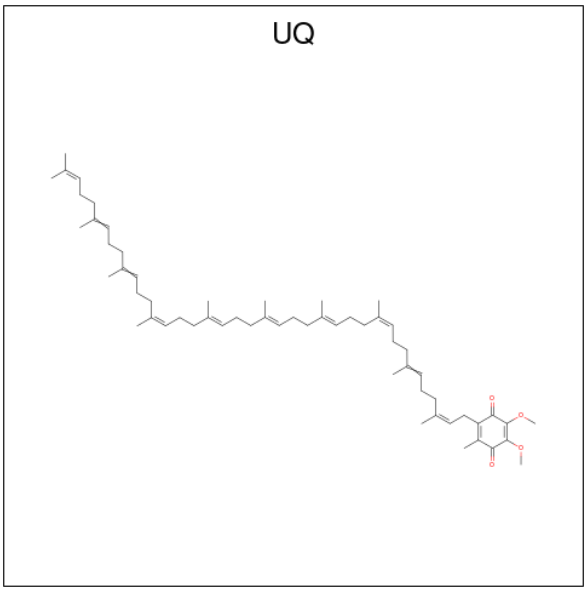
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 14 is methyl (2E)-{2-[(4-iodo-2,5-dimethylphenoxy)methyl]phenyl}(methoxyimino)ethanoate (CCD ID: IKR) (formula: $C_{19}H_{20}INO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
14	P	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

- Molecule 15 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$).



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

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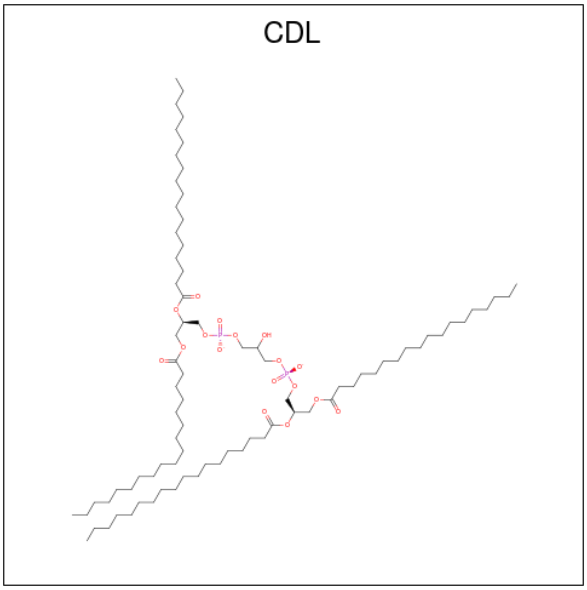
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	P	1	Total 19	C 15	O 4	0	0

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

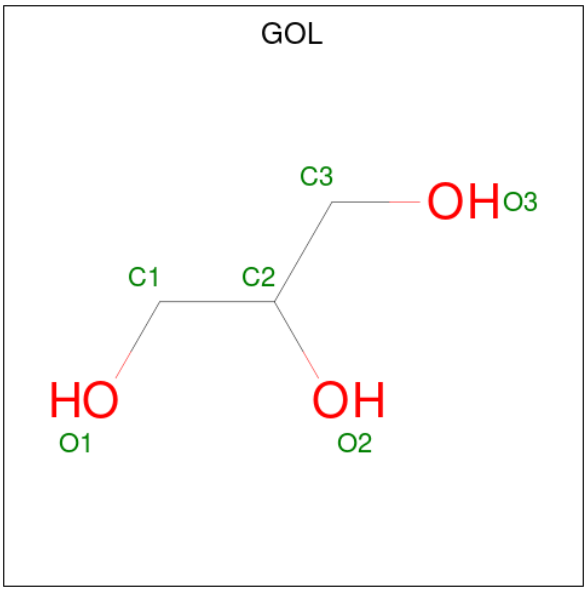


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total 40	C 21	O 17	P 2	0	0
16	D	1	Total 42	C 23	O 17	P 2	0	0
16	P	1	Total 40	C 21	O 17	P 2	0	0
16	Q	1	Total 42	C 23	O 17	P 2	0	0

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

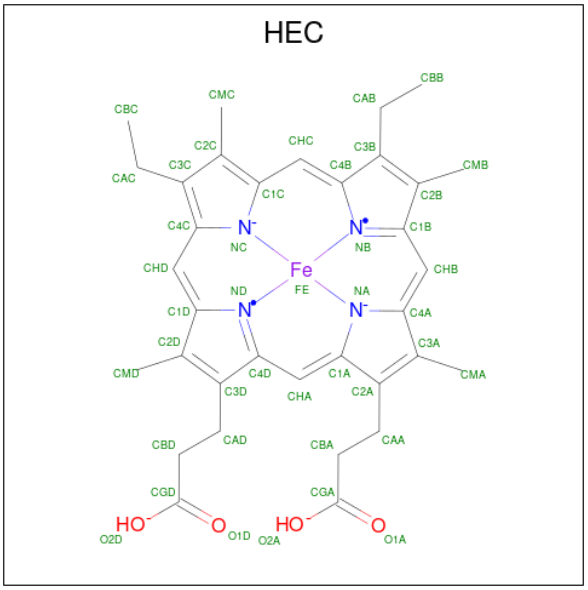
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	1	Total 1	Zn 1	0	0
17	P	1	Total 1	Zn 1	0	0

- Molecule 18 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



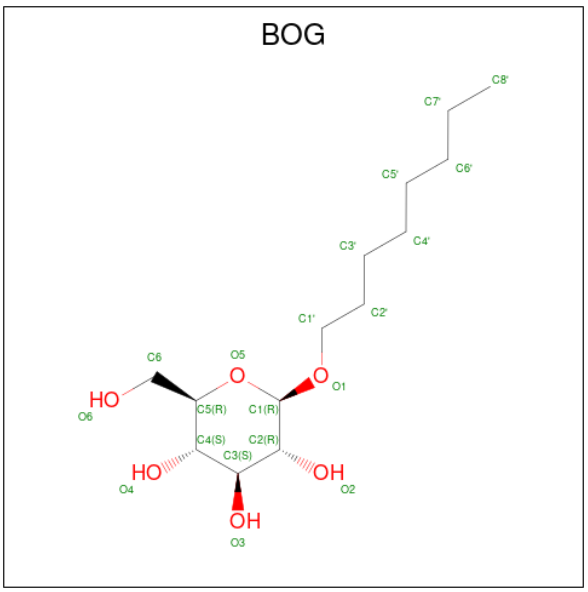
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	C	1	Total C O 6 3 3	0	0
18	P	1	Total C O 6 3 3	0	0

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



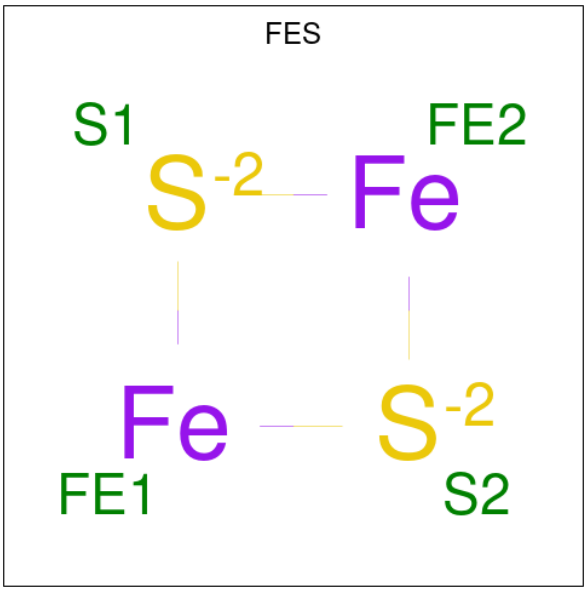
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total C Fe N O 43 34 1 4 4	0	0
19	Q	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 20 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C O 20 14 6	0	0
20	D	1	Total C O 13 7 6	0	0
20	P	1	Total C O 12 6 6	0	0
20	P	1	Total C O 13 7 6	0	0
20	Q	1	Total C O 20 14 6	0	0

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 22 is water.

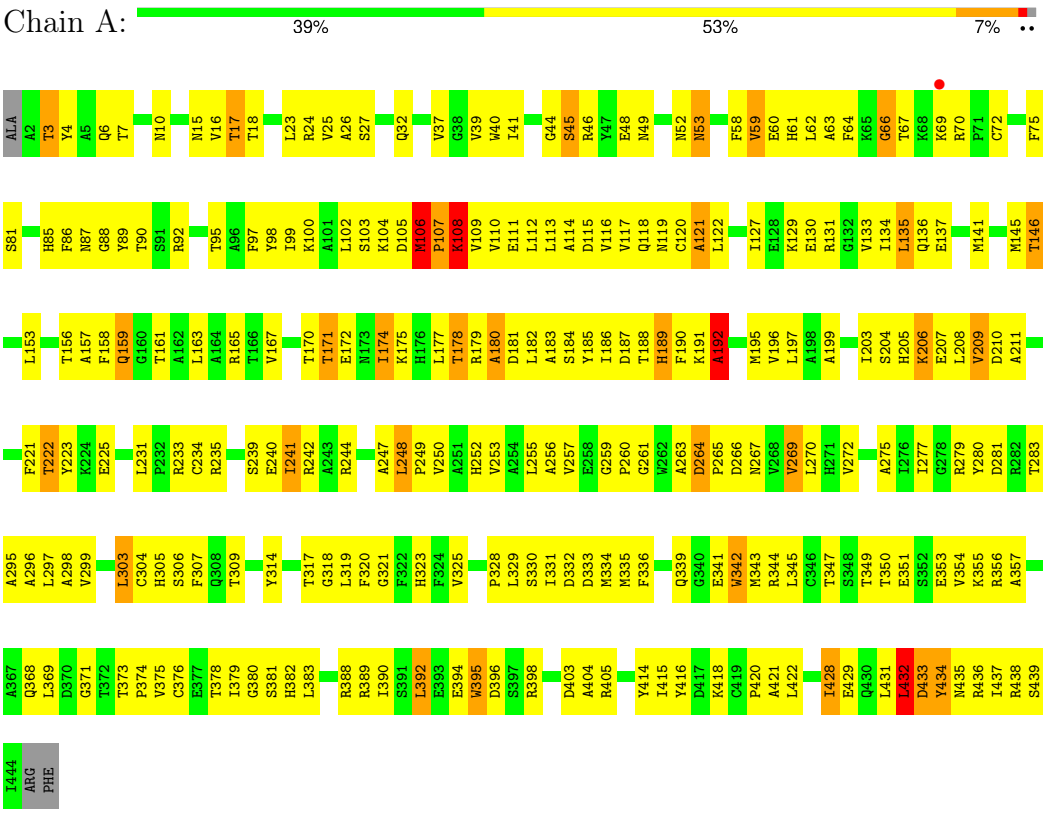
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total O 1 1	0	0
22	C	7	Total O 7 7	0	0
22	E	1	Total O 1 1	0	0
22	P	7	Total O 7 7	0	0
22	R	1	Total O 1 1	0	0

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.

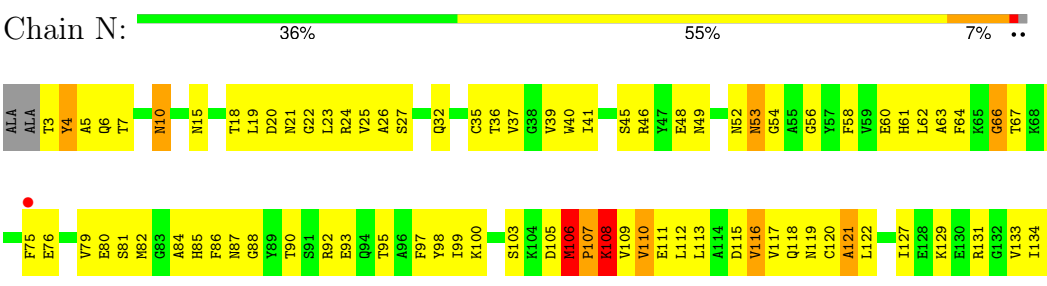
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

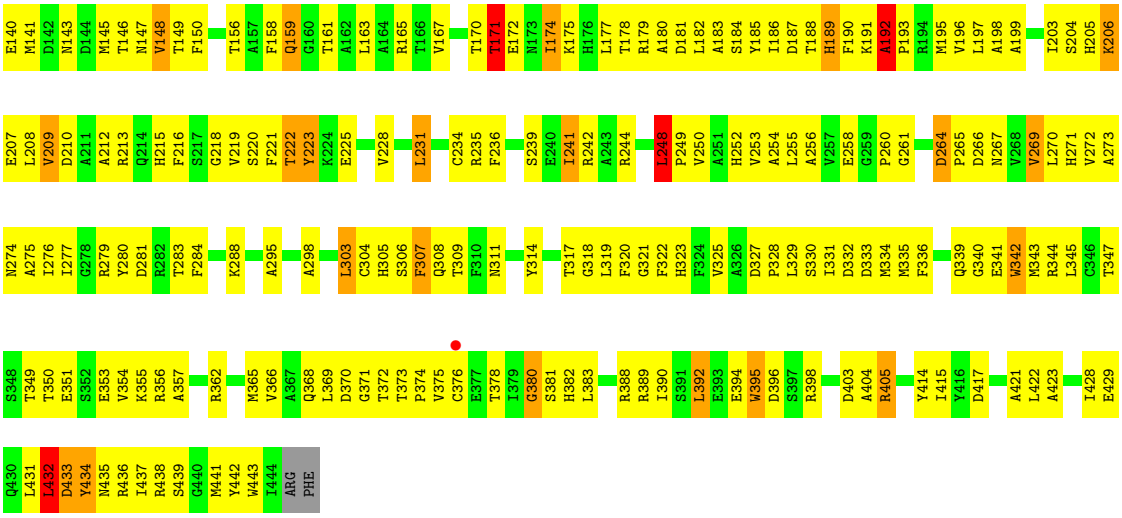
Chain A:



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

Chain N:

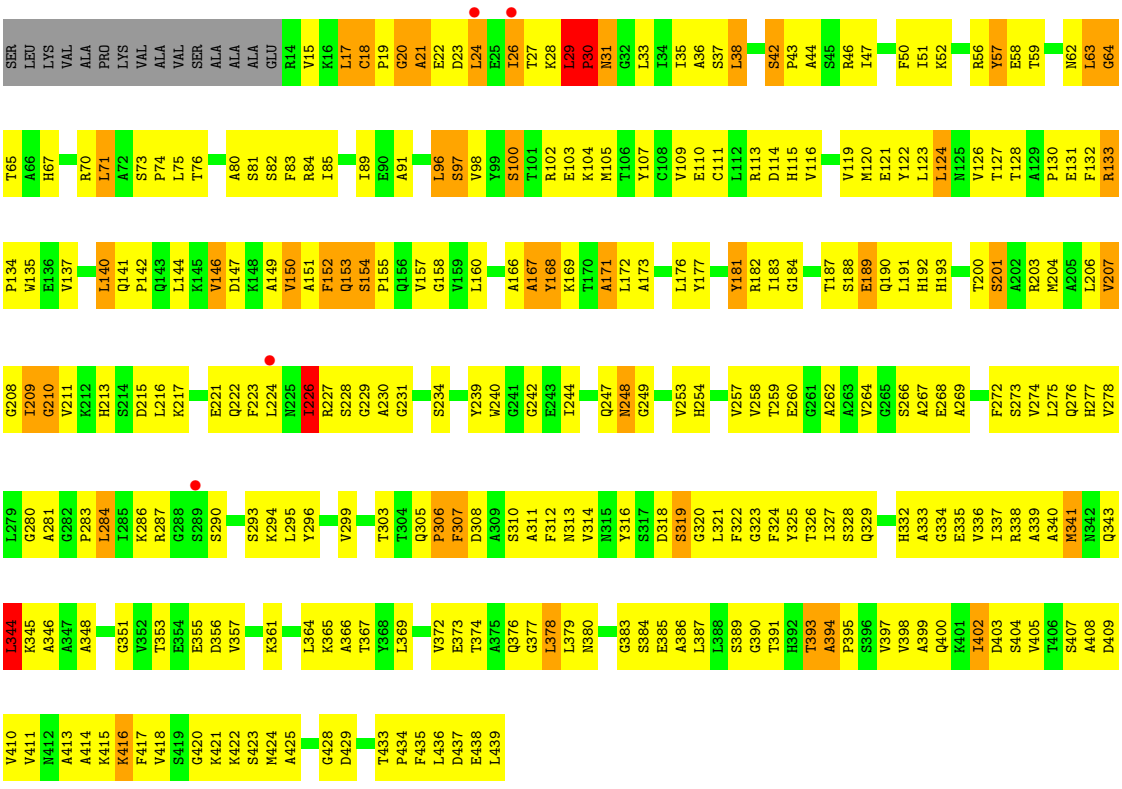




• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:

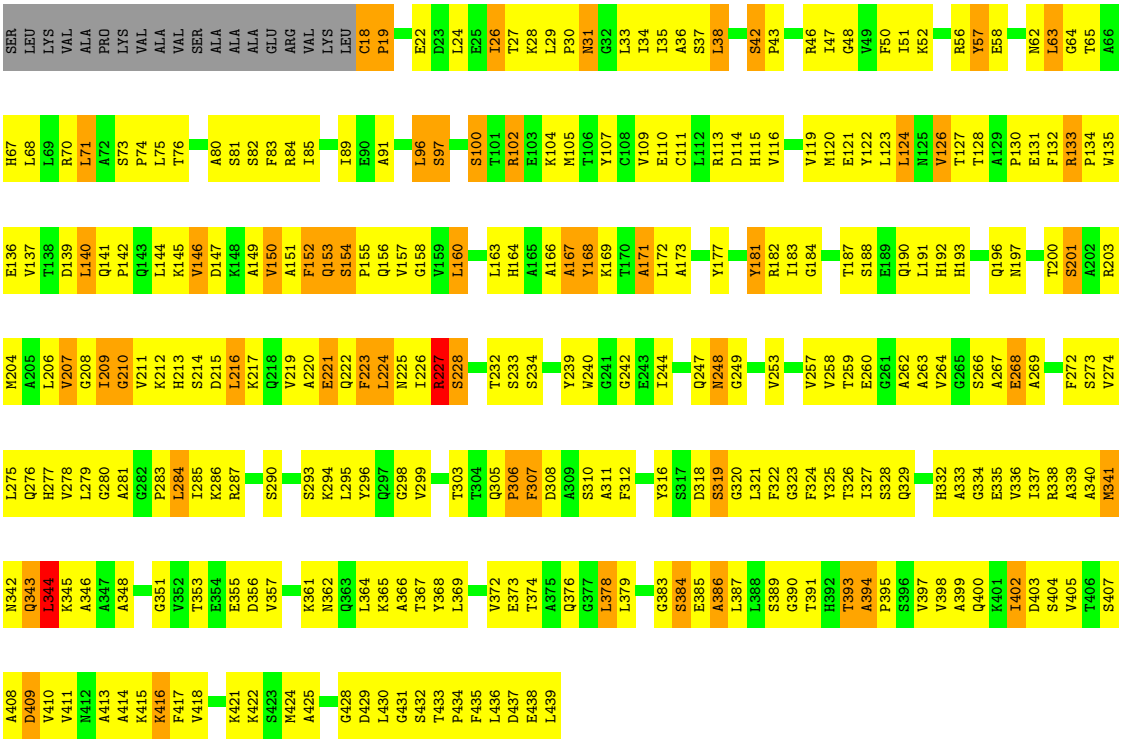




• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

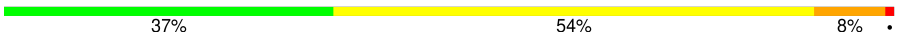
Chain O:

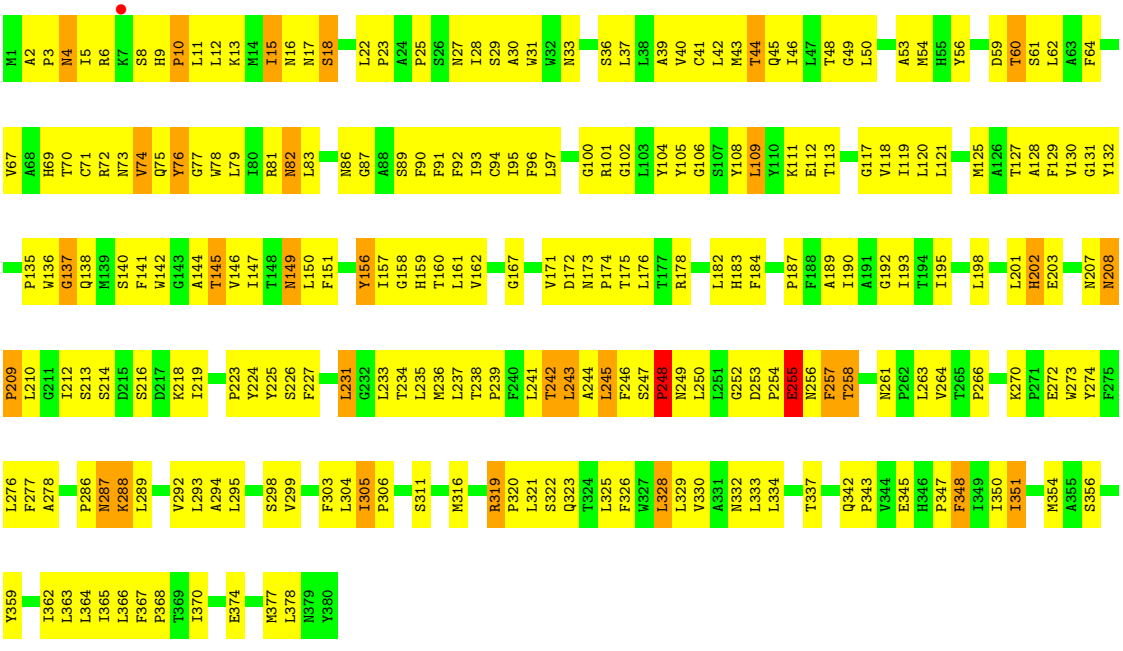




• Molecule 3: Cytochrome b

Chain C:

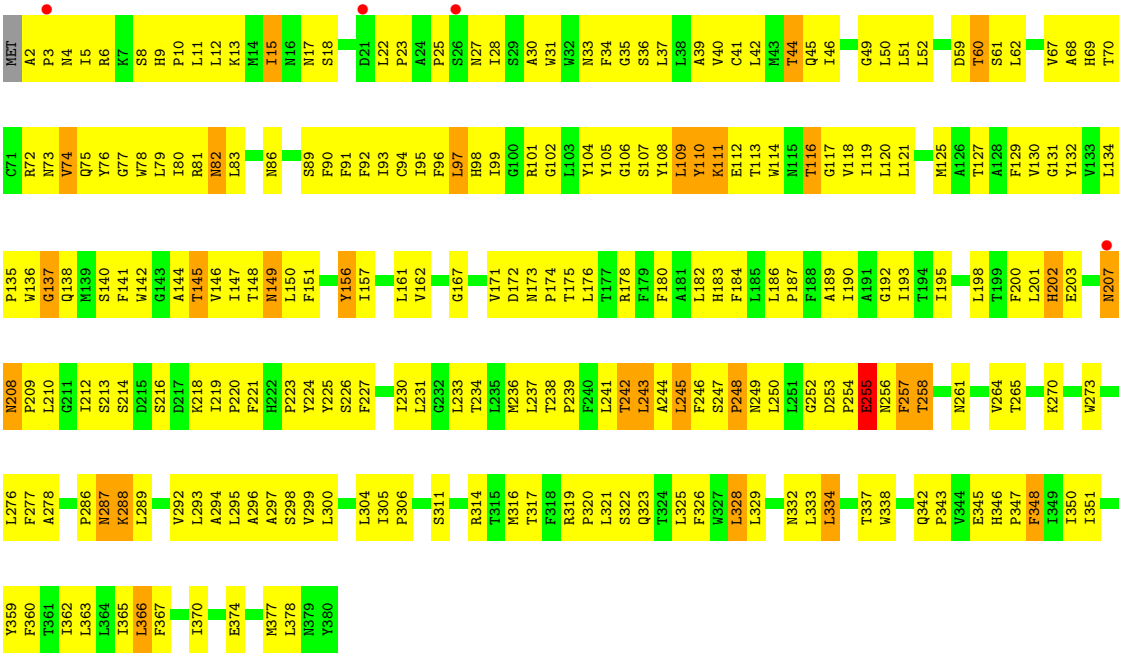




• Molecule 3: Cytochrome b

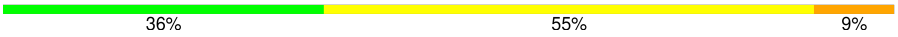
Chain P:

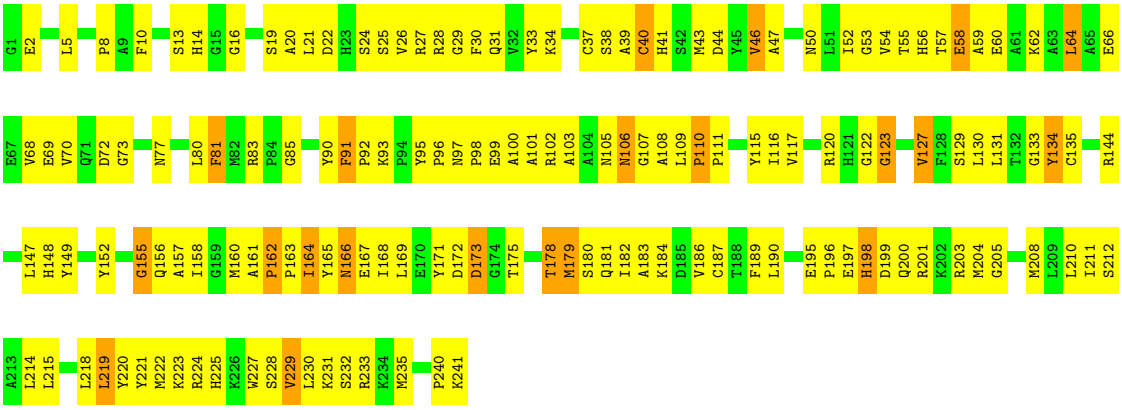




• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

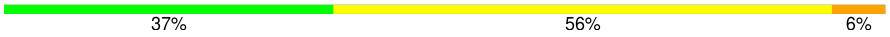
Chain D:

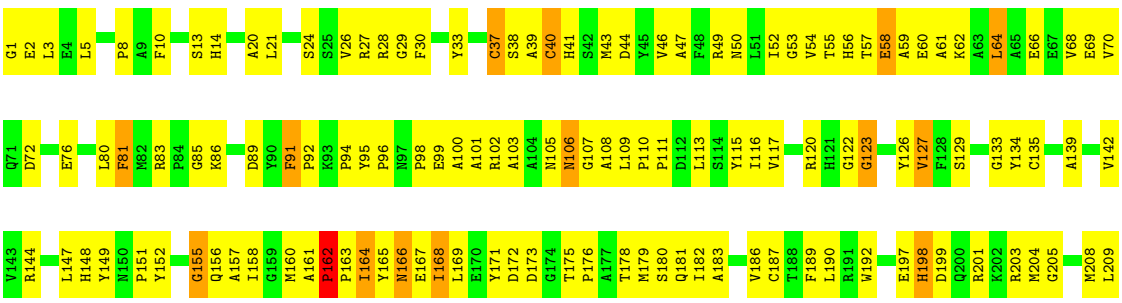


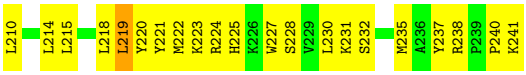


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

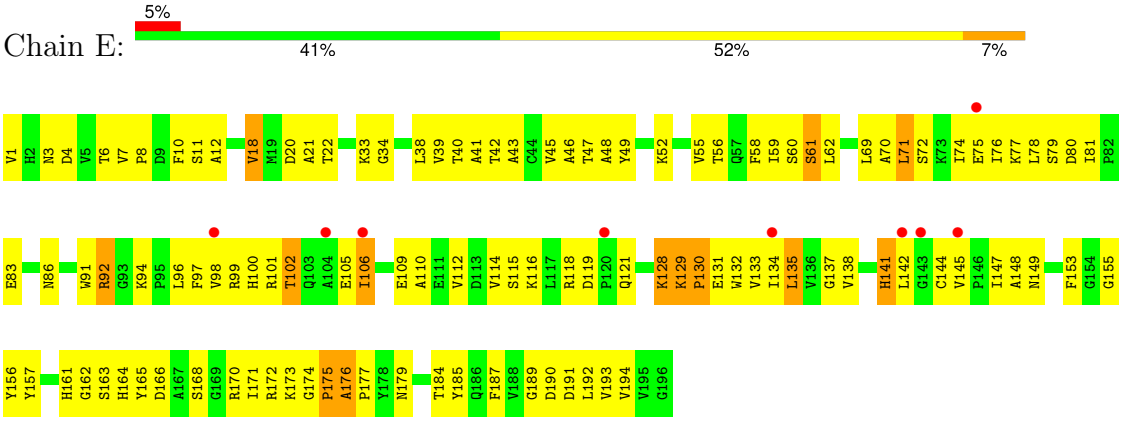
Chain Q:



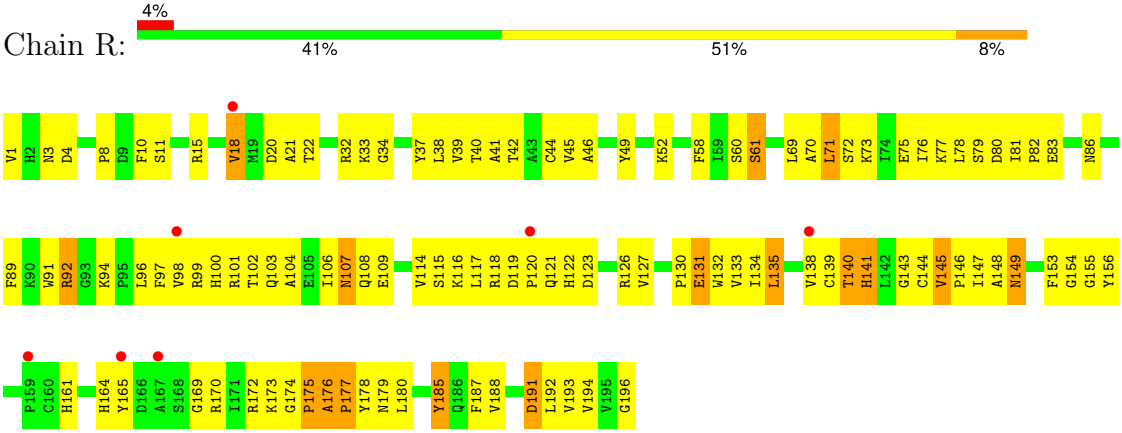




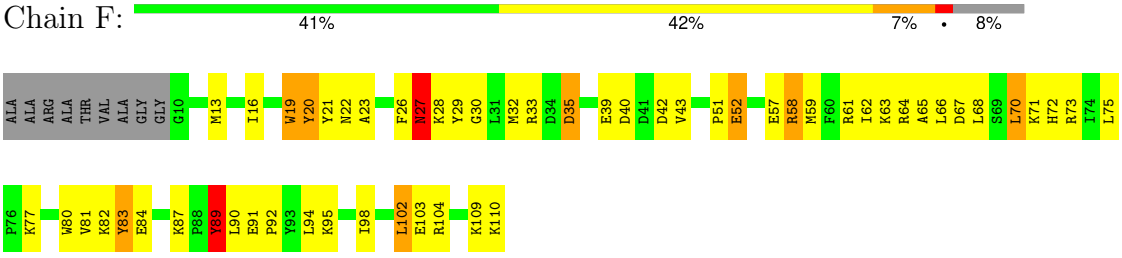
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



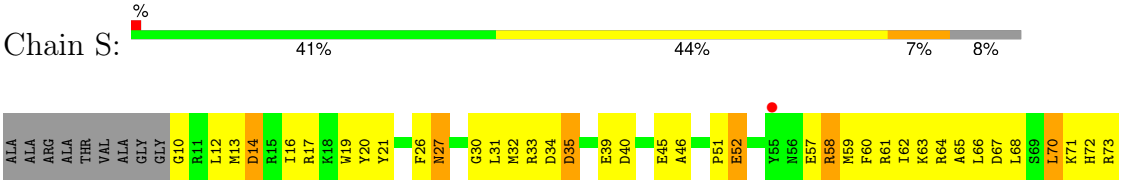
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



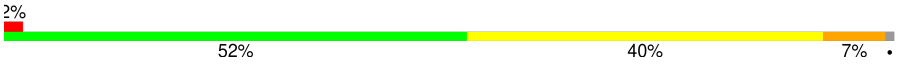
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

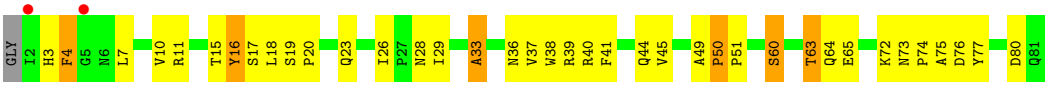




• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G:

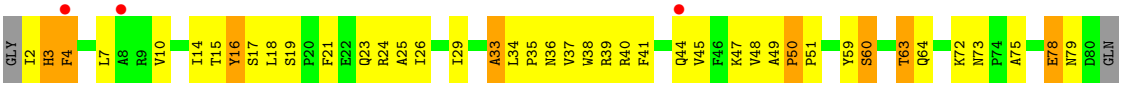




• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

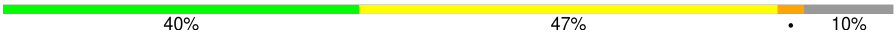
Chain T:

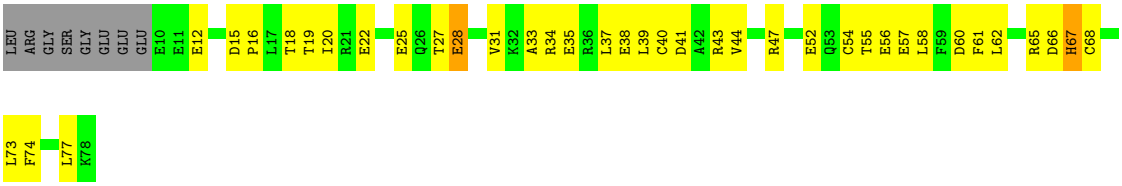




• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H:

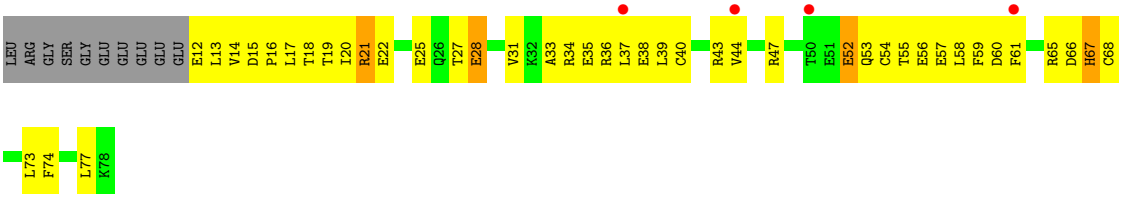




• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:

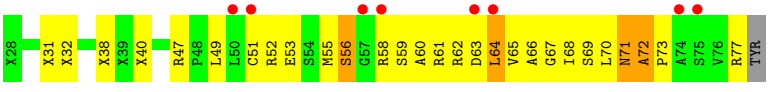




• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

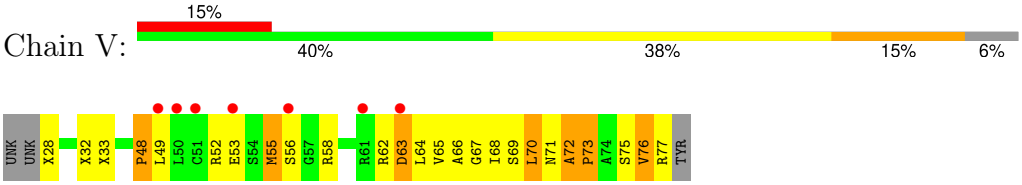
Chain I:





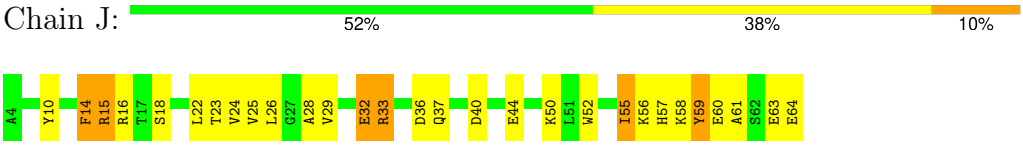
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



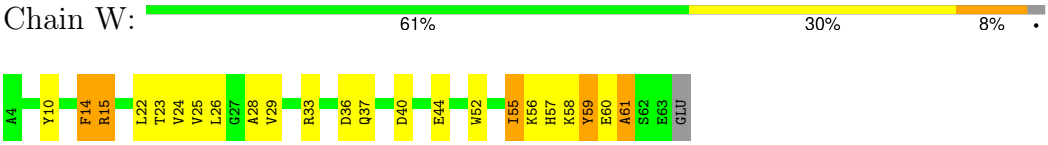
• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

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	171.72Å 181.30Å 241.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 3.48 18.00 – 3.48	Depositor EDS
% Data completeness (in resolution range)	89.7 (18.00-3.48) 89.0 (18.00-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.284 0.232 , 0.277	Depositor DCC
R_{free} test set	2570 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å^2)	101.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 82.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32673	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IKR, PEE, UNL, HEC, GOL, ZN, CDL, UQ, BOG, HEM, FES

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	0.57	0/3513	1.04	19/4760 (0.4%)
1	N	0.58	0/3508	1.05	22/4753 (0.5%)
2	B	0.49	0/3219	0.97	15/4364 (0.3%)
2	O	0.54	0/3202	1.01	18/4343 (0.4%)
3	C	0.68	1/3122 (0.0%)	1.08	21/4273 (0.5%)
3	P	0.58	0/3114	1.02	17/4263 (0.4%)
4	D	0.63	0/1956	1.11	16/2658 (0.6%)
4	Q	0.54	0/1956	1.06	13/2658 (0.5%)
5	E	0.47	0/1547	0.90	3/2103 (0.1%)
5	R	0.49	0/1547	0.94	2/2103 (0.1%)
6	F	0.57	0/911	0.98	5/1219 (0.4%)
6	S	0.50	0/911	0.93	4/1219 (0.3%)
7	G	0.64	0/694	1.10	2/941 (0.2%)
7	T	0.57	0/684	1.08	5/929 (0.5%)
8	H	0.56	0/579	0.95	1/775 (0.1%)
8	U	0.44	0/561	0.86	3/751 (0.4%)
9	I	0.54	0/218	1.10	3/293 (1.0%)
9	V	0.62	0/218	0.94	0/293
10	J	0.58	0/508	0.83	0/682
10	W	0.51	0/490	0.84	0/660
All	All	0.56	1/32458 (0.0%)	1.02	169/44040 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
4	D	0	1
6	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	354	MET	SD-CE	5.92	1.94	1.79

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	18	CYS	CA-C-N	8.90	130.96	119.84
2	O	18	CYS	C-N-CA	8.90	130.96	119.84
4	D	110	PRO	CA-C-N	8.51	128.55	119.78
4	D	110	PRO	C-N-CA	8.51	128.55	119.78
4	D	162	PRO	CA-C-N	8.33	128.02	119.19

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	56	TYR	Sidechain
3	C	76	TYR	Sidechain
4	D	134	TYR	Sidechain
6	F	20	TYR	Sidechain

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	3442	0	3354	281	0
1	N	3437	0	3349	303	0
2	B	3164	0	3158	322	0
2	O	3147	0	3146	356	0
3	C	3020	0	3070	260	0
3	P	3012	0	3058	257	0
4	D	1898	0	1846	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1898	0	1846	183	0
5	E	1513	0	1478	120	0
5	R	1513	0	1478	124	0
6	F	891	0	893	57	0
6	S	891	0	893	57	0
7	G	672	0	653	38	0
7	T	662	0	645	44	0
8	H	571	0	547	34	0
8	U	553	0	535	46	0
9	I	285	0	238	40	0
9	V	275	0	238	40	0
10	J	497	0	490	31	0
10	W	479	0	478	34	0
11	A	18	0	11	0	0
11	C	49	0	72	3	0
11	E	50	0	77	0	0
11	P	54	0	72	4	0
11	R	50	0	77	0	0
12	A	2	0	0	0	0
12	C	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
13	C	86	0	60	19	0
13	P	86	0	60	21	0
14	C	25	0	20	5	0
14	P	25	0	20	4	0
15	C	19	0	17	7	0
15	P	19	0	17	4	0
16	C	40	0	24	2	0
16	D	42	0	28	1	0
16	P	40	0	24	2	0
16	Q	42	0	28	3	0
17	C	1	0	0	0	0
17	P	1	0	0	0	0
18	C	6	0	8	1	0
18	P	6	0	8	1	0
19	D	43	0	30	2	0
19	Q	43	0	30	1	0
20	D	33	0	39	1	0
20	P	25	0	22	0	0
20	Q	20	0	28	0	0
21	E	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	R	4	0	0	2	0
22	A	1	0	0	0	0
22	C	7	0	0	1	0
22	E	1	0	0	0	0
22	P	7	0	0	3	0
22	R	1	0	0	1	0
All	All	32673	0	32165	2606	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 40.

The worst 5 of 2606 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)
2:B:209:ILE:HG22	2:B:210:GLY:H	1.08	1.09
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.31	1.08
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.28	1.07
2:O:209:ILE:HG22	2:O:210:GLY:H	1.09	1.07
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.38	1.06

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%)	335 (76%)	84 (19%)	22 (5%)	1 15
1	N	440/446 (99%)	330 (75%)	87 (20%)	23 (5%)	1 14
2	B	424/441 (96%)	315 (74%)	78 (18%)	31 (7%)	1 9
2	O	420/441 (95%)	313 (74%)	78 (19%)	29 (7%)	1 10
3	C	378/380 (100%)	298 (79%)	61 (16%)	19 (5%)	1 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	P	377/380 (99%)	294 (78%)	67 (18%)	16 (4%)	2 18
4	D	239/241 (99%)	177 (74%)	51 (21%)	11 (5%)	2 17
4	Q	239/241 (99%)	181 (76%)	47 (20%)	11 (5%)	2 17
5	E	194/196 (99%)	119 (61%)	60 (31%)	15 (8%)	1 8
5	R	194/196 (99%)	122 (63%)	50 (26%)	22 (11%)	0 5
6	F	99/110 (90%)	74 (75%)	21 (21%)	4 (4%)	2 19
6	S	99/110 (90%)	77 (78%)	19 (19%)	3 (3%)	3 25
7	G	78/81 (96%)	59 (76%)	16 (20%)	3 (4%)	2 20
7	T	77/81 (95%)	57 (74%)	15 (20%)	5 (6%)	1 11
8	H	67/77 (87%)	44 (66%)	22 (33%)	1 (2%)	8 37
8	U	65/77 (84%)	43 (66%)	20 (31%)	2 (3%)	3 25
9	I	29/47 (62%)	15 (52%)	10 (34%)	4 (14%)	0 3
9	V	29/47 (62%)	15 (52%)	9 (31%)	5 (17%)	0 2
10	J	59/61 (97%)	38 (64%)	16 (27%)	5 (8%)	0 7
10	W	58/61 (95%)	39 (67%)	14 (24%)	5 (9%)	0 7
All	All	4006/4160 (96%)	2945 (74%)	825 (21%)	236 (6%)	1 12

5 of 236 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	222	THR
1	A	432	LEU
2	B	15	VAL
2	B	17	LEU

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%)	345 (94%)	20 (6%)	19 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	365/368 (99%)	345 (94%)	20 (6%)	19	46
2	B	333/347 (96%)	309 (93%)	24 (7%)	13	38
2	O	333/347 (96%)	308 (92%)	25 (8%)	12	38
3	C	329/329 (100%)	314 (95%)	15 (5%)	24	50
3	P	328/329 (100%)	314 (96%)	14 (4%)	26	52
4	D	200/200 (100%)	191 (96%)	9 (4%)	24	51
4	Q	200/200 (100%)	192 (96%)	8 (4%)	28	54
5	E	166/166 (100%)	161 (97%)	5 (3%)	36	60
5	R	166/166 (100%)	161 (97%)	5 (3%)	36	60
6	F	93/96 (97%)	86 (92%)	7 (8%)	12	38
6	S	93/96 (97%)	86 (92%)	7 (8%)	12	38
7	G	71/71 (100%)	66 (93%)	5 (7%)	14	40
7	T	70/71 (99%)	66 (94%)	4 (6%)	18	45
8	H	65/71 (92%)	63 (97%)	2 (3%)	35	60
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	70
9	I	23/26 (88%)	22 (96%)	1 (4%)	26	52
9	V	23/26 (88%)	19 (83%)	4 (17%)	2	11
10	J	49/49 (100%)	47 (96%)	2 (4%)	27	53
10	W	47/49 (96%)	45 (96%)	2 (4%)	26	52
All	All	3382/3446 (98%)	3202 (95%)	180 (5%)	20	47

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	97	SER
3	P	243	LEU
2	O	139	ASP
2	O	341	MET
4	Q	37	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	339	GLN

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Mol	Chain	Res	Type
3	P	9	HIS
8	U	26	GLN
1	N	435	ASN
2	O	248	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 5 are unknown and 2 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
16	CDL	D	2003	-	41,41,99	1.16	1 (2%)	47,53,111	1.07	3 (6%)
11	PEE	C	2007	-	48,48,50	1.37	5 (10%)	51,53,55	0.80	2 (3%)
13	HEM	P	501	3	50,50,50	1.71	7 (14%)	67,82,82	1.79	15 (22%)
21	FES	R	501	5	0,4,4	-	-	-		
13	HEM	P	502	3	50,50,50	1.58	7 (14%)	67,82,82	1.38	10 (14%)
13	HEM	C	501	3	50,50,50	1.79	9 (18%)	67,82,82	2.00	26 (38%)
18	GOL	P	3011	-	5,5,5	1.36	0	5,5,5	0.60	0
18	GOL	C	2011	-	5,5,5	1.34	0	5,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	PEE	E	2005	-	49,49,50	1.56	10 (20%)	52,54,55	0.90	3 (5%)
11	PEE	R	3005	-	49,49,50	1.60	11 (22%)	52,54,55	0.88	3 (5%)
20	BOG	P	3091	-	13,13,20	1.33	2 (15%)	18,18,25	1.12	2 (11%)
11	PEE	P	3008	-	4,4,50	3.62	4 (100%)	6,6,55	0.66	0
16	CDL	P	3004	-	39,39,99	1.27	5 (12%)	45,51,111	1.16	5 (11%)
20	BOG	D	2009	-	20,20,20	1.09	2 (10%)	25,25,25	0.91	2 (8%)
14	IKR	P	3001	-	26,26,26	1.49	7 (26%)	33,35,35	1.70	6 (18%)
19	HEC	Q	501	4	50,50,50	1.51	10 (20%)	68,82,82	1.71	15 (22%)
15	UQ	P	3002	-	19,19,63	2.65	10 (52%)	24,26,79	1.37	3 (12%)
20	BOG	P	2010	-	12,12,20	1.45	2 (16%)	17,17,25	0.63	0
21	FES	E	501	5	0,4,4	-	-	-		
14	IKR	C	2001	-	26,26,26	1.52	6 (23%)	33,35,35	1.69	7 (21%)
11	PEE	A	2008	-	16,16,50	1.77	5 (31%)	18,20,55	0.54	0
16	CDL	C	2004	-	39,39,99	1.31	5 (12%)	45,51,111	1.17	5 (11%)
19	HEC	D	501	4	50,50,50	1.52	11 (22%)	68,82,82	2.00	19 (27%)
20	BOG	Q	3009	-	20,20,20	1.03	2 (10%)	25,25,25	1.01	1 (4%)
16	CDL	Q	3003	-	41,41,99	1.17	1 (2%)	47,53,111	1.08	4 (8%)
20	BOG	D	2091	-	13,13,20	1.46	3 (23%)	18,18,25	1.18	2 (11%)
13	HEM	C	502	3	50,50,50	1.88	11 (22%)	67,82,82	2.04	21 (31%)
15	UQ	C	2002	-	19,19,63	2.52	10 (52%)	24,26,79	1.35	3 (12%)
11	PEE	P	3007	-	48,48,50	1.35	5 (10%)	51,53,55	0.77	2 (3%)

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
16	CDL	D	2003	-	-	18/51/51/110	-
11	PEE	C	2007	-	-	18/52/52/54	-
13	HEM	P	501	3	-	8/14/54/54	-
21	FES	R	501	5	-	-	0/1/1/1
13	HEM	P	502	3	-	9/14/54/54	-
13	HEM	C	501	3	-	6/14/54/54	-
18	GOL	P	3011	-	-	2/4/4/4	-
18	GOL	C	2011	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PEE	E	2005	-	-	24/53/53/54	-
11	PEE	R	3005	-	-	26/53/53/54	-
20	BOG	P	3091	-	-	4/4/24/31	0/1/1/1
16	CDL	P	3004	-	-	19/49/49/110	-
20	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
14	IKR	P	3001	-	-	1/18/18/18	0/2/2/2
19	HEC	Q	501	4	1/1/3/7	5/14/54/54	-
15	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
20	BOG	P	2010	-	-	1/2/22/31	0/1/1/1
21	FES	E	501	5	-	-	0/1/1/1
14	IKR	C	2001	-	-	0/18/18/18	0/2/2/2
11	PEE	A	2008	-	-	2/19/19/54	-
16	CDL	C	2004	-	-	19/49/49/110	-
19	HEC	D	501	4	1/1/3/7	5/14/54/54	-
20	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
16	CDL	Q	3003	-	-	18/51/51/110	-
20	BOG	D	2091	-	-	1/4/24/31	0/1/1/1
13	HEM	C	502	3	-	10/14/54/54	-
15	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
11	PEE	P	3007	-	-	17/52/52/54	-

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEM	CBC-CAC	6.36	1.60	1.30
15	P	3002	UQ	C7-C6	5.31	1.61	1.51
13	P	501	HEM	CBC-CAC	5.20	1.55	1.30
15	P	3002	UQ	C6-C5	5.14	1.44	1.35
13	P	502	HEM	CBC-CAC	5.06	1.54	1.30

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	502	HEM	C3B-C2B-C1B	-6.93	101.20	106.41
13	C	501	HEM	C3B-C4B-NB	5.72	113.57	109.47
13	C	502	HEM	CMB-C2B-C1B	5.68	133.91	125.03
14	P	3001	IKR	C40-C2-C1	5.43	127.29	123.40
14	C	2001	IKR	C40-C2-C1	5.13	127.08	123.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	D	501	HEC	NA
19	Q	501	HEC	NA

5 of 234 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O3P
11	E	2005	PEE	C4-O4P-P-O1P
11	E	2005	PEE	O4P-C4-C5-N
11	R	3005	PEE	C11-C10-O2-C2

There are no ring outliers.

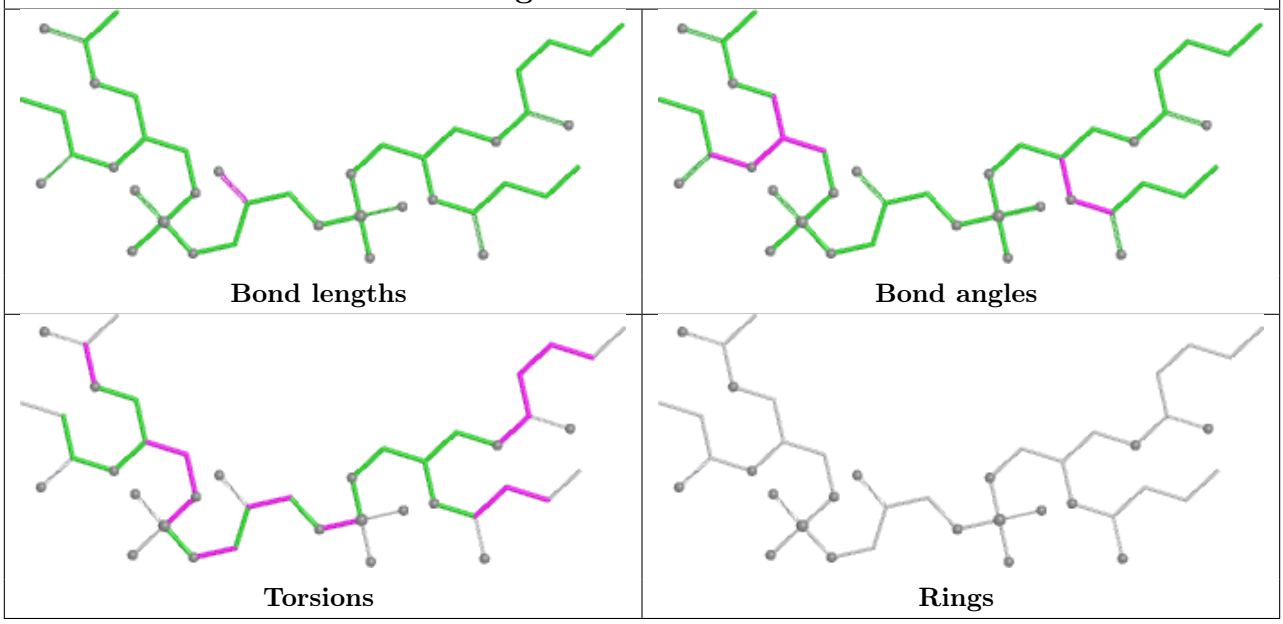
21 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	2003	CDL	1	0
11	C	2007	PEE	3	0
13	P	501	HEM	9	0
21	R	501	FES	2	0
13	P	502	HEM	12	0
13	C	501	HEM	6	0
18	P	3011	GOL	1	0
18	C	2011	GOL	1	0
16	P	3004	CDL	2	0
14	P	3001	IKR	4	0
19	Q	501	HEC	1	0
15	P	3002	UQ	4	0
21	E	501	FES	3	0
14	C	2001	IKR	5	0
16	C	2004	CDL	2	0
19	D	501	HEC	2	0
16	Q	3003	CDL	3	0
20	D	2091	BOG	1	0
13	C	502	HEM	13	0
15	C	2002	UQ	7	0
11	P	3007	PEE	4	0

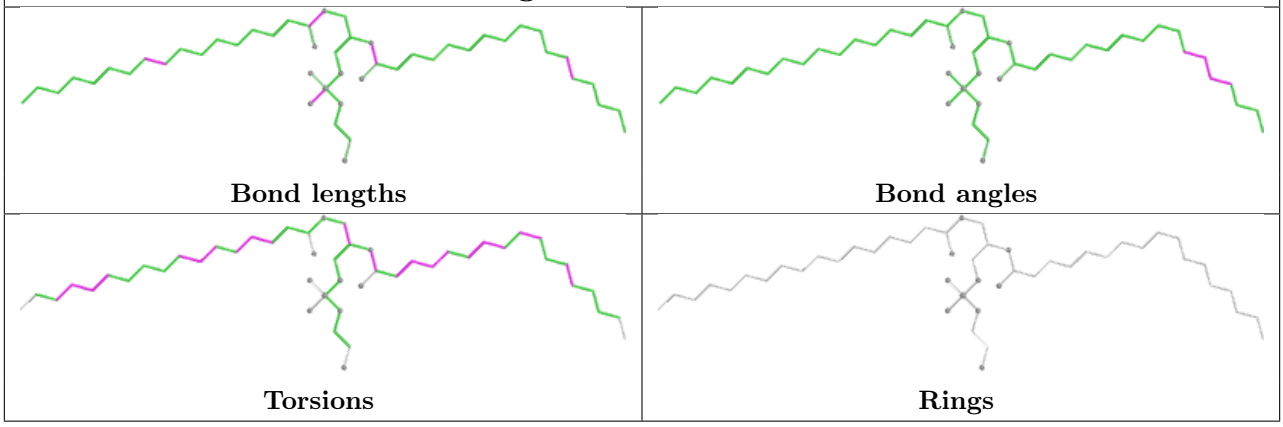
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 CDL D 2003



Ligand PEE C 2007



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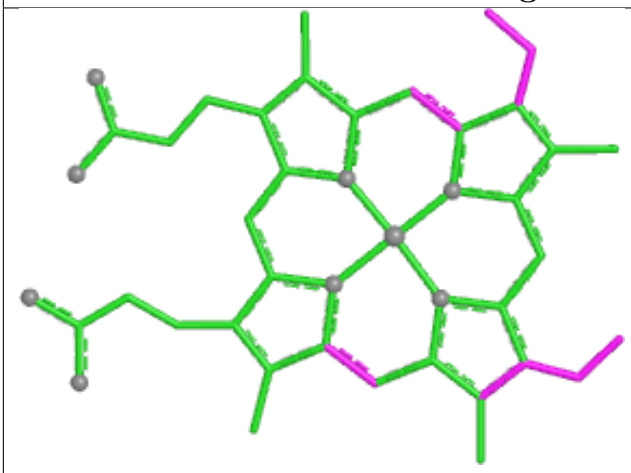
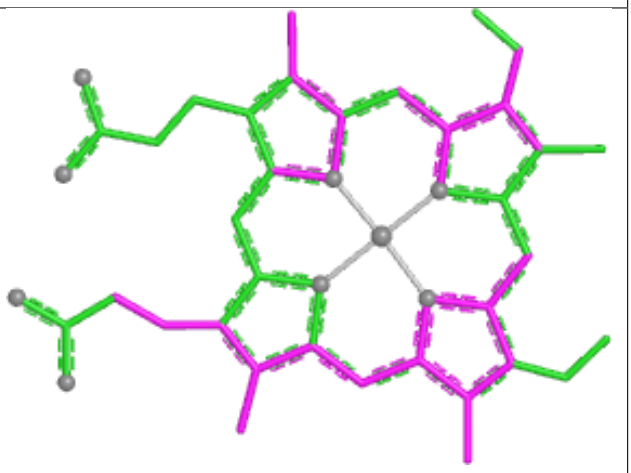
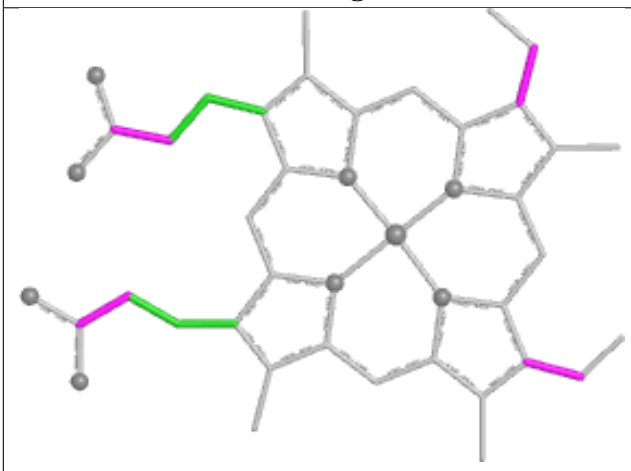


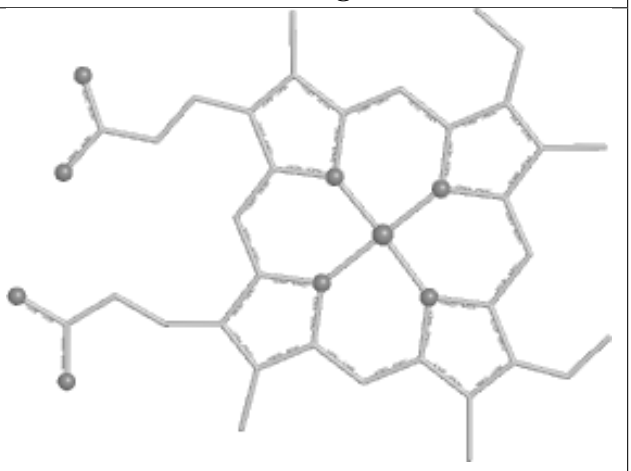
Bond lengths



Bond angles

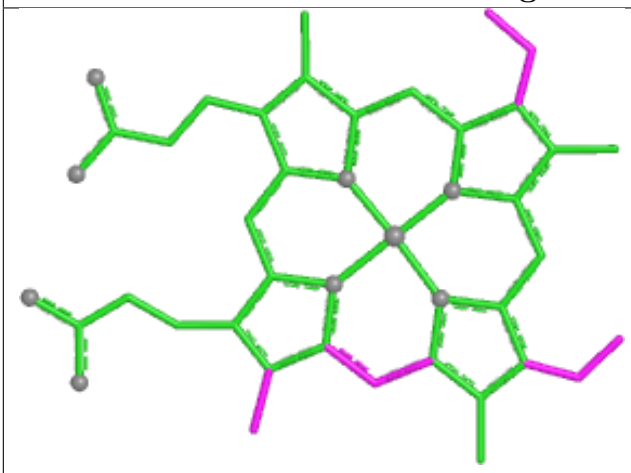


Torsions



Rings

Ligand HEM P 502



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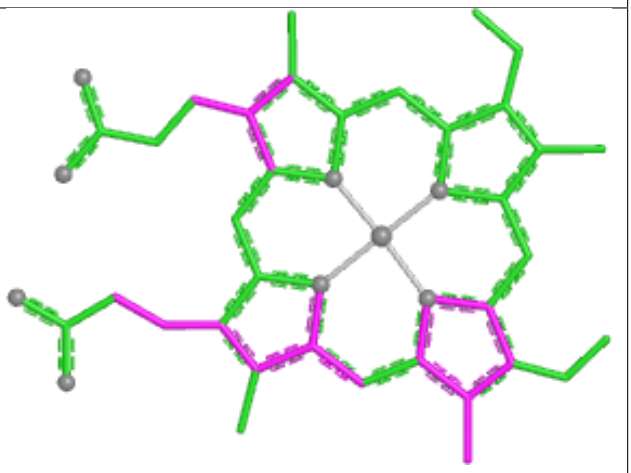

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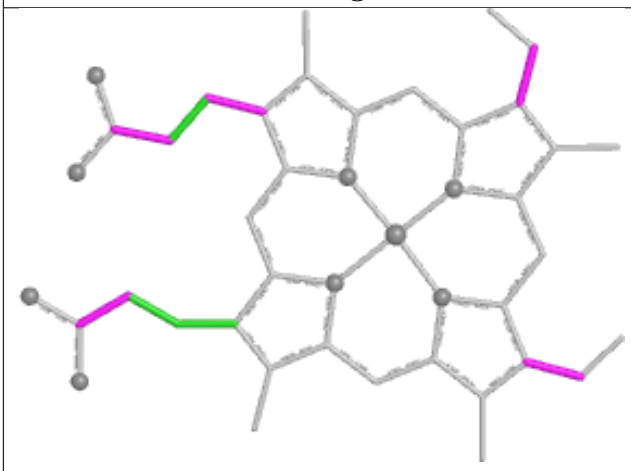

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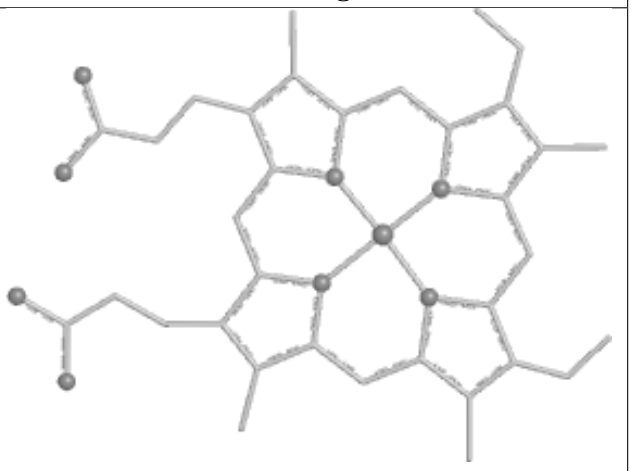
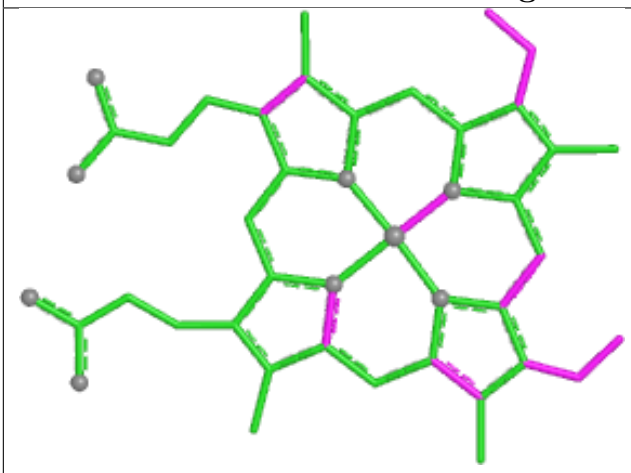


Rings

Ligand HEM C 501



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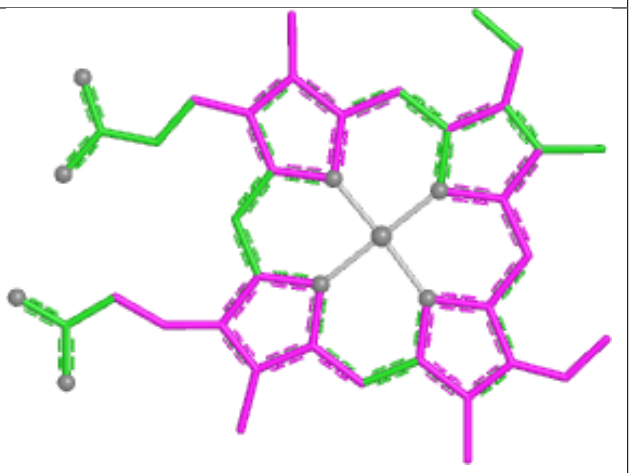

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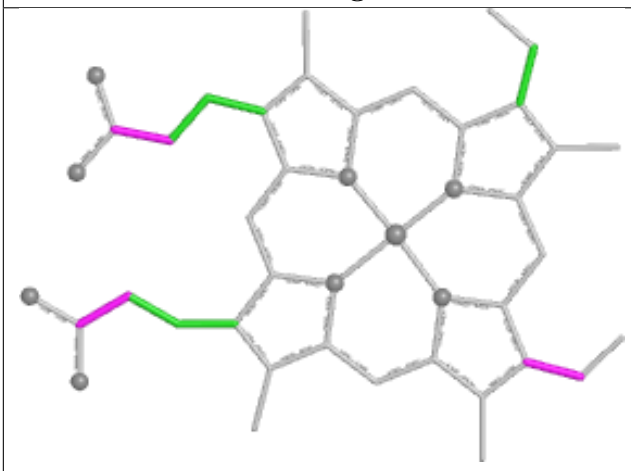

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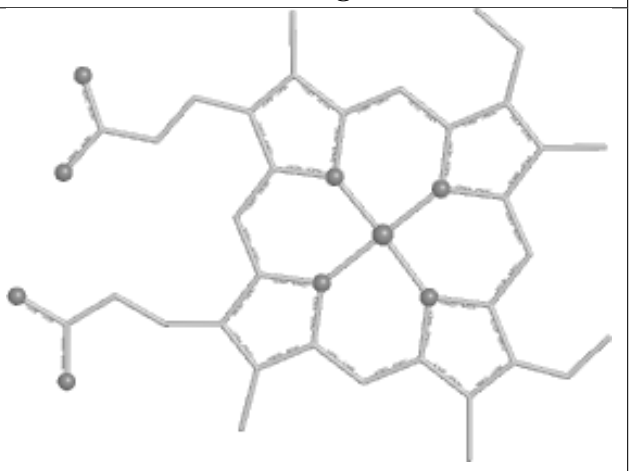

Rings

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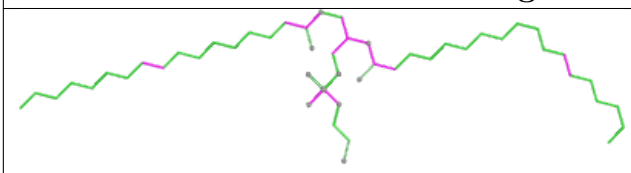
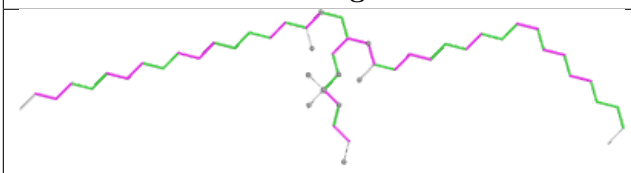


Bond lengths



Bond angles



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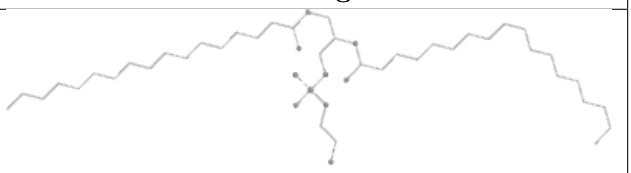
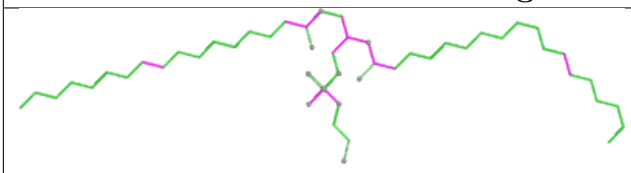


Rings

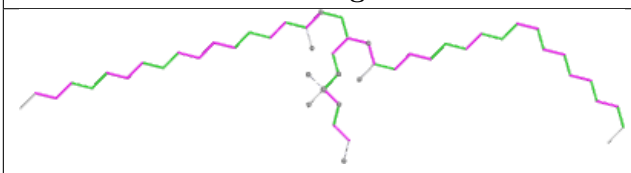
Ligand PEE R 3005



Bond lengths



Bond angles



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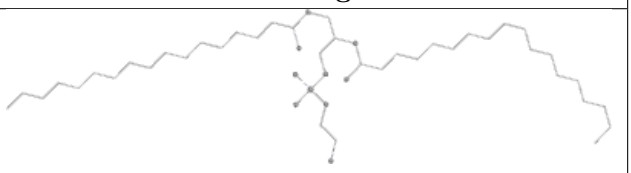
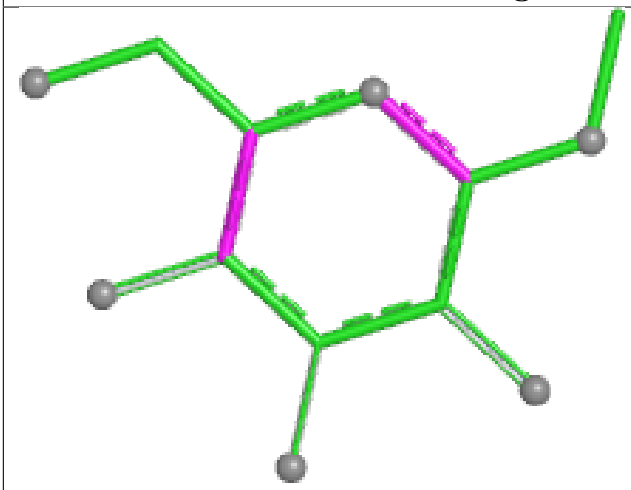
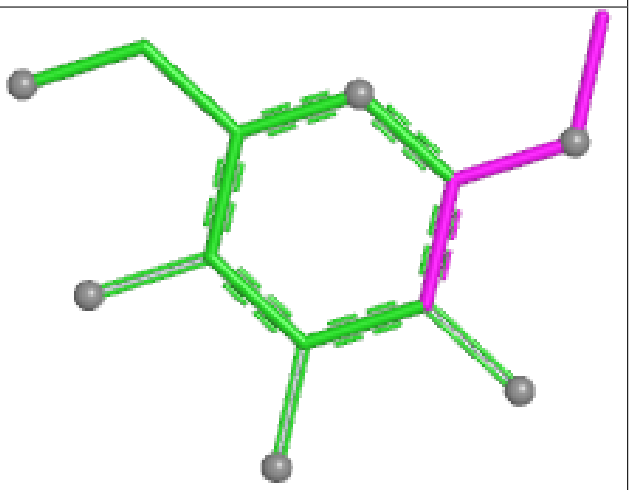


Rings

Ligand BOG P 3091



Bond lengths



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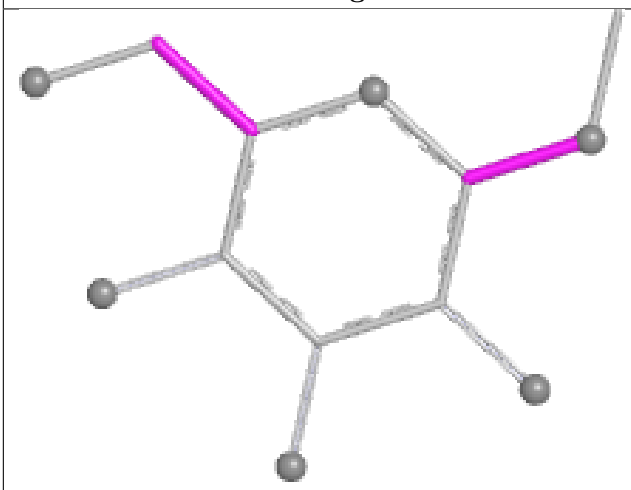

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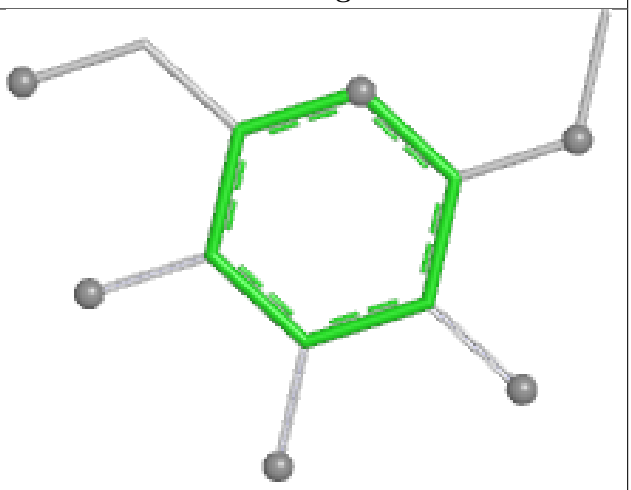
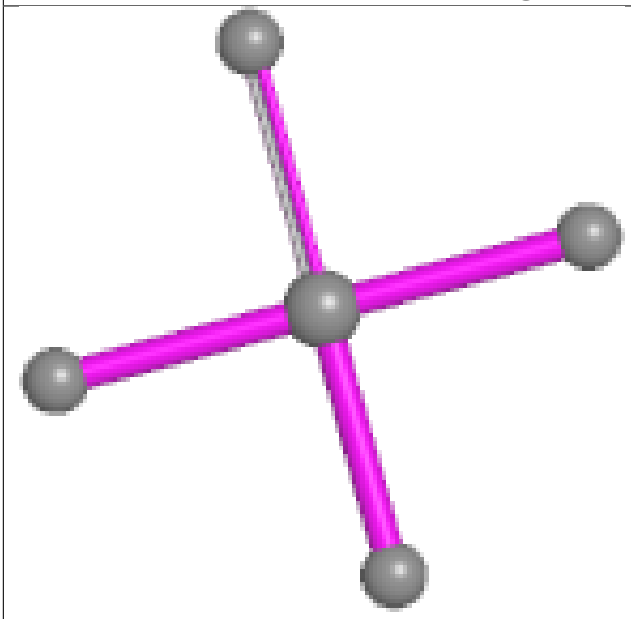


Rings

Ligand PEE P 3008



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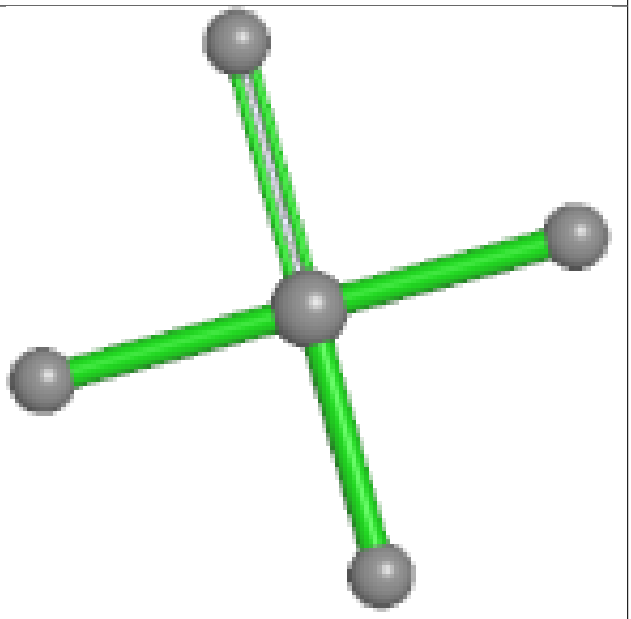
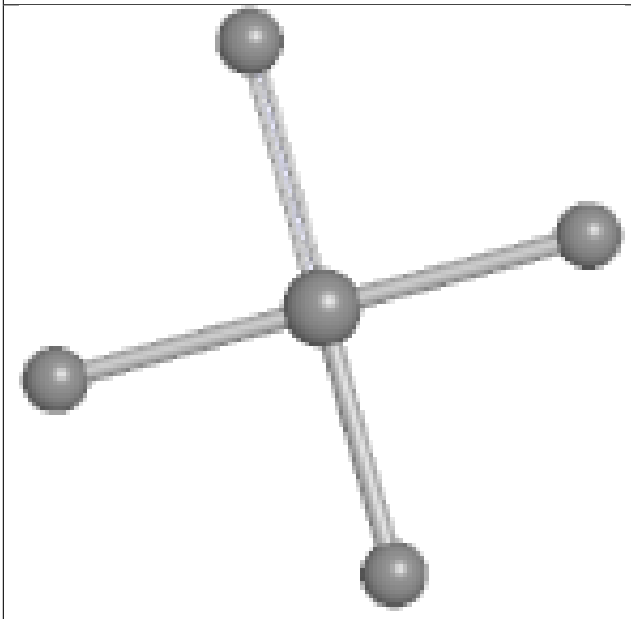


Bond angles



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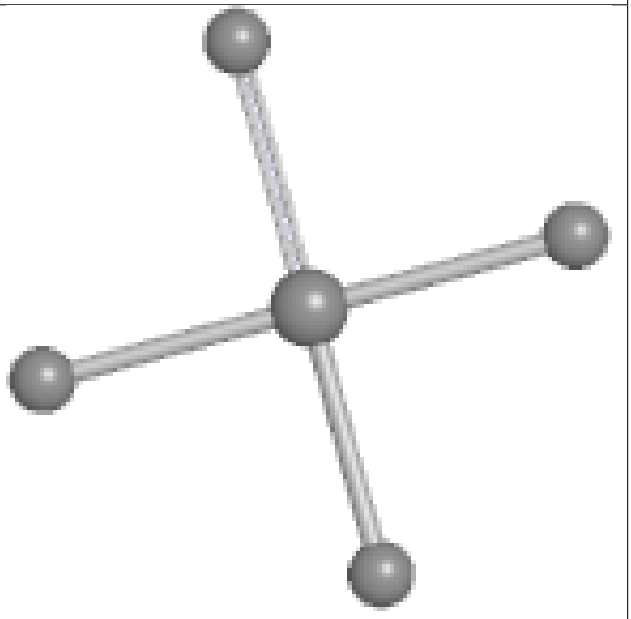
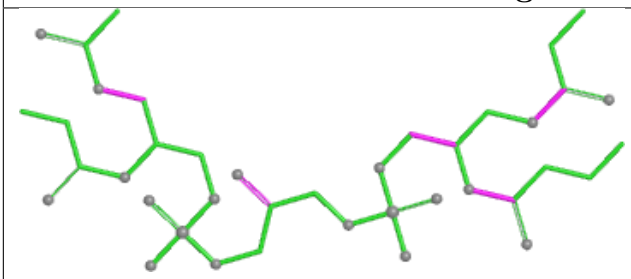
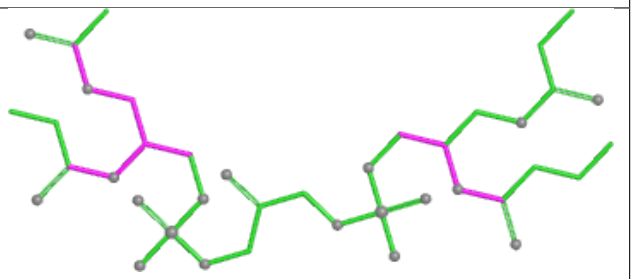


Rings

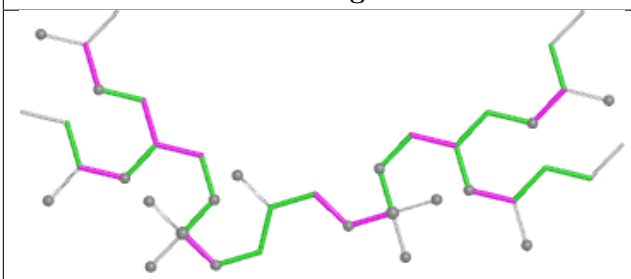
Ligand CDL P 3004



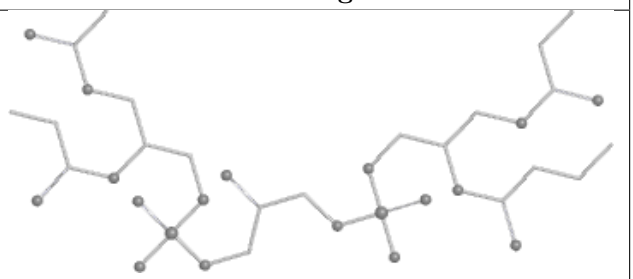
Bond lengths



Bond angles

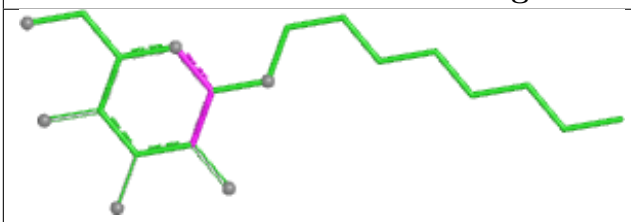


Torsions



Rings

Ligand BOG D 2009



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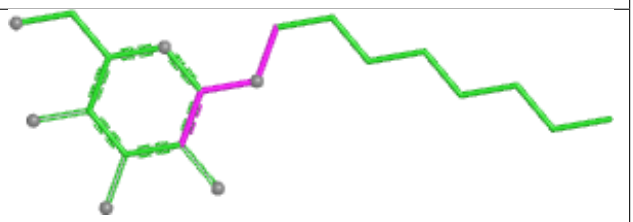

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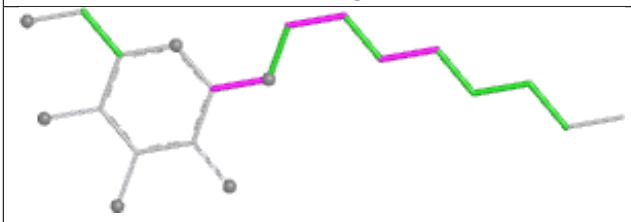
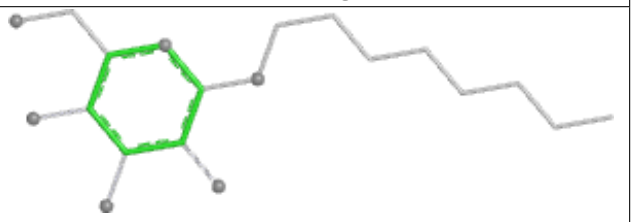
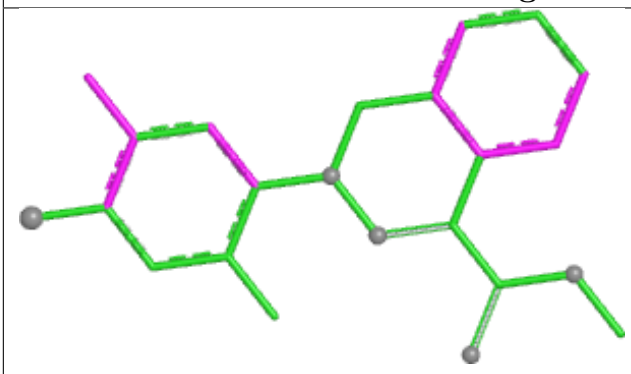


Torsions



Rings

Ligand IKR P 3001



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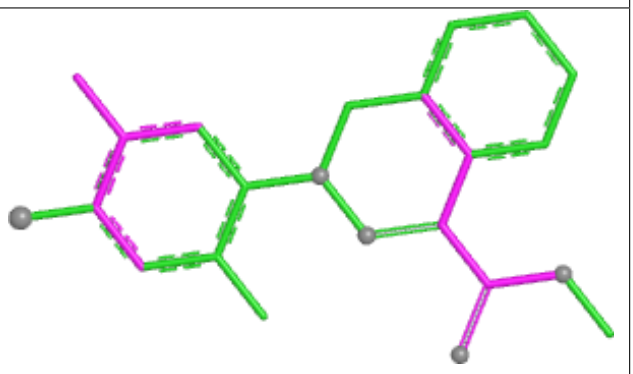

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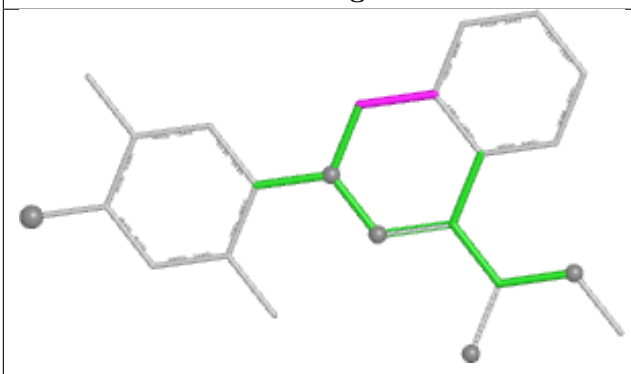

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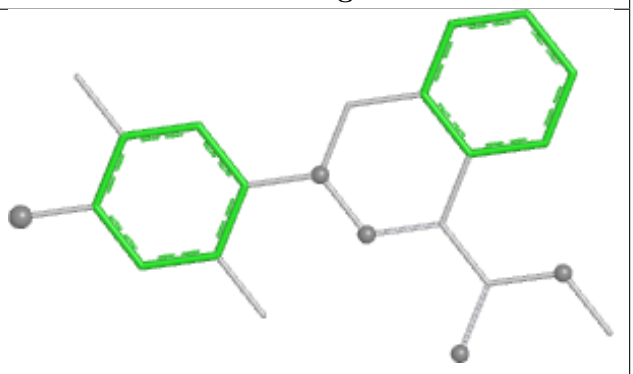
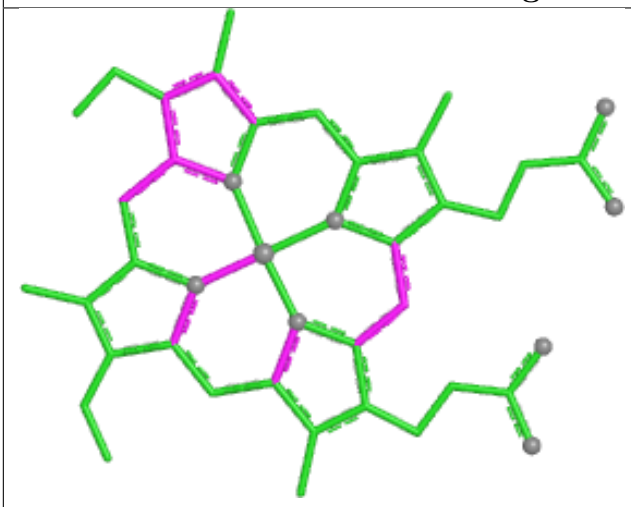


Rings

Ligand HEC Q 501



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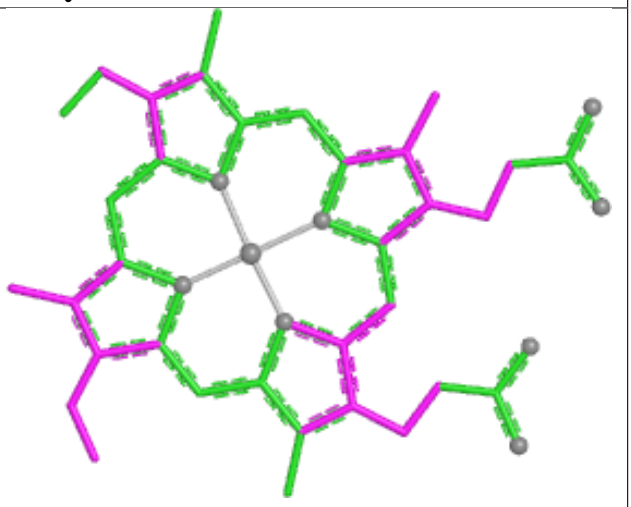

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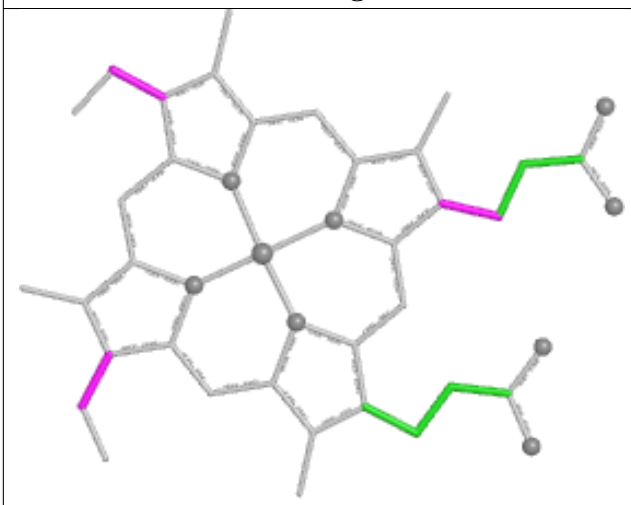

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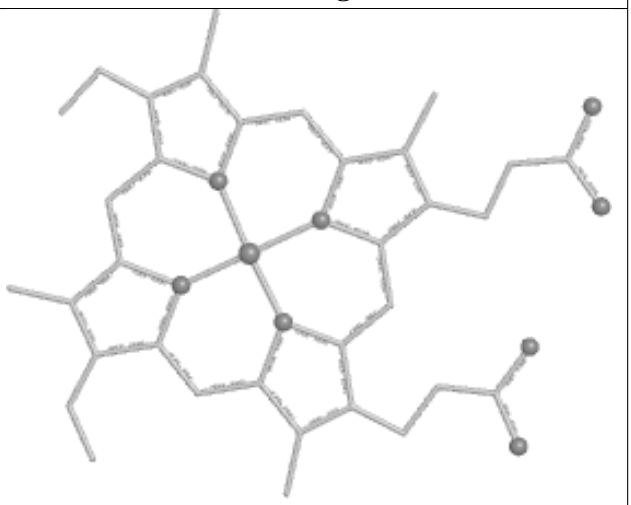
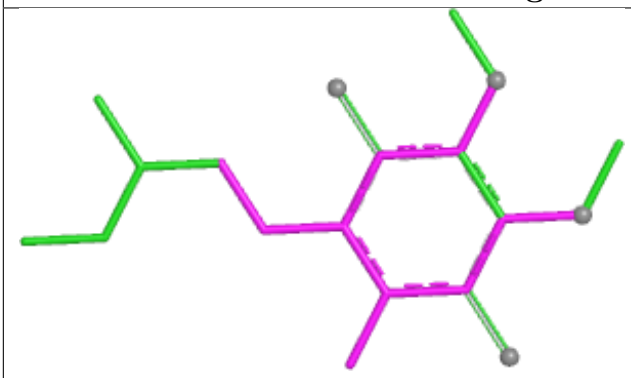


Rings

Ligand UQ P 3002



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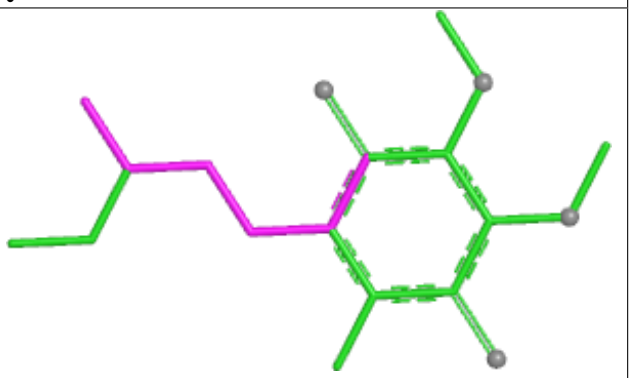
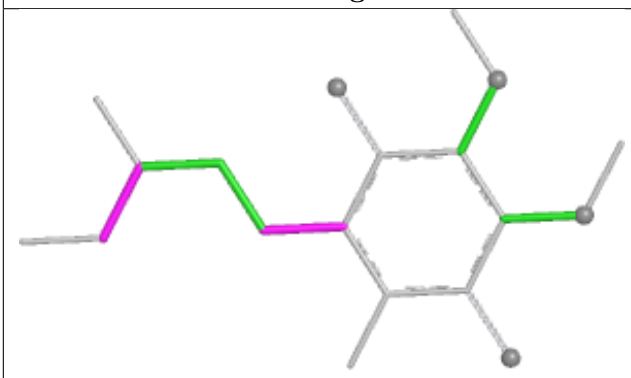


Bond angles



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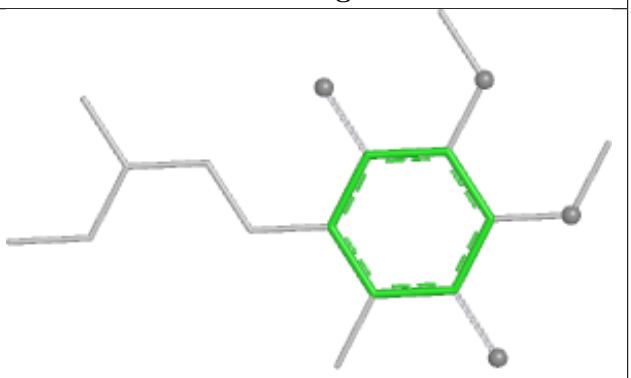
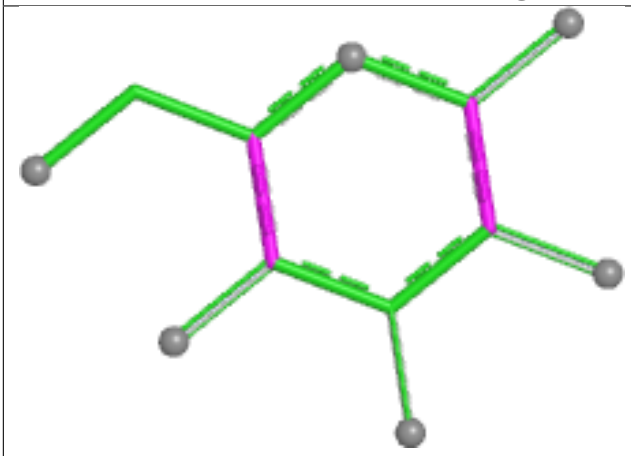


Rings

Ligand BOG P 2010



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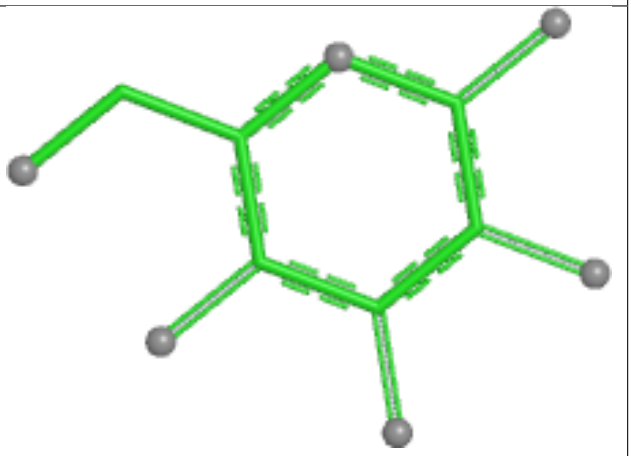

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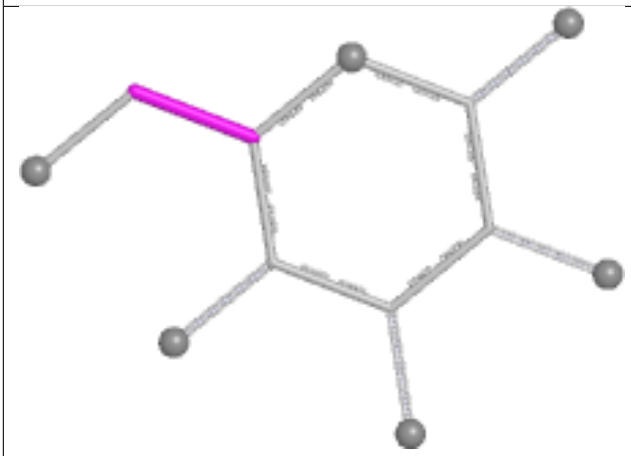

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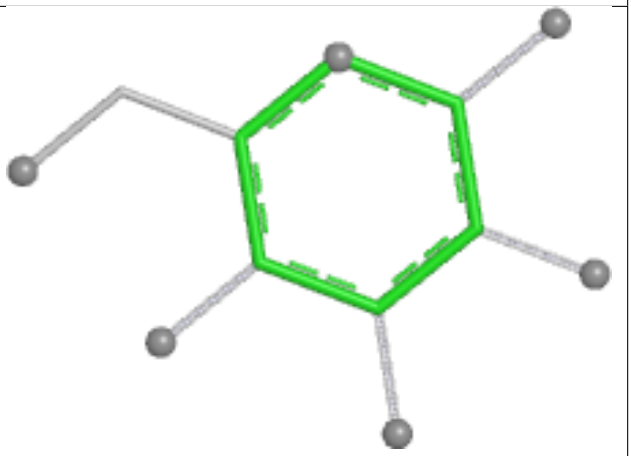
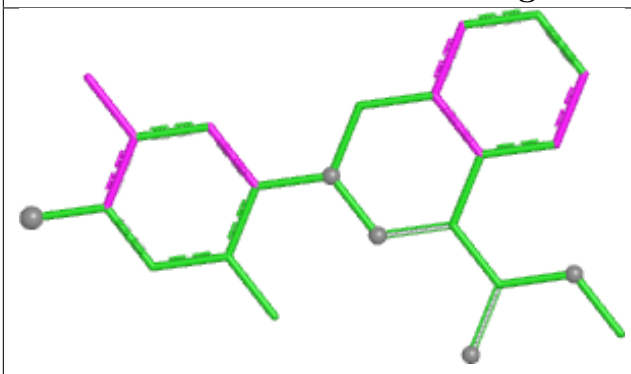


Rings

Ligand IKR C 2001



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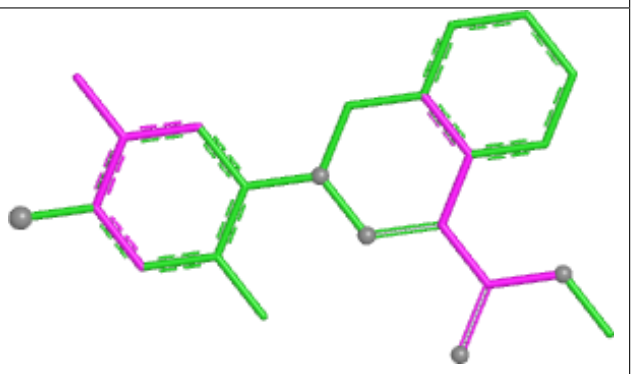
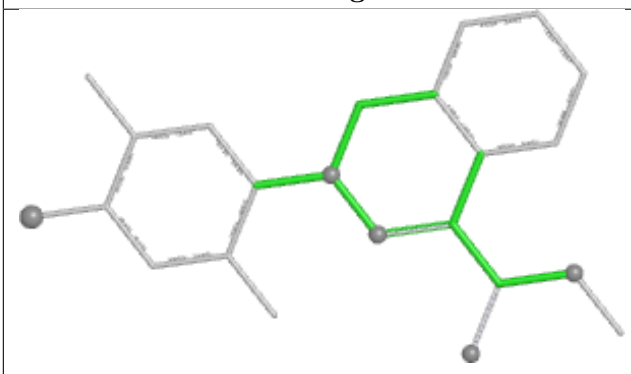


Bond angles



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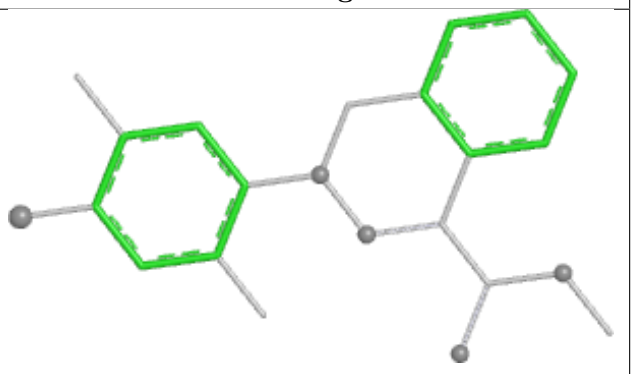
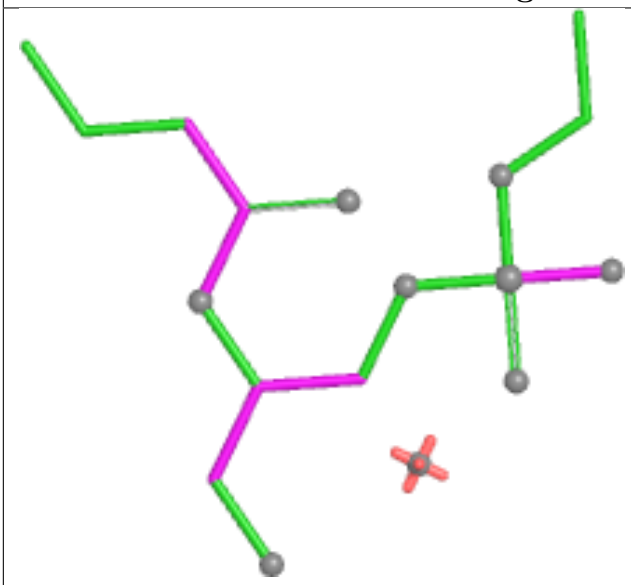


Rings

Ligand PEE A 2008



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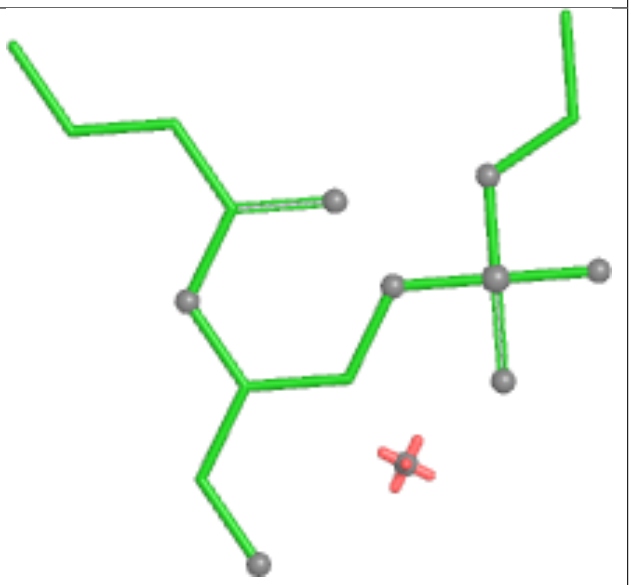

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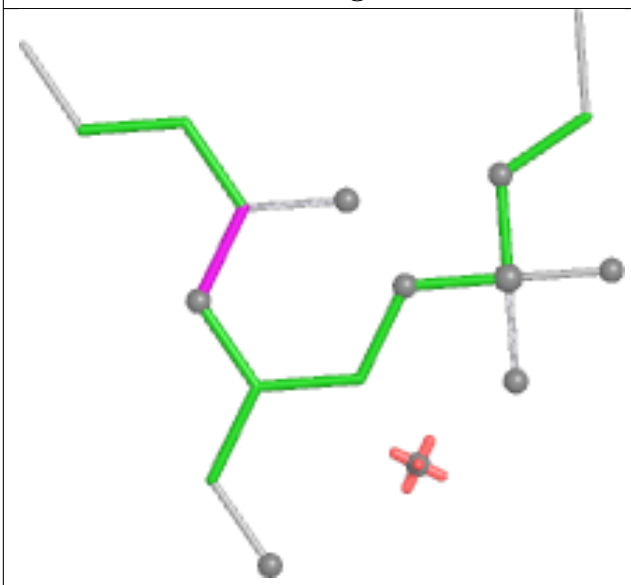

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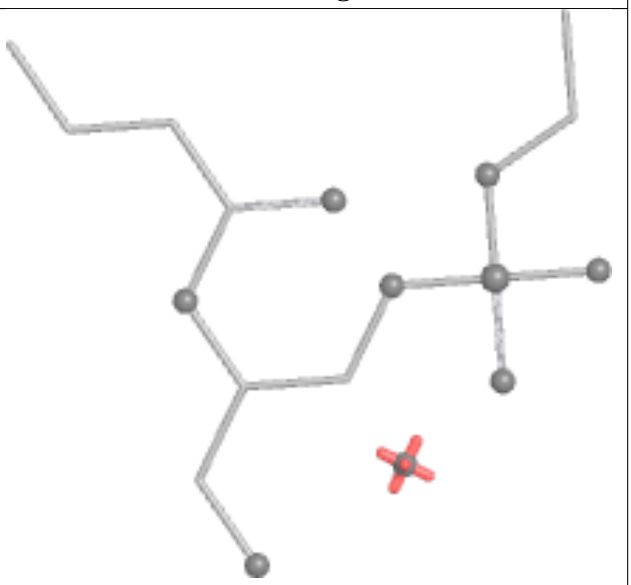
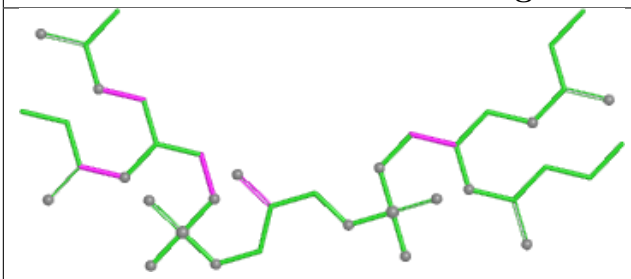


Rings

Ligand CDL C 2004



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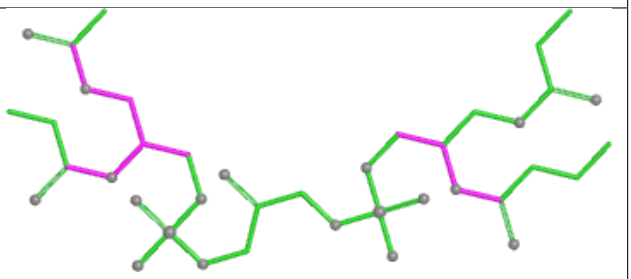

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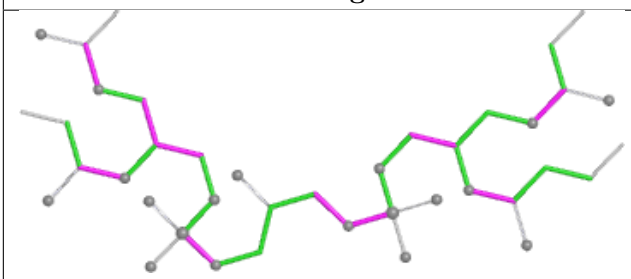

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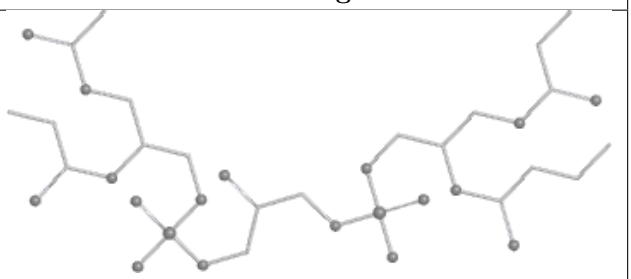
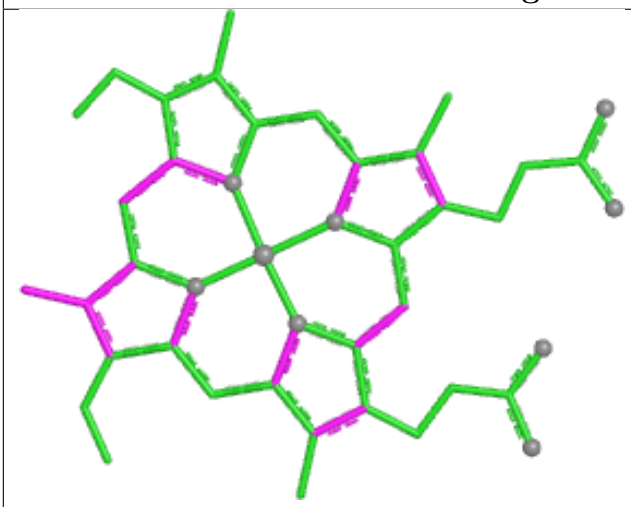


Rings

Ligand HEC D 501



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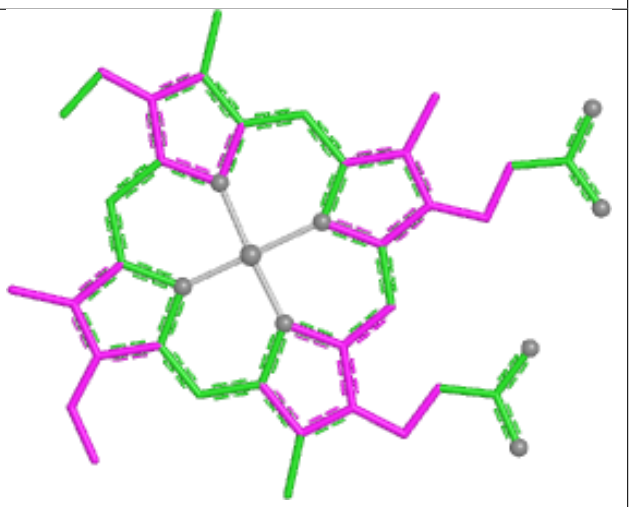
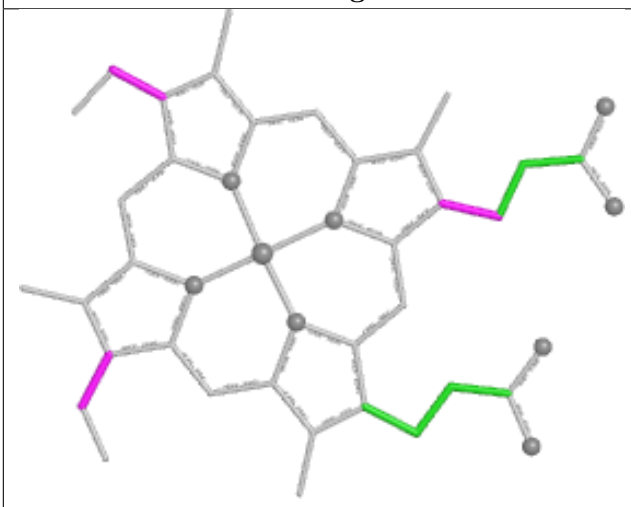


Bond angles



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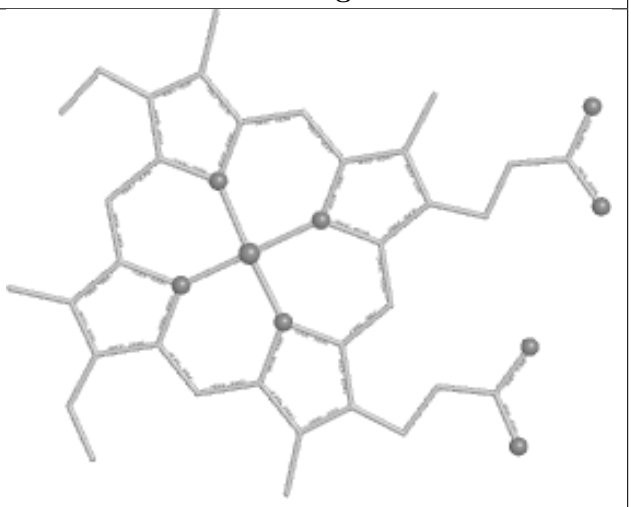
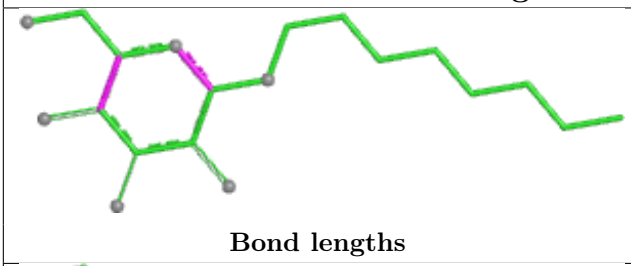


Rings

Ligand BOG Q 3009



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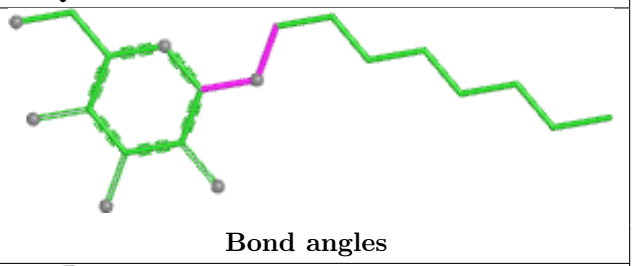

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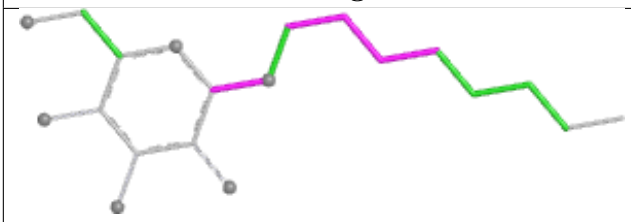

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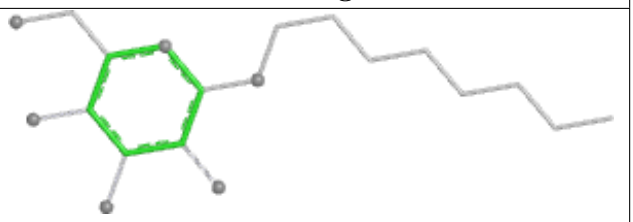
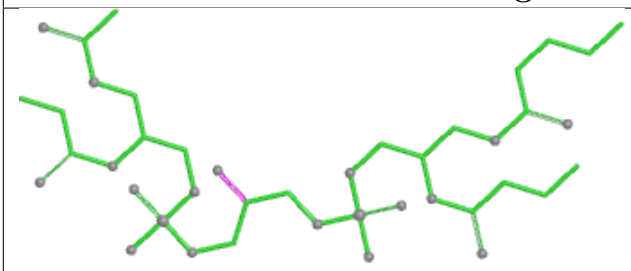


Rings

Ligand CDL Q 3003



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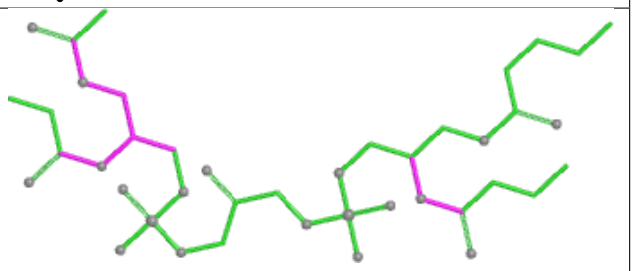
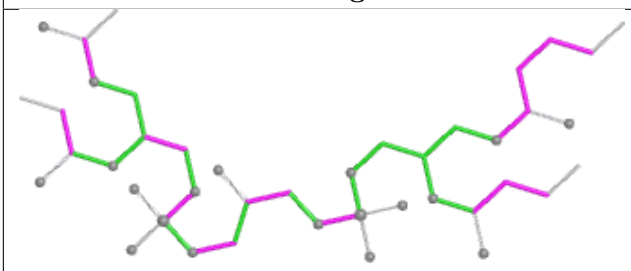


Bond angles



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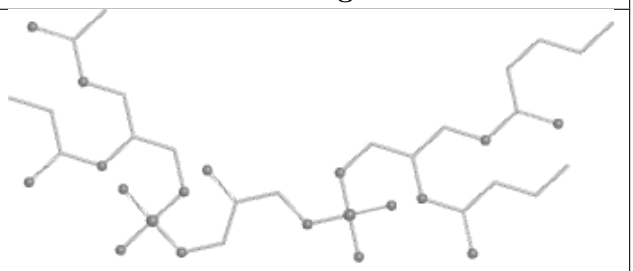
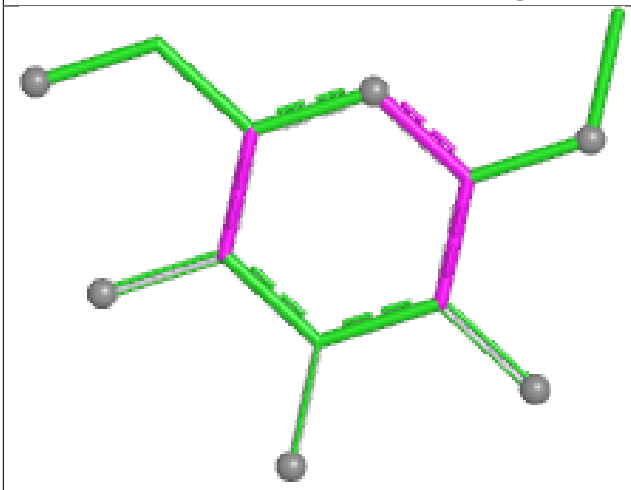


Rings

Ligand BOG D 2091



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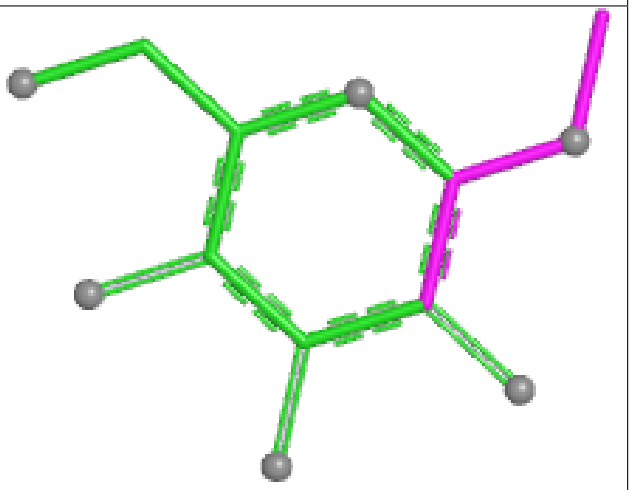
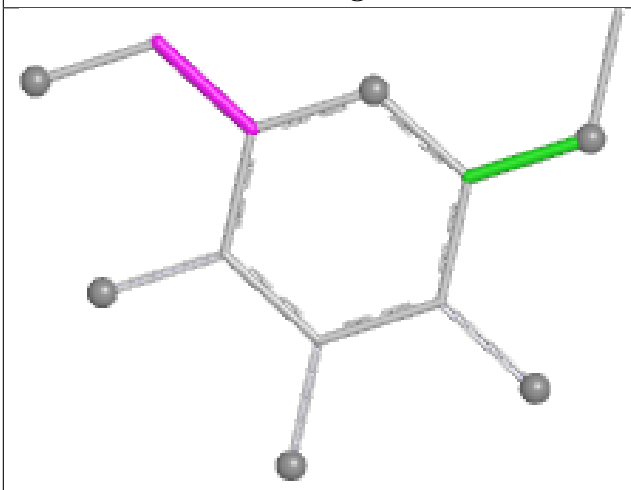


Bond angles



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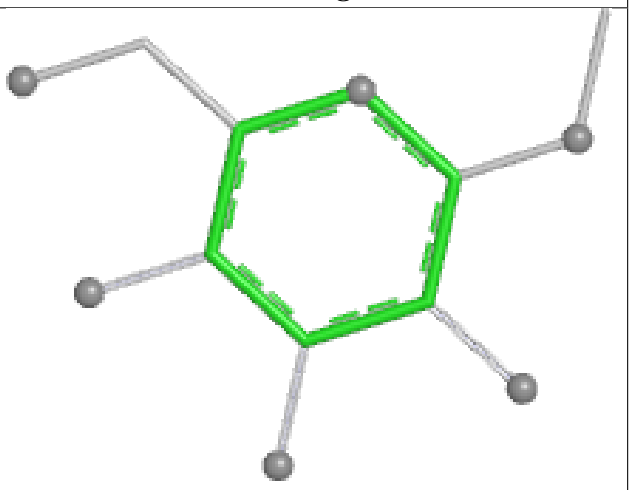
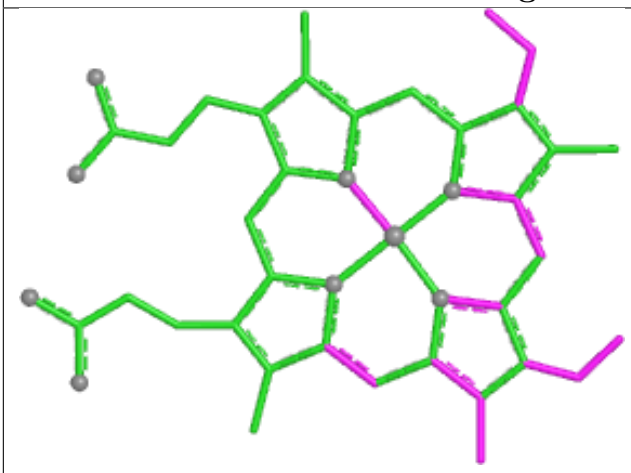


Rings

Ligand HEM C 502



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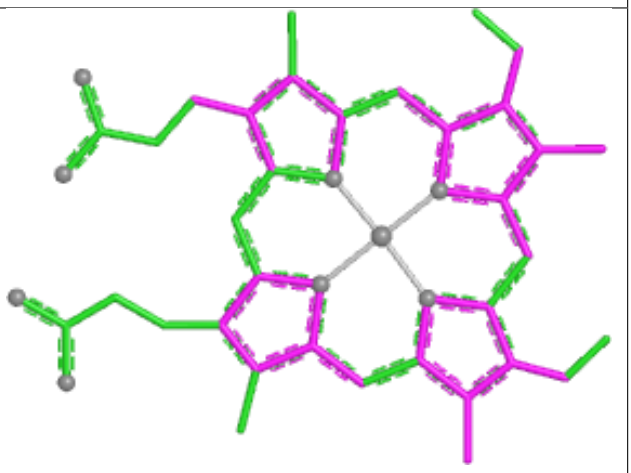

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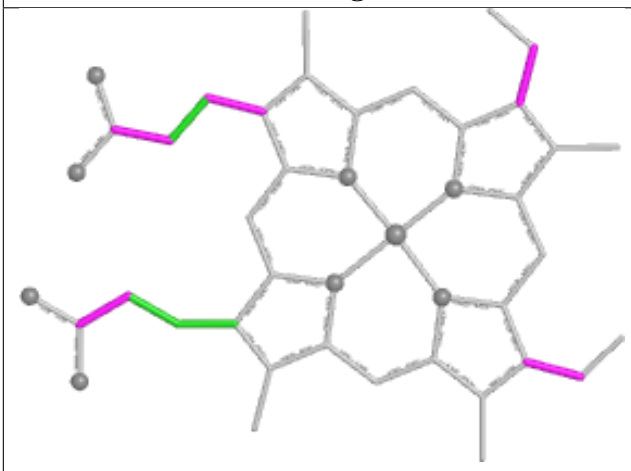

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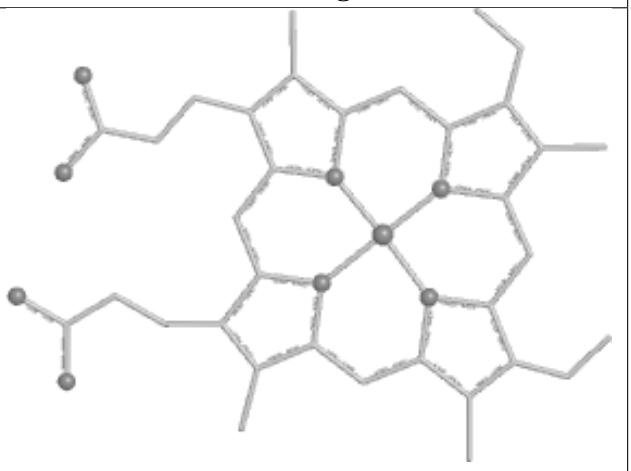
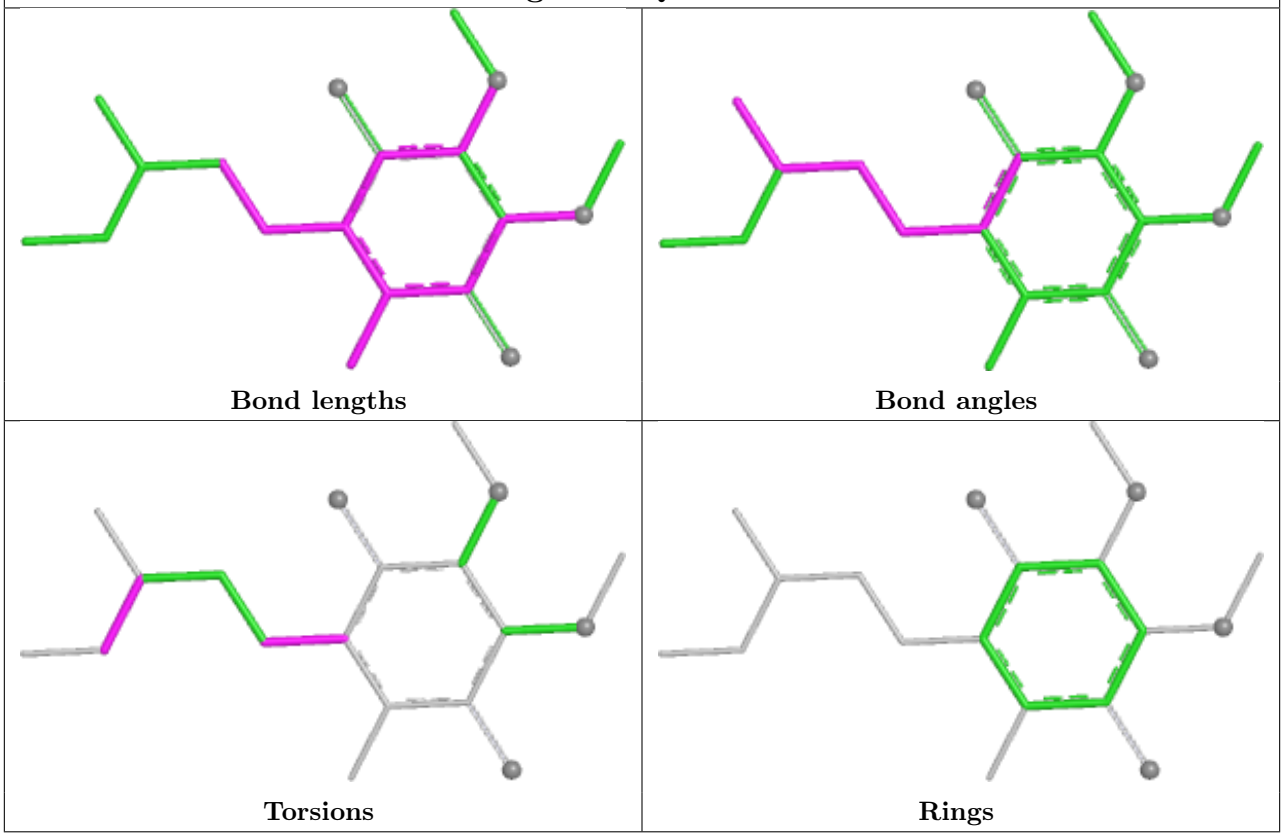
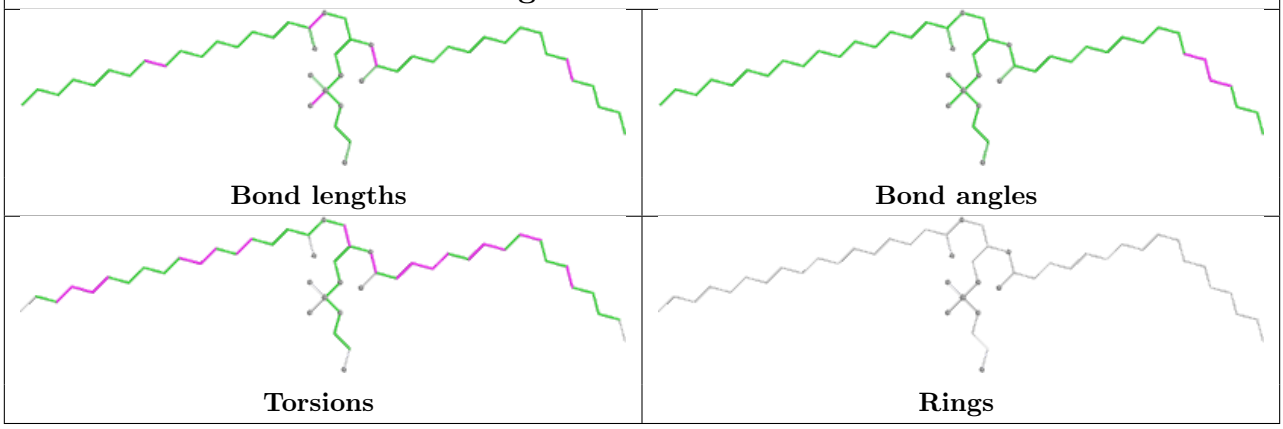


Rings

Ligand UQ C 2002



Ligand PEE P 3007



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, 95th 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%)	-0.40	1 (0%) 91 82	56, 103, 147, 160	0
1	N	442/446 (99%)	-0.29	2 (0%) 87 69	65, 100, 132, 147	0
2	B	426/441 (96%)	-0.19	4 (0%) 81 58	85, 126, 182, 218	0
2	O	422/441 (95%)	-0.29	0 100 100	70, 108, 147, 161	0
3	C	380/380 (100%)	-0.65	1 (0%) 90 77	40, 64, 131, 204	0
3	P	379/380 (99%)	-0.32	4 (1%) 78 54	52, 97, 148, 187	0
4	D	241/241 (100%)	-0.64	0 100 100	48, 72, 121, 138	0
4	Q	241/241 (100%)	-0.17	0 100 100	74, 108, 149, 167	0
5	E	196/196 (100%)	0.31	9 (4%) 37 21	57, 169, 205, 207	125 (63%)
5	R	196/196 (100%)	0.15	7 (3%) 46 26	64, 172, 215, 220	1 (0%)
6	F	101/110 (91%)	-0.66	0 100 100	56, 75, 97, 116	0
6	S	101/110 (91%)	-0.26	1 (0%) 79 57	87, 124, 174, 190	0
7	G	80/81 (98%)	-0.41	2 (2%) 58 35	58, 86, 158, 166	0
7	T	79/81 (97%)	0.22	3 (3%) 44 25	81, 126, 222, 227	0
8	H	69/77 (89%)	-0.42	0 100 100	70, 98, 119, 154	0
8	U	67/77 (87%)	0.20	4 (5%) 27 17	133, 165, 209, 211	0
9	I	31/47 (65%)	1.74	8 (25%) 1 2	147, 185, 257, 259	0
9	V	31/47 (65%)	1.21	7 (22%) 2 2	121, 163, 242, 244	0
10	J	61/61 (100%)	-0.48	0 100 100	75, 93, 139, 177	0
10	W	60/61 (98%)	-0.37	0 100 100	84, 108, 157, 165	0
All	All	4046/4160 (97%)	-0.26	53 (1%) 75 51	40, 104, 189, 259	126 (3%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	63	ASP	5.0
9	I	51	CYS	5.0
9	I	50	LEU	4.9
5	E	142	LEU	4.1
8	U	50	THR	3.6

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 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, 95th 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
20	BOG	P	3091	13/20	0.42	0.17	298,299,299,300	0
11	PEE	P	3008	5/51	0.59	0.10	184,184,184,185	0
11	PEE	A	2008	18/51	0.69	0.20	89,197,198,199	0
16	CDL	Q	3003	42/100	0.73	0.20	183,193,208,208	0
20	BOG	P	2010	12/20	0.73	0.18	248,249,250,250	0
16	CDL	P	3004	40/100	0.73	0.16	147,157,162,162	0
21	FES	R	501	4/4	0.84	0.11	201,201,201,202	0
21	FES	E	501	4/4	0.85	0.12	257,257,257,257	4
11	PEE	R	3005	50/51	0.86	0.19	114,131,139,141	0
16	CDL	D	2003	42/100	0.87	0.17	134,141,153,153	0
12	UNL	A	3231	1/-	0.87	0.08	45,45,45,45	0
20	BOG	Q	3009	20/20	0.87	0.14	103,118,120,121	0
16	CDL	C	2004	40/100	0.87	0.12	103,110,126,128	0
20	BOG	D	2091	13/20	0.87	0.15	191,192,193,193	0
12	UNL	P	4236	1/-	0.88	0.07	94,94,94,94	0
11	PEE	E	2005	50/51	0.89	0.16	113,127,137,139	0
11	PEE	P	3007	49/51	0.89	0.13	102,116,140,141	0
15	UQ	P	3002	19/63	0.91	0.22	134,146,148,149	0
11	PEE	C	2007	49/51	0.92	0.12	68,80,102,104	0

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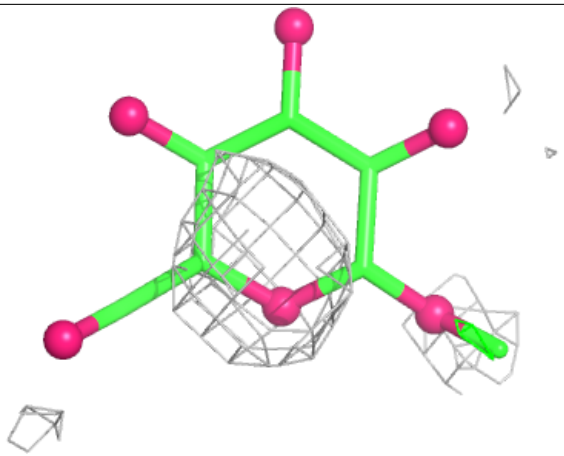
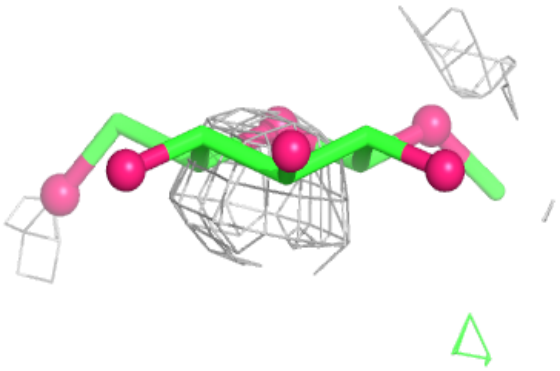
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	BOG	D	2009	20/20	0.93	0.11	93,104,108,108	0
12	UNL	C	4234	1/-	0.94	0.09	58,58,58,58	0
12	UNL	A	3284	1/-	0.94	0.12	31,31,31,31	0
12	UNL	N	4231	1/-	0.95	0.13	90,90,90,90	0
18	GOL	P	3011	6/6	0.95	0.14	103,108,109,110	0
15	UQ	C	2002	19/63	0.95	0.15	107,111,115,115	0
18	GOL	C	2011	6/6	0.96	0.12	69,72,75,78	0
19	HEC	Q	501	43/43	0.97	0.09	87,91,97,99	0
14	IKR	P	3001	25/25	0.97	0.11	86,89,108,116	0
17	ZN	C	2012	1/1	0.98	0.03	104,104,104,104	0
13	HEM	P	502	43/43	0.98	0.09	68,73,82,82	0
13	HEM	P	501	43/43	0.98	0.08	65,72,79,81	0
19	HEC	D	501	43/43	0.98	0.07	57,60,68,70	0
17	ZN	P	3012	1/1	0.99	0.04	121,121,121,121	0
14	IKR	C	2001	25/25	0.99	0.08	65,67,75,79	0
13	HEM	C	501	43/43	0.99	0.06	48,52,62,66	0
13	HEM	C	502	43/43	0.99	0.07	41,46,56,61	0

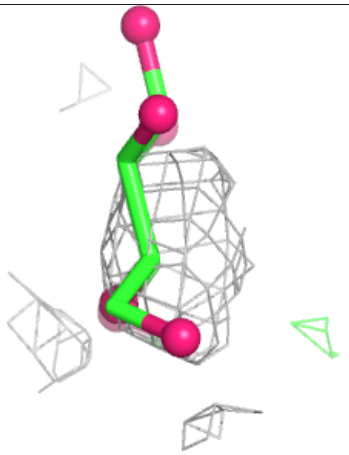
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG P 3091:

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

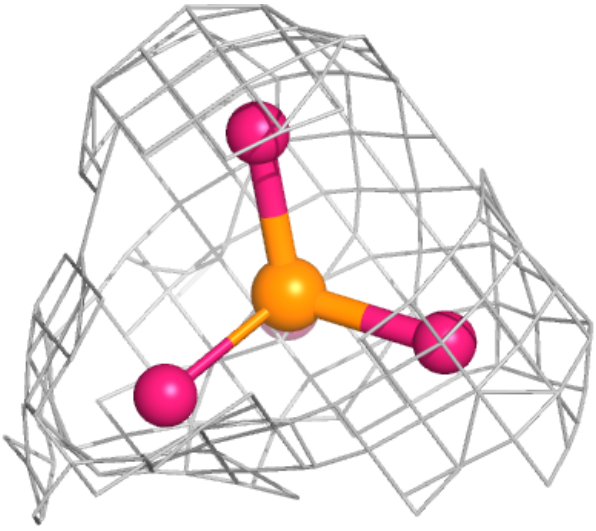


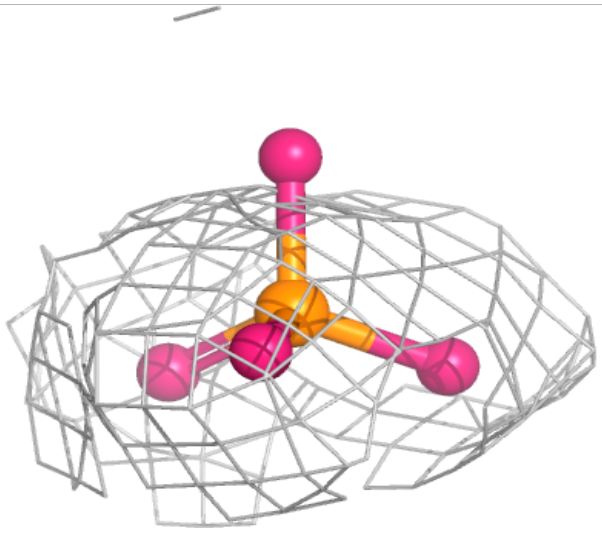


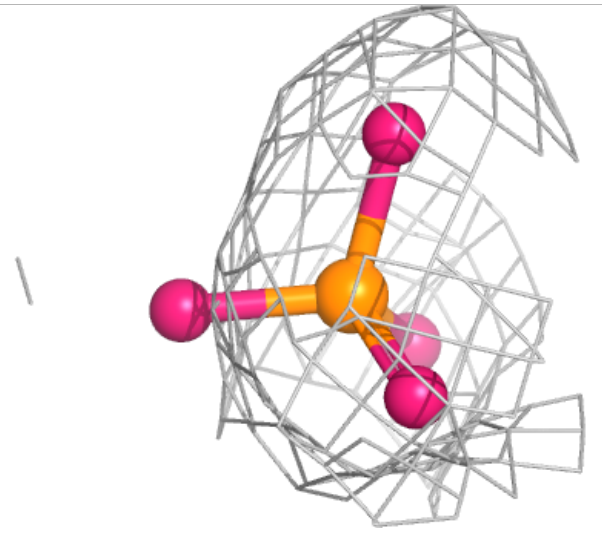


Electron density around PEE P 3008:

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

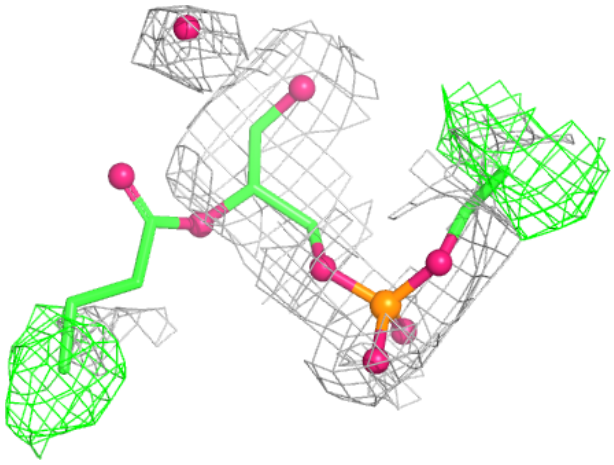


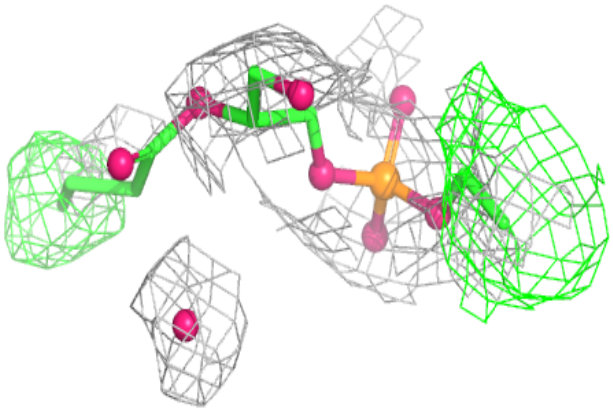


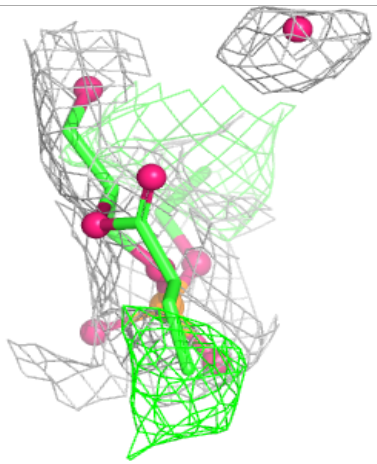


Electron density around PEE A 2008:

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

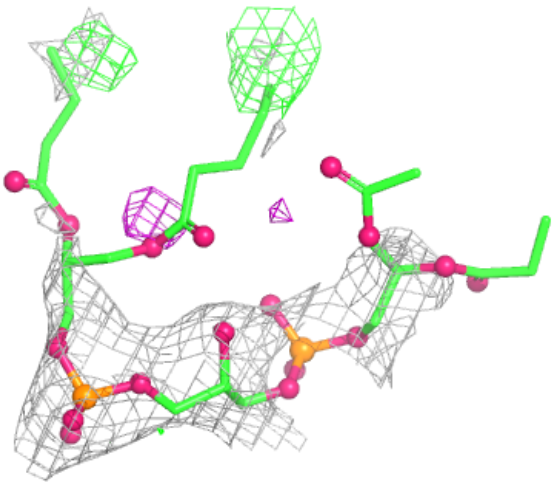


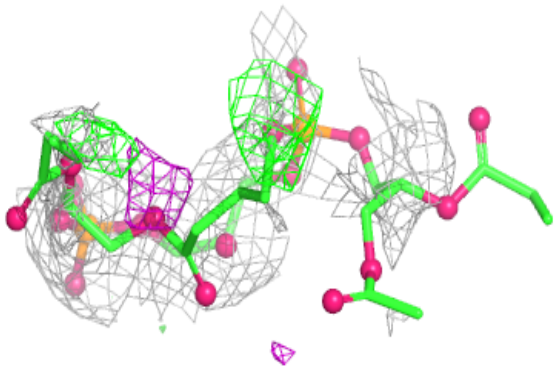


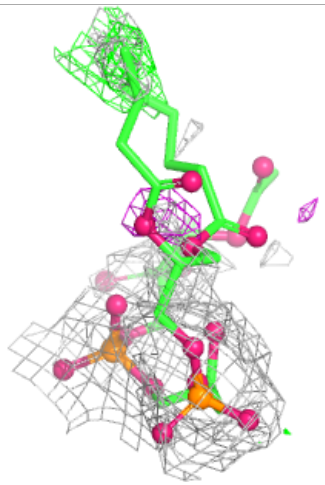


Electron density around CDL Q 3003:

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

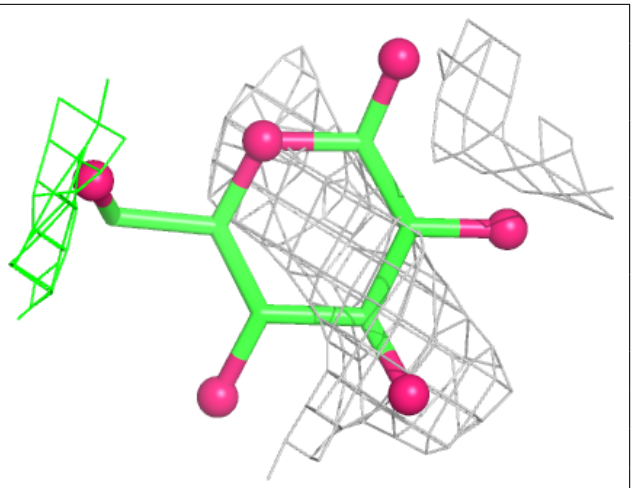


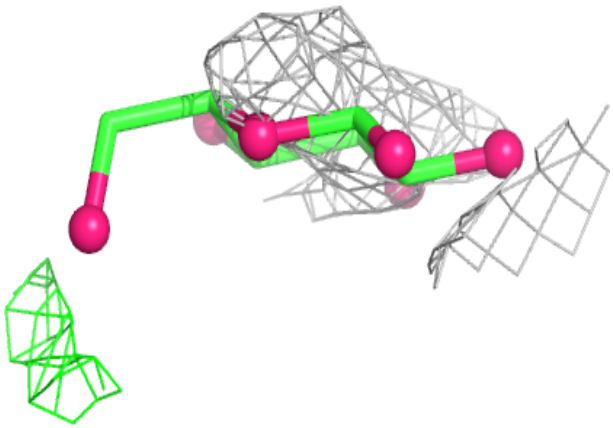


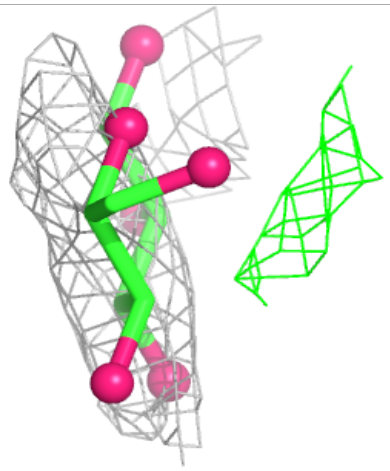


Electron density around BOG P 2010:

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

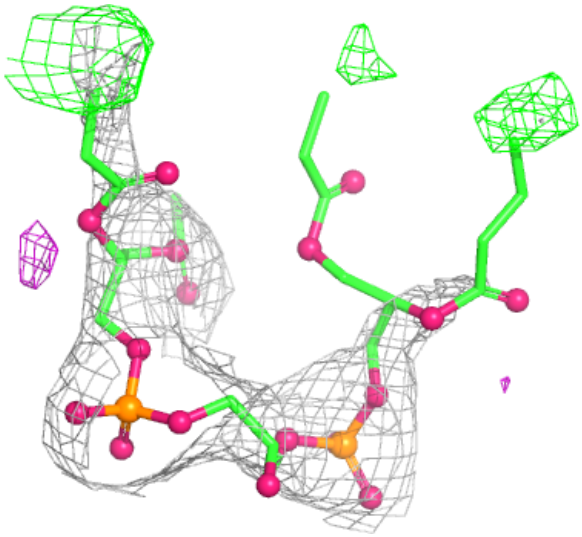


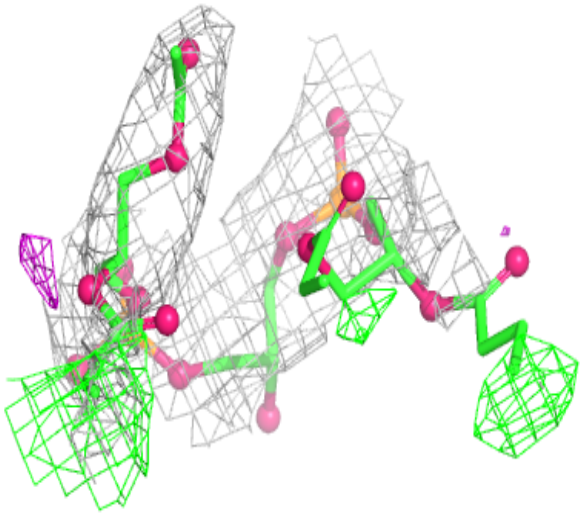


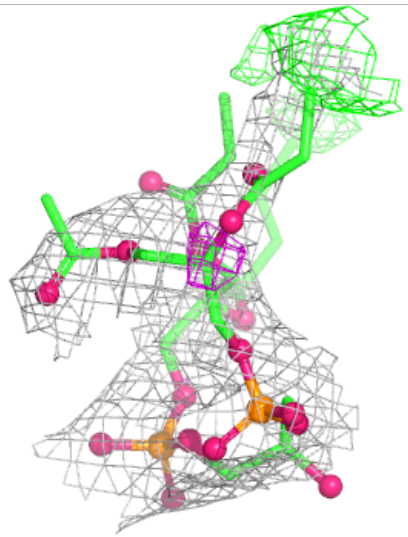


Electron density around CDL P 3004:

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

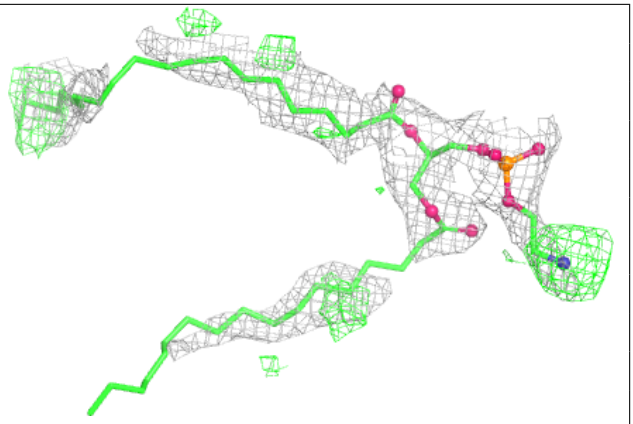


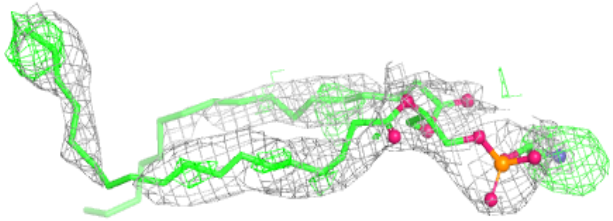


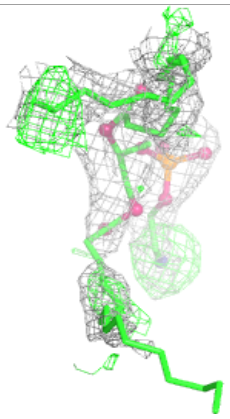


Electron density around PEE R 3005:

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

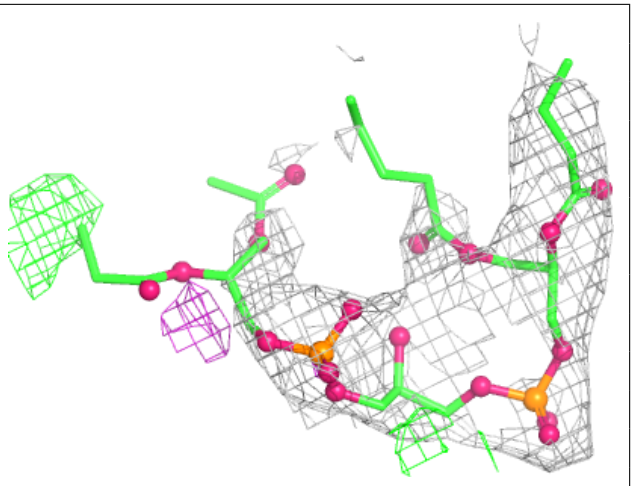


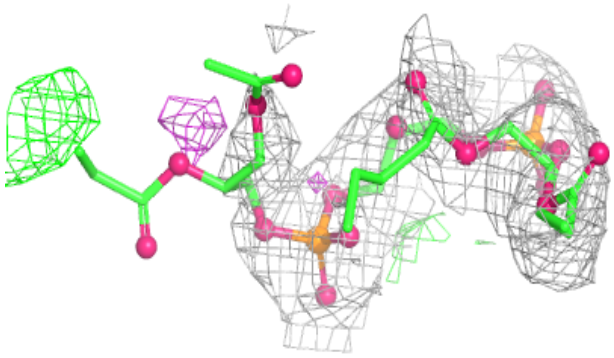


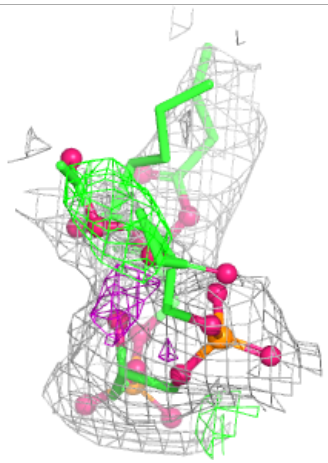


Electron density around CDL D 2003:

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

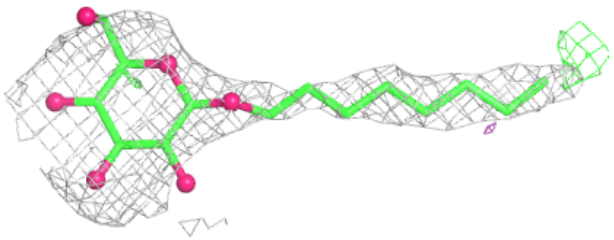


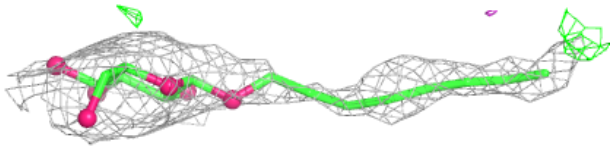


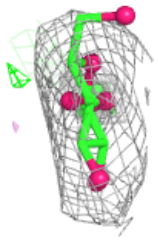


Electron density around BOG Q 3009:

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

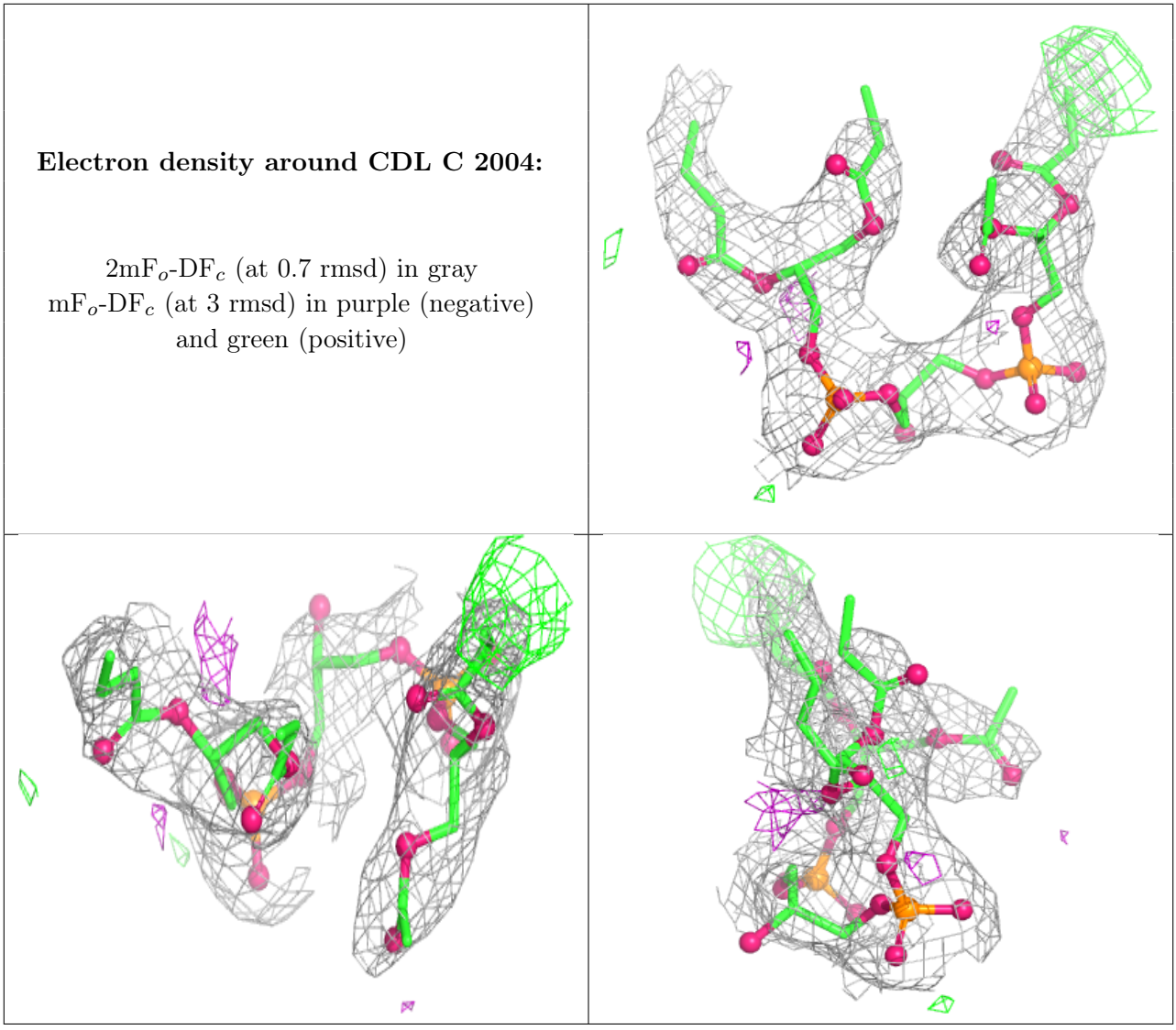






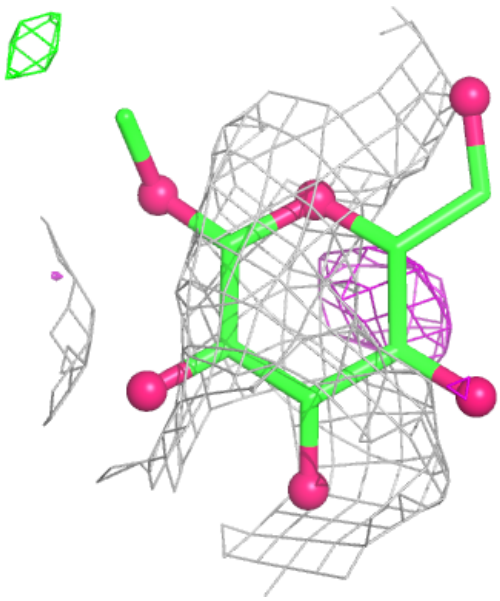
Electron density around CDL C 2004:

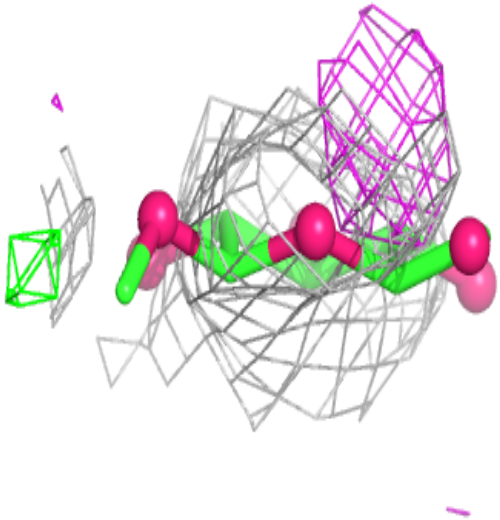
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BOG 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)

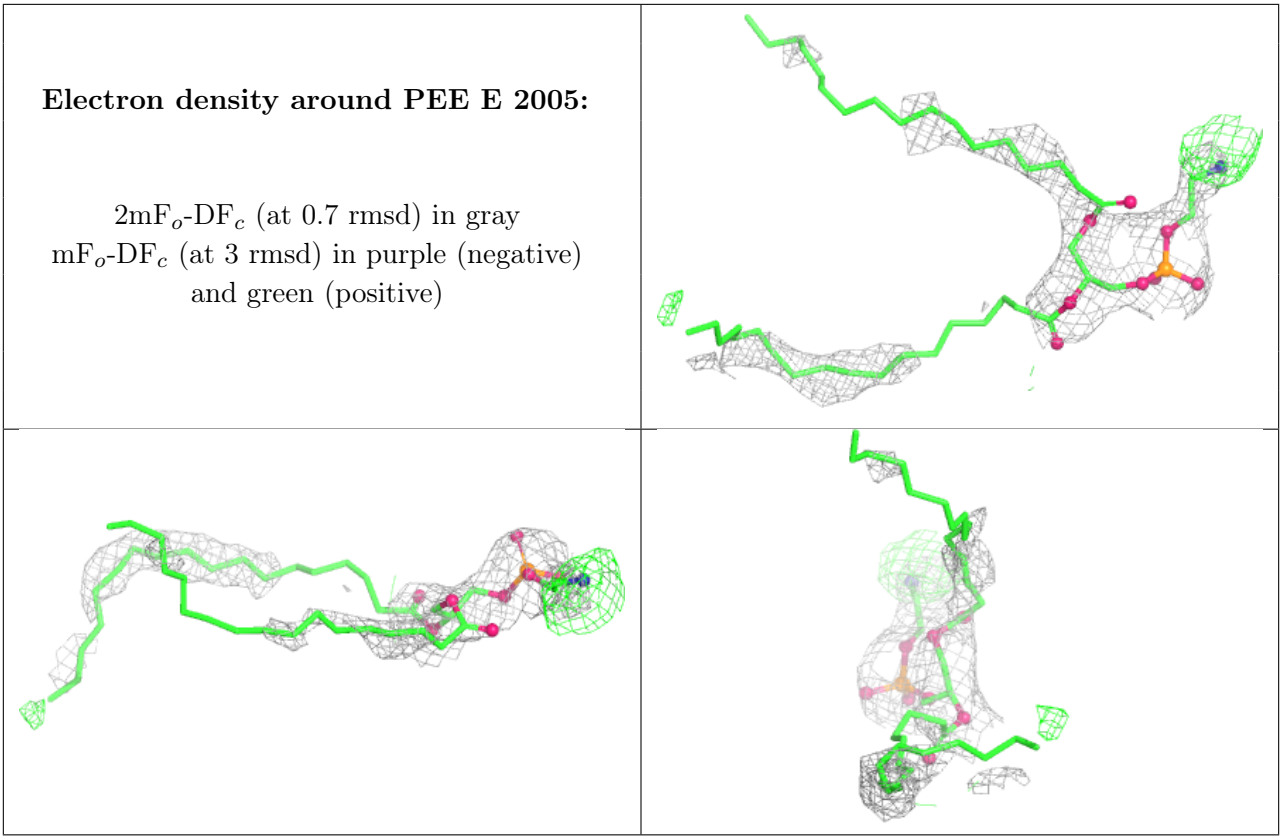






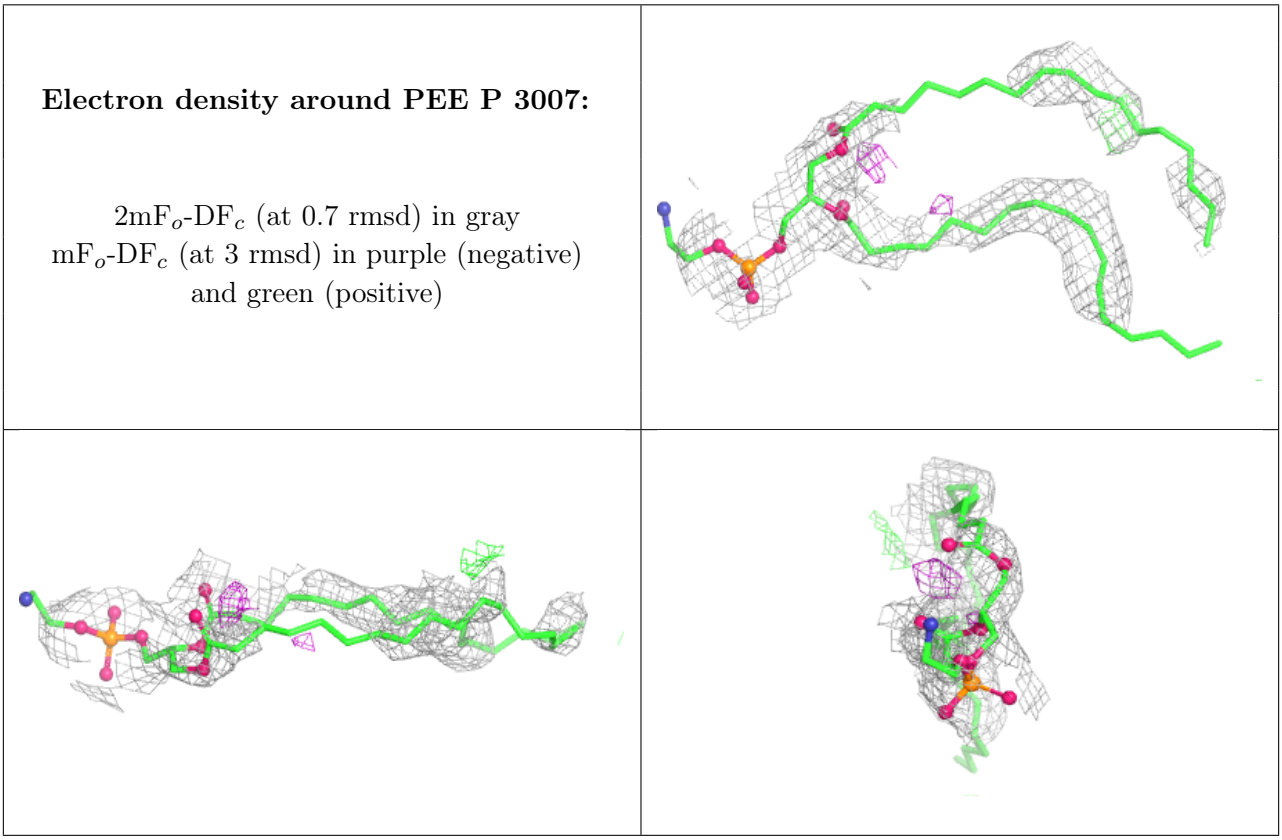
Electron density around PEE E 2005:

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



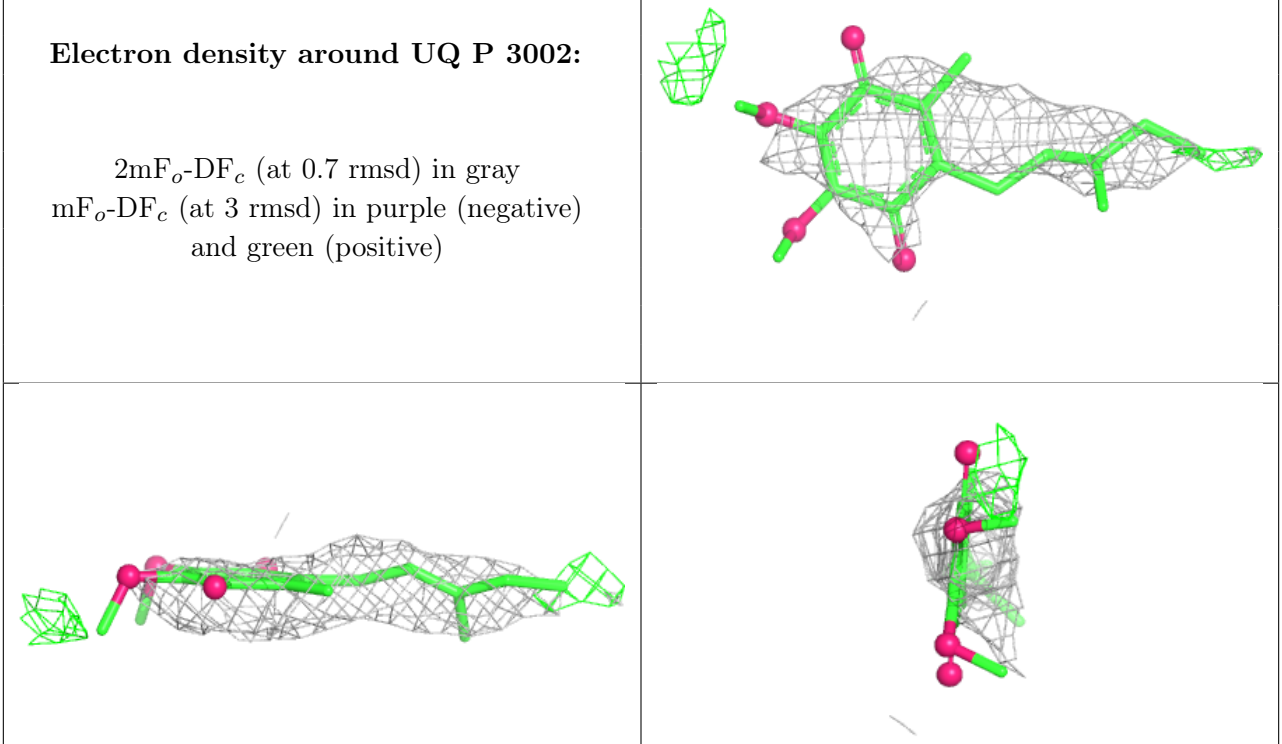
Electron density around PEE P 3007:

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



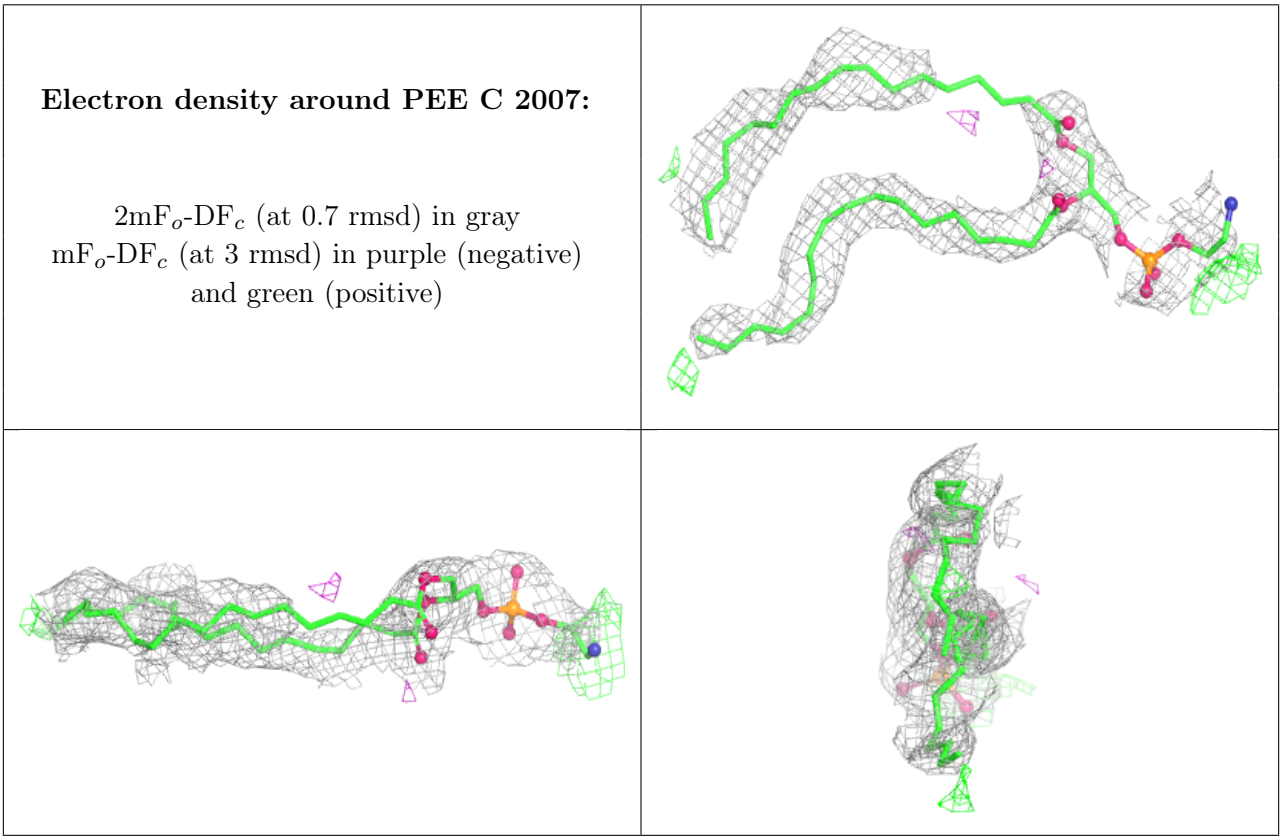
Electron density around UQ P 3002:

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



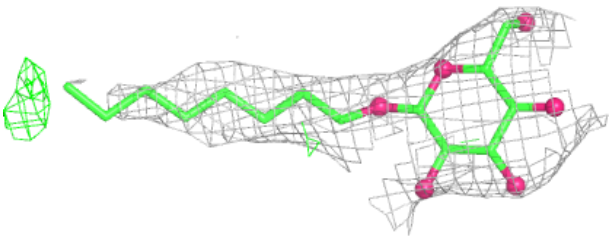
Electron density around PEE C 2007:

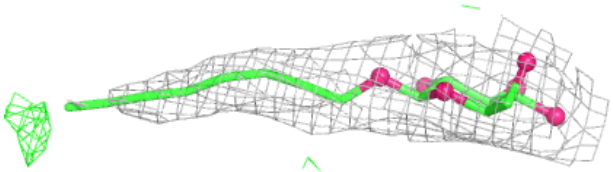
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

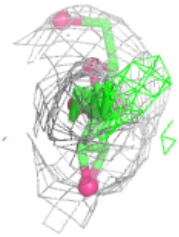


Electron density around BOG D 2009:

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

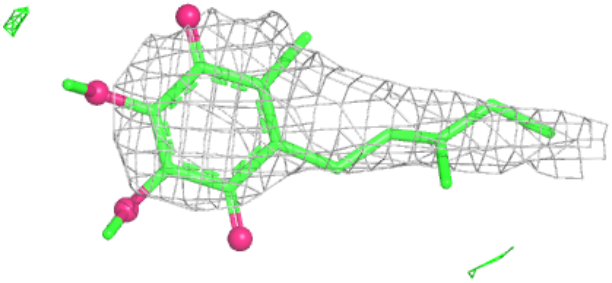


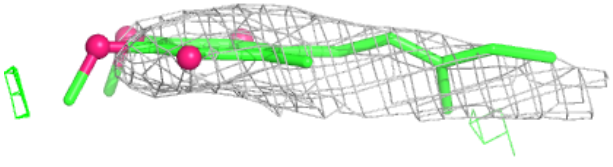


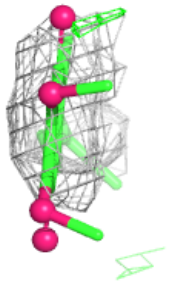


Electron density around UQ C 2002:

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

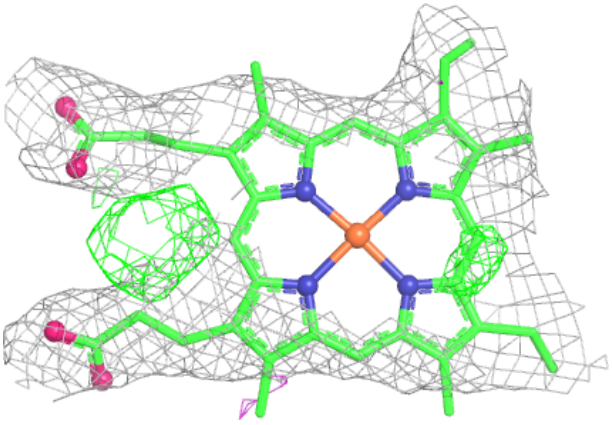


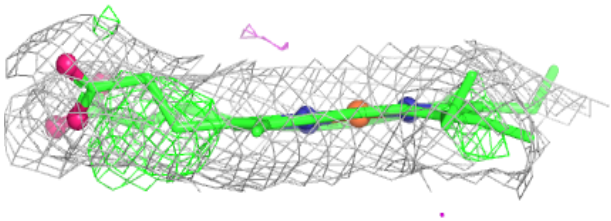


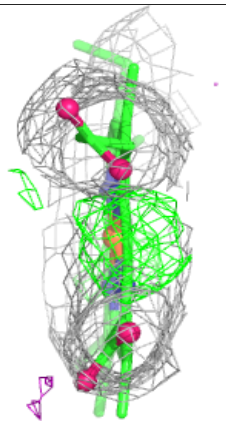


Electron density around HEC Q 501:

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

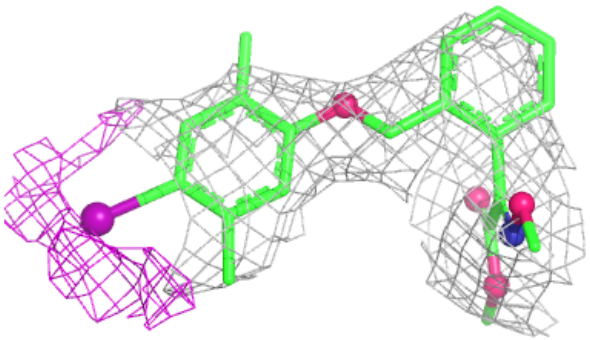


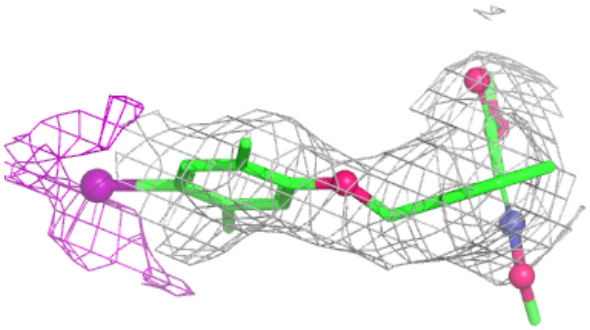


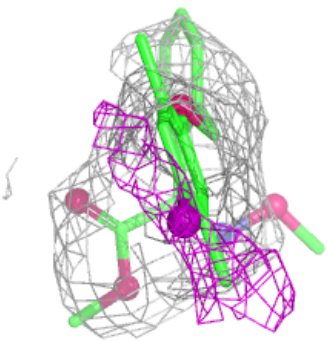


Electron density around IKR P 3001:

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

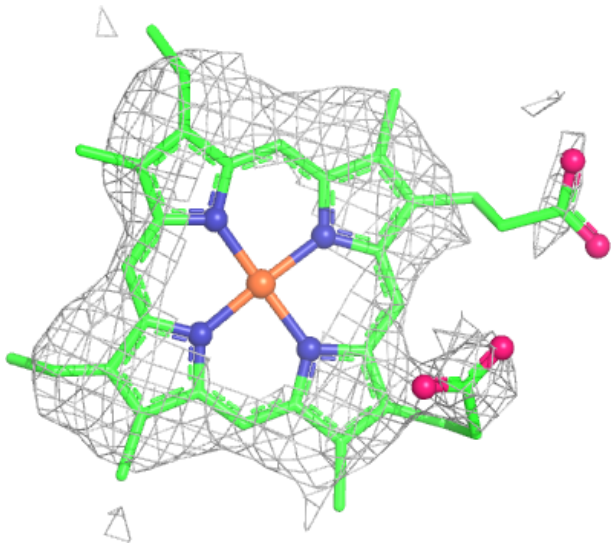


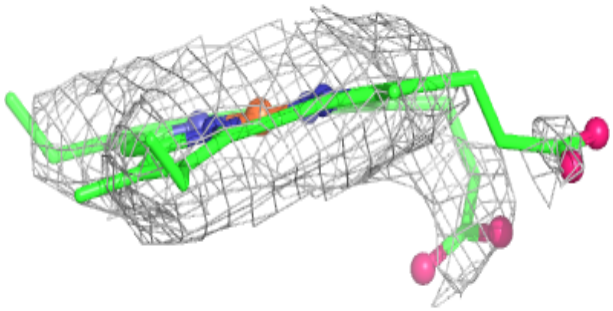


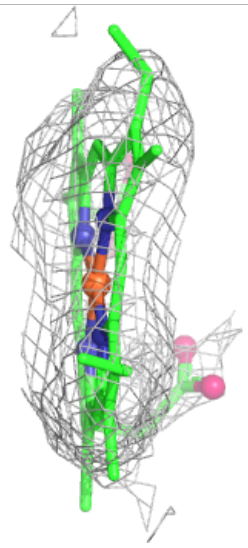


Electron density around HEM P 502:

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

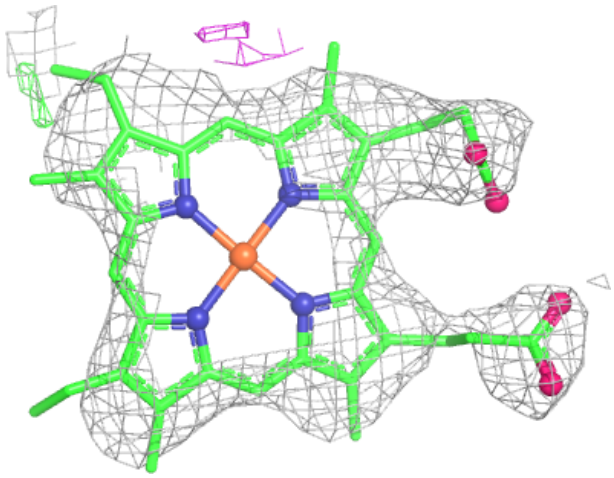


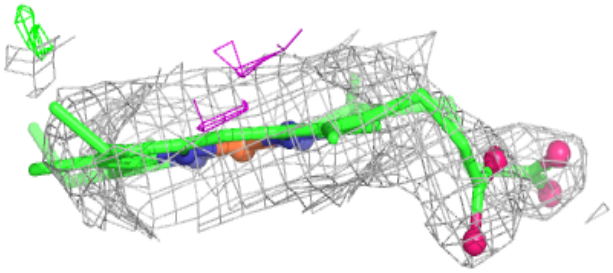


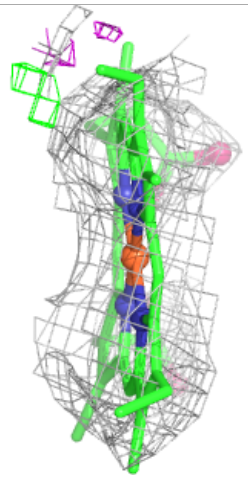


Electron density around HEM P 501:

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

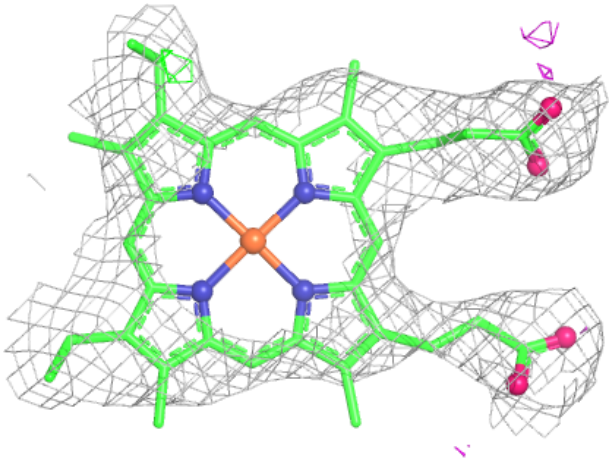


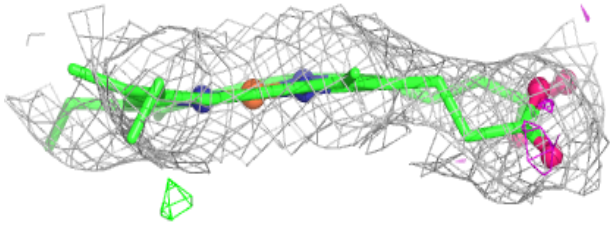


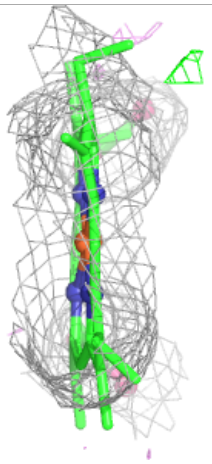


Electron density around HEC D 501:

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

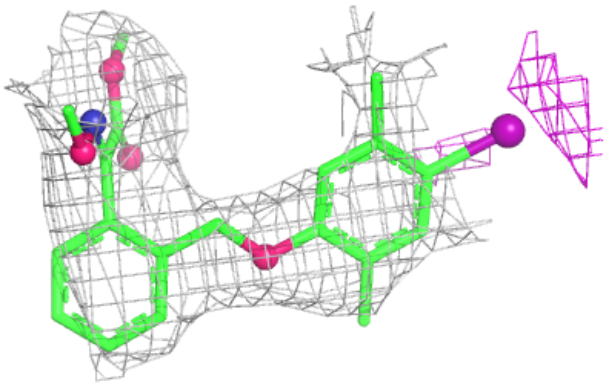


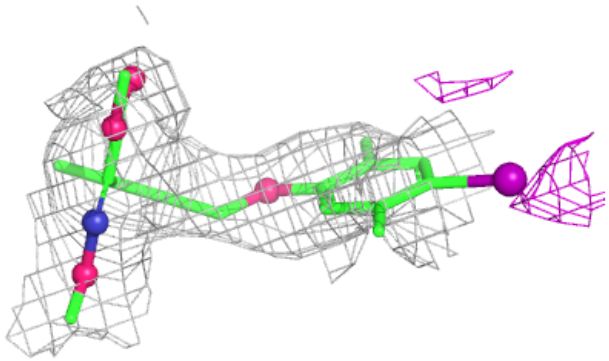




Electron density around IKR C 2001:

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

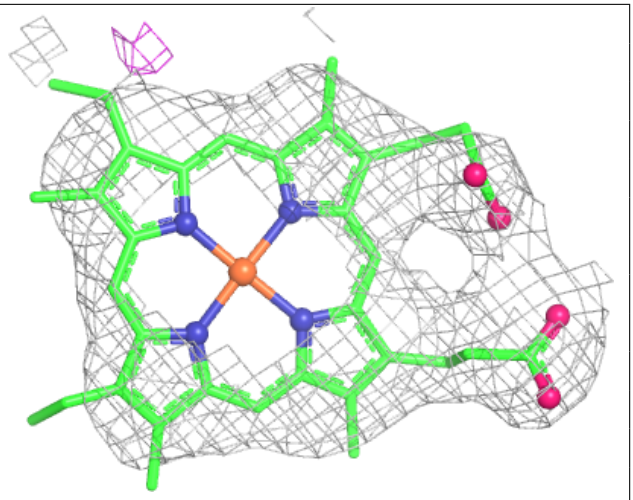


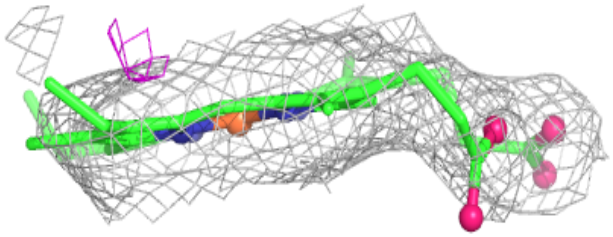


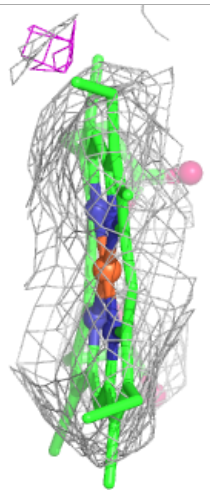


Electron density around HEM C 501:

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

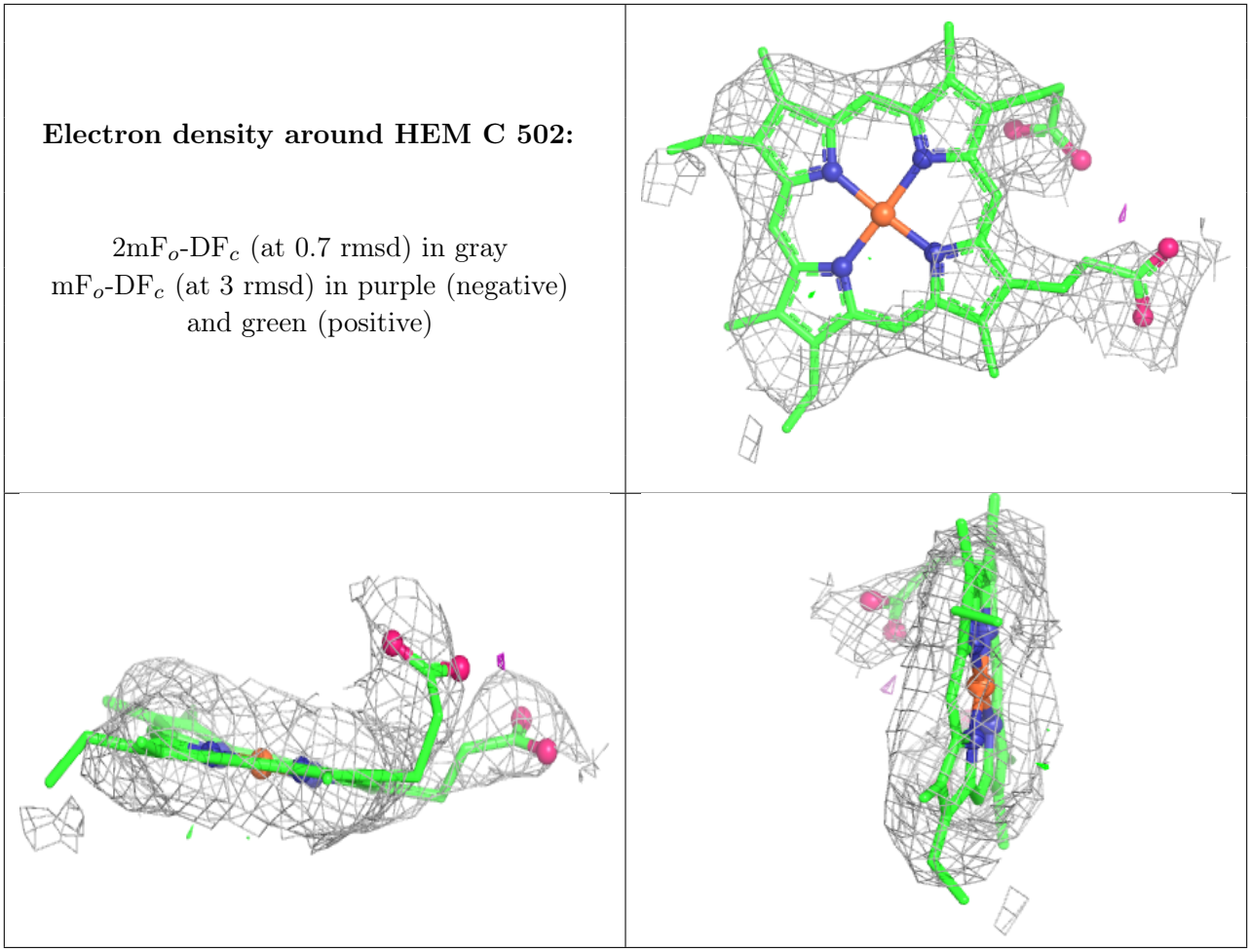






Electron density around HEM C 502:

$2mF_o$-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.