wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 11:09 AM EDT

PDB ID	:	3TGU / pdb_00003tgu
Title	:	Cytochrome bc1 complex from chicken with pfvs-designed moa inhibitor bound
Authors	:	Huang, L.-S.; Yang, G.-F.; Berry, E.A.
Deposited on	:	2011-08-17
Resolution	:	2.70 Å(reported)

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

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

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

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

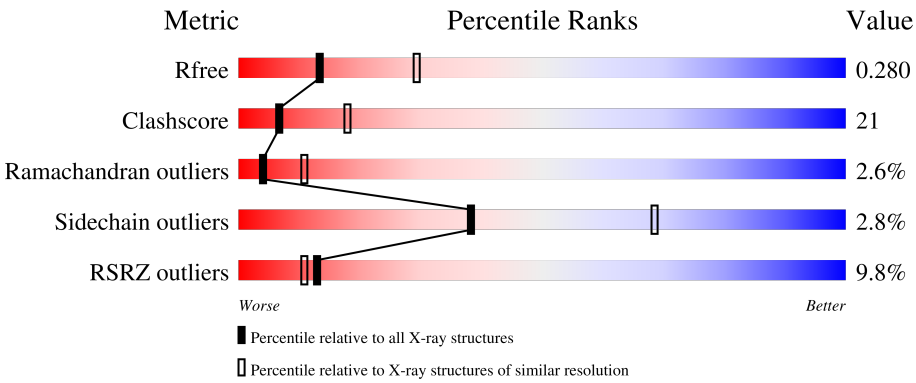
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	4%, 62%, 34%, • •
1	N	446	7%, 61%, 35%, • •
2	B	441	7%, 51%, 41%, •, 5%
2	O	441	7%, 50%, 39%, 6%, •
3	C	380	3%, 72%, 25%, •

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Mol	Chain	Length	Quality of chain
3	P	380	6% 69% 27%
4	D	241	2% 65% 32%
4	Q	241	7% 63% 34%
5	E	196	32% 44% 47% 9%
5	R	196	22% 50% 44% 6%
6	F	110	72% 19% 8%
6	S	110	10% 61% 26% 5% 8%
7	G	81	4% 56% 36% 7%
7	T	81	16% 54% 36% 7%
8	H	77	5% 58% 30% 9%
8	U	77	43% 47% 36% 13%
9	I	76	37% 33% 30% 5% 32%
9	V	76	39% 30% 32% 34%
10	J	61	2% 70% 26%
10	W	61	3% 59% 30% 10%

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
16	PEE	N	502	-	X	-	-
18	HEC	D	501	X	-	-	-
18	HEC	Q	501	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 32733 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
			Total	C	N	O	S			
1	A	443	3442	2157	606	658	21	0	0	0
1	N	442	3437	2154	605	657	21	0	0	0

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

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

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	380	3021	2025	478	505	13	0	0	0
3	P	379	3012	2019	477	504	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	-	initiating methionine	UNP P18946
P	1	FME	-	initiating methionine	UNP P18946

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

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

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1513	952	263	292	6	0	0	0
5	R	196	1509	950	263	290	6	0	0	0

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	891	570	159	159	3	0	0	0
6	S	101	891	570	159	159	3	0	0	0

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	G	80	672	437	119	116	0	0	0
7	T	79	662	432	117	113	0	0	0

- 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
			Total	C	N	O	S			
8	H	70	574	350	105	114	5	0	0	0
8	U	67	553	338	103	107	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	52	319	190	65	61	3	0	0	2
9	V	50	311	186	63	59	3	0	0	2

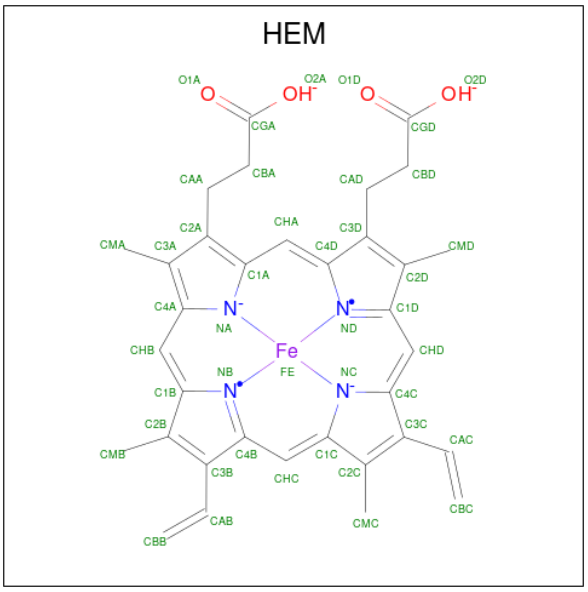
- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	61	497	321	87	89	0	0	0
10	W	60	479	311	86	82	0	0	1

- Molecule 11 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

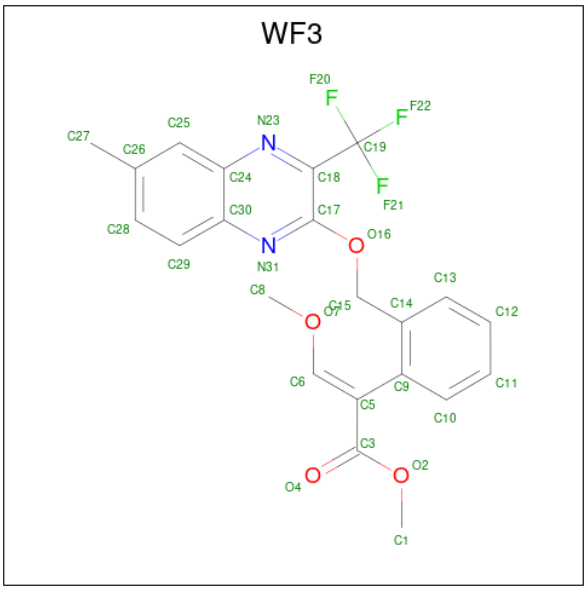
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	1	1	1	0	0
11	N	1	1	1	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



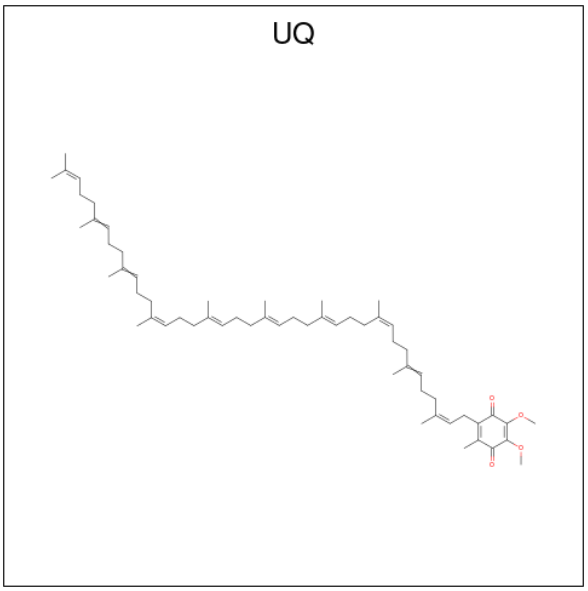
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0

- Molecule 13 is methyl (2E)-3-methoxy-2-[2-({[6-methyl-3-(trifluoromethyl)quinoxalin-2-yl]oxy}methyl)phenyl]prop-2-enoate (CCD ID: WF3) (formula: $C_{22}H_{19}F_3N_2O_4$).



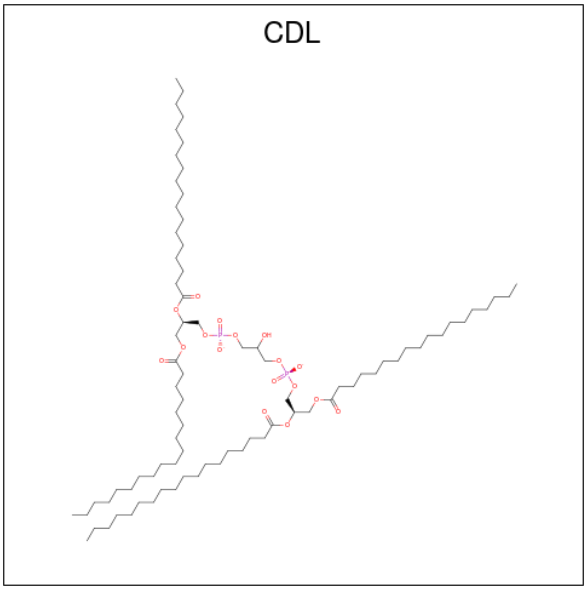
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
13	C	1	31	22	3	2	4	0	0
			Total	C	F	N	O		
13	P	1	31	22	3	2	4	0	0

- Molecule 14 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
			Total	C	O		
14	C	1	19	15	4	0	0
			Total	C	O		
14	P	1	19	15	4	0	0

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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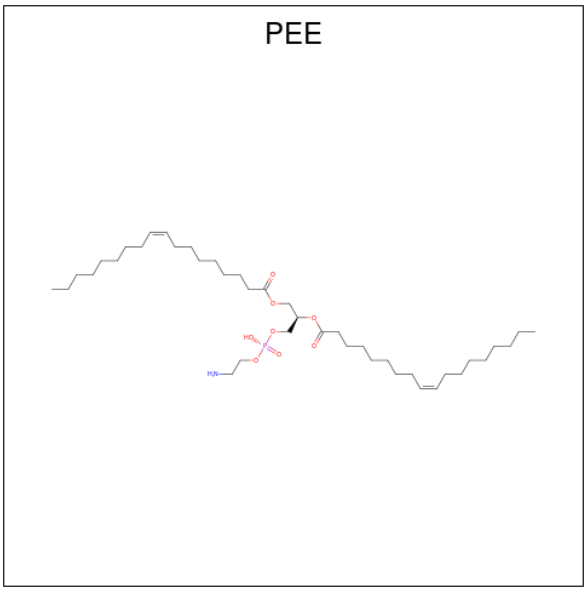
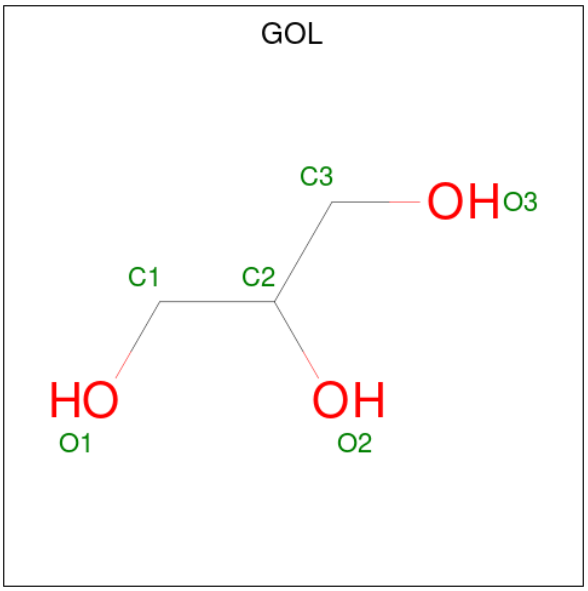
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
15	P	1	40	21	17	2	0	0
			Total	C	O	P		
15	Q	1	42	23	17	2	0	0

- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



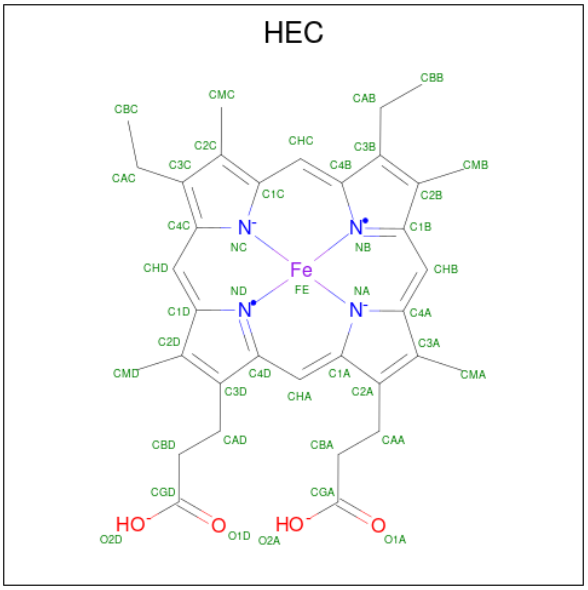
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	C	1	49	39	1	8	1	0	0
			Total	C	O	P			
16	C	1	21	12	8	1		0	0
			Total	C	N	O	P		
16	E	1	50	40	1	8	1	0	0
			Total	O	P				
16	N	1	5	4	1			0	0
			Total	C	N	O	P		
16	P	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
16	R	1	49	39	1	8	1	0	0

- Molecule 17 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



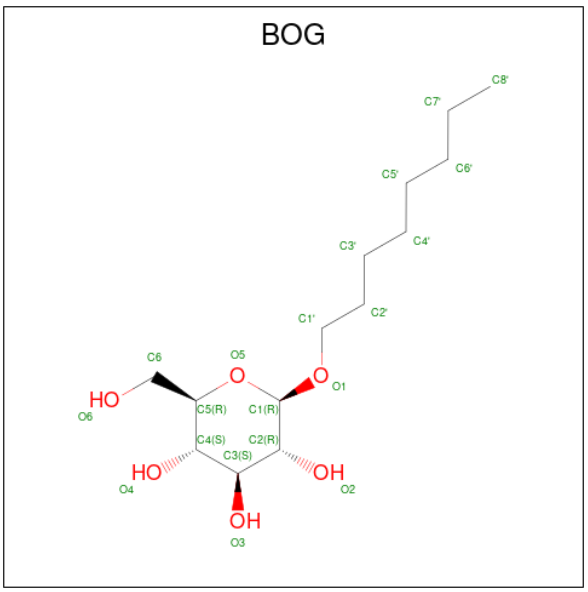
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
17	C	1	6	3	3	0	0
			Total	C	O		
17	P	1	6	3	3	0	0

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



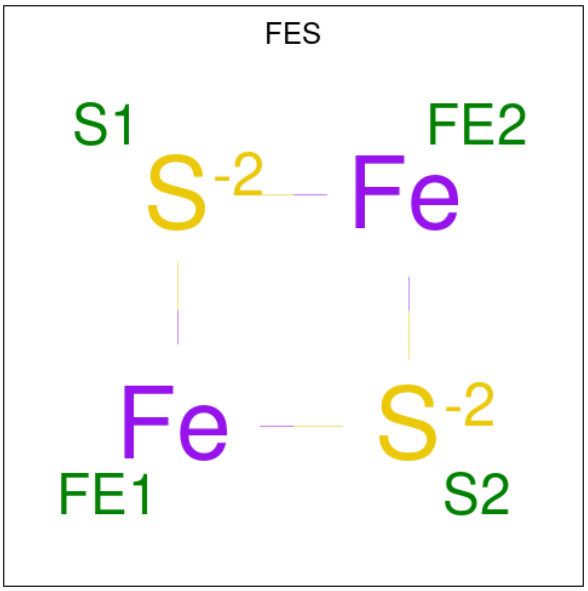
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
18	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
18	Q	1	43	34	1	4	4	0	0

- Molecule 19 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 21 is water.

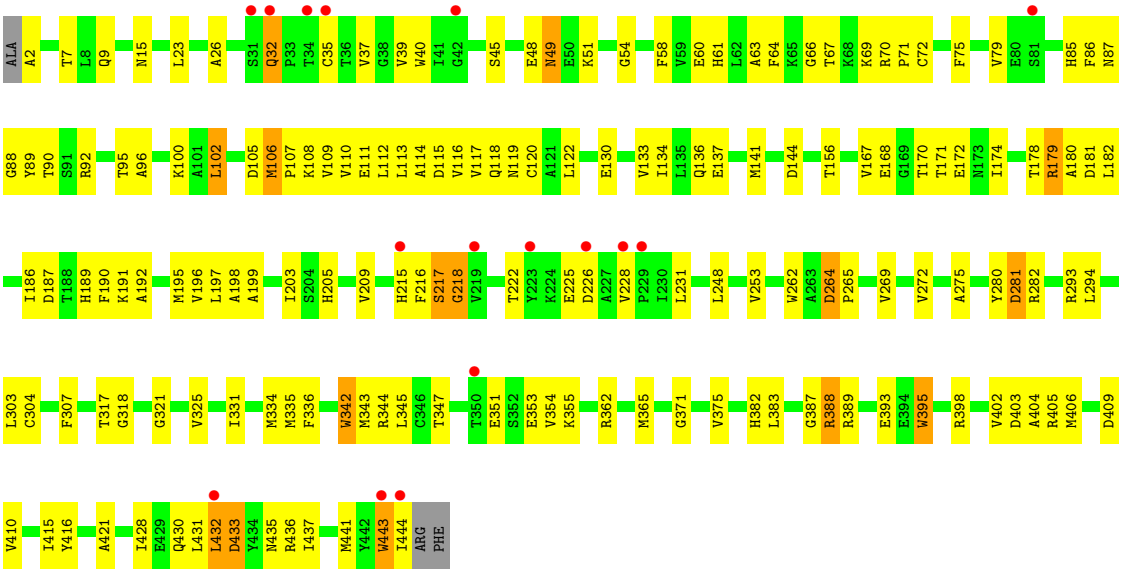
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
21	C	9	9	9	0	0
21	E	1	1	1	0	0
21	P	10	10	10	0	0
21	R	1	1	1	0	0

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.

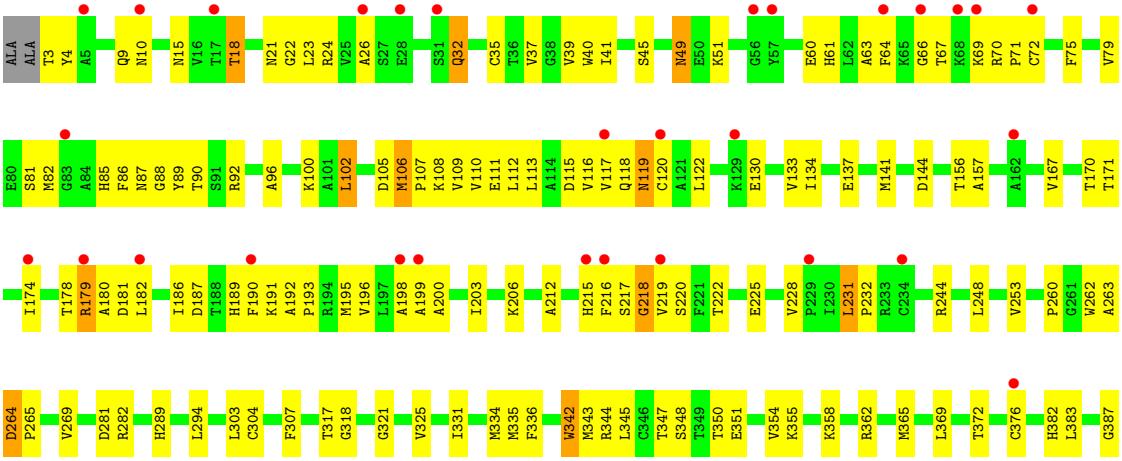
• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

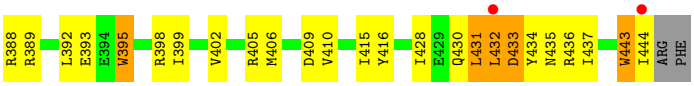
Chain A:



• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

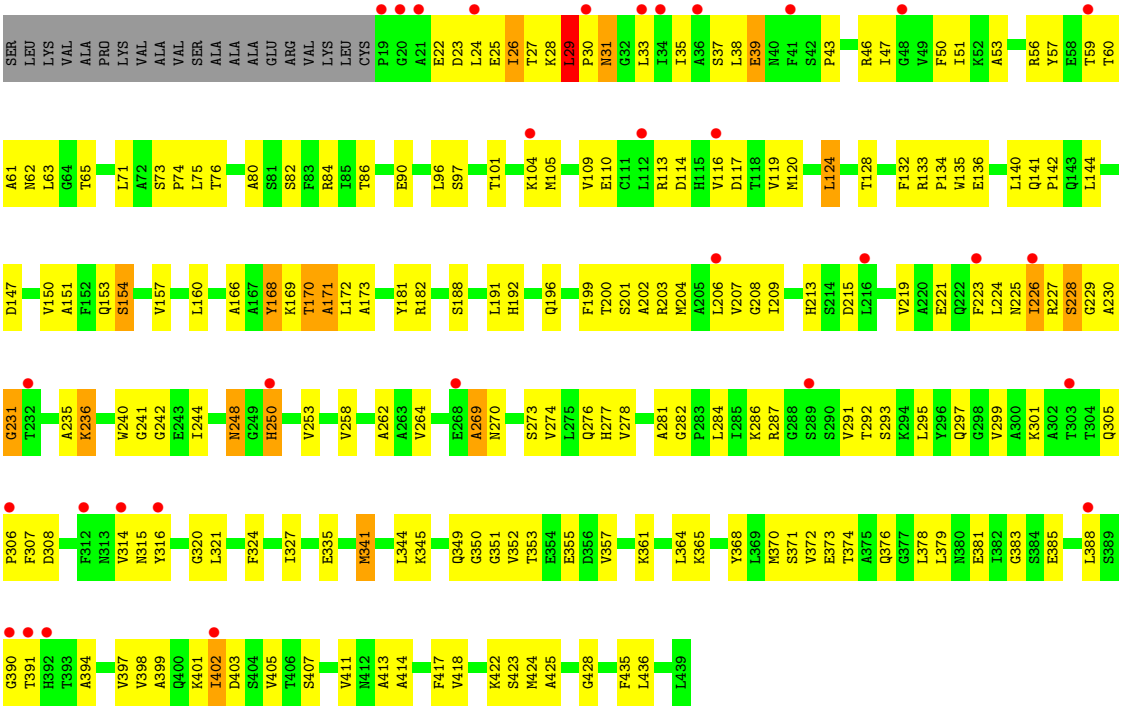
Chain N:





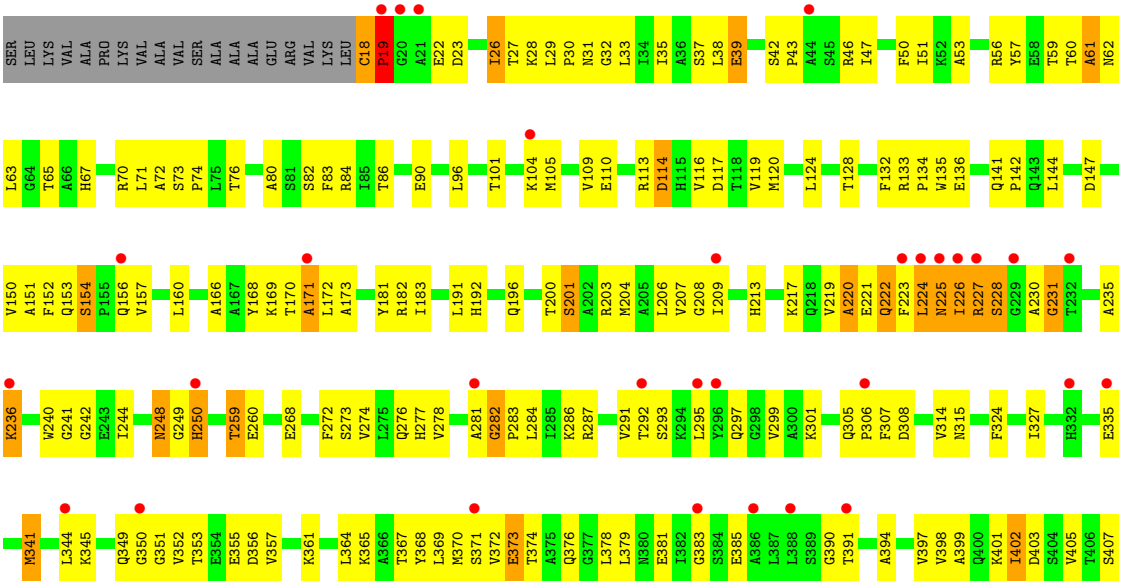
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

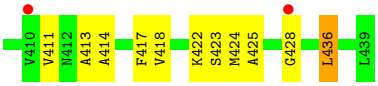
Chain B:



• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

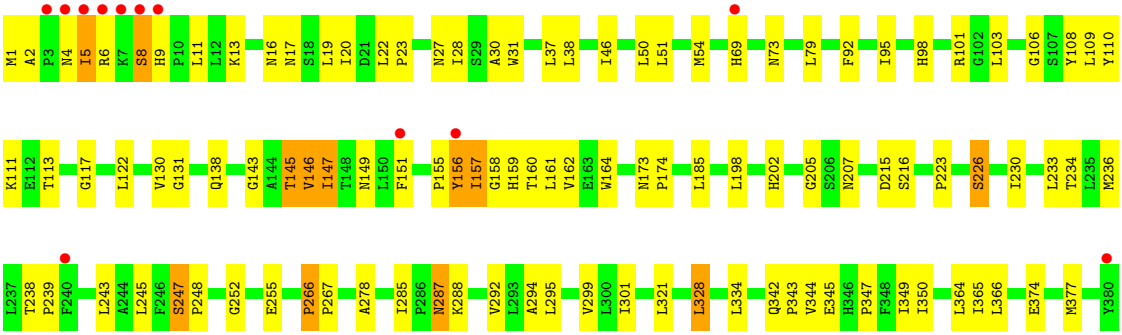
Chain O:





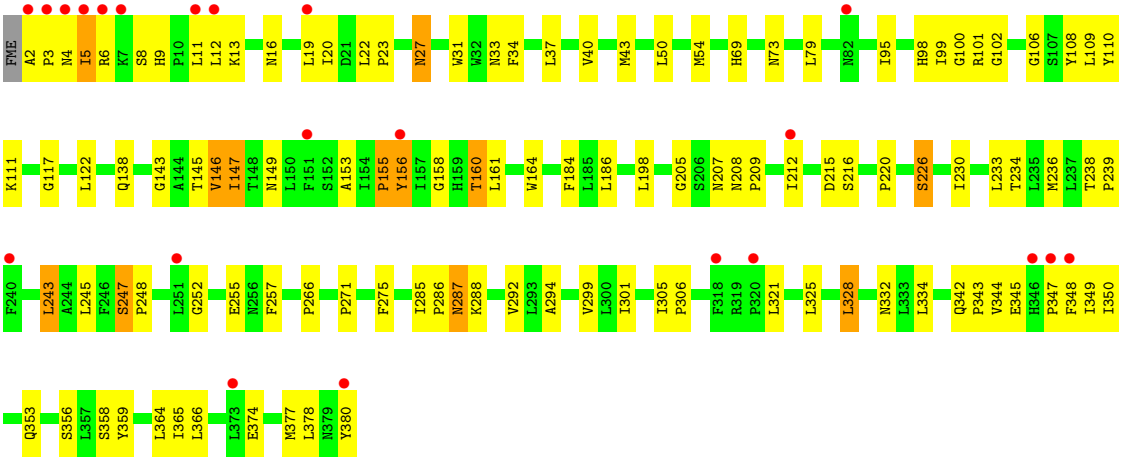
• Molecule 3: Cytochrome b

Chain C:



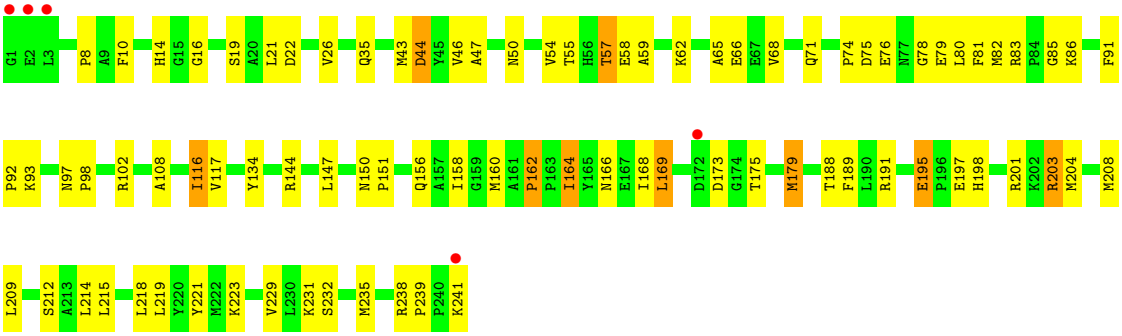
• Molecule 3: Cytochrome b

Chain P:



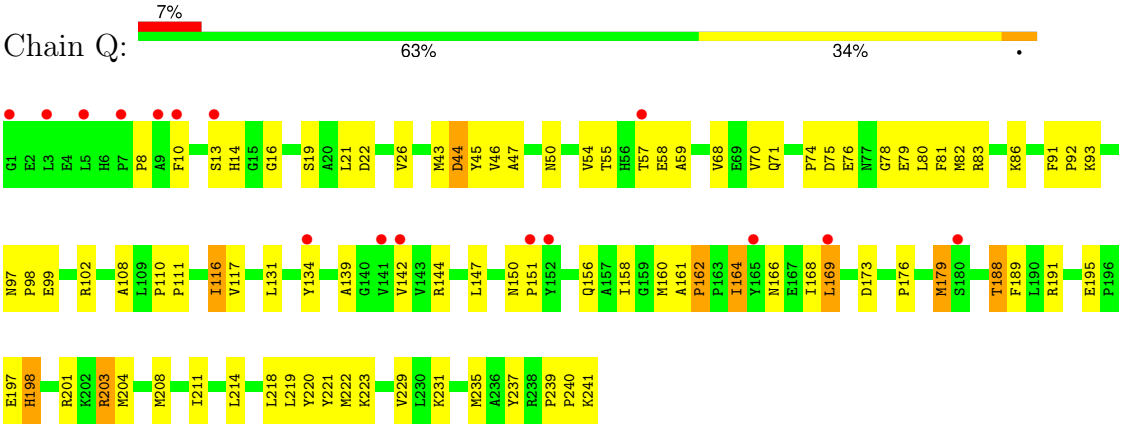
• Molecule 4: Mitochondrial cytochrome c1, heme protein

Chain D:



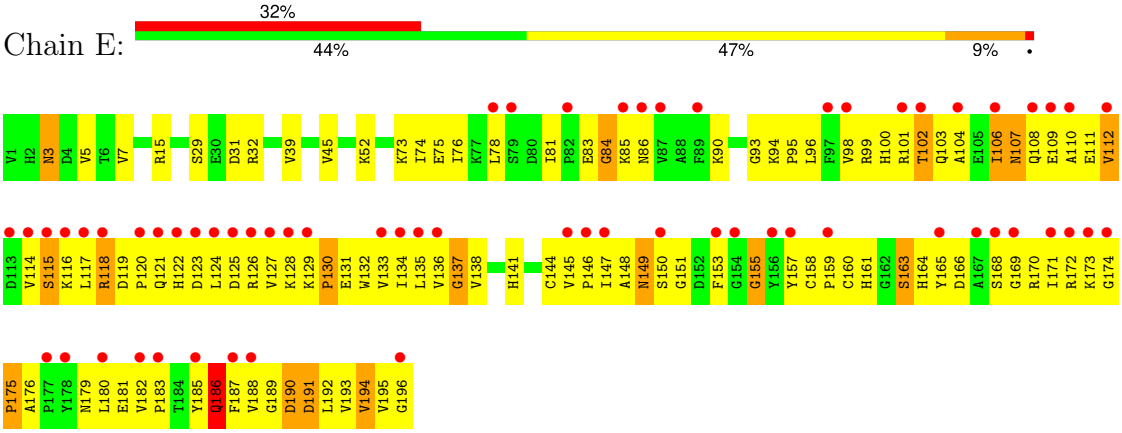
• Molecule 4: Mitochondrial cytochrome c1, heme protein

Chain Q:



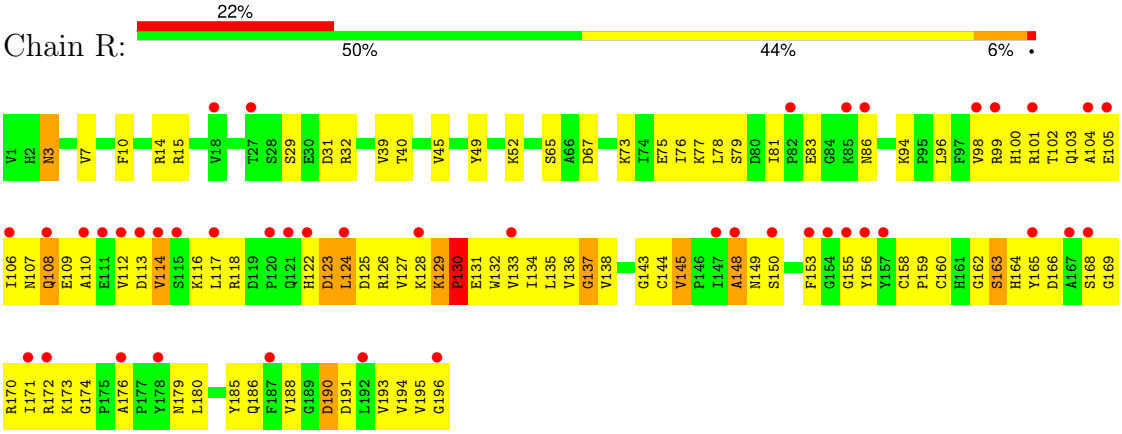
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



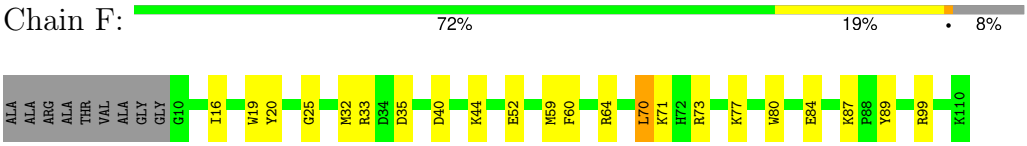
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:



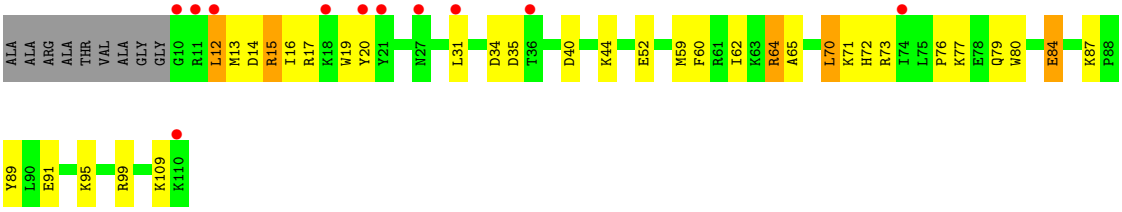
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain F:



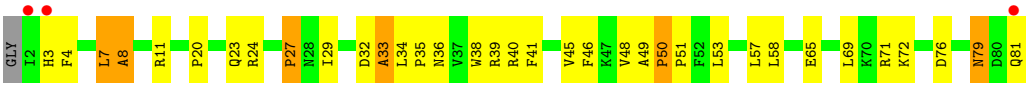
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain S:



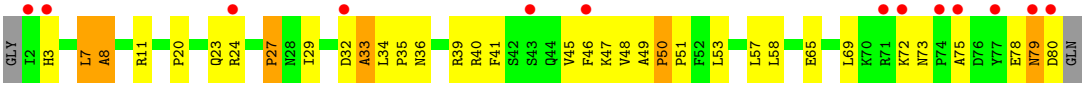
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain G:



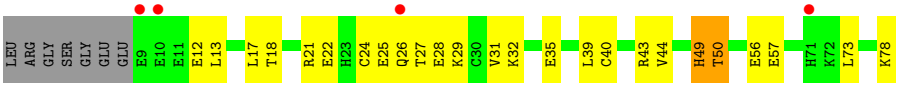
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain T:



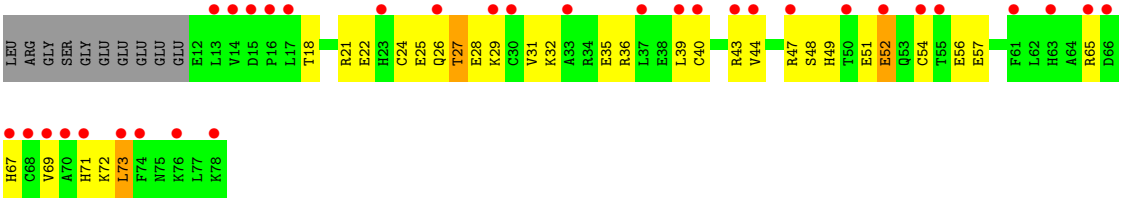
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain H:



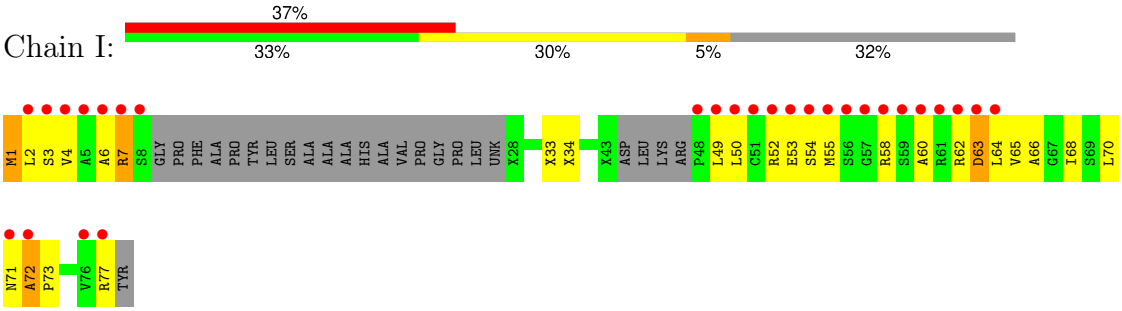
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain U:



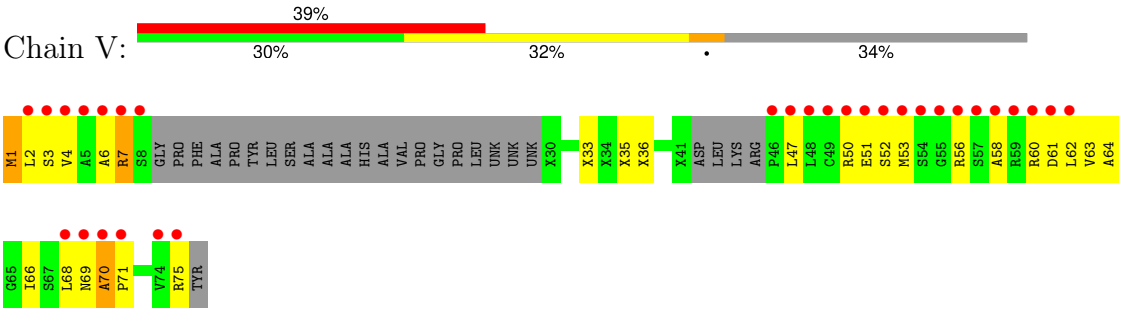
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



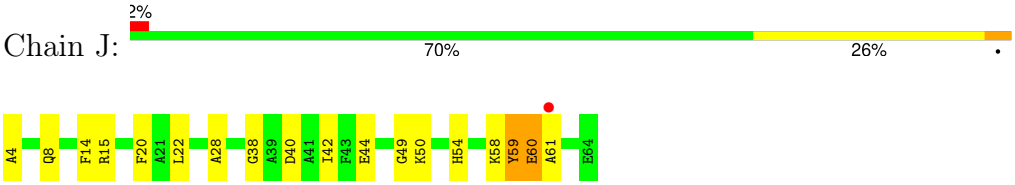
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



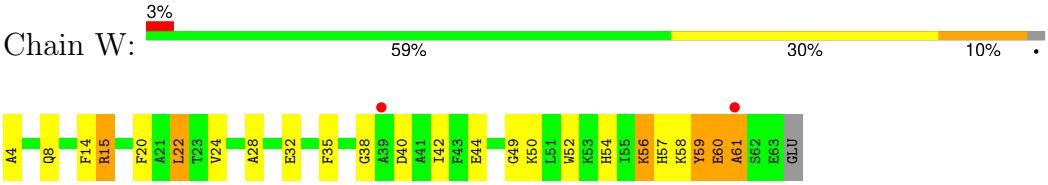
- Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

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	172.68Å 183.31Å 241.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.70 24.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.1 (24.98-2.70) 91.0 (24.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.289 0.246 , 0.280	Depositor DCC
R_{free} test set	3737 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 70.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32733	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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: FME, AME, HEM, UNL, WF3, UQ, BOG, CDL, PEE, GOL, FES, HEC

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	0.47	0/3513	1.00	20/4760 (0.4%)
1	N	0.46	0/3508	1.01	26/4753 (0.5%)
2	B	0.43	0/3196	0.96	8/4334 (0.2%)
2	O	0.47	0/3202	0.99	11/4343 (0.3%)
3	C	0.56	0/3114	1.01	18/4263 (0.4%)
3	P	0.50	0/3114	1.00	17/4263 (0.4%)
4	D	0.53	0/1956	1.02	8/2658 (0.3%)
4	Q	0.45	0/1956	0.97	7/2658 (0.3%)
5	E	0.43	0/1547	0.89	4/2103 (0.2%)
5	R	0.42	0/1543	0.96	10/2098 (0.5%)
6	F	0.53	0/911	0.89	1/1219 (0.1%)
6	S	0.42	0/911	0.94	2/1219 (0.2%)
7	G	0.47	0/694	1.01	2/941 (0.2%)
7	T	0.43	0/684	1.00	4/929 (0.4%)
8	H	0.47	0/582	0.91	0/779
8	U	0.37	0/561	0.88	2/751 (0.3%)
9	I	0.51	0/251	1.07	3/336 (0.9%)
9	V	0.49	0/251	0.95	0/336
10	J	0.48	0/508	0.86	0/682
10	W	0.46	0/490	0.84	1/660 (0.2%)
All	All	0.47	0/32492	0.98	144/44085 (0.3%)

There are no bond length outliers.

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	116	ILE	N-CA-C	7.59	117.71	110.42
5	E	106	ILE	N-CA-C	-7.58	104.08	112.80
1	A	248	LEU	CA-C-N	7.53	126.80	118.97
1	A	248	LEU	C-N-CA	7.53	126.80	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	GLN	N-CA-C	7.31	118.01	109.60

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	3442	0	3354	129	0
1	N	3437	0	3349	142	0
2	B	3141	0	3142	204	0
2	O	3147	0	3146	221	0
3	C	3021	0	3068	84	0
3	P	3012	0	3058	90	0
4	D	1898	0	1846	70	0
4	Q	1898	0	1846	75	0
5	E	1513	0	1478	113	0
5	R	1509	0	1474	102	0
6	F	891	0	893	21	0
6	S	891	0	893	34	0
7	G	672	0	653	31	0
7	T	662	0	645	33	0
8	H	574	0	548	19	0
8	U	553	0	535	31	0
9	I	319	0	281	45	0
9	V	311	0	283	50	0
10	J	497	0	490	14	0
10	W	479	0	478	22	0
11	A	1	0	0	0	0
11	N	1	0	0	0	0
12	C	86	0	60	4	0
12	P	86	0	60	5	0
13	C	31	0	19	1	0
13	P	31	0	19	1	0
14	C	19	0	17	3	0
14	P	19	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	42	0	28	1	0
15	G	40	0	24	1	0
15	P	40	0	24	3	0
15	Q	42	0	28	1	0
16	C	70	0	85	2	0
16	E	50	0	77	0	0
16	N	5	0	0	0	0
16	P	49	0	72	2	0
16	R	49	0	71	1	0
17	C	6	0	8	0	0
17	P	6	0	8	0	0
18	D	43	0	30	1	0
18	Q	43	0	30	1	0
19	D	33	0	39	0	0
19	P	12	0	11	0	0
19	Q	33	0	39	0	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	C	9	0	0	0	0
21	E	1	0	0	0	0
21	P	10	0	0	2	0
21	R	1	0	0	0	0
All	All	32733	0	32226	1395	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 21.

The worst 5 of 1395 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:O:76:THR:HG22	2:O:82:SER:H	1.05	1.19
1:N:178:THR:HG22	1:N:180:ALA:H	1.10	1.14
1:A:178:THR:HG22	1:A:180:ALA:H	1.11	1.13
2:B:76:THR:HG22	2:B:82:SER:H	1.12	1.12
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.12	1.10

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%)	408 (92%)	25 (6%)	8 (2%)	6	18
1	N	440/446 (99%)	409 (93%)	24 (6%)	7 (2%)	7	20
2	B	419/441 (95%)	351 (84%)	52 (12%)	16 (4%)	2	5
2	O	420/441 (95%)	359 (86%)	46 (11%)	15 (4%)	2	6
3	C	378/380 (100%)	350 (93%)	24 (6%)	4 (1%)	11	29
3	P	377/380 (99%)	348 (92%)	23 (6%)	6 (2%)	7	20
4	D	239/241 (99%)	222 (93%)	16 (7%)	1 (0%)	30	54
4	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	9	25
5	E	194/196 (99%)	147 (76%)	31 (16%)	16 (8%)	0	1
5	R	194/196 (99%)	151 (78%)	32 (16%)	11 (6%)	1	2
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	G	78/81 (96%)	65 (83%)	11 (14%)	2 (3%)	4	11
7	T	77/81 (95%)	66 (86%)	9 (12%)	2 (3%)	4	11
8	H	68/77 (88%)	63 (93%)	4 (6%)	1 (2%)	8	22
8	U	65/77 (84%)	55 (85%)	8 (12%)	2 (3%)	3	8
9	I	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0	0
9	V	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0	0
10	J	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
10	W	58/61 (95%)	52 (90%)	4 (7%)	2 (3%)	3	7
All	All	4012/4218 (95%)	3556 (89%)	352 (9%)	104 (3%)	4	11

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY

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Mol	Chain	Res	Type
1	A	433	ASP
2	B	26	ILE
2	B	39	GLU
2	B	226	ILE

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%)	355 (97%)	10 (3%)	39	69
1	N	365/368 (99%)	353 (97%)	12 (3%)	33	63
2	B	332/347 (96%)	319 (96%)	13 (4%)	28	57
2	O	333/347 (96%)	321 (96%)	12 (4%)	31	60
3	C	328/328 (100%)	323 (98%)	5 (2%)	57	81
3	P	328/328 (100%)	325 (99%)	3 (1%)	70	87
4	D	200/200 (100%)	195 (98%)	5 (2%)	42	71
4	Q	200/200 (100%)	197 (98%)	3 (2%)	57	81
5	E	166/166 (100%)	160 (96%)	6 (4%)	31	60
5	R	165/166 (99%)	161 (98%)	4 (2%)	43	72
6	F	93/96 (97%)	90 (97%)	3 (3%)	34	64
6	S	93/96 (97%)	88 (95%)	5 (5%)	20	45
7	G	71/71 (100%)	68 (96%)	3 (4%)	26	55
7	T	70/71 (99%)	67 (96%)	3 (4%)	26	54
8	H	65/71 (92%)	64 (98%)	1 (2%)	57	81
8	U	63/71 (89%)	63 (100%)	0	100	100
9	I	26/45 (58%)	26 (100%)	0	100	100
9	V	26/45 (58%)	26 (100%)	0	100	100
10	J	49/49 (100%)	46 (94%)	3 (6%)	17	40
10	W	47/49 (96%)	44 (94%)	3 (6%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3385/3482 (97%)	3291 (97%)	94 (3%)	38 68

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	395	TRP
2	O	341	MET
1	N	432	LEU
2	O	124	LEU
3	P	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	343	GLN
4	Q	50	ASN
2	O	362	ASN
3	P	159	HIS
5	R	107	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	AME	V	1	9	7,8,11	2.10	1 (14%)	5,8,13	1.56	1 (20%)
3	FME	C	1	3	7,8,10	2.12	1 (14%)	5,8,11	1.45	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	AME	I	1	9	7,8,11	2.09	1 (14%)	5,8,13	1.48	1 (20%)

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
9	AME	V	1	9	-	0/5/8/12	-
3	FME	C	1	3	-	1/5/8/11	-
9	AME	I	1	9	-	0/5/8/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	AME	CT1-N	-5.41	1.33	1.46
9	I	1	AME	CT1-N	-5.40	1.33	1.46
3	C	1	FME	CN-N	-5.36	1.33	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	AME	CT1-N-CA	2.72	121.83	113.70
3	C	1	FME	CN-N-CA	2.71	121.79	113.70
9	I	1	AME	CT1-N-CA	2.66	121.66	113.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	AME	4	0
9	I	1	AME	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 2 are unknown - 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	$\#\|Z\| > 2$
18	HEC	Q	501	4	50,50,50	1.04	1 (2%)	68,82,82	1.56	10 (14%)
12	HEM	C	502	3	50,50,50	1.38	4 (8%)	67,82,82	1.43	9 (13%)
14	UQ	P	505	-	19,19,63	2.59	10 (52%)	24,26,79	1.05	2 (8%)
12	HEM	P	501	3	50,50,50	1.47	5 (10%)	67,82,82	1.21	6 (8%)
19	BOG	D	502	-	20,20,20	0.86	0	25,25,25	0.89	1 (4%)
15	CDL	P	506	-	39,39,99	1.23	2 (5%)	45,51,111	1.14	4 (8%)
16	PEE	N	502	-	4,4,50	3.62	4 (100%)	6,6,55	0.59	0
12	HEM	C	501	3	50,50,50	1.51	6 (12%)	67,82,82	1.33	7 (10%)
15	CDL	C	505	-	41,41,99	1.19	2 (4%)	47,53,111	1.08	4 (8%)
19	BOG	Q	503	-	20,20,20	0.94	2 (10%)	25,25,25	0.90	1 (4%)
16	PEE	P	507	-	48,48,50	1.36	5 (10%)	51,53,55	0.76	2 (3%)
18	HEC	D	501	4	50,50,50	1.21	6 (12%)	68,82,82	1.67	11 (16%)
19	BOG	P	503	-	12,12,20	1.40	3 (25%)	17,17,25	0.53	0
13	WF3	C	503	-	32,33,33	2.97	15 (46%)	43,47,47	2.48	15 (34%)
15	CDL	G	101	-	39,39,99	1.22	1 (2%)	45,51,111	1.14	4 (8%)
15	CDL	Q	502	-	41,41,99	1.20	1 (2%)	47,53,111	1.09	4 (8%)
13	WF3	P	504	-	32,33,33	3.11	15 (46%)	43,47,47	2.47	15 (34%)
16	PEE	C	507	-	20,20,50	1.79	6 (30%)	23,25,55	0.63	0
16	PEE	C	506	-	48,48,50	1.39	6 (12%)	51,53,55	0.79	2 (3%)
19	BOG	D	503	-	13,13,20	1.39	2 (15%)	18,18,25	1.20	2 (11%)
20	FES	E	501	5	0,4,4	-	-	-		
16	PEE	E	502	-	49,49,50	1.55	10 (20%)	52,54,55	0.92	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	GOL	P	508	-	5,5,5	1.46	1 (20%)	5,5,5	0.68	0
14	UQ	C	504	-	19,19,63	2.61	9 (47%)	24,26,79	1.07	2 (8%)
19	BOG	Q	504	-	13,13,20	1.30	2 (15%)	18,18,25	1.11	2 (11%)
17	GOL	C	508	-	5,5,5	1.43	0	5,5,5	0.68	0
12	HEM	P	502	3	50,50,50	1.41	4 (8%)	67,82,82	1.22	7 (10%)
20	FES	R	501	5	0,4,4	-	-	-		
16	PEE	R	502	-	47,47,50	1.49	8 (17%)	49,51,55	0.73	1 (2%)

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
18	HEC	Q	501	4	1/1/3/7	9/14/54/54	-
12	HEM	C	502	3	-	6/14/54/54	-
14	UQ	P	505	-	-	3/11/35/87	0/1/1/1
12	HEM	P	501	3	-	5/14/54/54	-
19	BOG	D	502	-	-	4/11/31/31	0/1/1/1
15	CDL	P	506	-	-	19/49/49/110	-
12	HEM	C	501	3	-	4/14/54/54	-
15	CDL	C	505	-	-	16/51/51/110	-
19	BOG	Q	503	-	-	4/11/31/31	0/1/1/1
16	PEE	P	507	-	-	20/52/52/54	-
18	HEC	D	501	4	1/1/3/7	10/14/54/54	-
19	BOG	P	503	-	-	0/2/22/31	0/1/1/1
13	WF3	C	503	-	-	1/24/24/24	0/3/3/3
15	CDL	G	101	-	-	17/49/49/110	-
15	CDL	Q	502	-	-	16/51/51/110	-
13	WF3	P	504	-	-	6/24/24/24	0/3/3/3
16	PEE	C	507	-	-	7/24/24/54	-
16	PEE	C	506	-	-	19/52/52/54	-
19	BOG	D	503	-	-	0/4/24/31	0/1/1/1
20	FES	E	501	5	-	-	0/1/1/1
16	PEE	E	502	-	-	27/53/53/54	-
17	GOL	P	508	-	-	3/4/4/4	-
14	UQ	C	504	-	-	3/11/35/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BOG	Q	504	-	-	4/4/24/31	0/1/1/1
17	GOL	C	508	-	-	4/4/4/4	-
12	HEM	P	502	3	-	5/14/54/54	-
20	FES	R	501	5	-	-	0/1/1/1
16	PEE	R	502	-	-	25/49/49/54	-

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	504	WF3	C6-C5	9.85	1.54	1.34
13	C	503	WF3	C6-C5	9.44	1.53	1.34
13	P	504	WF3	C18-N23	6.30	1.38	1.30
13	P	504	WF3	C9-C5	-5.84	1.42	1.49
13	C	503	WF3	C18-N23	5.74	1.37	1.30

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	504	WF3	O2-C3-C5	9.95	125.61	112.05
13	C	503	WF3	O2-C3-C5	9.67	125.22	112.05
18	D	501	HEC	CAC-C3C-C2C	4.92	134.68	126.89
18	Q	501	HEC	CAC-C3C-C2C	4.81	134.50	126.89
18	Q	501	HEC	CAC-C3C-C4C	-4.55	118.65	124.91

All (2) chirality outliers are listed below:

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

5 of 237 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	P	504	WF3	O2-C3-C5-C6
13	P	504	WF3	O4-C3-C5-C6
15	C	505	CDL	O1-C1-CB2-OB2
15	C	505	CDL	CB2-OB2-PB2-OB3
15	C	505	CDL	CB2-OB2-PB2-OB4

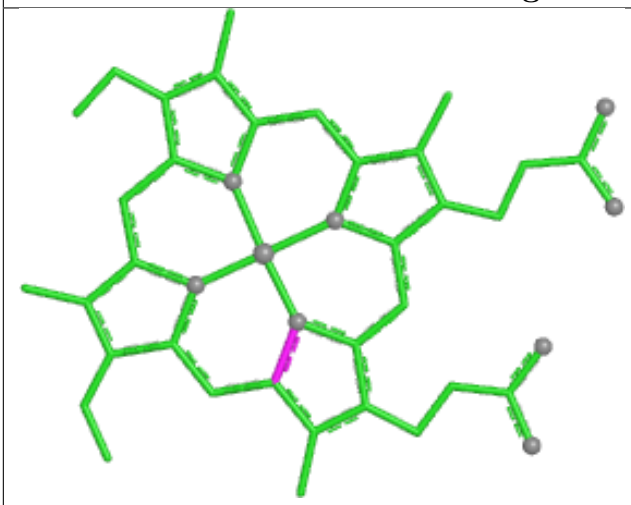
There are no ring outliers.

17 monomers are involved in 28 short contacts:

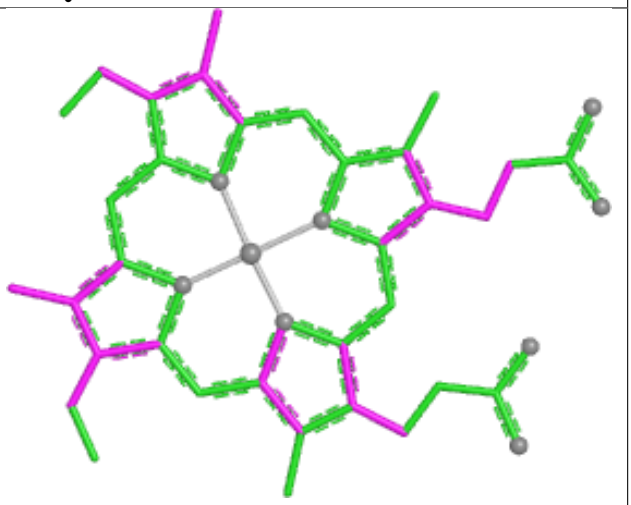
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Q	501	HEC	1	0
12	C	502	HEM	3	0
14	P	505	UQ	1	0
12	P	501	HEM	2	0
15	P	506	CDL	3	0
12	C	501	HEM	1	0
15	C	505	CDL	1	0
16	P	507	PEE	2	0
18	D	501	HEC	1	0
13	C	503	WF3	1	0
15	G	101	CDL	1	0
15	Q	502	CDL	1	0
13	P	504	WF3	1	0
16	C	506	PEE	2	0
14	C	504	UQ	3	0
12	P	502	HEM	3	0
16	R	502	PEE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

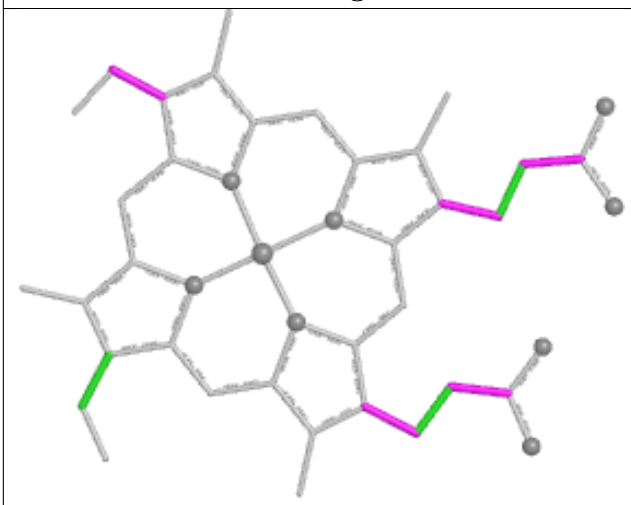
Ligand HEC Q 501



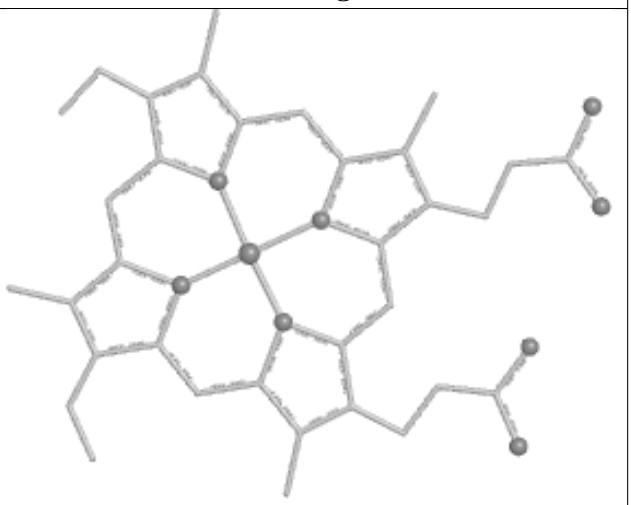
Bond lengths



Bond angles

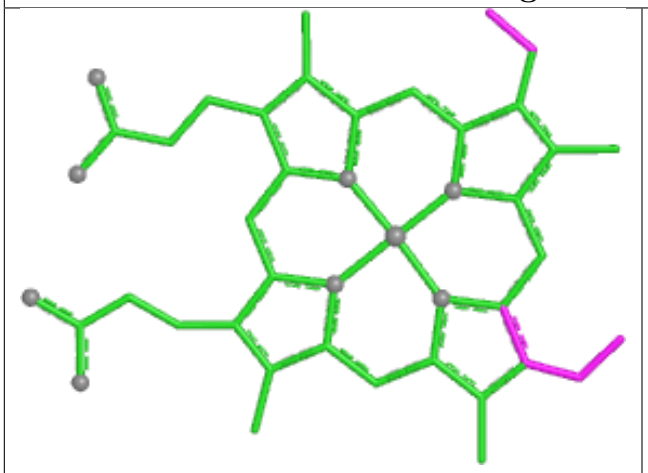


Torsions



Rings

Ligand HEM C 502



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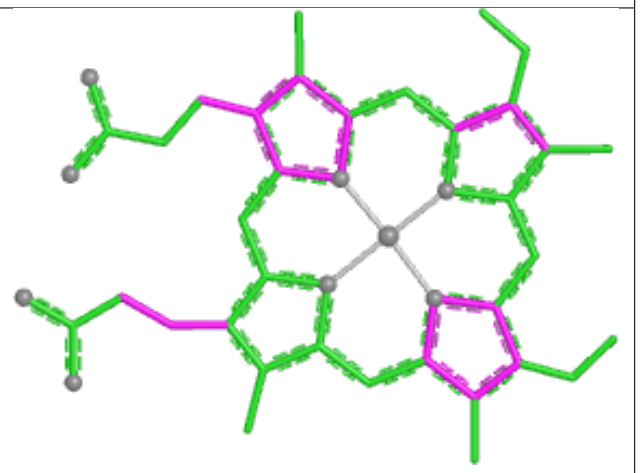

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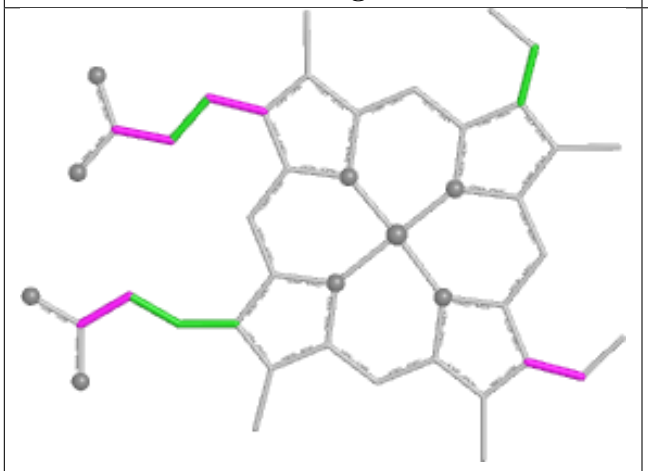

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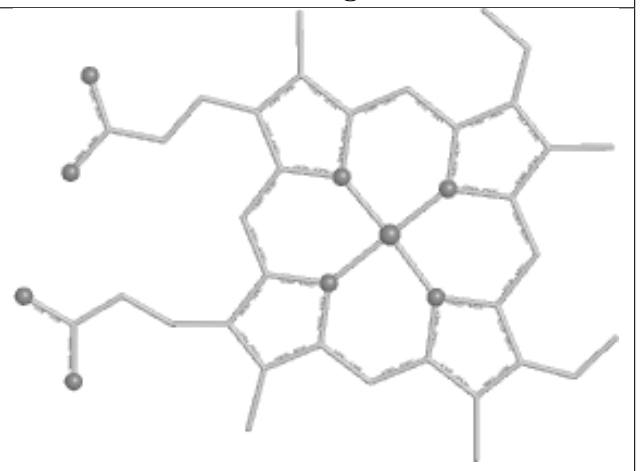
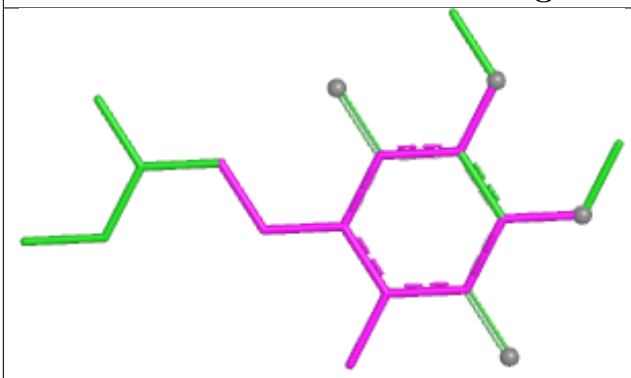


Rings

Ligand UQ P 505



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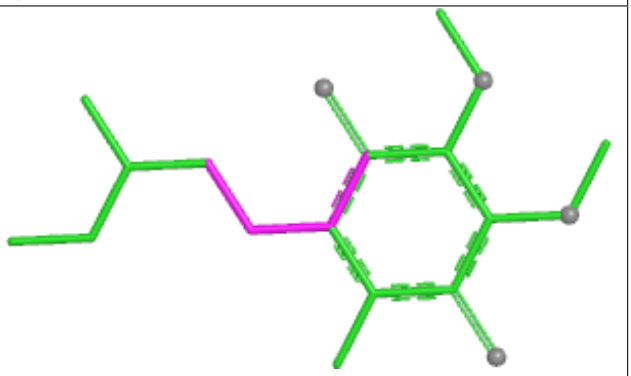

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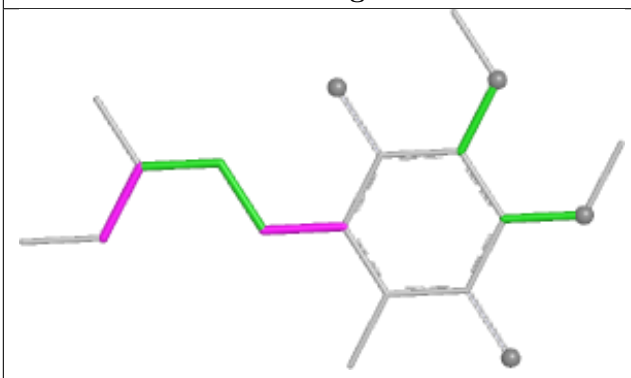

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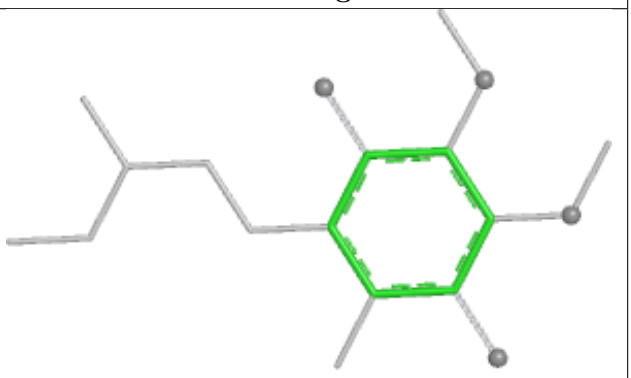
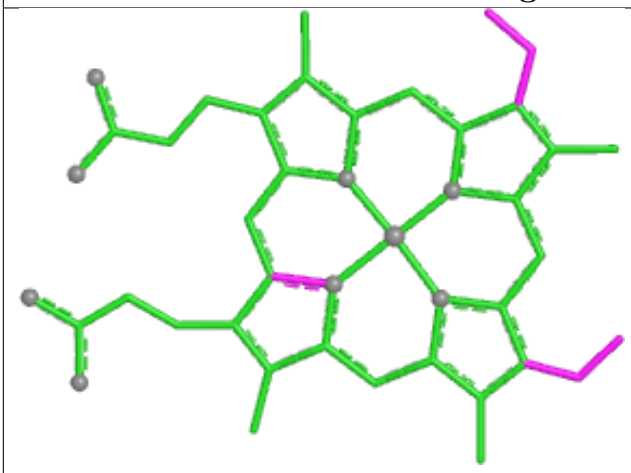


Rings

Ligand HEM P 501



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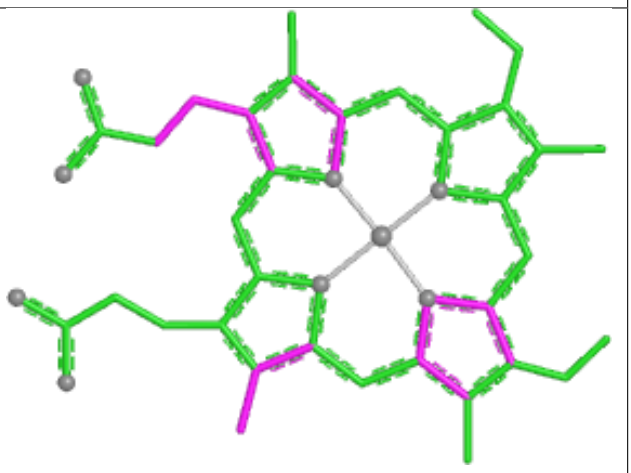

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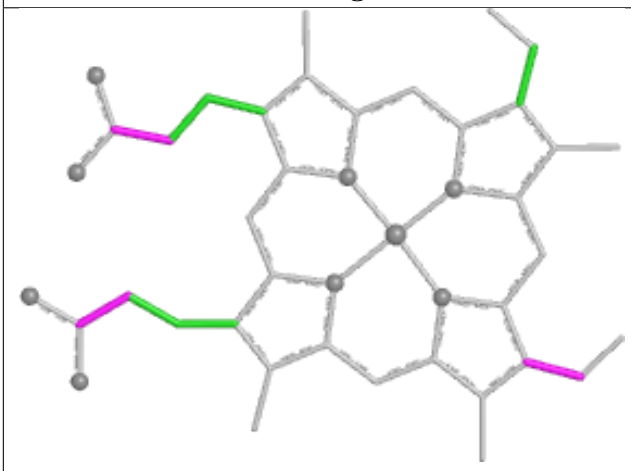

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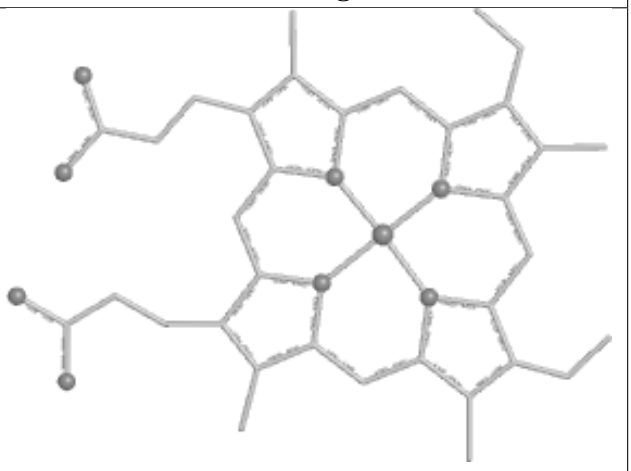
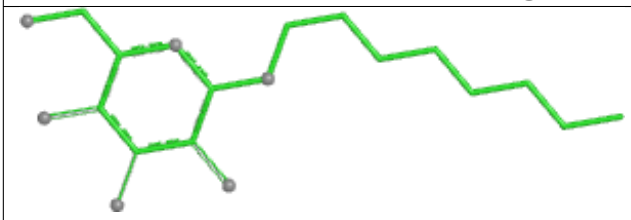


Rings

Ligand BOG D 502



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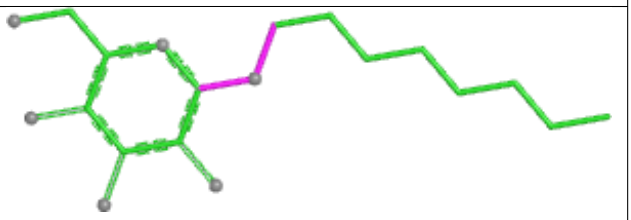

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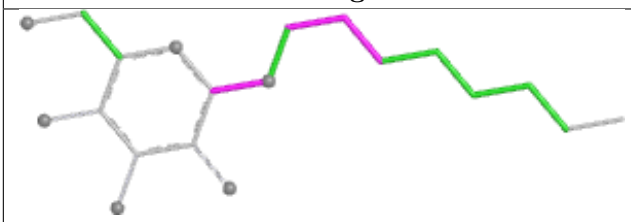

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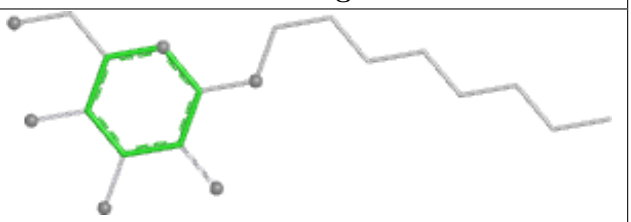
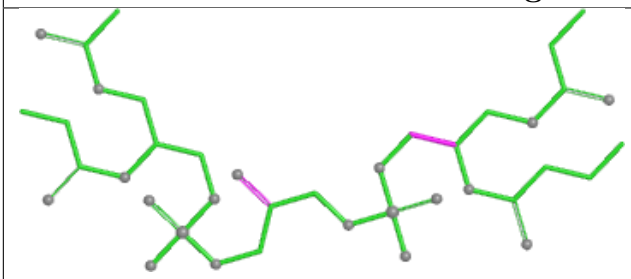


Rings

Ligand CDL P 506



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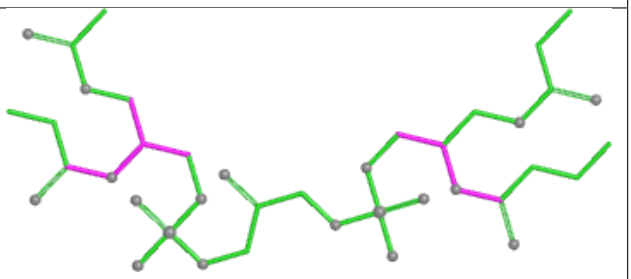

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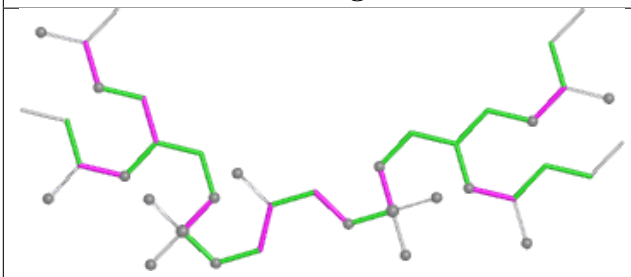

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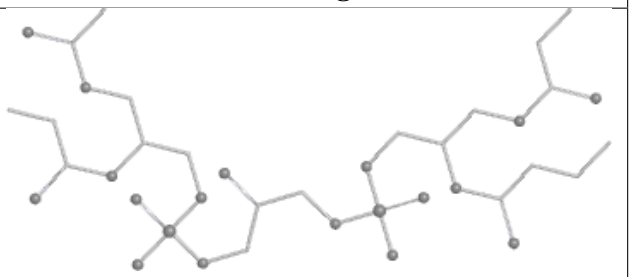
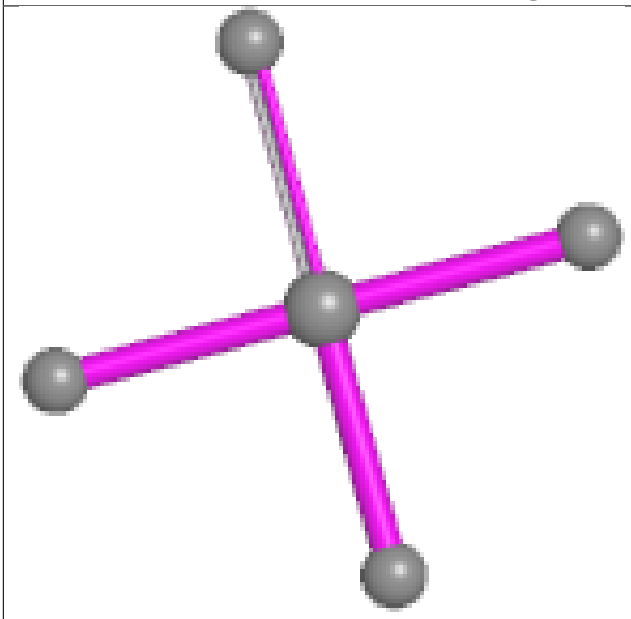


Rings

Ligand PEE N 502



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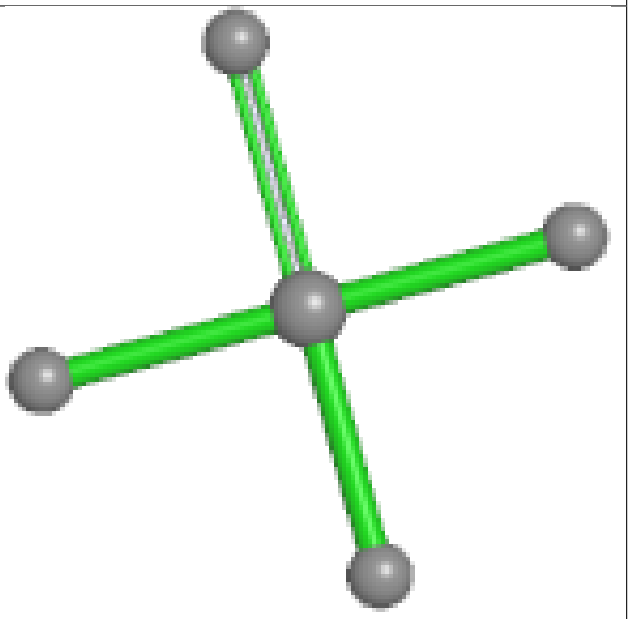

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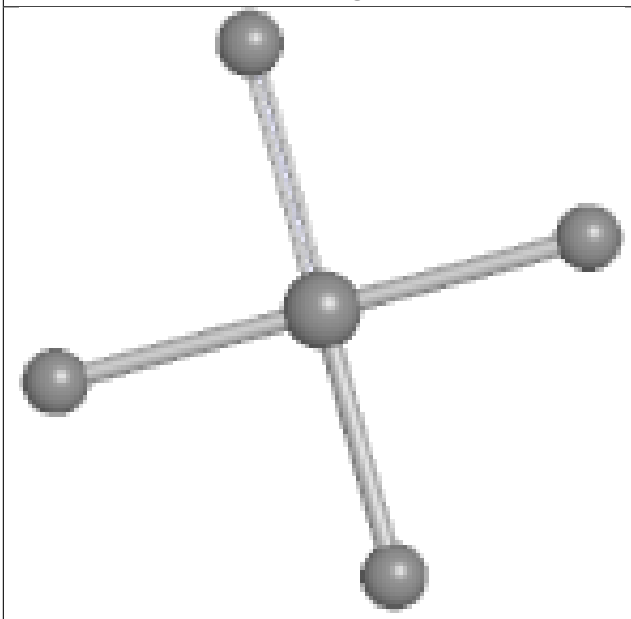

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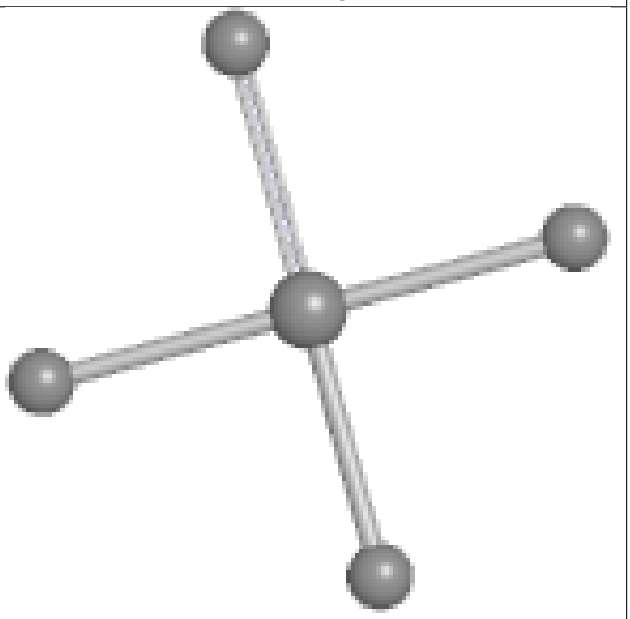
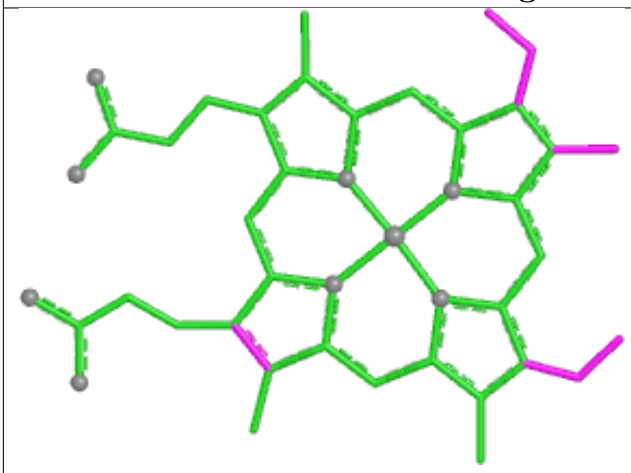


Rings

Ligand HEM C 501



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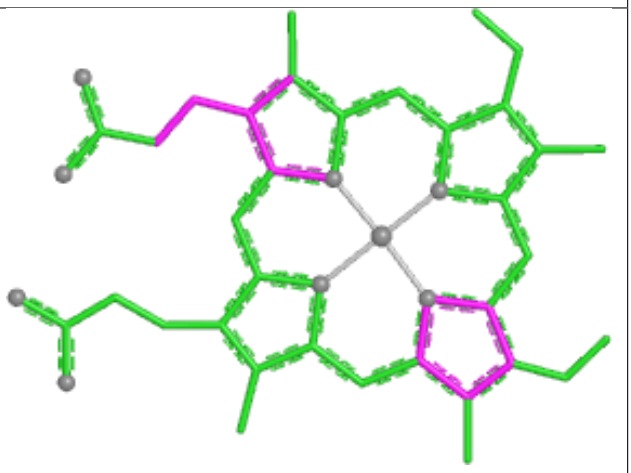

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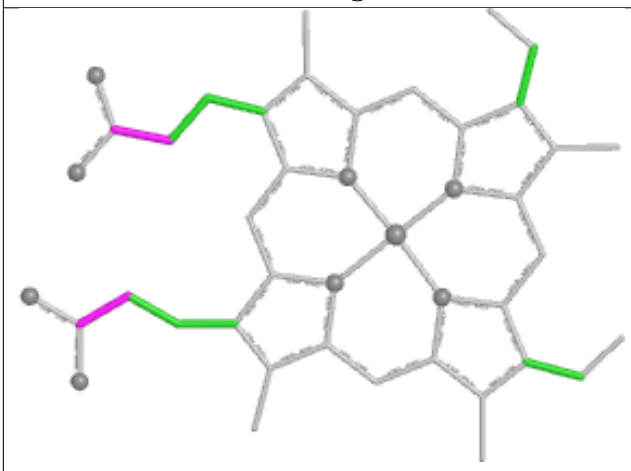

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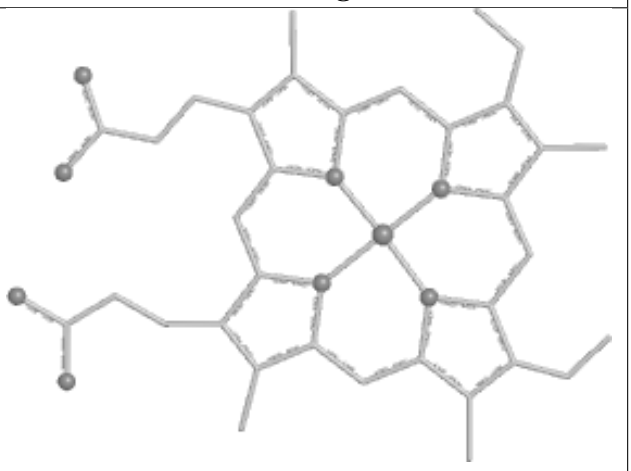
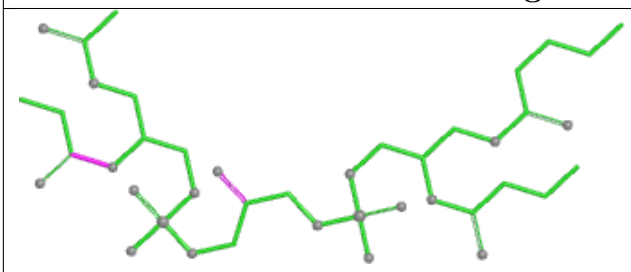


Rings

Ligand CDL C 505



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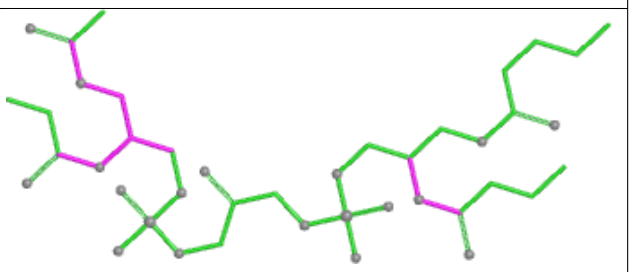
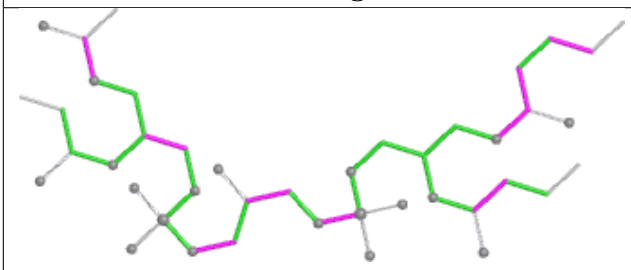


Bond angles



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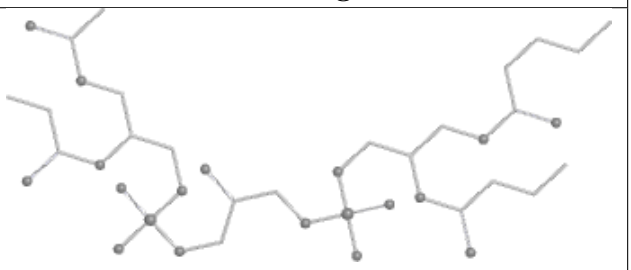
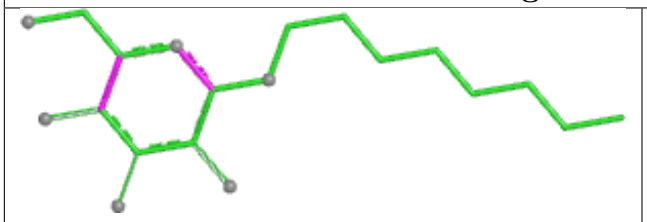


Rings

Ligand BOG Q 503



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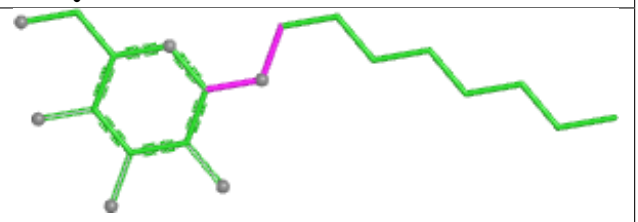
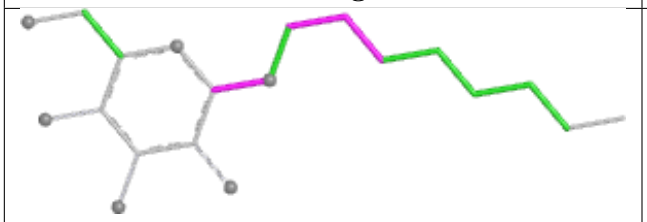
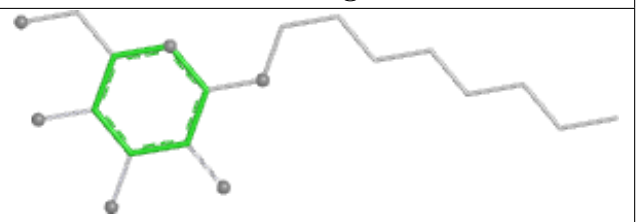


Bond angles

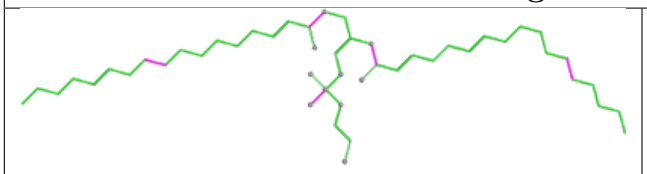


Torsions

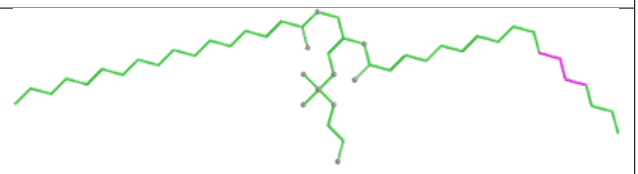


Rings

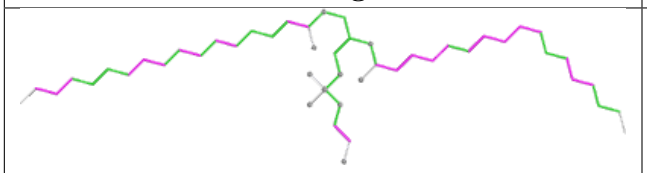
Ligand PEE P 507



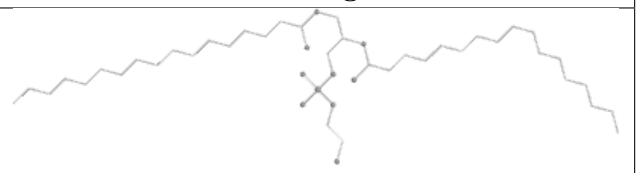
Bond lengths



Bond angles

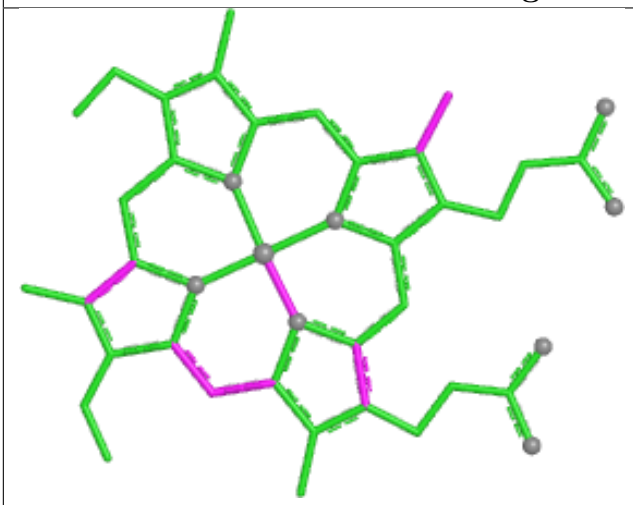


Torsions



Rings

Ligand HEC D 501



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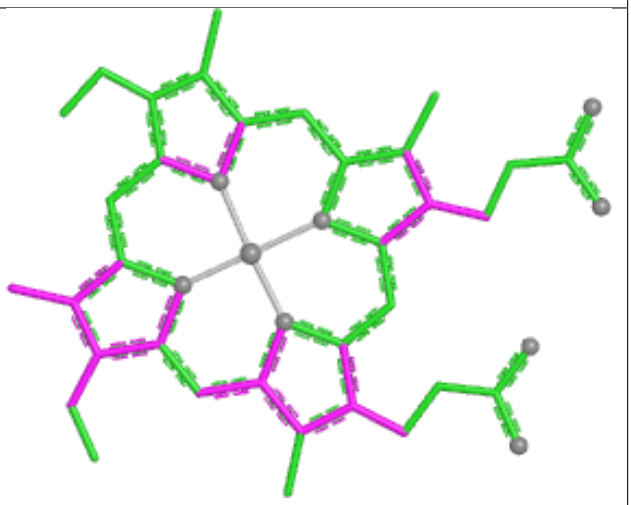

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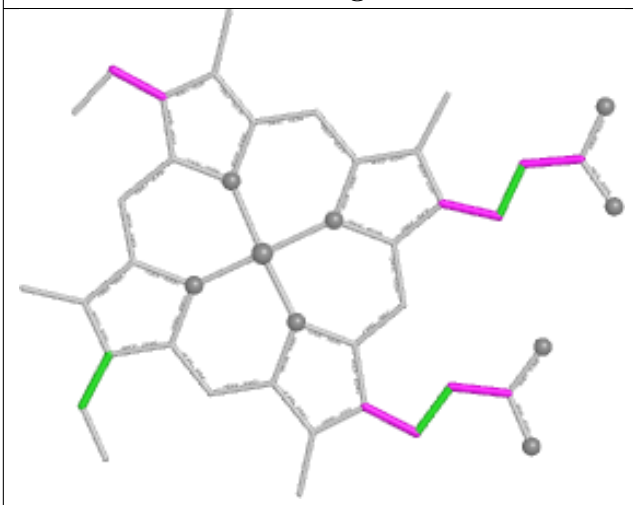

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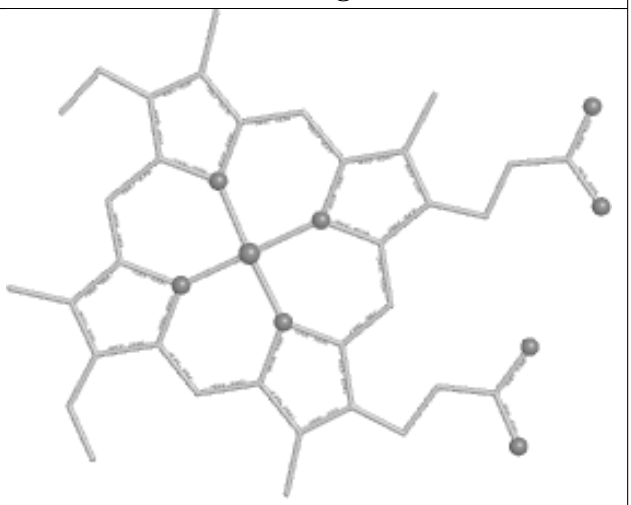
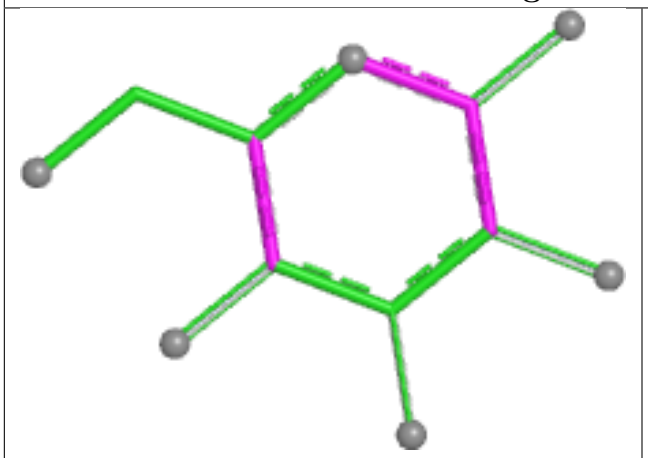


Rings

Ligand BOG P 503



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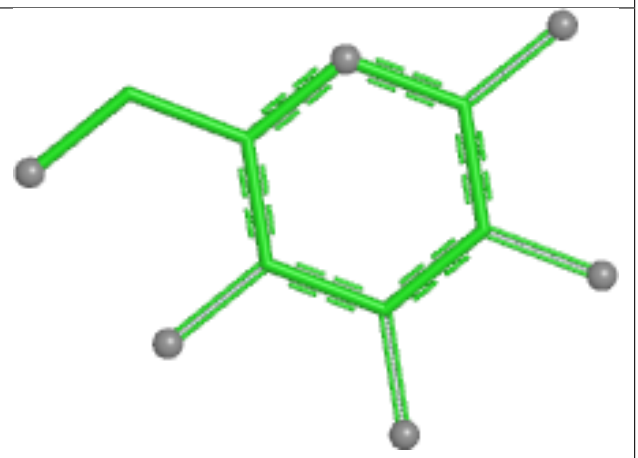
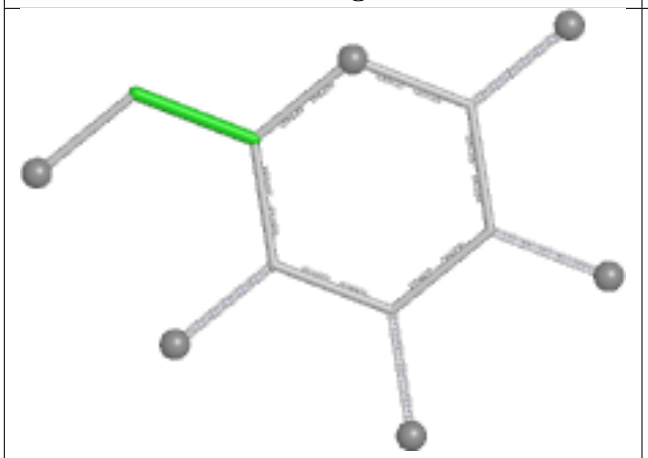
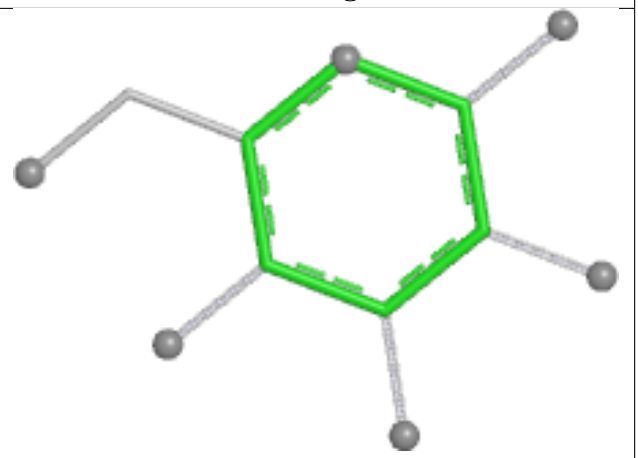


Bond angles

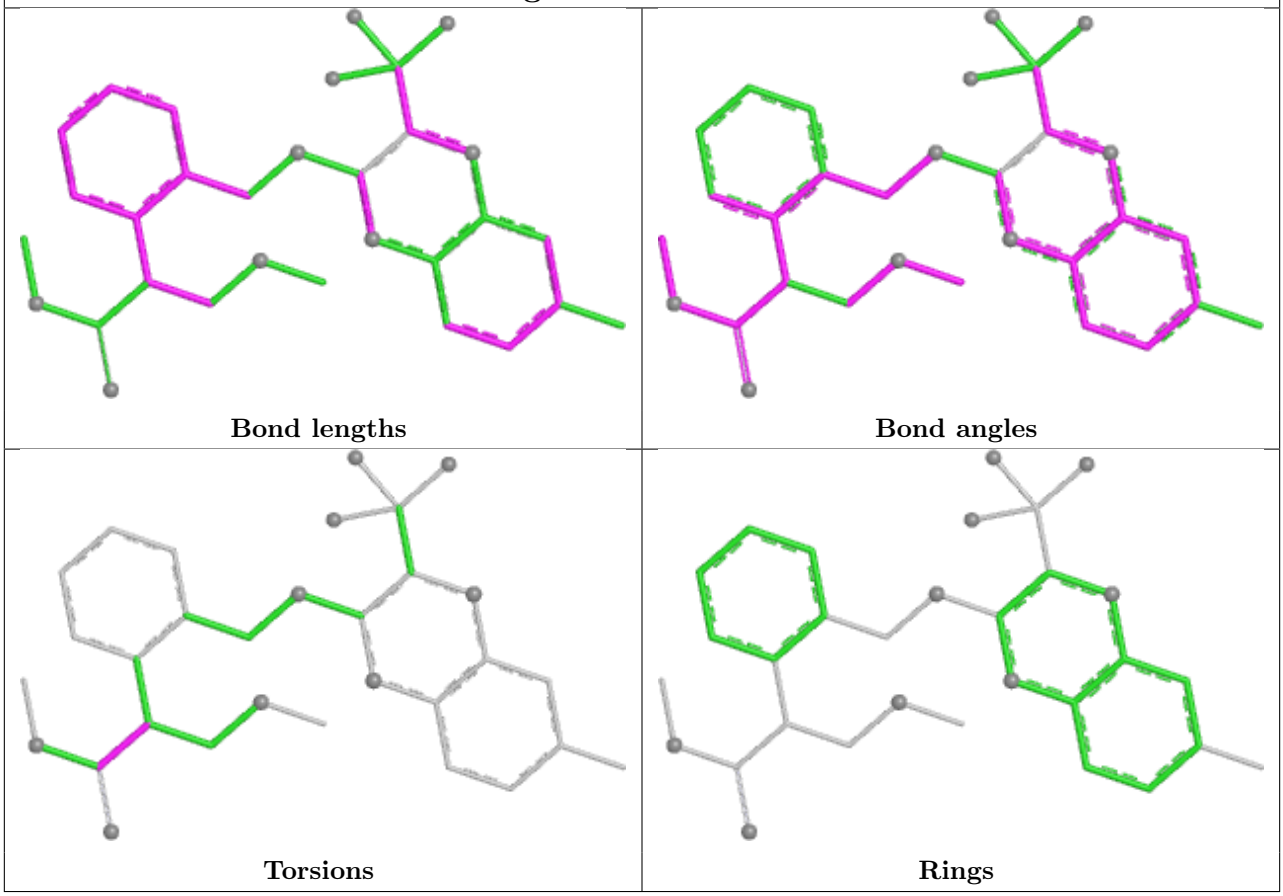


Torsions

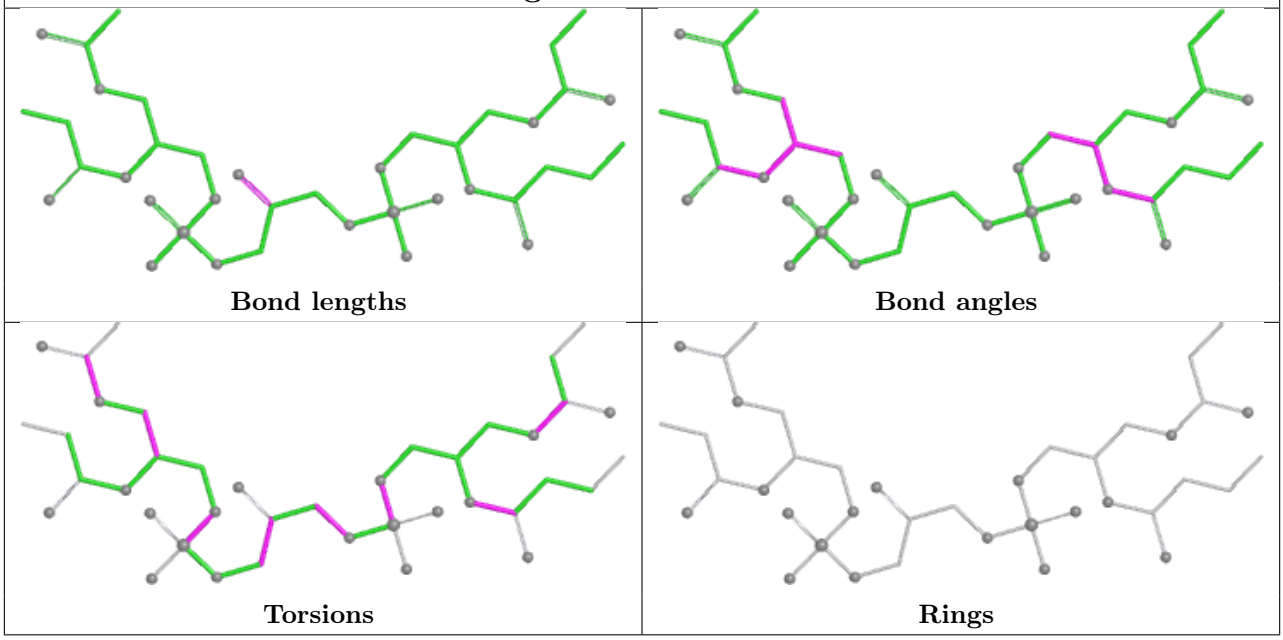


Rings

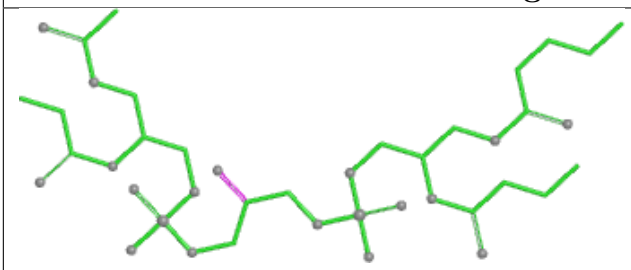
Ligand WF3 C 503



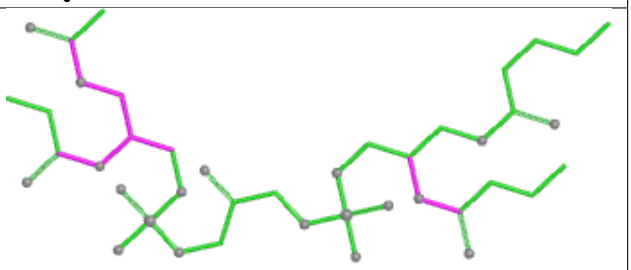
Ligand CDL G 101



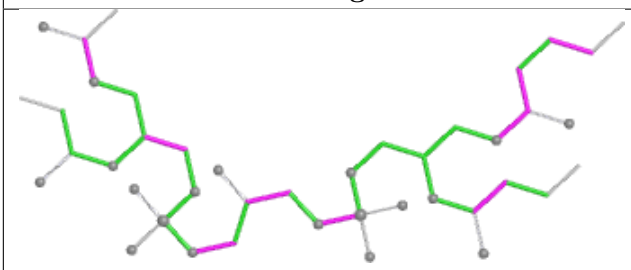
Ligand CDL Q 502



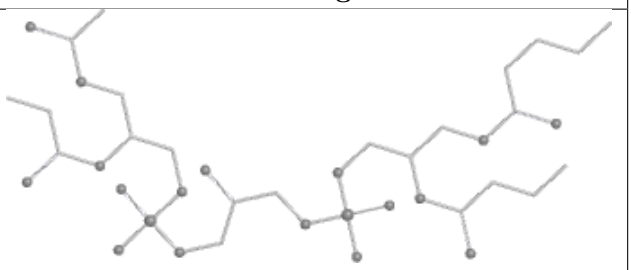
Bond lengths



Bond angles

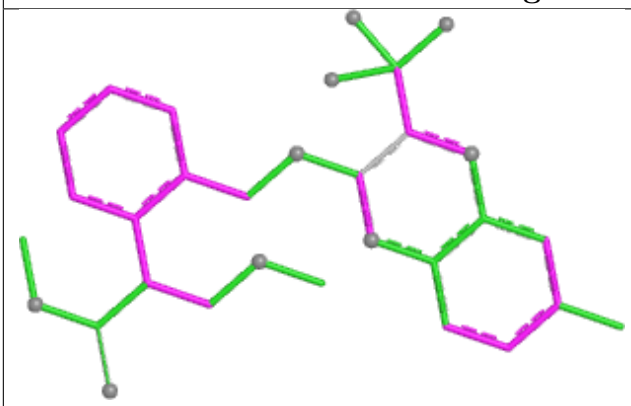


Torsions



Rings

Ligand WF3 P 504



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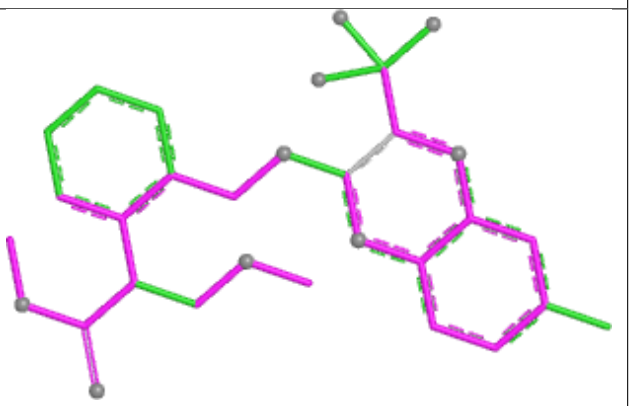
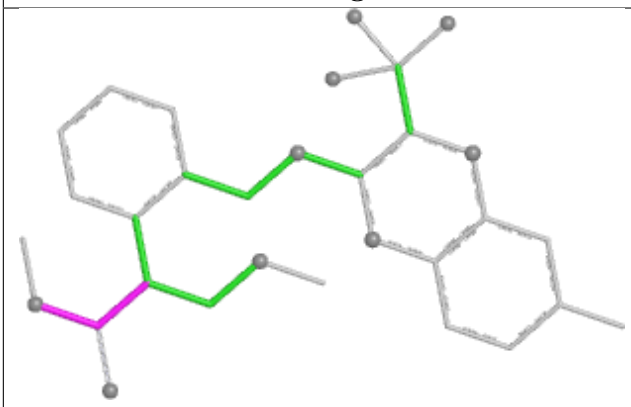


Bond angles



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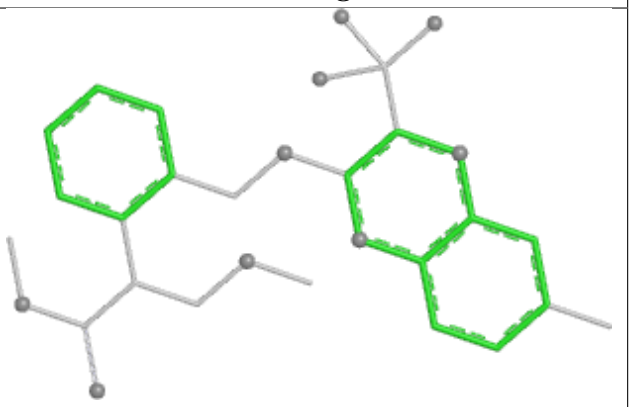
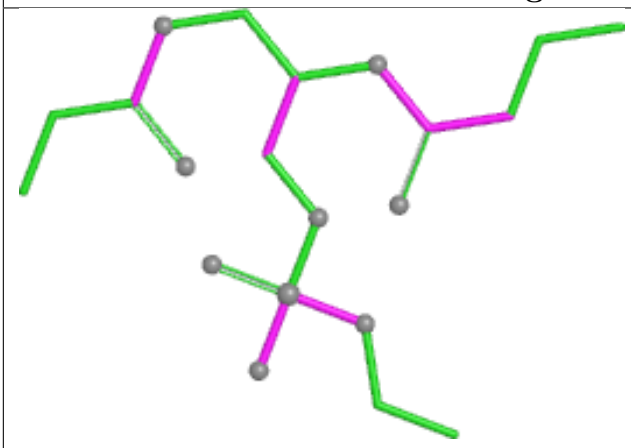


Rings

Ligand PEE C 507



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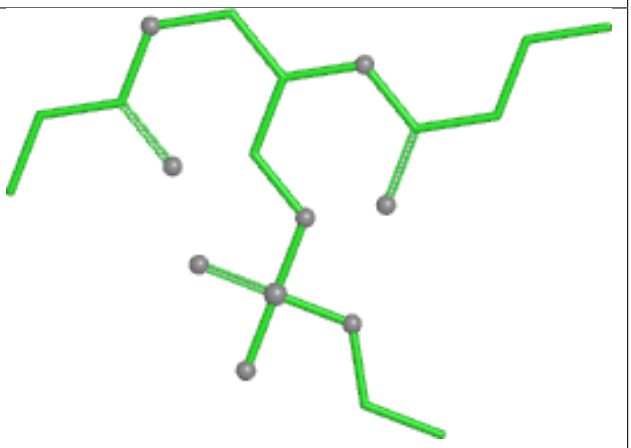
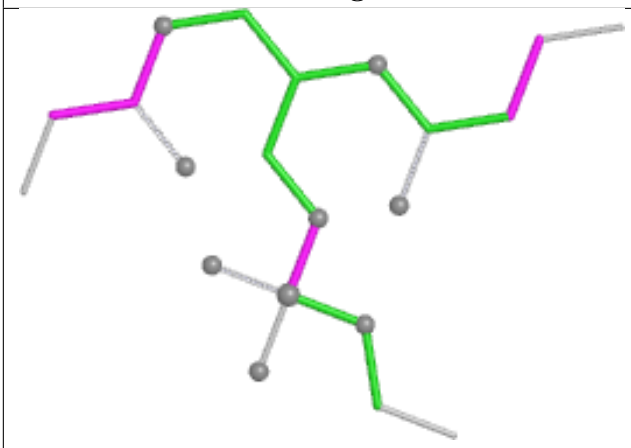
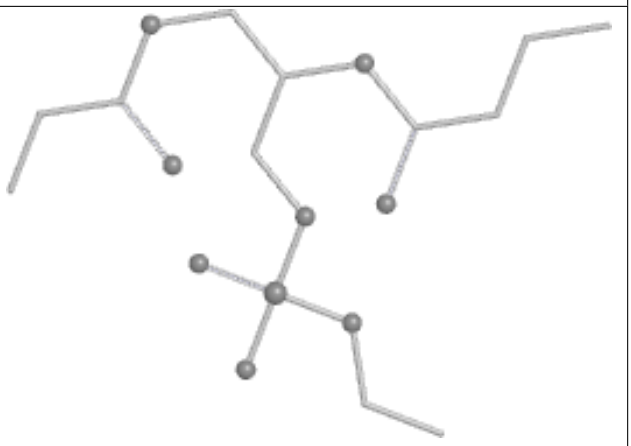


Bond angles



Torsions



Rings

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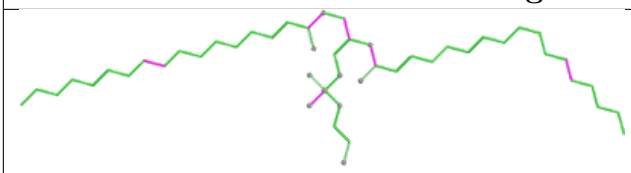

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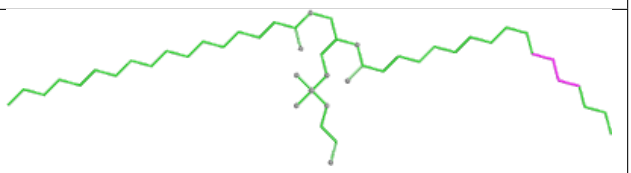
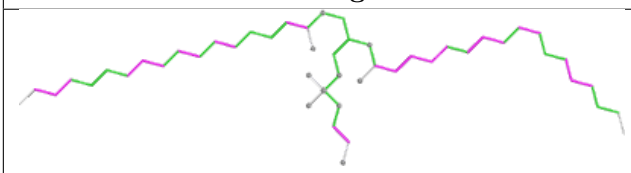


Bond angles



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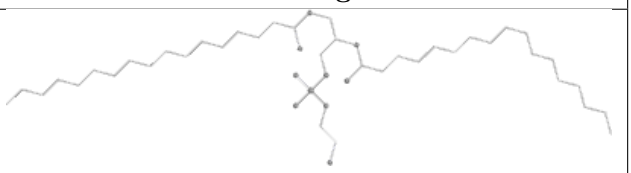
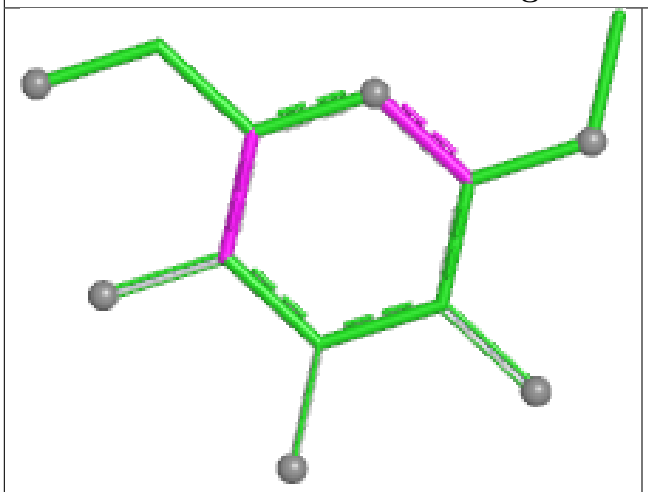


Rings

Ligand BOG D 503



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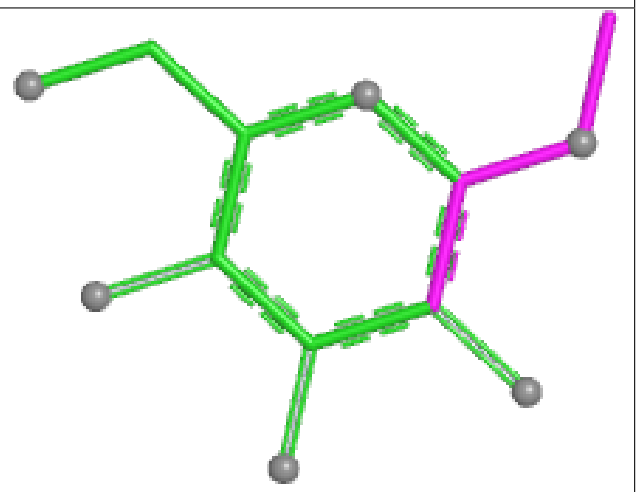

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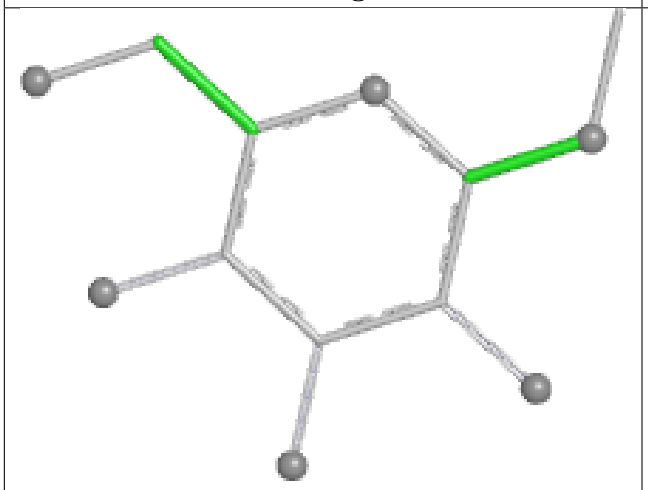
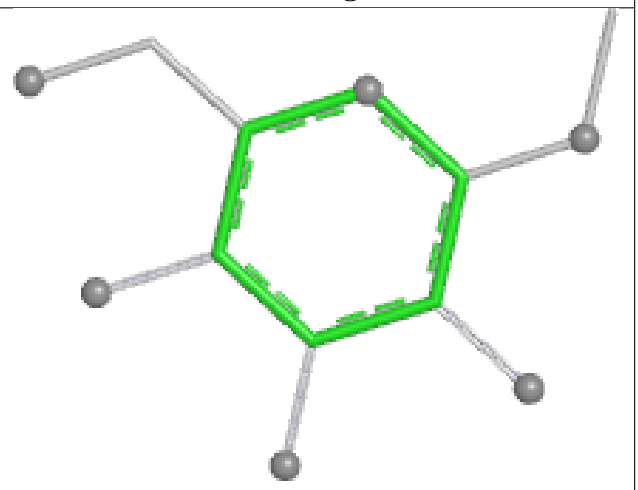
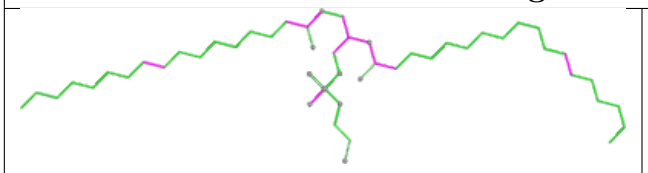


Torsions



Rings

Ligand PEE E 502



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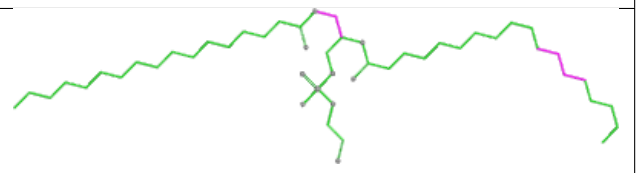
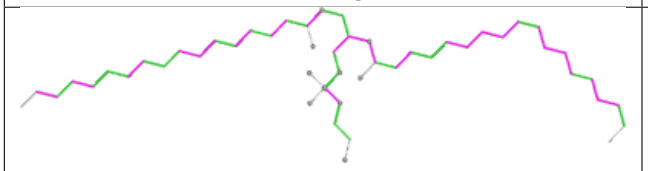
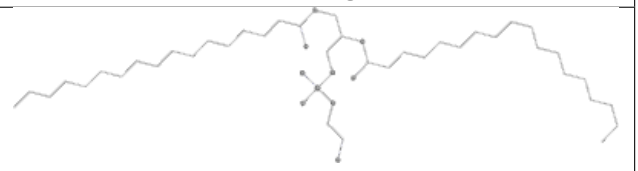


Bond angles

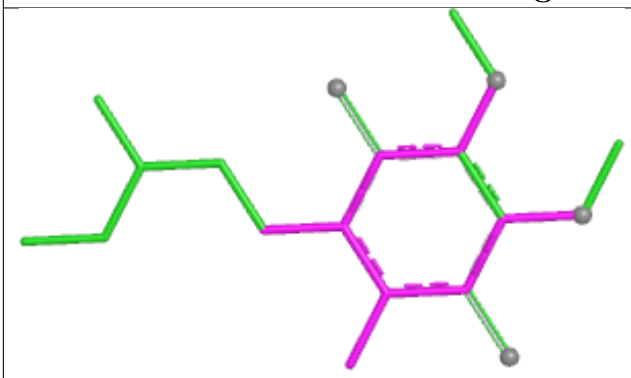


Torsions

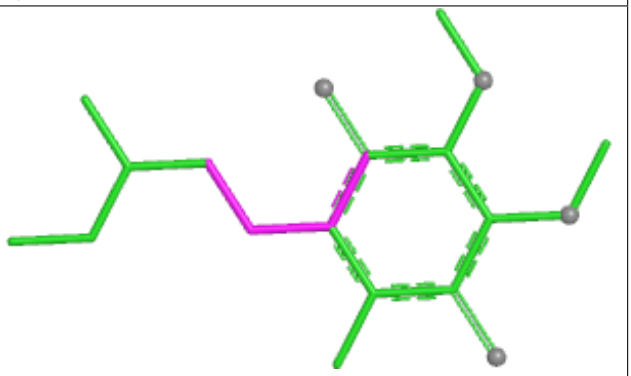


Rings

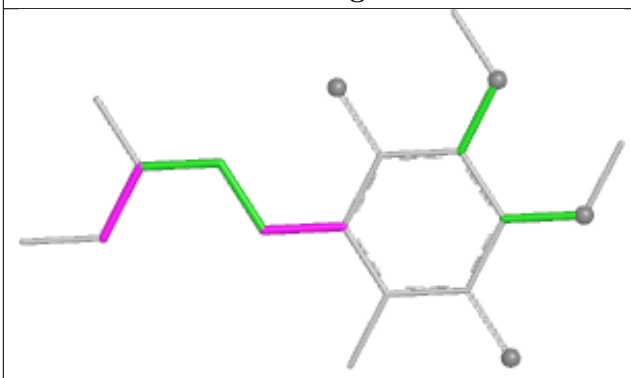
Ligand UQ C 504



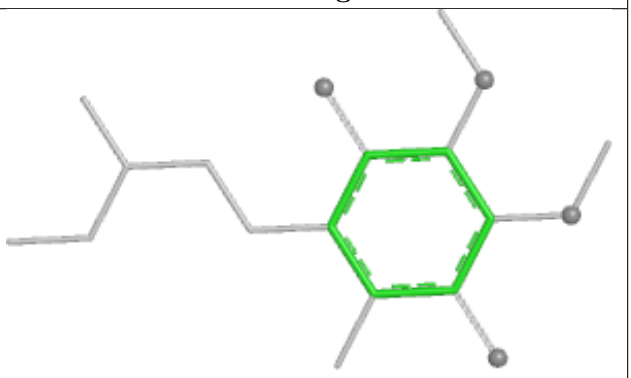
Bond lengths



Bond angles

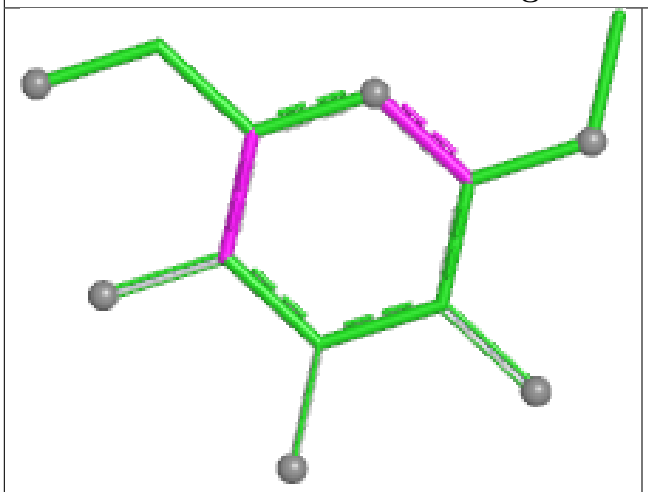


Torsions



Rings

Ligand BOG Q 504



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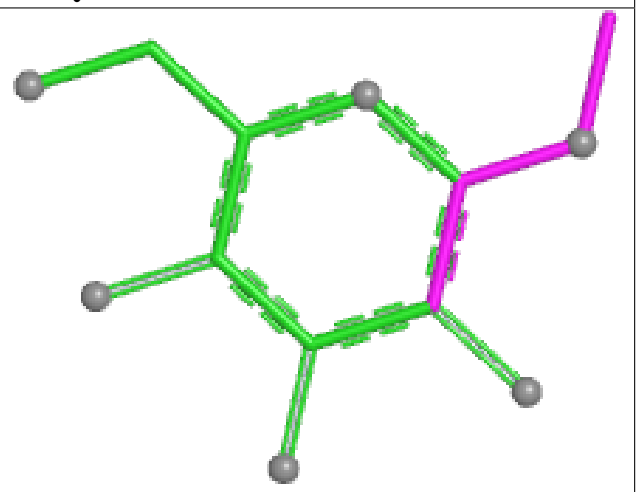
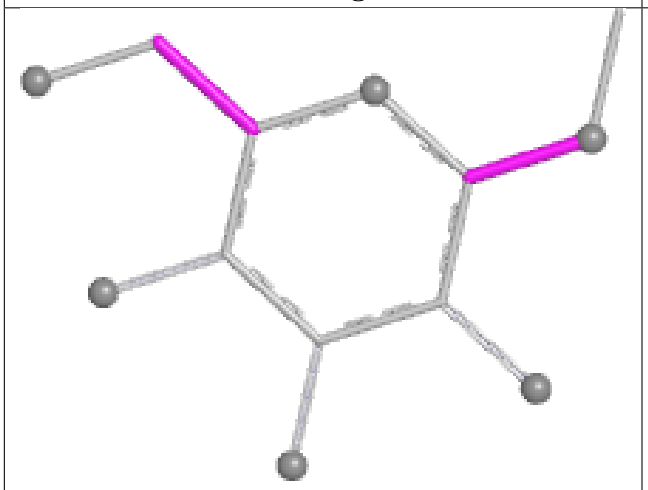
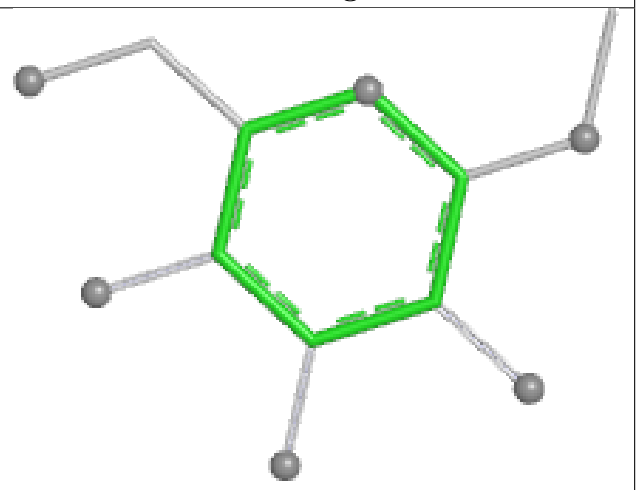


Bond angles

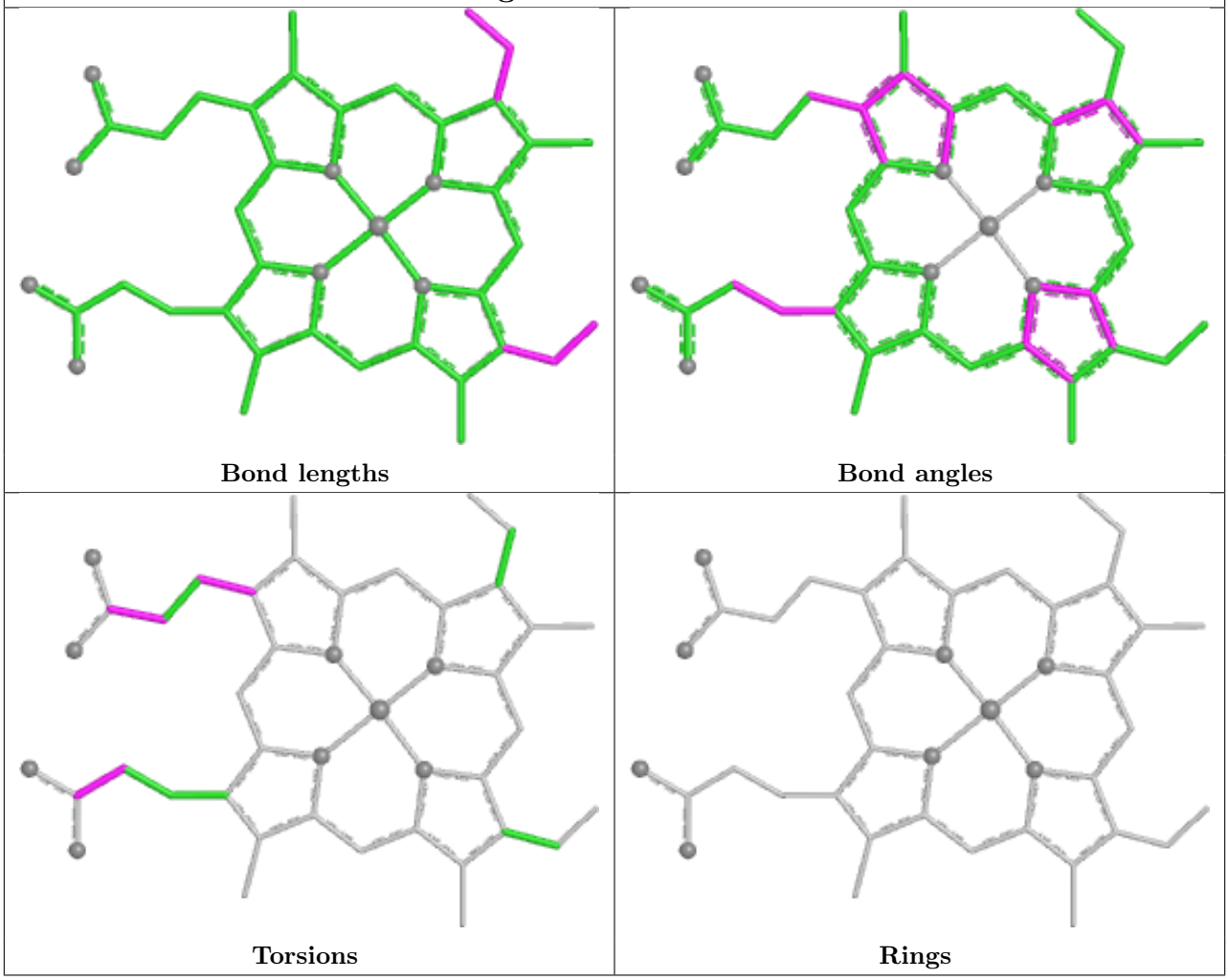


Torsions

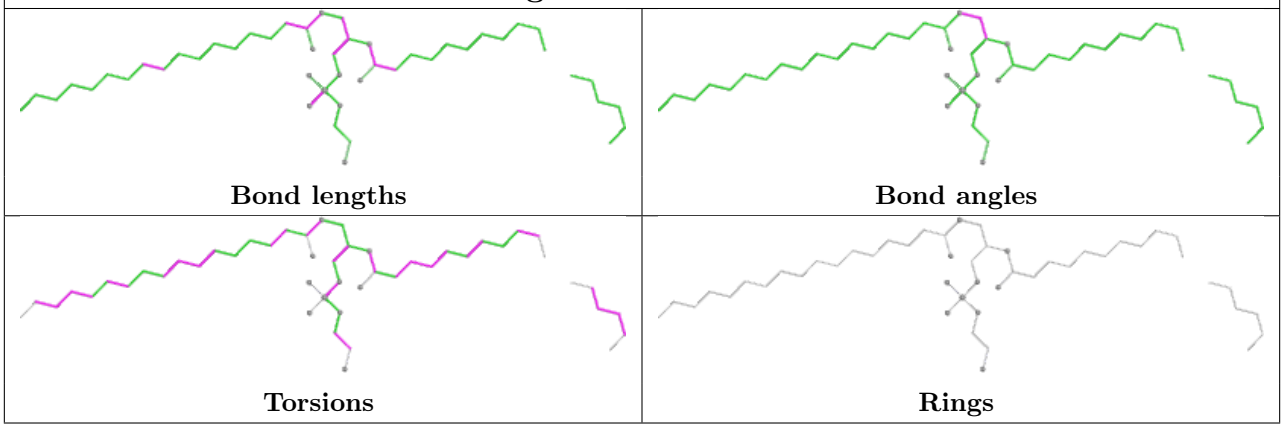


Rings

Ligand HEM P 502



Ligand PEE R 502



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.33	16 (3%)	46	42	40, 70, 101, 123	0
1	N	442/446 (99%)	0.72	32 (7%)	21	18	44, 76, 104, 117	0
2	B	421/441 (95%)	0.85	32 (7%)	20	17	55, 88, 120, 147	0
2	O	422/441 (95%)	0.69	33 (7%)	19	16	49, 81, 114, 133	0
3	C	379/380 (99%)	-0.22	12 (3%)	50	46	29, 47, 92, 135	0
3	P	379/380 (99%)	0.36	22 (5%)	29	25	37, 68, 106, 127	0
4	D	241/241 (100%)	-0.23	5 (2%)	63	61	37, 49, 89, 118	0
4	Q	241/241 (100%)	0.88	16 (6%)	24	21	51, 82, 115, 128	0
5	E	196/196 (100%)	1.32	63 (32%)	1	1	41, 109, 159, 174	0
5	R	196/196 (100%)	1.18	43 (21%)	2	2	49, 96, 148, 168	0
6	F	101/110 (91%)	-0.35	0	100	100	31, 51, 71, 100	0
6	S	101/110 (91%)	0.75	11 (10%)	10	9	60, 79, 123, 146	0
7	G	80/81 (98%)	0.23	3 (3%)	44	40	37, 62, 116, 128	0
7	T	79/81 (97%)	1.26	13 (16%)	4	4	55, 91, 150, 165	0
8	H	70/77 (90%)	0.48	4 (5%)	29	26	45, 69, 101, 145	0
8	U	67/77 (87%)	2.05	33 (49%)	0	0	96, 129, 149, 155	0
9	I	37/76 (48%)	3.30	28 (75%)	0	0	80, 124, 163, 166	0
9	V	37/76 (48%)	3.30	30 (81%)	0	0	61, 126, 162, 163	0
10	J	61/61 (100%)	0.13	1 (1%)	70	68	46, 65, 107, 170	0
10	W	60/61 (98%)	0.72	2 (3%)	49	45	62, 81, 128, 138	0
All	All	4053/4218 (96%)	0.60	399 (9%)	13	11	29, 74, 131, 174	0

The worst 5 of 399 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	9	GLU	7.8
9	V	59	ARG	7.3
2	O	226	ILE	7.1
9	V	54	SER	7.0
9	I	2	LEU	6.3

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	FME	C	1	9/11	0.44	0.25	139,141,148,153	0
9	AME	V	1	9/12	0.77	0.25	136,148,153,154	0
9	AME	I	1	9/12	0.80	0.24	150,155,160,160	0

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
19	BOG	Q	504	13/20	0.37	0.27	179,186,190,192	0
19	BOG	D	503	13/20	0.56	0.30	140,156,162,164	0
16	PEE	C	507	21/51	0.57	0.25	64,135,154,156	0
16	PEE	N	502	5/51	0.63	0.15	132,134,139,140	0
15	CDL	Q	502	42/100	0.67	0.34	79,169,202,203	0
19	BOG	P	503	12/20	0.69	0.22	126,144,149,158	0
15	CDL	C	505	42/100	0.72	0.31	65,134,159,163	0
15	CDL	P	506	40/100	0.72	0.23	110,125,138,141	0
11	UNL	N	501	1/-	0.77	0.12	47,47,47,47	0
11	UNL	A	501	1/-	0.81	0.15	48,48,48,48	0
16	PEE	R	502	49/51	0.84	0.23	51,98,121,125	0

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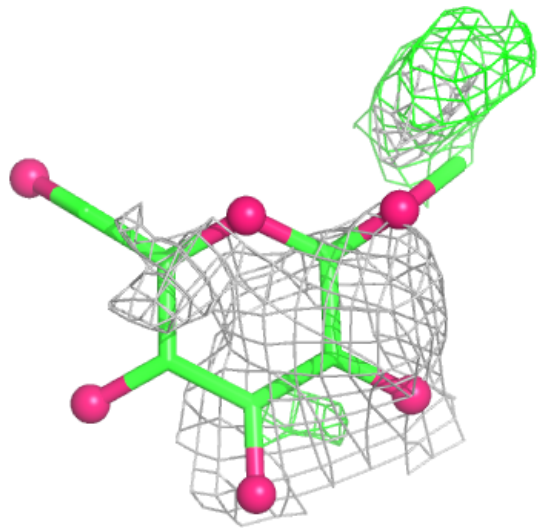
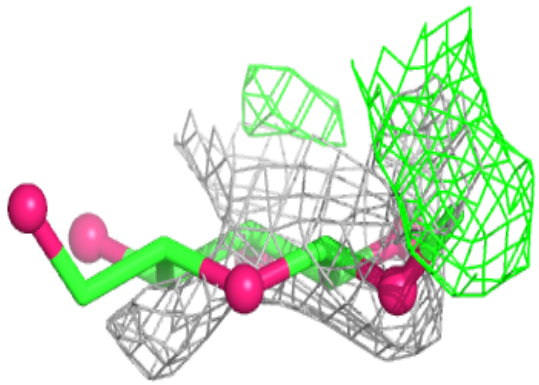
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	UQ	P	505	19/63	0.85	0.33	80,127,140,146	0
15	CDL	G	101	40/100	0.85	0.16	46,83,125,131	0
16	PEE	E	502	50/51	0.86	0.19	59,86,114,117	0
14	UQ	C	504	19/63	0.86	0.28	73,96,104,108	0
16	PEE	P	507	49/51	0.88	0.20	72,91,119,123	0
19	BOG	Q	503	20/20	0.89	0.17	72,100,105,113	0
16	PEE	C	506	49/51	0.92	0.14	33,60,91,103	0
19	BOG	D	502	20/20	0.92	0.10	44,64,72,76	0
17	GOL	C	508	6/6	0.93	0.16	64,72,75,76	0
17	GOL	P	508	6/6	0.94	0.15	67,76,82,84	0
13	WF3	P	504	31/31	0.94	0.10	51,64,73,78	0
20	FES	E	501	4/4	0.96	0.07	125,129,129,130	0
13	WF3	C	503	31/31	0.97	0.07	30,40,53,60	0
12	HEM	P	501	43/43	0.98	0.10	39,58,68,81	0
12	HEM	P	502	43/43	0.98	0.07	36,50,69,74	0
18	HEC	Q	501	43/43	0.98	0.08	48,60,77,85	0
20	FES	R	501	4/4	0.98	0.05	78,88,91,94	0
18	HEC	D	501	43/43	0.99	0.05	7,31,49,55	0
12	HEM	C	501	43/43	0.99	0.07	23,41,51,66	0
12	HEM	C	502	43/43	0.99	0.07	21,39,48,59	0

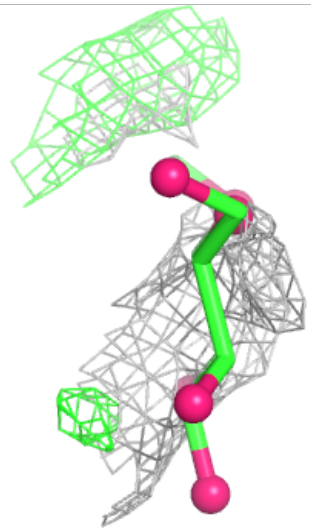
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG Q 504:

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







Electron density around BOG D 503:

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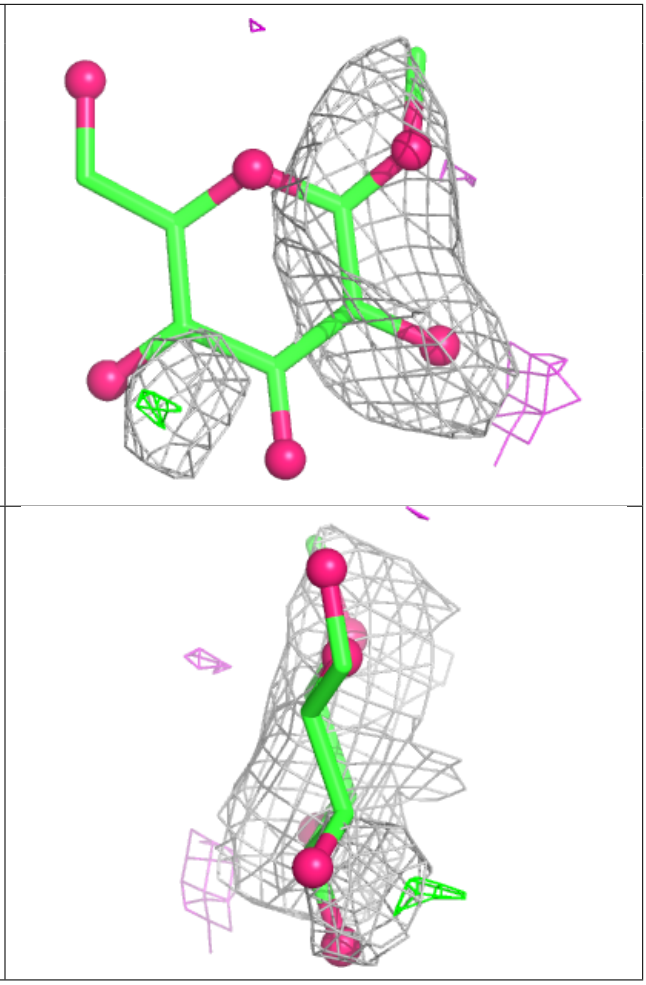
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEE C 507:

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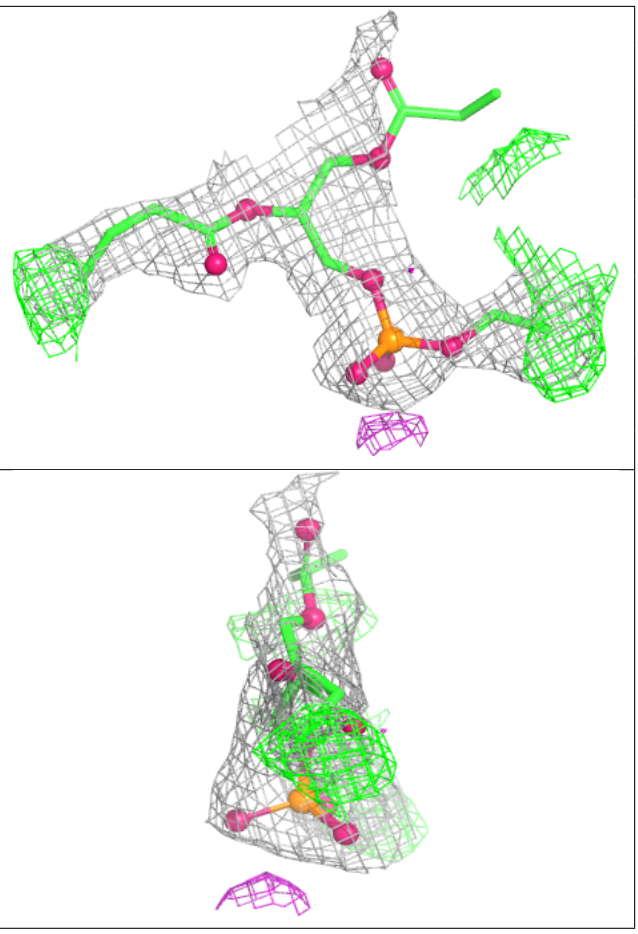
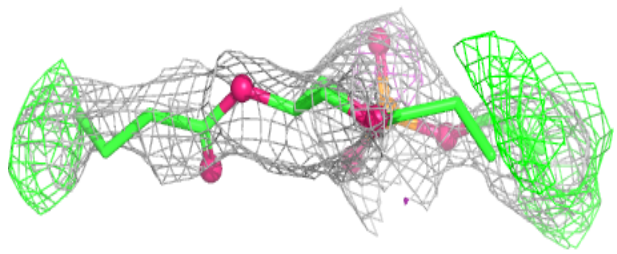
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around PEE N 502:

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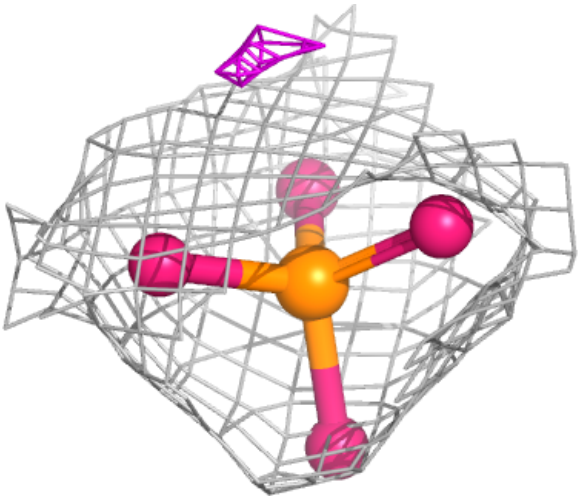
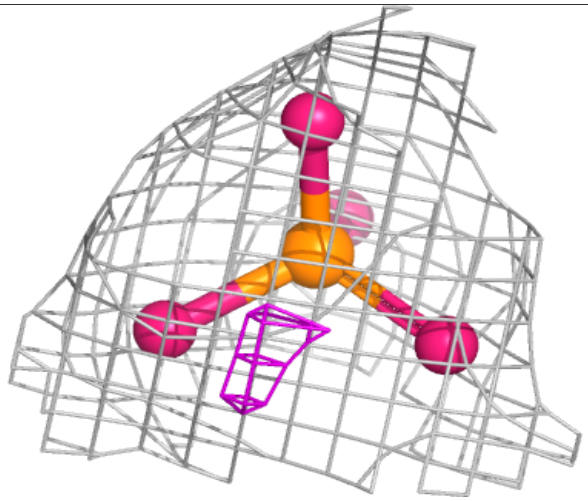
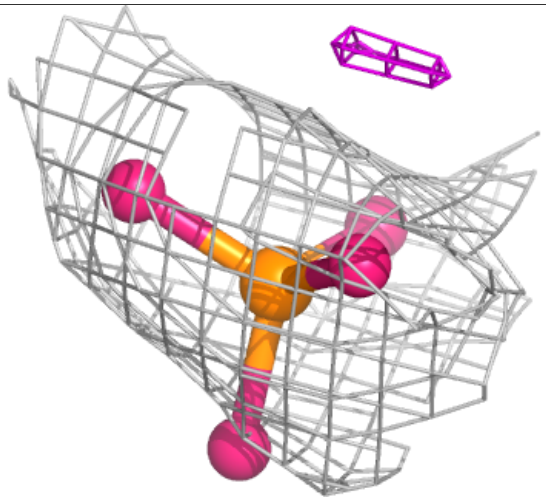
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around CDL Q 502:

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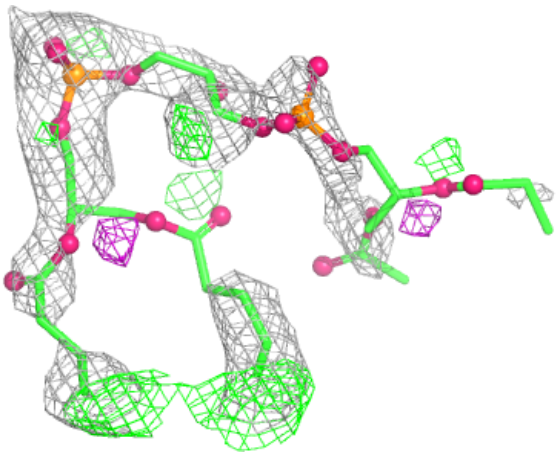
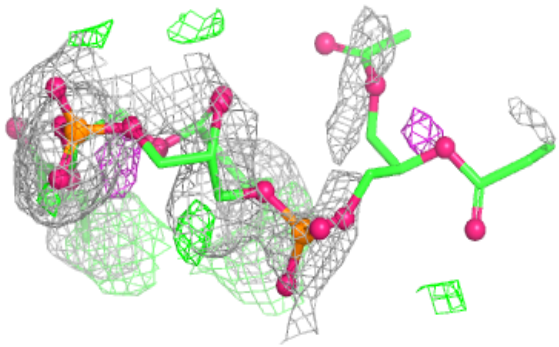
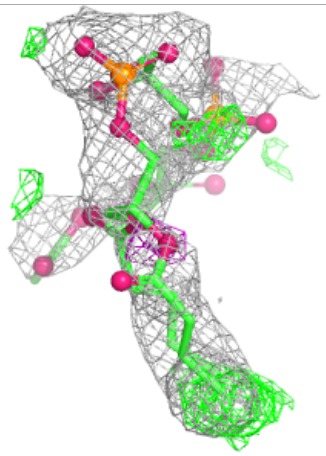
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BOG P 503:

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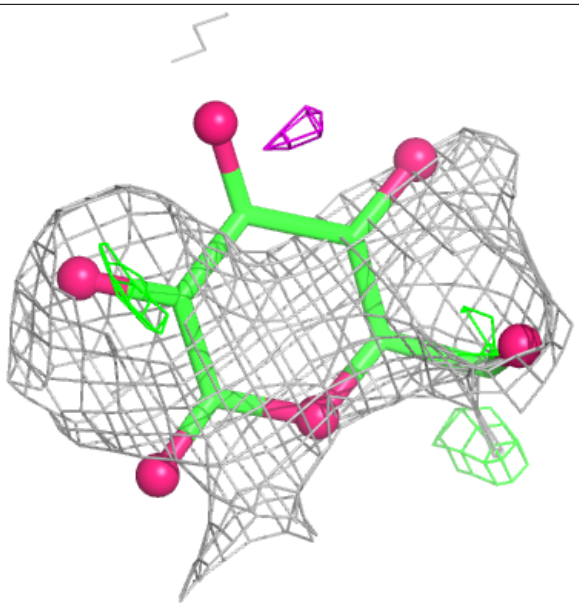
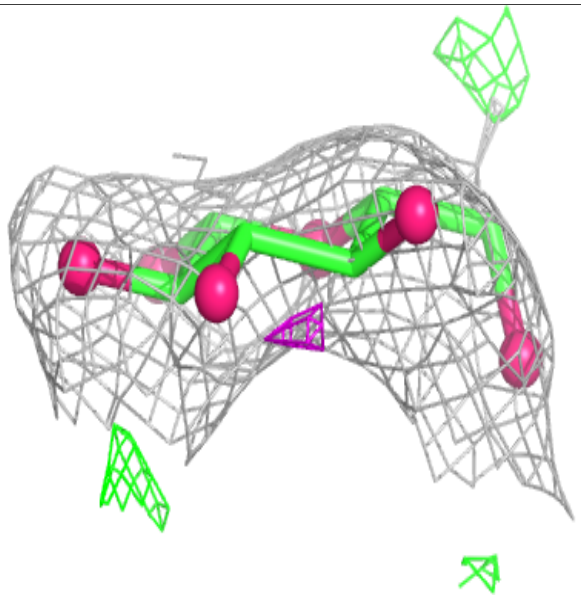
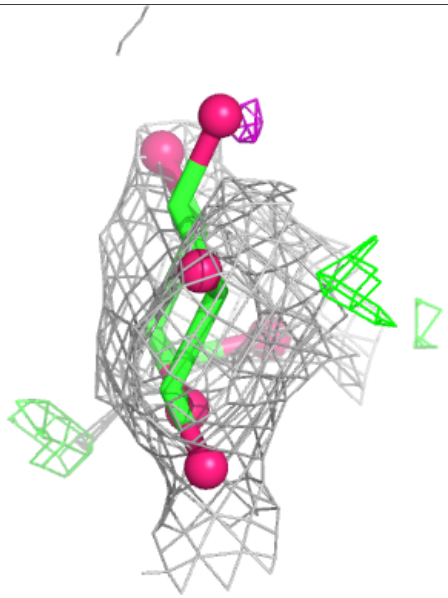
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

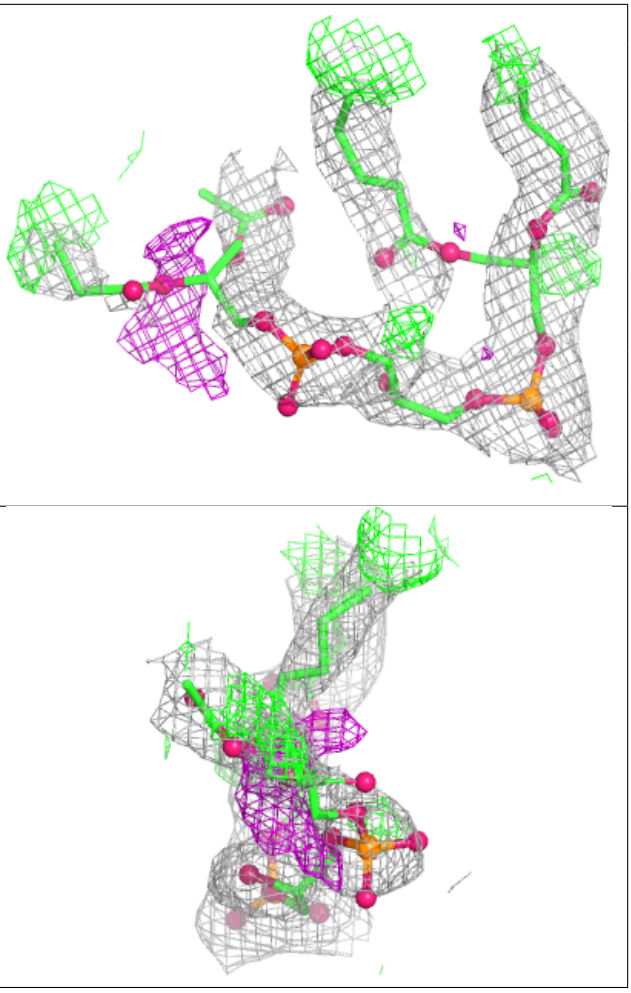






Electron density around CDL C 505:

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



Electron density around CDL P 506:

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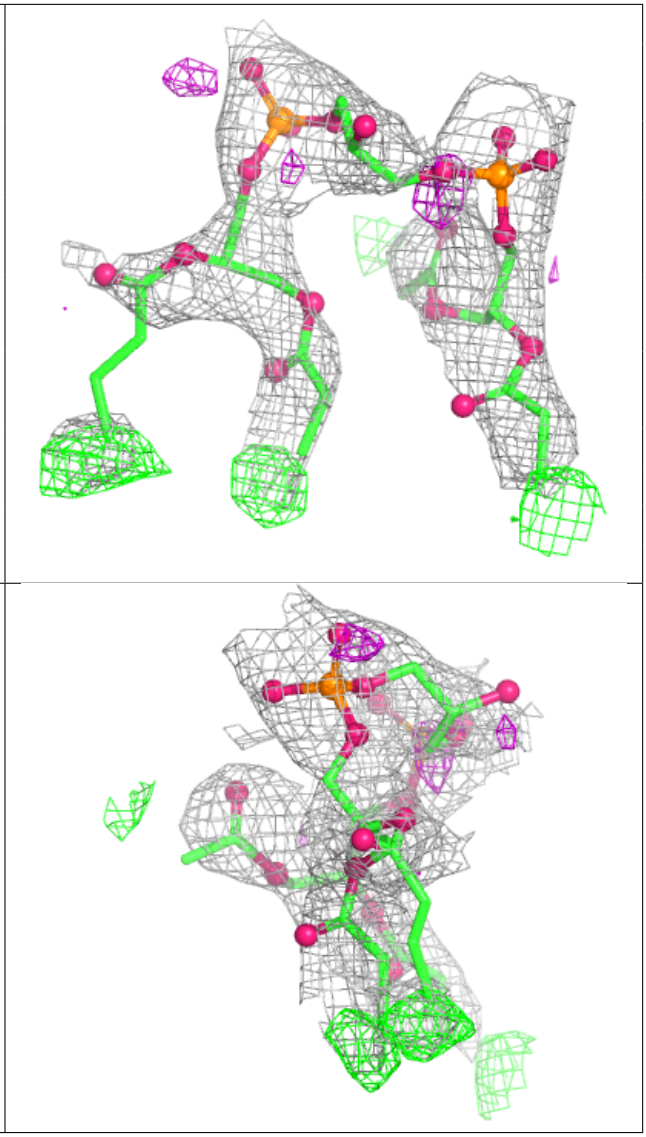
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEE R 502:

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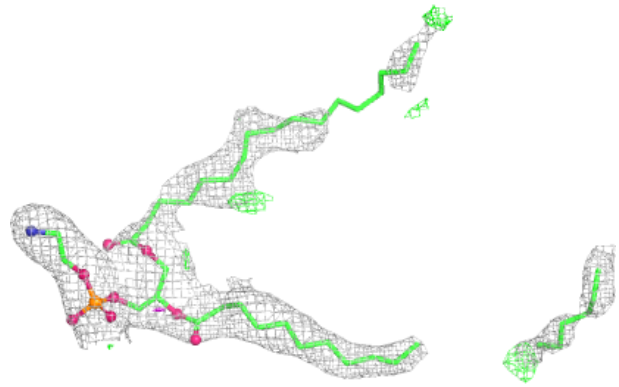
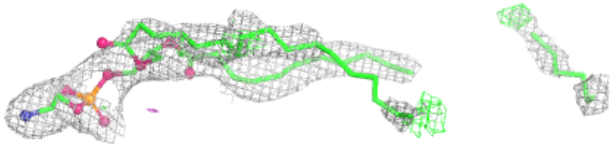
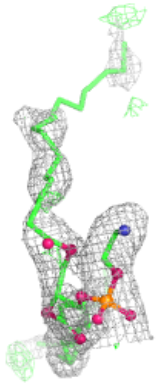
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

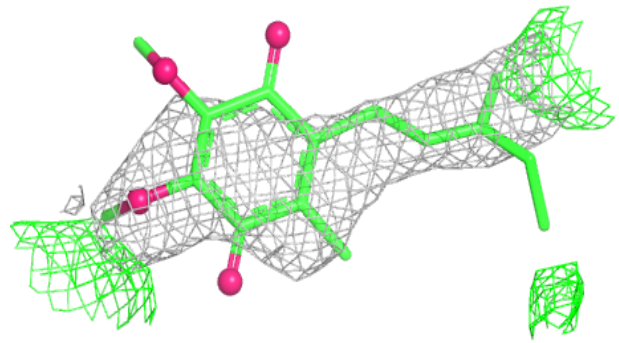


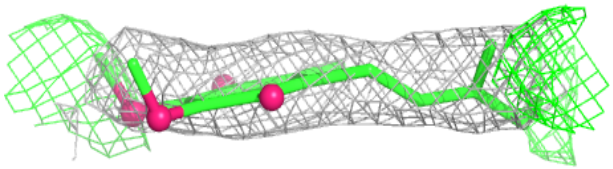


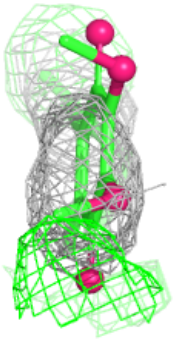


Electron density around UQ P 505:

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







Electron density around CDL G 101:

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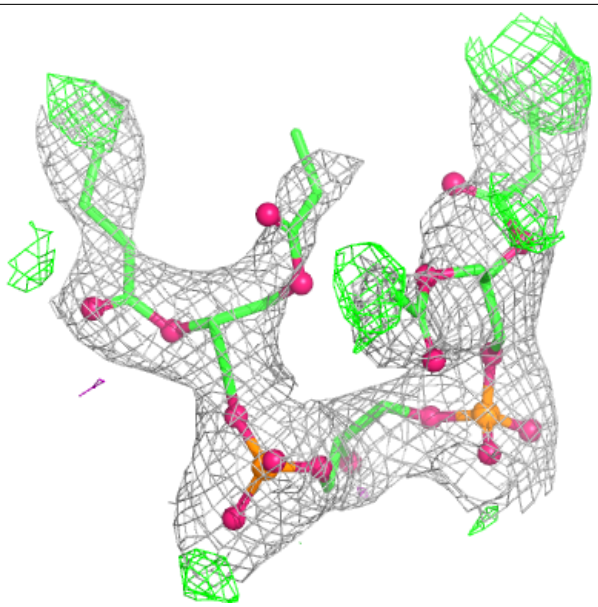
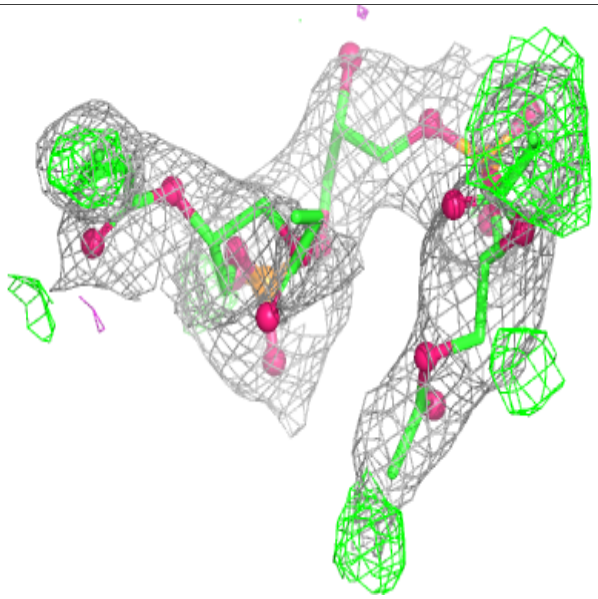
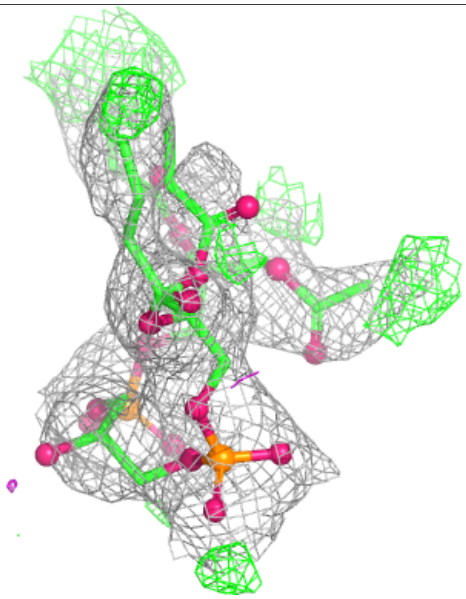
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around PEE E 502:

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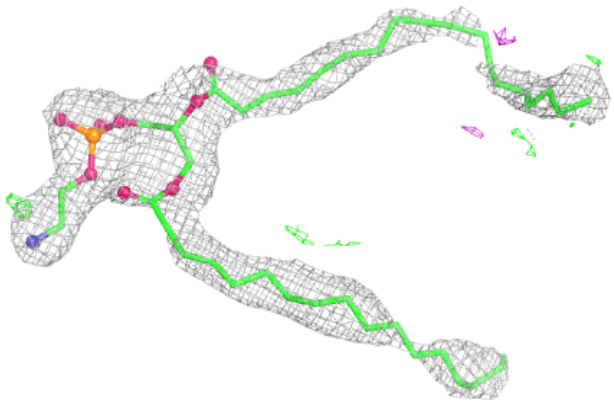
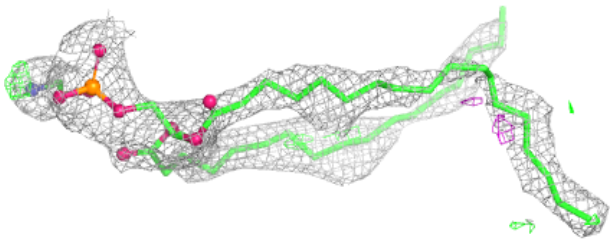
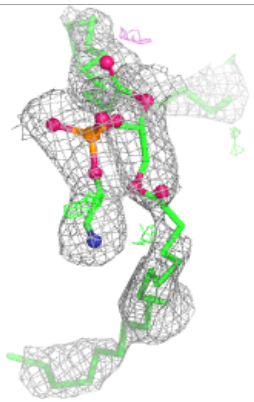
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UQ C 504:

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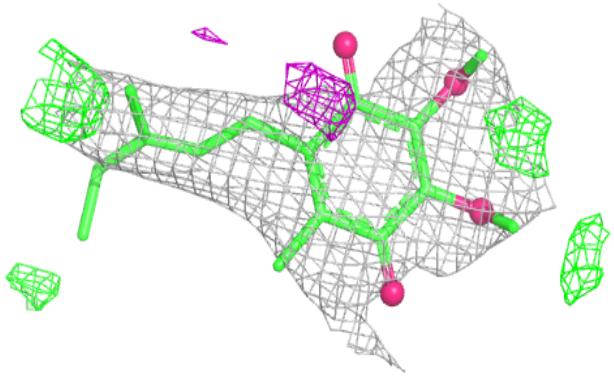
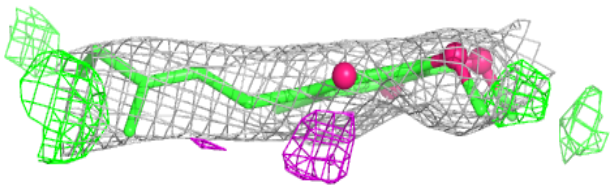
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around PEE P 507:

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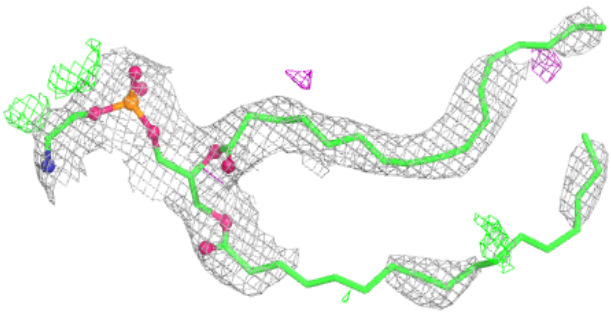
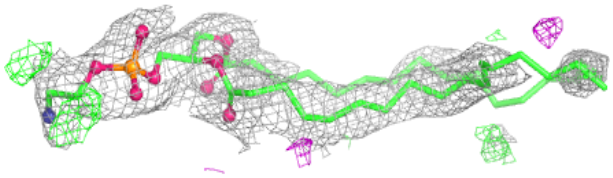
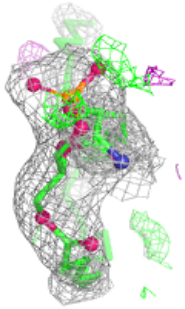
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BOG Q 503:

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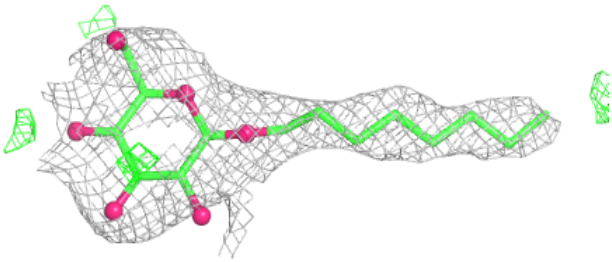
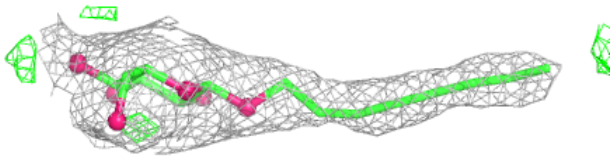
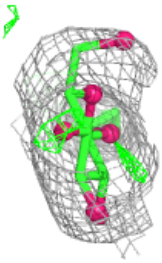
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around PEE C 506:

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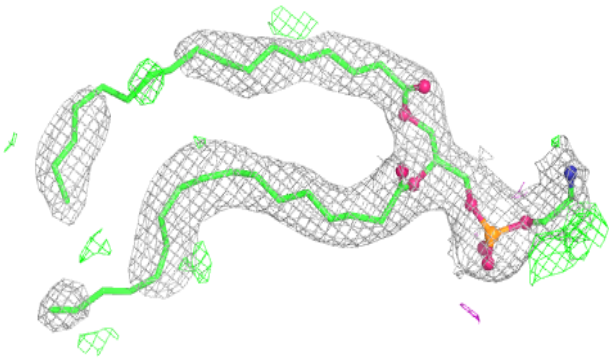
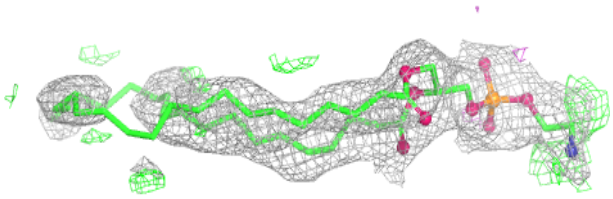
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around BOG D 502:

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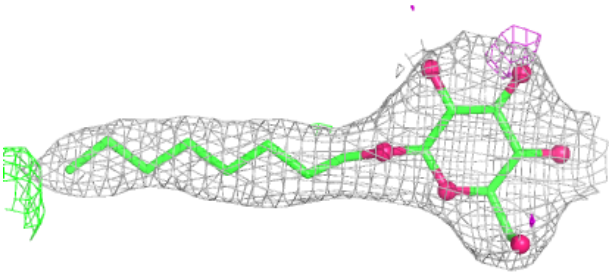
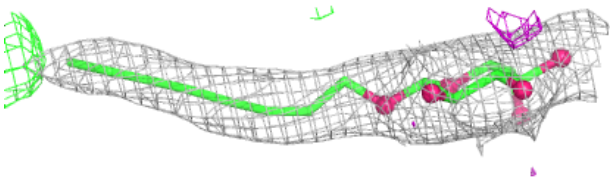
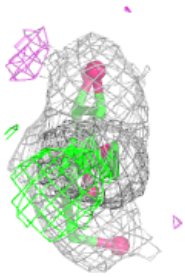
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

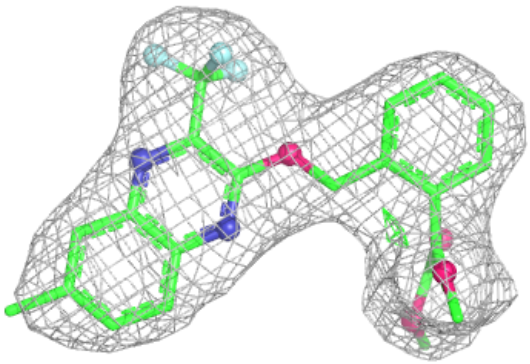


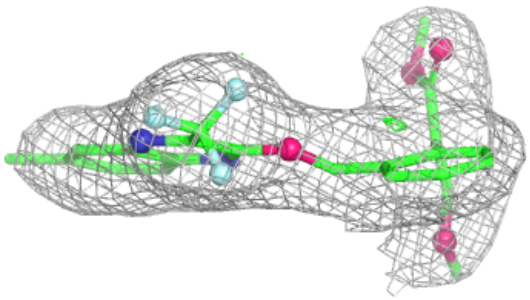


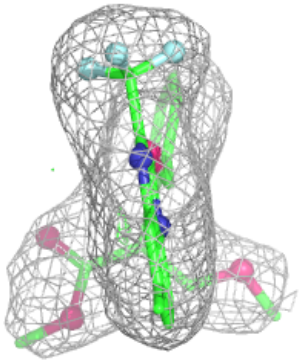


Electron density around WF3 P 504:

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

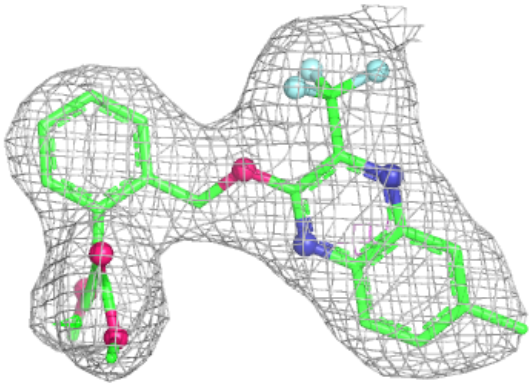


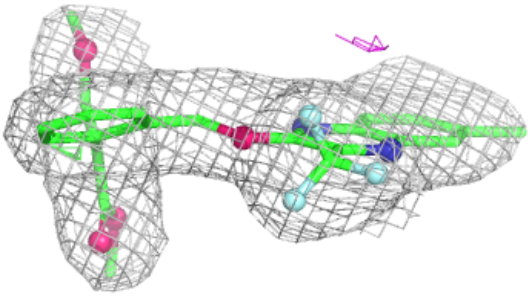


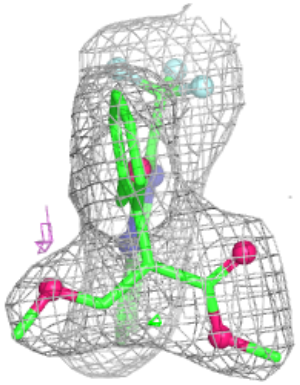


Electron density around WF3 C 503:

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

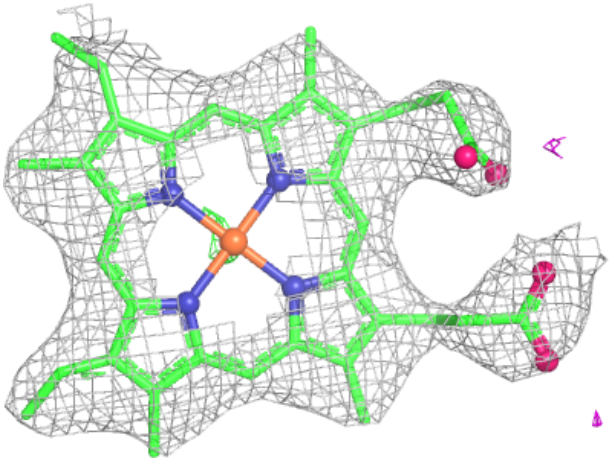


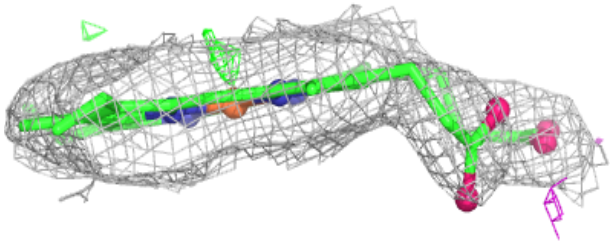


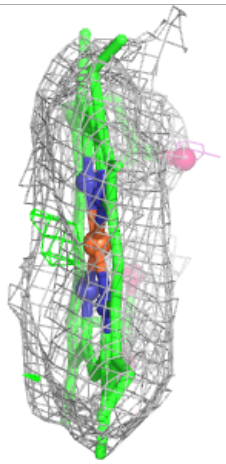


Electron density around HEM P 501:

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

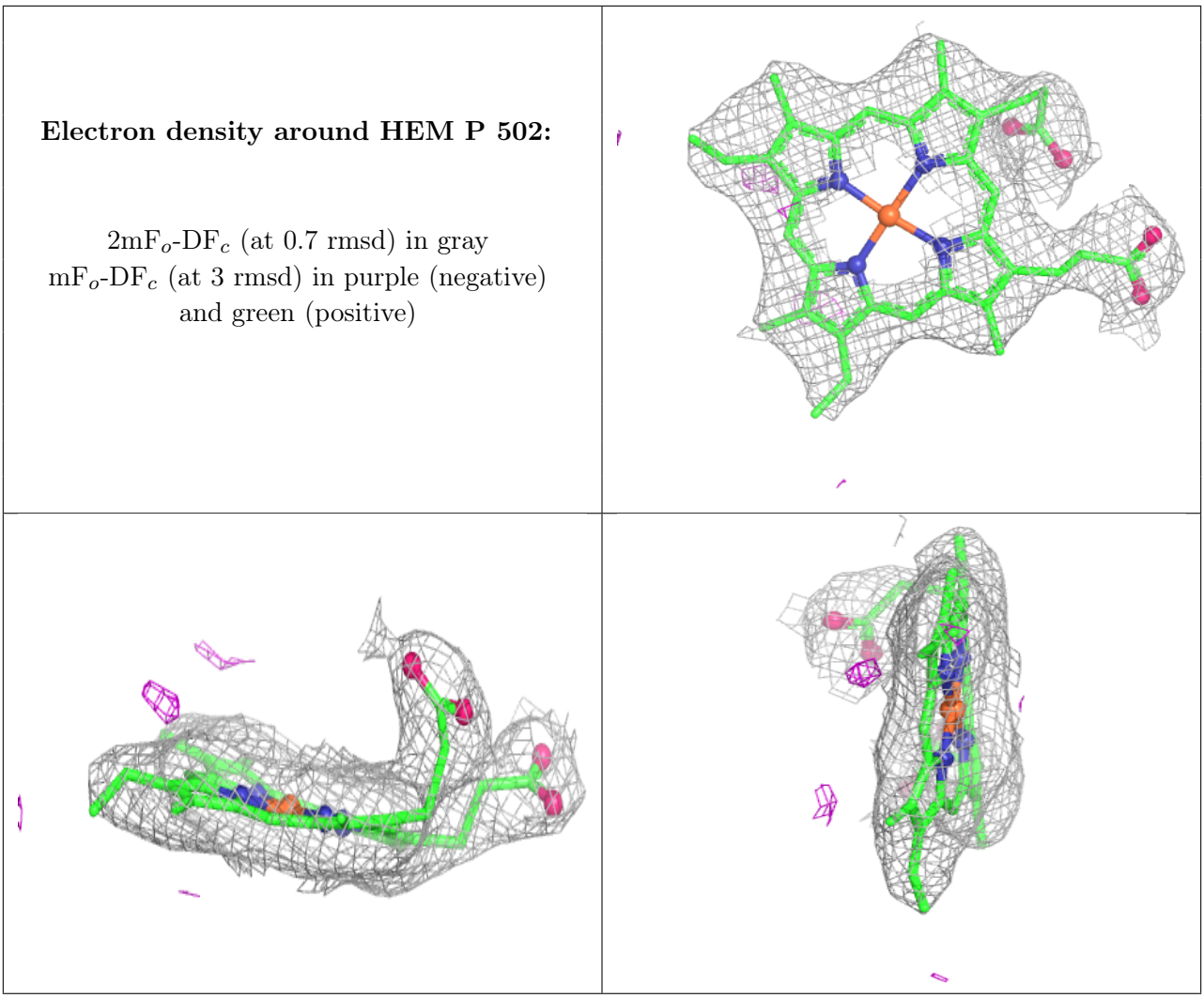






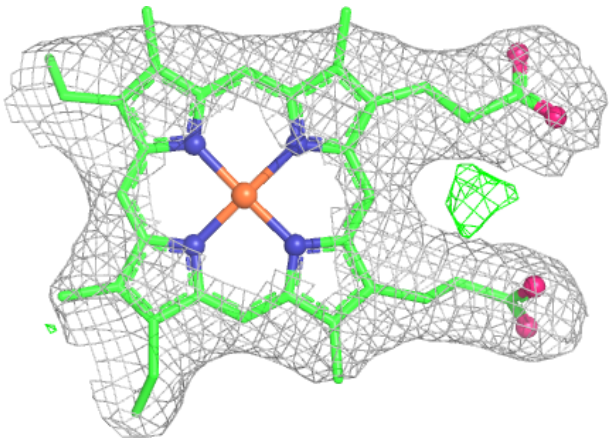
Electron density around HEM P 502:

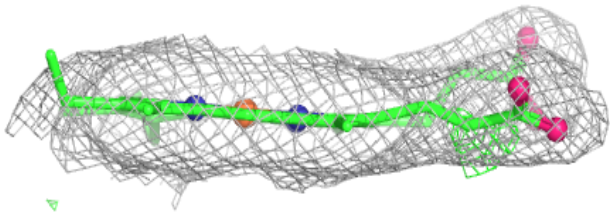
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

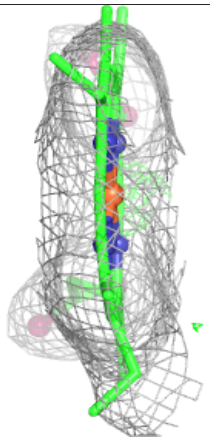


Electron density around HEC Q 501:

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

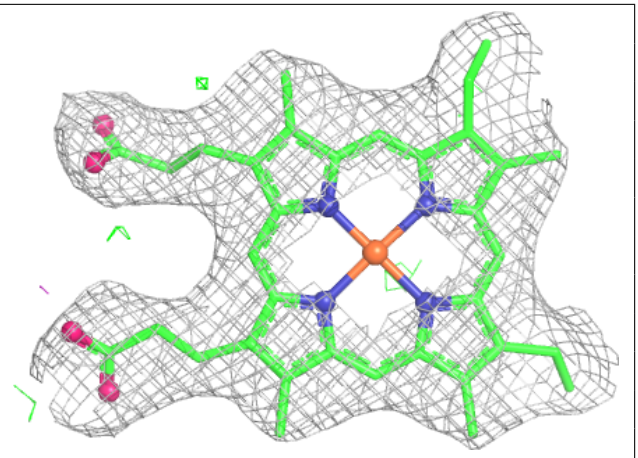


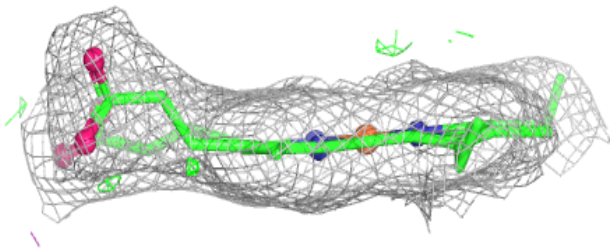


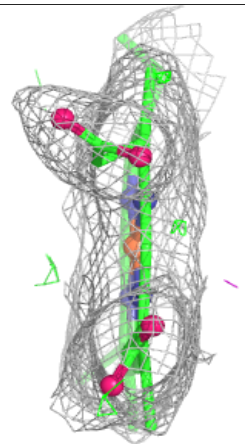


Electron density around HEC D 501:

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

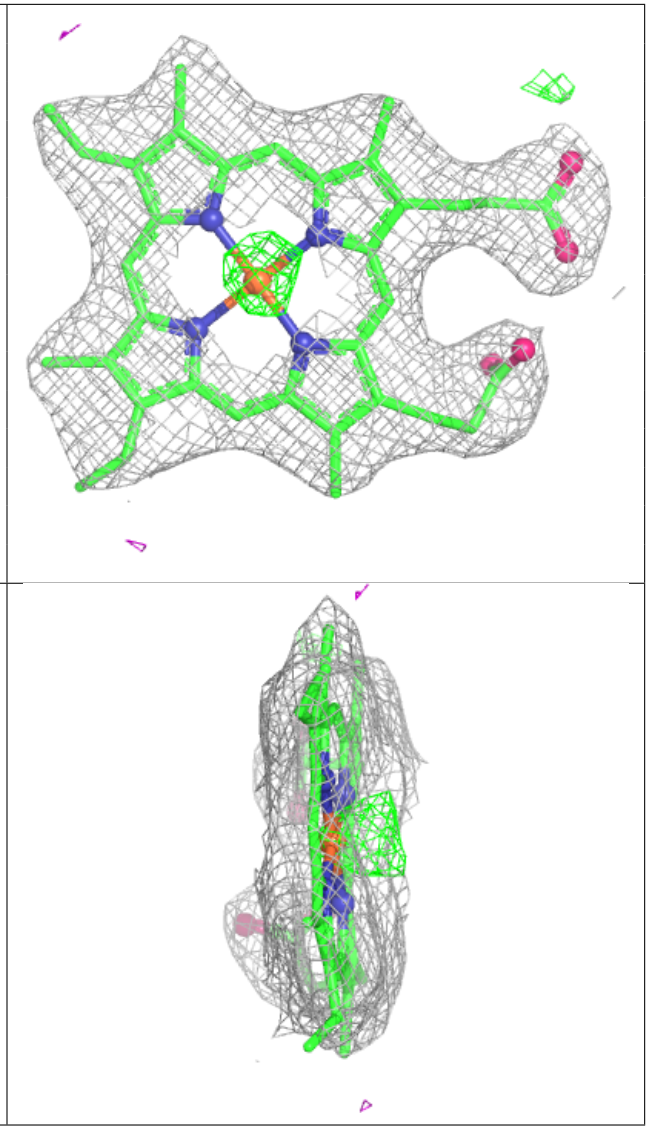






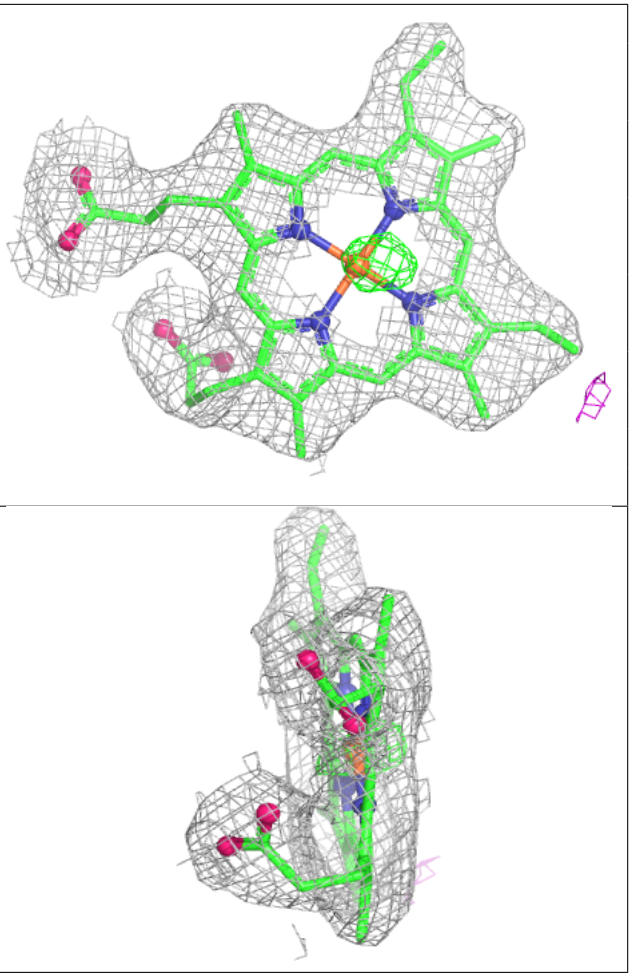
Electron density around HEM C 501:

$2mF_o$-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.