wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 06:34 AM EDT

PDB ID	:	3L70
Title	:	Cytochrome BC1 complex from chicken with trifloxystrobin bound
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-27
Resolution	:	2.75 Å(reported)

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

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

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

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

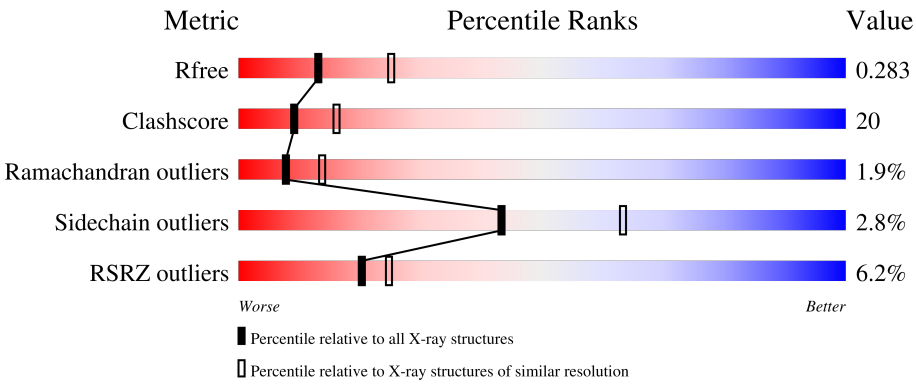
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	2%, 64%, 33%
1	N	446	2%, 61%, 35%
2	B	441	4%, 54%, 38%, 5%
2	O	441	4%, 57%, 35%
3	C	380	%, 75%, 24%

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Mol	Chain	Length	Quality of chain
3	P	380	2%, 73%, 26%
4	D	241	%, 74%, 25%
4	Q	241	5%, 70%, 29%
5	E	196	38%, 48%, 44%, 8%
5	R	196	13%, 56%, 40%
6	F	110	65%, 25%, 8%
6	S	110	4%, 62%, 27%, 8%
7	G	81	2%, 60%, 35%
7	T	81	15%, 57%, 37%
8	H	77	3%, 68%, 23%, 9%
8	U	77	17%, 61%, 25%, 13%
9	I	47	26%, 43%, 49%, 6%
9	V	47	36%, 38%, 51%, 9%
10	J	61	7%, 74%, 25%
10	W	61	5%, 67%, 30%

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	N	3008	-	X	-	-
11	PEE	R	3005	-	-	-	X
18	BOG	D	2091	-	-	-	X
18	BOG	Q	3091	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 32653 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	444	3447	2160	607	659	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	420	3133	1968	544	612	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	3017	2022	478	505	12	0	0	0
3	P	379	3012	2019	477	504	12	0	0	0

- 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

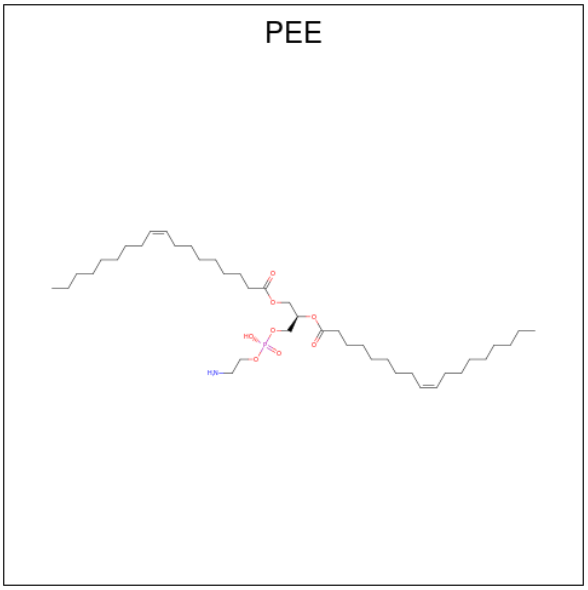
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	46	287	171	58	56	2	0	0	0
9	V	43	277	167	55	53	2	0	0	0

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

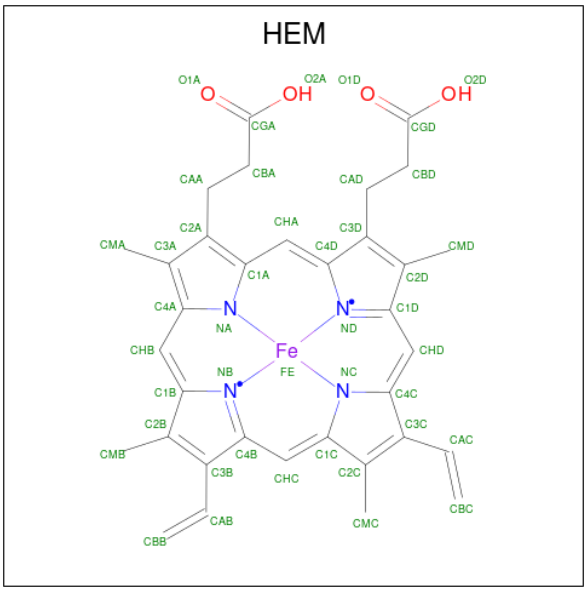
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	61	497	321	87	89	0	0	0
			Total	C	N	O			
10	W	60	479	311	86	82	0	0	1

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



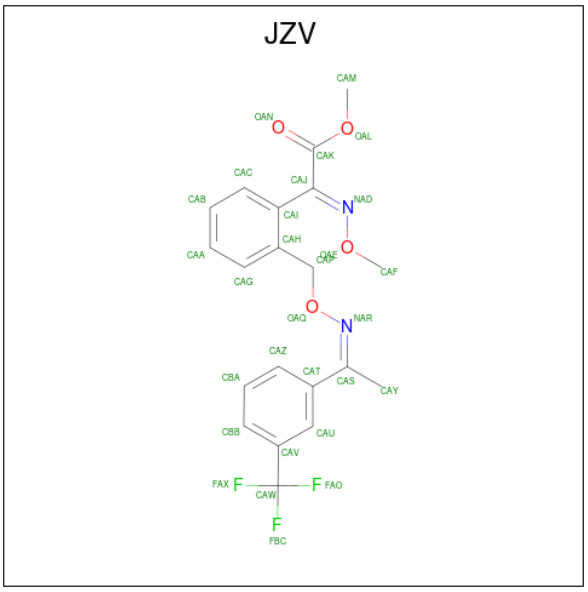
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O	P			
11	A	1	21	12	8	1		0	0
			Total	C	N	O	P		
11	C	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
11	E	1	50	40	1	8	1	0	0
			Total	O	P				
11	N	1	5	4	1			0	0
			Total	C	N	O	P		
11	P	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
11	R	1	50	40	1	8	1	0	0

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



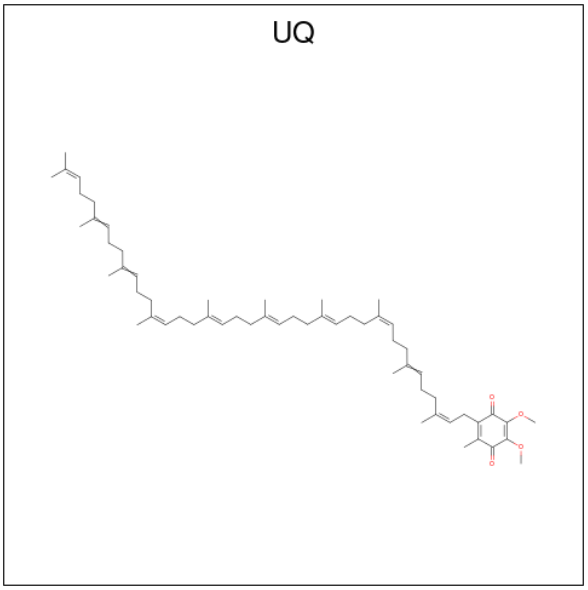
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0

- Molecule 13 is methyl (2E)-(methoxyimino)(2-{[({(1Z)-1-[3-(trifluoromethyl)phenyl]ethylidene}amino)oxy]methyl}phenyl)ethanoate (three-letter code: JZV) (formula: $C_{20}H_{19}F_3N_2O_4$).



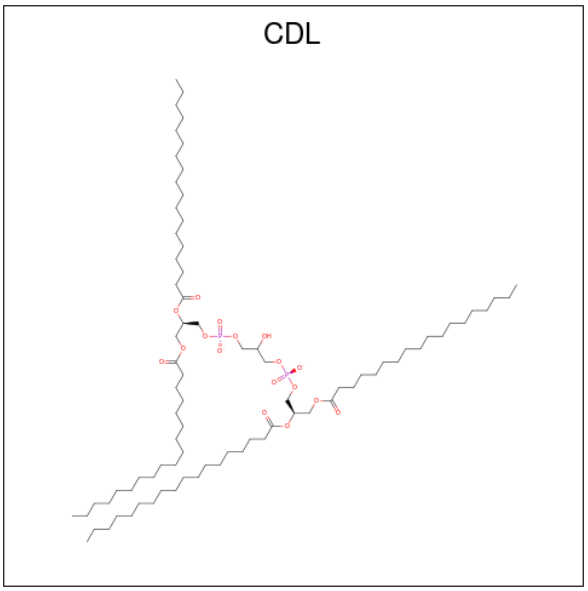
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
13	C	1	29	20	3	2	4	0	0
			Total	C	F	N	O		
13	P	1	29	20	3	2	4	0	0

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



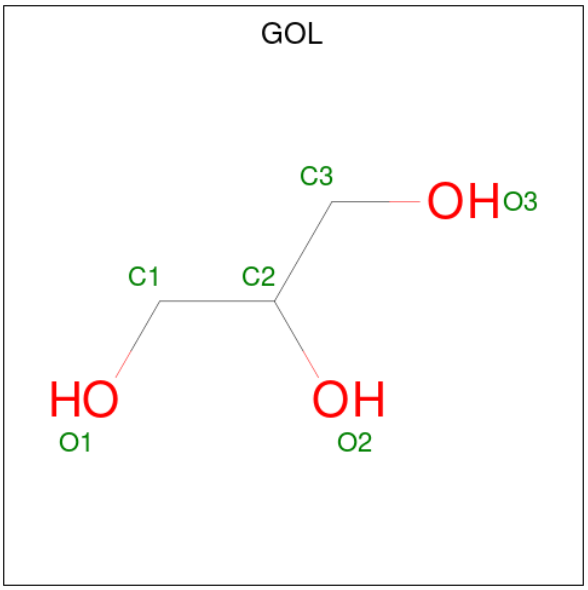
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	C	1	19	15	4	0	0
			Total	C	O		
14	P	1	19	15	4	0	0

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



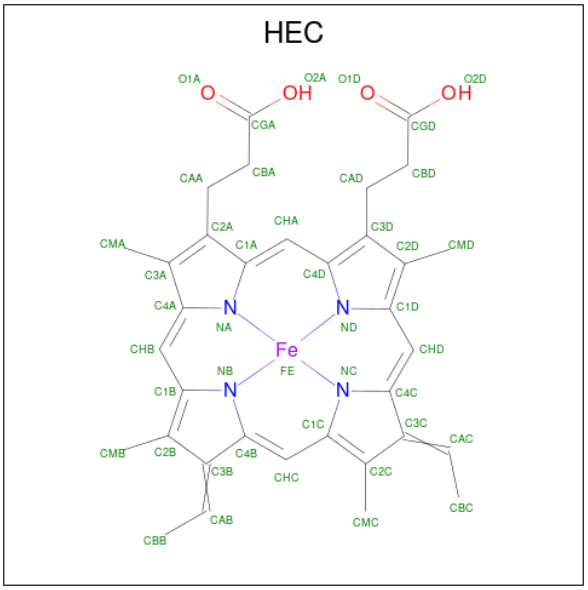
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O	P	0	0
			40	21	17	2		
15	D	1	Total	C	O	P	0	0
			42	23	17	2		
15	P	1	Total	C	O	P	0	0
			40	21	17	2		
15	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



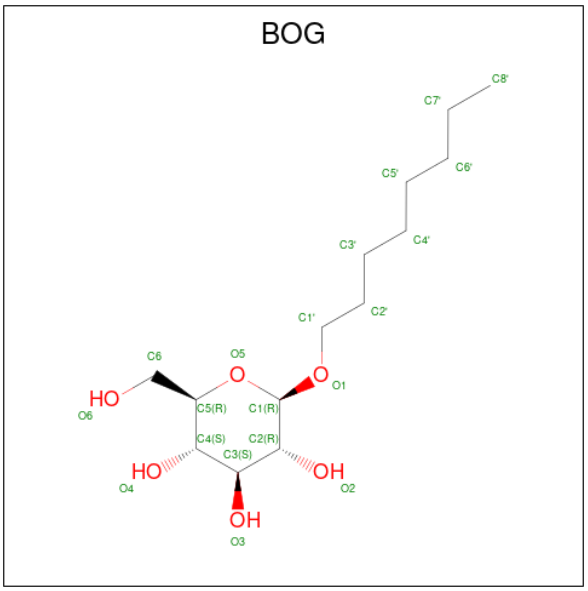
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
16	C	1	6	3	3	0	0
			Total	C	O		
16	P	1	6	3	3	0	0

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



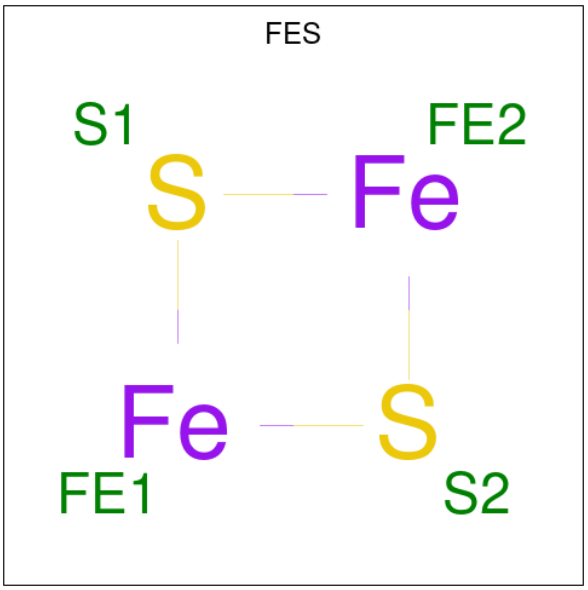
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
17	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
17	Q	1	43	34	1	4	4	0	0

- Molecule 18 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

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



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

- Molecule 20 is water.

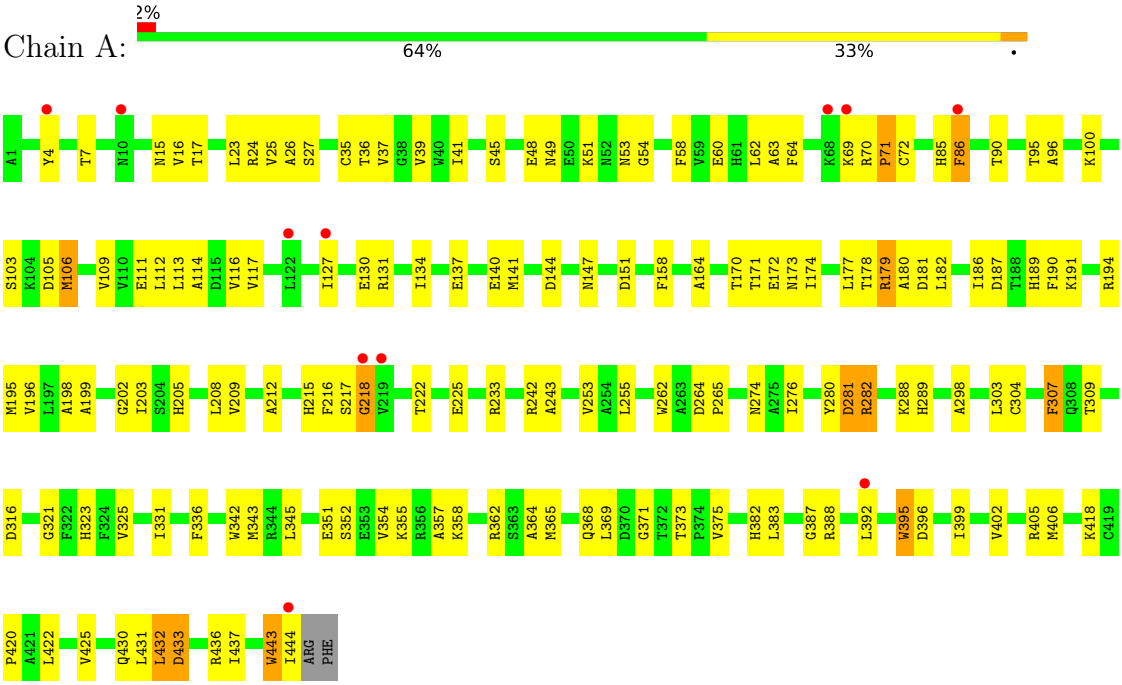
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	C	8	8	8	0	0
			Total	O		
20	E	1	1	1	0	0
			Total	O		
20	P	9	9	9	0	0
			Total	O		
20	R	1	1	1	0	0

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.

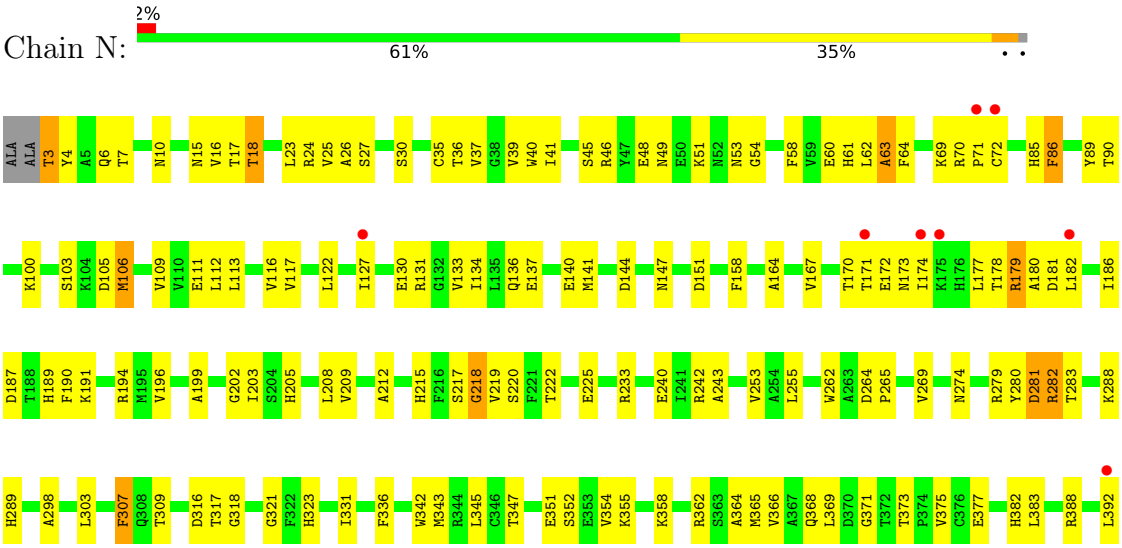
• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

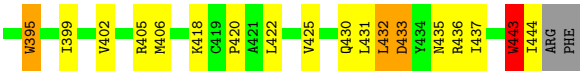
Chain A:



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

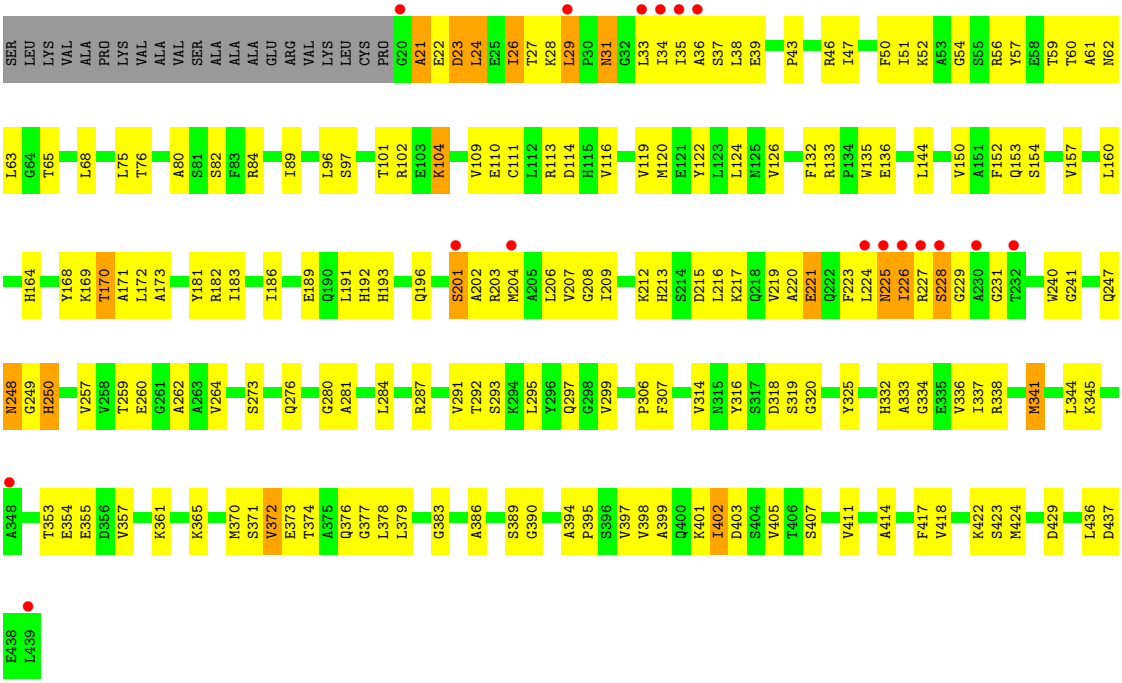
Chain N:





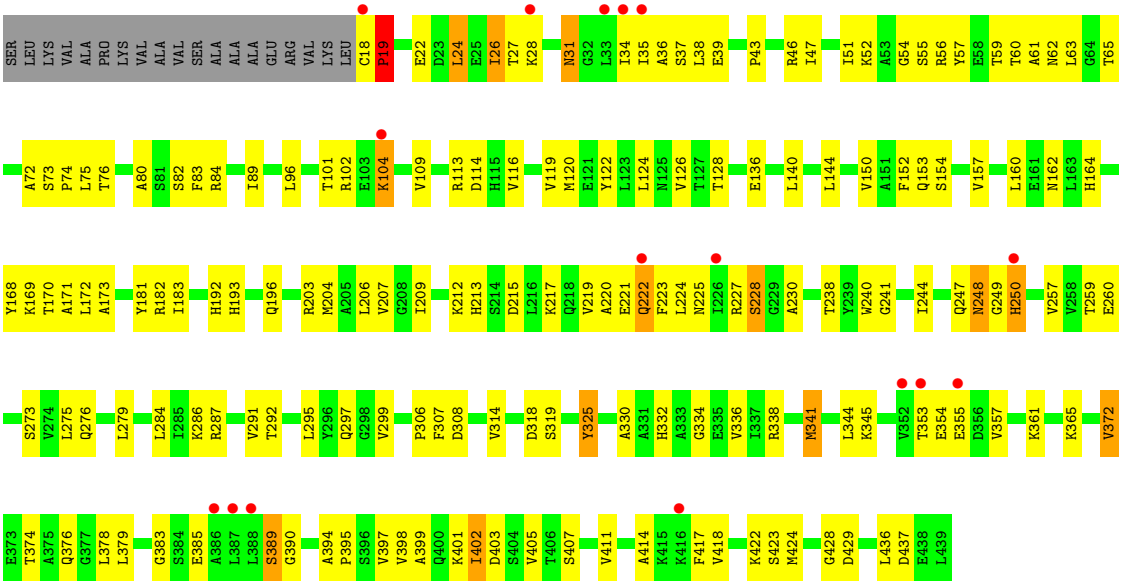
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain B:



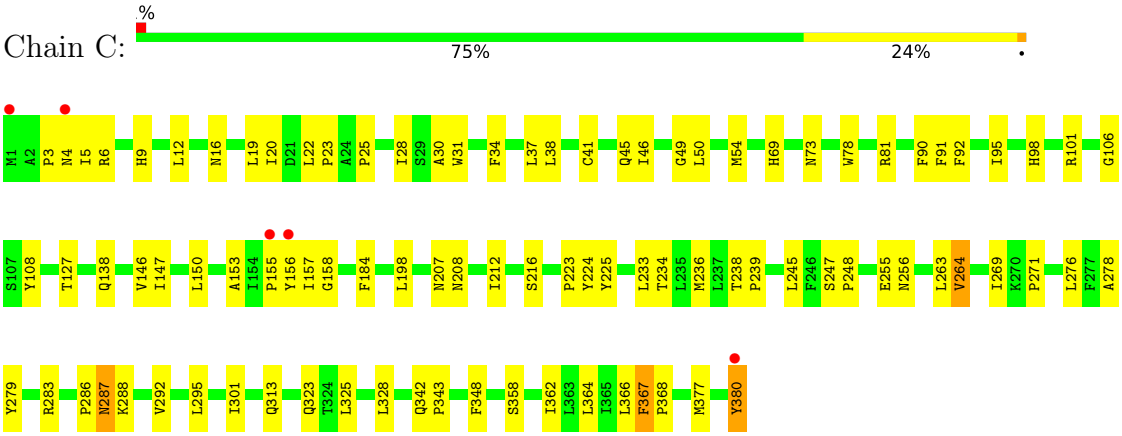
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain O:



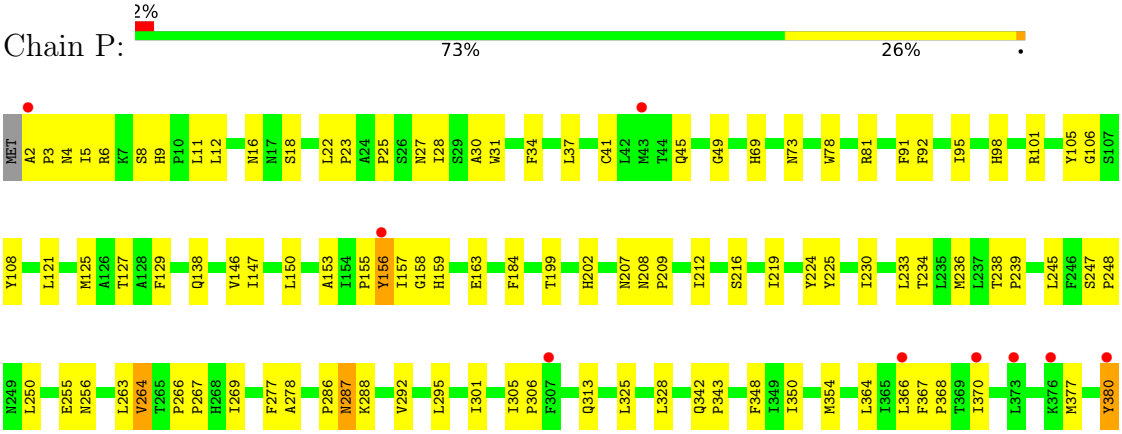
• Molecule 3: Cytochrome b

Chain C:



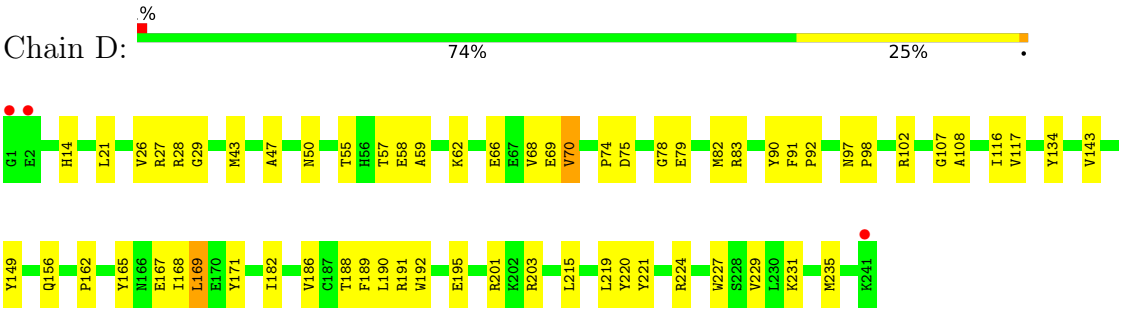
• Molecule 3: Cytochrome b

Chain P:



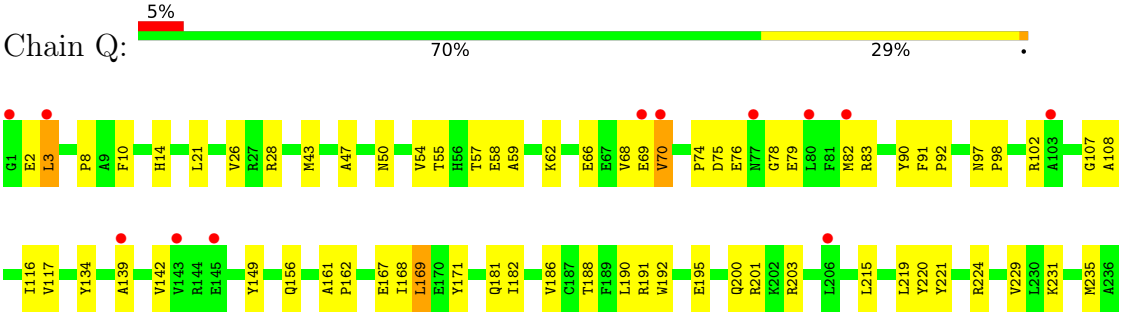
• Molecule 4: Mitochondrial cytochrome c1, heme protein

Chain D:



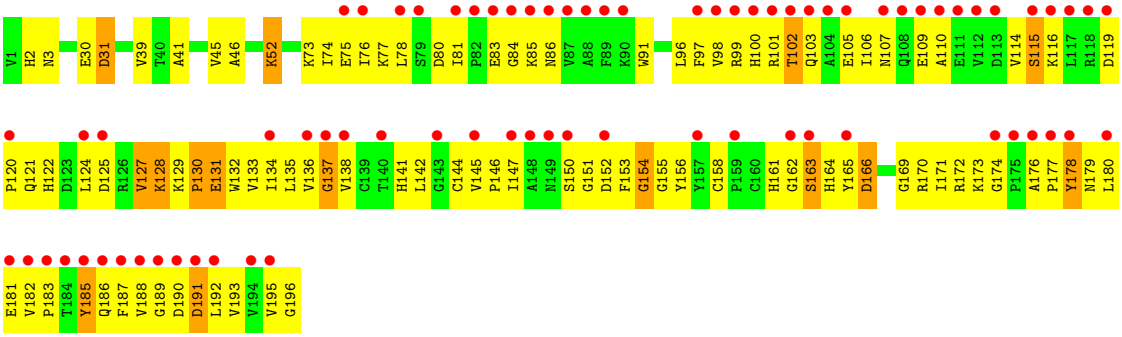
• Molecule 4: Mitochondrial cytochrome c1, heme protein

Chain Q:



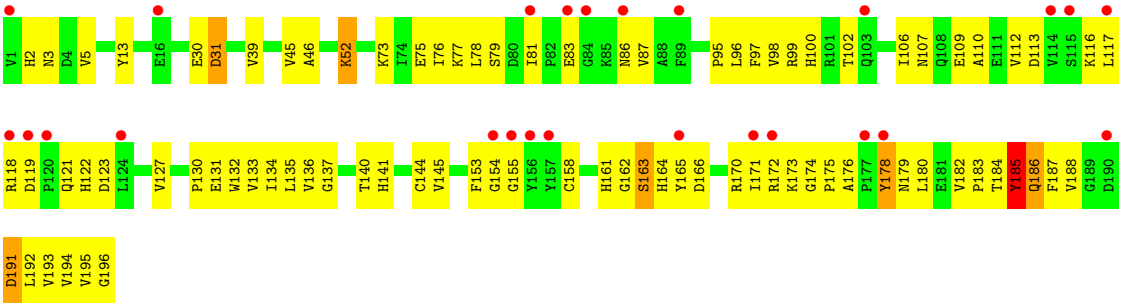
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



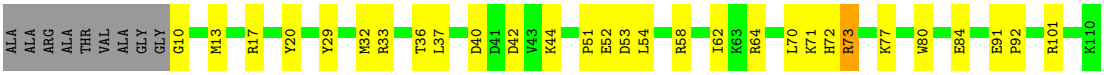
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:



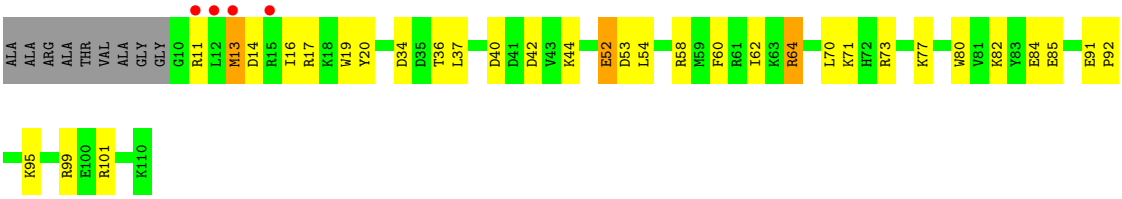
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain F:



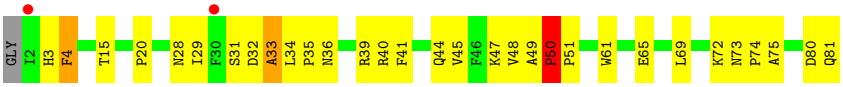
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain S:



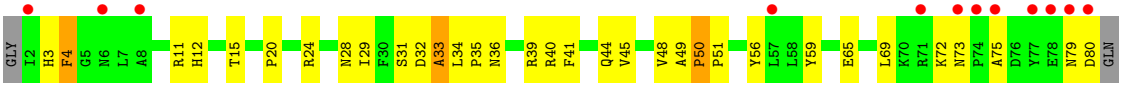
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain G:



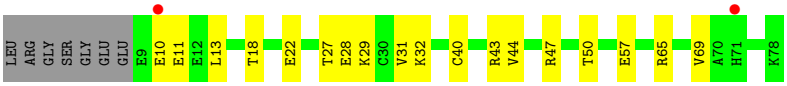
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain T:



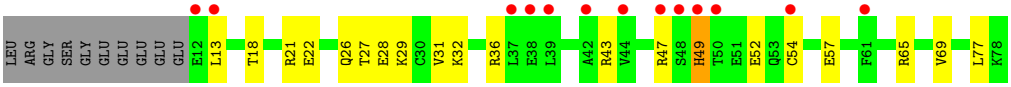
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain H:



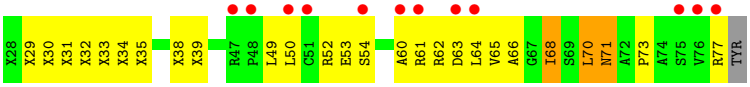
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain U:



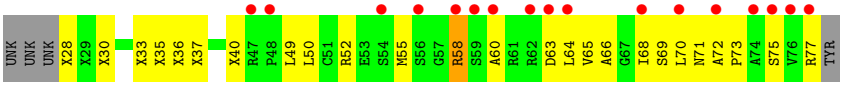
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



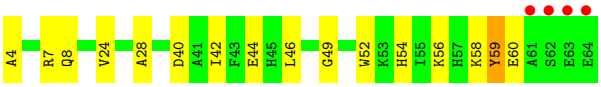
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

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	169.61Å 181.99Å 240.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 2.75 58.26 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.99-2.75) 98.8 (58.26-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.297 0.255 , 0.283	Depositor DCC
R_{free} test set	10214 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.7	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	0.91	EDS
Total number of atoms	32653	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: PEE, GOL, FES, HEC, CDL, JZV, UQ, BOG, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	0/3518	0.65	0/4767
1	N	0.42	0/3508	0.64	0/4753
2	B	0.38	0/3187	0.63	0/4321
2	O	0.40	0/3202	0.63	0/4343
3	C	0.50	0/3119	0.66	0/4270
3	P	0.45	0/3114	0.64	0/4263
4	D	0.48	0/1956	0.64	0/2658
4	Q	0.39	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.59	0/2103
5	R	0.37	0/1543	0.60	0/2098
6	F	0.54	1/911 (0.1%)	0.67	0/1219
6	S	0.43	0/911	0.61	0/1219
7	G	0.49	0/694	0.69	0/941
7	T	0.43	0/684	0.64	0/929
8	H	0.44	0/582	0.63	0/779
8	U	0.31	0/561	0.56	0/751
9	I	0.39	0/218	0.60	0/293
9	V	0.36	0/218	0.59	0/293
10	J	0.43	0/508	0.60	0/682
10	W	0.40	0/490	0.60	0/660
All	All	0.43	1/32427 (0.0%)	0.63	0/44000

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	10	GLY	N-CA	5.16	1.53	1.46

There are no bond angle outliers.

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	3447	0	3362	126	0
1	N	3437	0	3349	143	0
2	B	3133	0	3130	187	0
2	O	3147	0	3146	181	0
3	C	3017	0	3063	76	0
3	P	3012	0	3058	95	0
4	D	1898	0	1846	55	0
4	Q	1898	0	1846	67	0
5	E	1513	0	1478	122	0
5	R	1509	0	1474	94	0
6	F	891	0	893	20	0
6	S	891	0	893	33	0
7	G	672	0	653	32	0
7	T	662	0	645	35	0
8	H	574	0	548	16	0
8	U	553	0	535	22	0
9	I	287	0	250	37	0
9	V	277	0	251	32	0
10	J	497	0	490	16	0
10	W	479	0	478	16	0
11	A	21	0	13	0	0
11	C	49	0	72	4	0
11	E	50	0	77	1	0
11	N	5	0	0	0	0
11	P	49	0	72	3	0
11	R	50	0	77	2	0
12	C	86	0	60	9	0
12	P	86	0	60	7	0
13	C	29	0	19	4	0
13	P	29	0	19	4	0
14	C	19	0	17	4	0
14	P	19	0	17	5	0
15	C	40	0	24	4	0
15	D	42	0	28	4	0
15	P	40	0	24	4	0
15	Q	42	0	28	3	0
16	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	6	0	8	0	0
17	D	43	0	30	3	0
17	Q	43	0	30	1	0
18	D	33	0	39	0	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	1	0
20	R	1	0	0	0	0
All	All	32653	0	32160	1298	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 20.

The worst 5 of 1298 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)
9:V:35:UNK:HG3	9:V:36:UNK:H	1.05	1.14
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.15	1.13
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.34	1.07
2:B:76:THR:HG22	2:B:82:SER:H	1.18	1.07
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07

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	442/446 (99%)	414 (94%)	22 (5%)	6 (1%)	11	19
1	N	440/446 (99%)	414 (94%)	19 (4%)	7 (2%)	9	16
2	B	418/441 (95%)	358 (86%)	46 (11%)	14 (3%)	4	5
2	O	420/441 (95%)	370 (88%)	40 (10%)	10 (2%)	6	9
3	C	378/380 (100%)	363 (96%)	10 (3%)	5 (1%)	12	21
3	P	377/380 (99%)	358 (95%)	14 (4%)	5 (1%)	12	21
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	34	53
5	E	194/196 (99%)	152 (78%)	28 (14%)	14 (7%)	1	1
5	R	194/196 (99%)	165 (85%)	22 (11%)	7 (4%)	3	5
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
6	S	99/110 (90%)	91 (92%)	8 (8%)	0	100	100
7	G	78/81 (96%)	69 (88%)	6 (8%)	3 (4%)	3	4
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	5	8
8	H	68/77 (88%)	64 (94%)	4 (6%)	0	100	100
8	U	65/77 (84%)	60 (92%)	3 (5%)	2 (3%)	4	6
9	I	29/47 (62%)	27 (93%)	2 (7%)	0	100	100
9	V	29/47 (62%)	28 (97%)	1 (3%)	0	100	100
10	J	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	16
All	All	4002/4160 (96%)	3659 (91%)	266 (7%)	77 (2%)	8	14

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY
2	B	21	ALA
2	B	24	LEU
2	B	26	ILE
2	B	29	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%)	354 (97%)	11 (3%)	41	61
1	N	365/368 (99%)	352 (96%)	13 (4%)	35	55
2	B	331/347 (95%)	321 (97%)	10 (3%)	41	61
2	O	333/347 (96%)	324 (97%)	9 (3%)	44	65
3	C	328/329 (100%)	320 (98%)	8 (2%)	49	68
3	P	328/329 (100%)	322 (98%)	6 (2%)	59	75
4	D	200/200 (100%)	197 (98%)	3 (2%)	65	78
4	Q	200/200 (100%)	197 (98%)	3 (2%)	65	78
5	E	166/166 (100%)	161 (97%)	5 (3%)	41	61
5	R	165/166 (99%)	161 (98%)	4 (2%)	49	68
6	F	93/96 (97%)	88 (95%)	5 (5%)	22	38
6	S	93/96 (97%)	88 (95%)	5 (5%)	22	38
7	G	71/71 (100%)	69 (97%)	2 (3%)	43	63
7	T	70/71 (99%)	69 (99%)	1 (1%)	67	79
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	62	77
9	I	23/26 (88%)	20 (87%)	3 (13%)	4	6
9	V	23/26 (88%)	20 (87%)	3 (13%)	4	6
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	72
10	W	47/49 (96%)	46 (98%)	1 (2%)	53	71
All	All	3378/3446 (98%)	3284 (97%)	94 (3%)	43	63

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

Mol	Chain	Res	Type
1	N	395	TRP
3	P	91	PHE
1	N	432	LEU
2	O	248	ASN
3	P	380	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	297	GLN
4	Q	50	ASN
2	O	343	GLN
3	P	82	ASN
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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	GOL	P	3011	-	5,5,5	1.38	1 (20%)	5,5,5	0.65	0
18	BOG	Q	3009	-	20,20,20	0.98	1 (5%)	25,25,25	0.89	1 (4%)
19	FES	R	501	5	0,4,4	-	-	-		
15	CDL	P	3004	-	39,39,99	1.21	2 (5%)	45,51,111	1.11	4 (8%)
12	HEM	P	501	3	41,50,50	1.59	6 (14%)	45,82,82	1.46	7 (15%)
11	PEE	P	3007	-	48,48,50	1.39	7 (14%)	51,53,55	0.82	2 (3%)
19	FES	E	501	5	0,4,4	-	-	-		
15	CDL	C	2004	-	39,39,99	1.20	2 (5%)	45,51,111	1.09	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	HEC	D	501	4	32,50,50	1.68	3 (9%)	24,82,82	1.21	2 (8%)
18	BOG	Q	3091	-	13,13,20	1.41	2 (15%)	18,18,25	1.13	2 (11%)
11	PEE	E	2005	-	49,49,50	1.54	10 (20%)	52,54,55	0.88	3 (5%)
14	UQ	C	2002	-	19,19,63	2.71	10 (52%)	23,26,79	1.28	3 (13%)
16	GOL	C	2011	-	5,5,5	1.27	0	5,5,5	0.61	0
14	UQ	P	3002	-	19,19,63	2.69	10 (52%)	23,26,79	1.28	3 (13%)
12	HEM	C	501	3	41,50,50	1.49	4 (9%)	45,82,82	1.60	12 (26%)
12	HEM	P	502	3	41,50,50	1.65	6 (14%)	45,82,82	1.71	9 (20%)
11	PEE	A	2008	-	20,20,50	1.86	6 (30%)	23,25,55	0.67	0
11	PEE	N	3008	-	4,4,50	3.61	4 (100%)	6,6,55	0.65	0
13	JZV	C	2001	-	30,30,30	1.92	5 (16%)	40,41,41	3.73	11 (27%)
11	PEE	C	2007	-	48,48,50	1.42	7 (14%)	51,53,55	0.85	2 (3%)
18	BOG	P	2010	-	12,12,20	1.37	2 (16%)	17,17,25	0.58	0
12	HEM	C	502	3	41,50,50	1.71	7 (17%)	45,82,82	1.91	12 (26%)
18	BOG	D	2009	-	20,20,20	0.95	2 (10%)	25,25,25	0.82	2 (8%)
13	JZV	P	3001	-	30,30,30	1.96	5 (16%)	40,41,41	3.82	11 (27%)
15	CDL	D	2003	-	41,41,99	1.20	4 (9%)	47,53,111	1.03	2 (4%)
18	BOG	D	2091	-	13,13,20	1.31	2 (15%)	18,18,25	1.10	2 (11%)
17	HEC	Q	501	4	32,50,50	2.10	3 (9%)	24,82,82	1.34	2 (8%)
15	CDL	Q	3003	-	41,41,99	1.20	2 (4%)	47,53,111	1.04	2 (4%)
11	PEE	R	3005	-	49,49,50	1.51	10 (20%)	52,54,55	0.87	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	GOL	P	3011	-	-	3/4/4/4	-
18	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
15	CDL	P	3004	-	-	21/49/49/110	-
12	HEM	P	501	3	-	4/12/54/54	-
11	PEE	P	3007	-	-	26/52/52/54	-
19	FES	E	501	5	-	-	0/1/1/1
15	CDL	C	2004	-	-	21/49/49/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEC	D	501	4	-	6/10/54/54	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
11	PEE	E	2005	-	-	27/53/53/54	-
14	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
16	GOL	C	2011	-	-	4/4/4/4	-
14	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
12	HEM	C	501	3	-	6/12/54/54	-
12	HEM	P	502	3	-	6/12/54/54	-
11	PEE	A	2008	-	-	12/24/24/54	-
13	JZV	C	2001	-	-	3/29/29/29	0/2/2/2
11	PEE	C	2007	-	-	23/52/52/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
12	HEM	C	502	3	-	5/12/54/54	-
18	BOG	D	2009	-	-	5/11/31/31	0/1/1/1
13	JZV	P	3001	-	-	3/29/29/29	0/2/2/2
15	CDL	D	2003	-	-	24/51/51/110	-
18	BOG	D	2091	-	-	2/4/24/31	0/1/1/1
17	HEC	Q	501	4	-	6/10/54/54	-
15	CDL	Q	3003	-	-	25/51/51/110	-
11	PEE	R	3005	-	-	27/53/53/54	-

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C2B-C3B	-7.39	1.33	1.40
17	Q	501	HEC	C3C-C2C	-7.29	1.33	1.40
17	D	501	HEC	C3C-C2C	-6.41	1.34	1.40
13	P	3001	JZV	CAT-CAS	-6.21	1.39	1.49
13	C	2001	JZV	CAT-CAS	-6.00	1.39	1.49

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	3001	JZV	OAQ-NAR-CAS	14.28	133.72	111.91
13	C	2001	JZV	OAQ-NAR-CAS	12.49	131.00	111.91
13	P	3001	JZV	CAT-CAS-NAR	10.28	133.75	115.28
13	C	2001	JZV	CAT-CAS-NAR	10.15	133.53	115.28
13	C	2001	JZV	CAY-CAS-NAR	-9.97	108.61	123.88

There are no chirality outliers.

5 of 276 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O2P

There are no ring outliers.

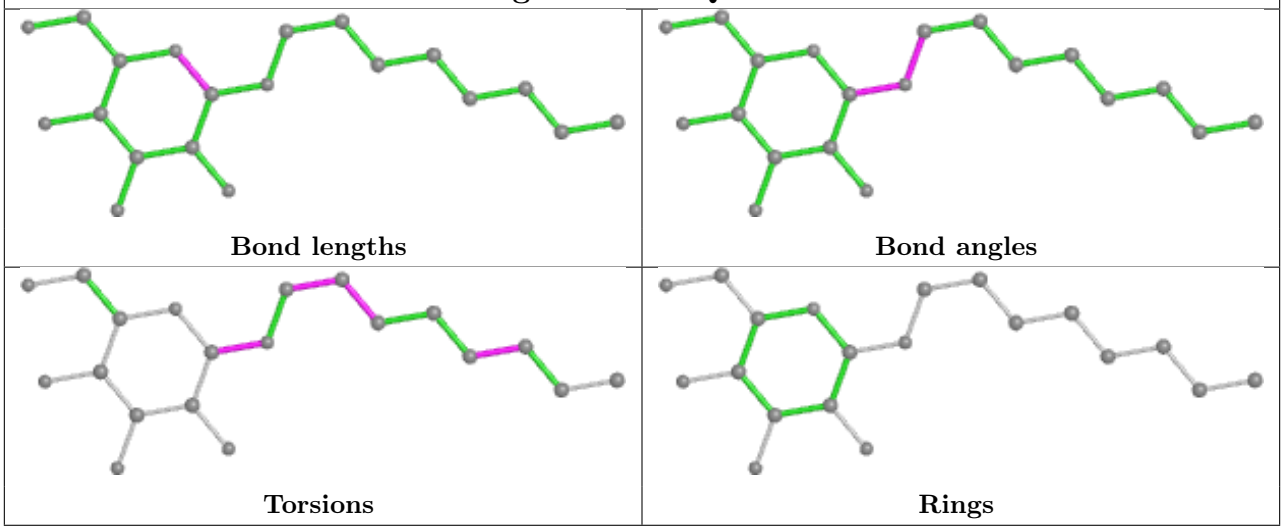
22 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	R	501	FES	2	0
15	P	3004	CDL	4	0
12	P	501	HEM	4	0
11	P	3007	PEE	3	0
19	E	501	FES	2	0
15	C	2004	CDL	4	0
17	D	501	HEC	3	0
18	Q	3091	BOG	1	0
11	E	2005	PEE	1	0
14	C	2002	UQ	4	0
14	P	3002	UQ	5	0
12	C	501	HEM	5	0
12	P	502	HEM	3	0
13	C	2001	JZV	4	0
11	C	2007	PEE	4	0
18	P	2010	BOG	1	0
12	C	502	HEM	4	0
13	P	3001	JZV	4	0
15	D	2003	CDL	4	0
17	Q	501	HEC	1	0
15	Q	3003	CDL	3	0
11	R	3005	PEE	2	0

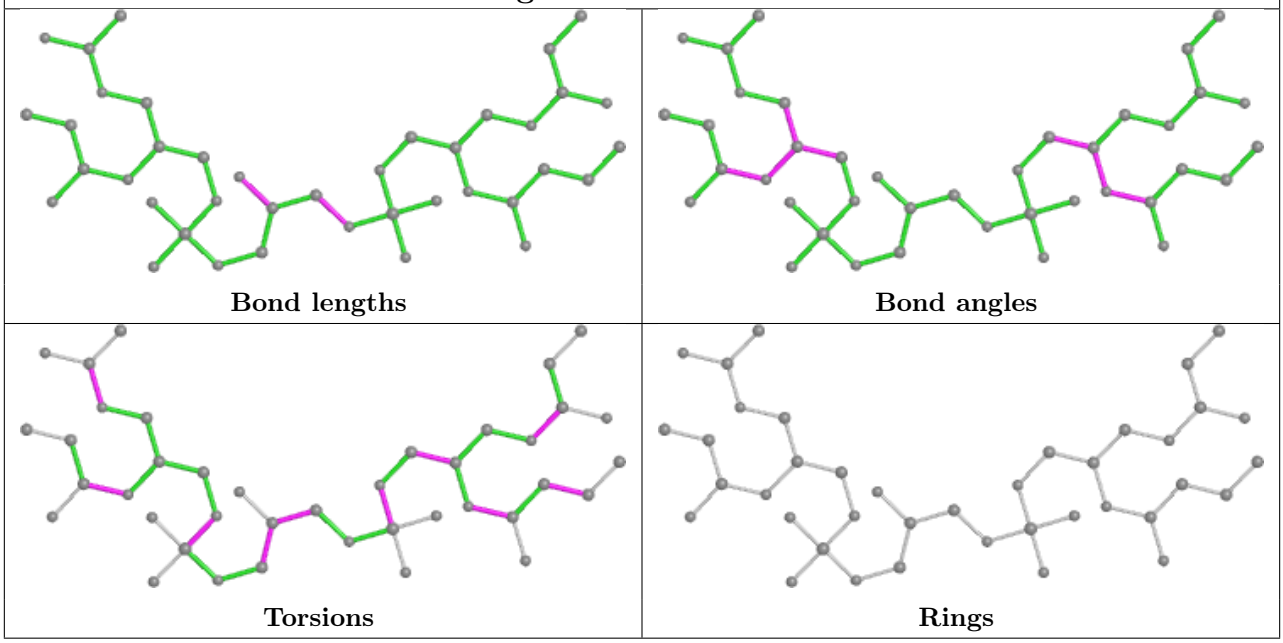
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

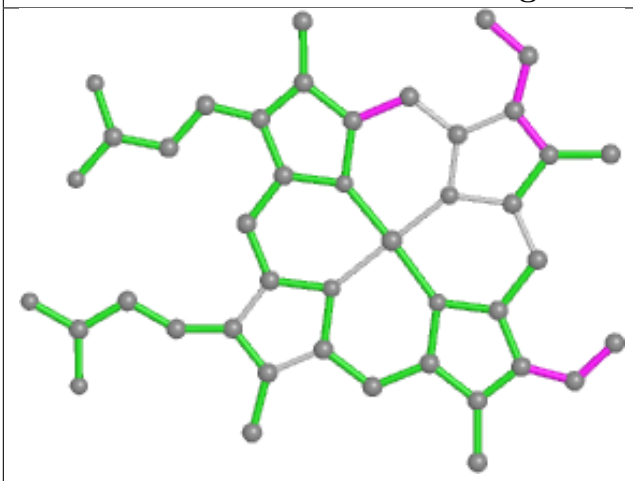
Ligand BOG Q 3009



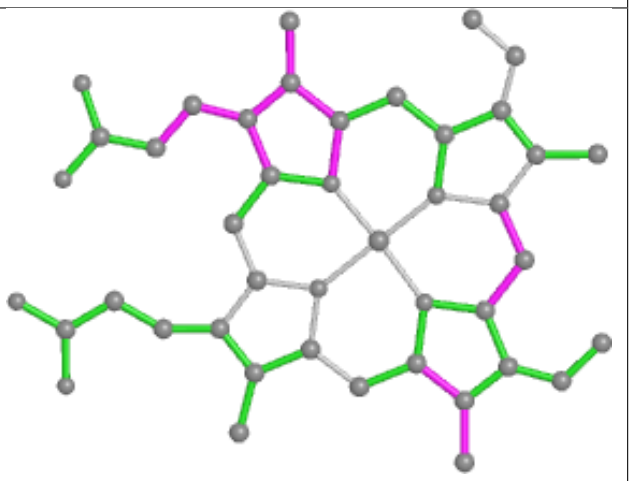
Ligand CDL P 3004



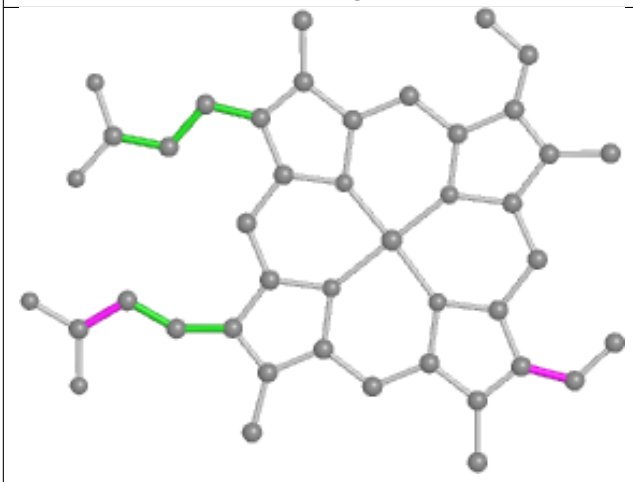
Ligand HEM P 501



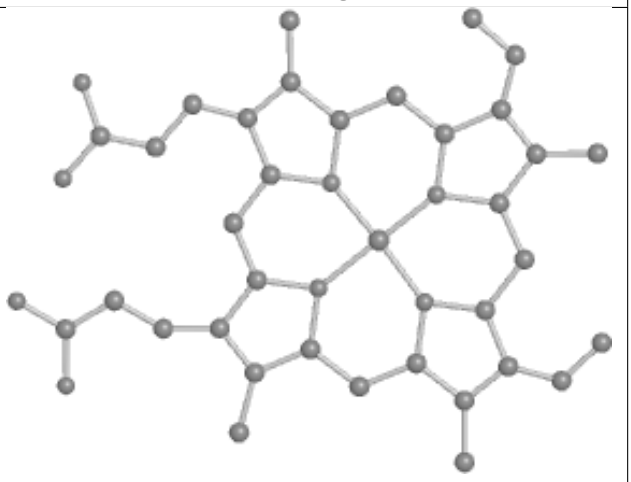
Bond lengths



Bond angles

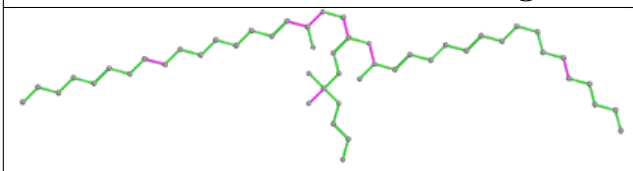


Torsions



Rings

Ligand PEE P 3007



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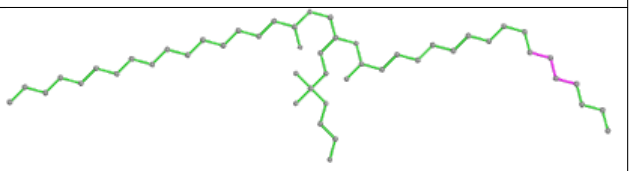

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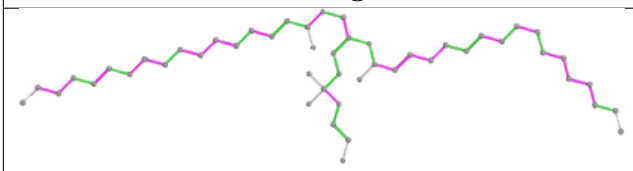
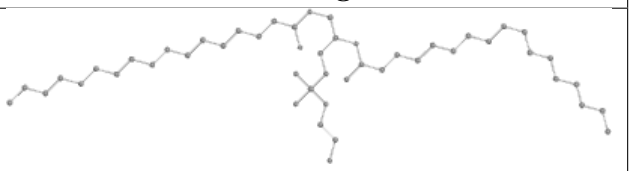
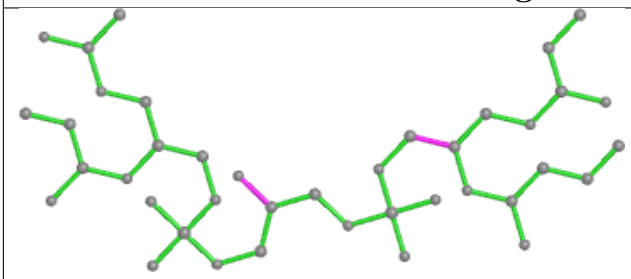


Torsions



Rings

Ligand CDL C 2004



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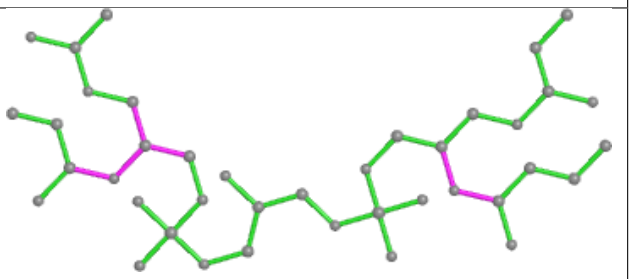

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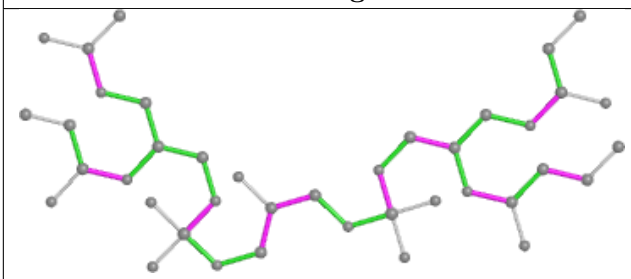
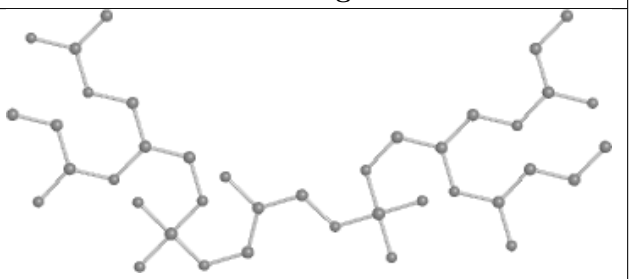
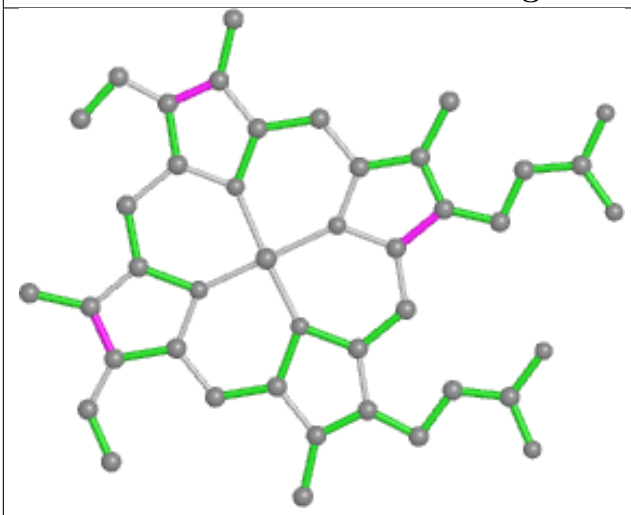


Torsions



Rings

Ligand HEC D 501



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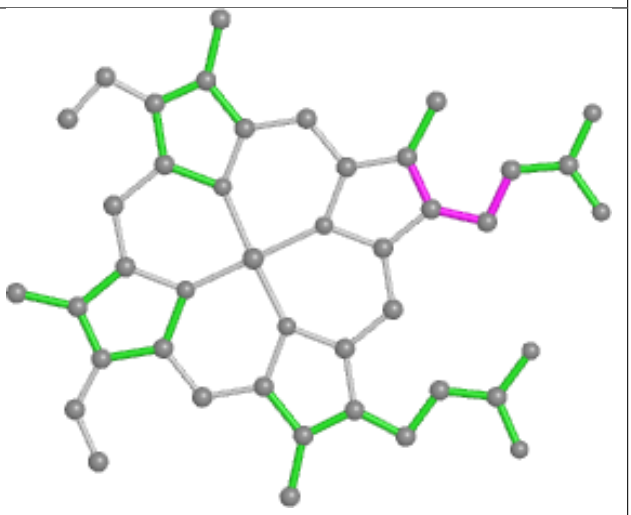

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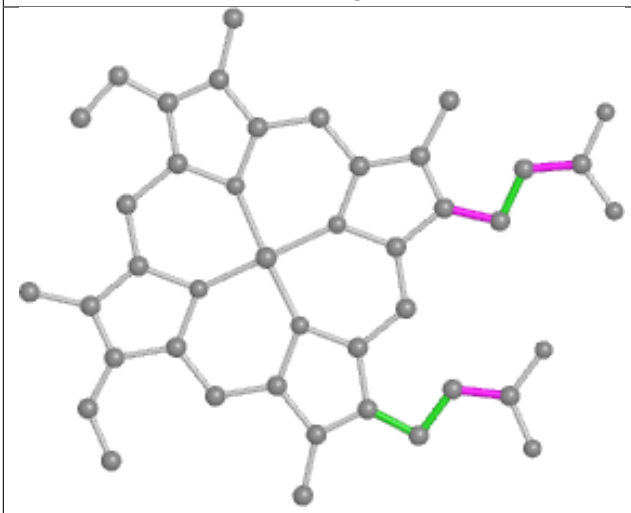

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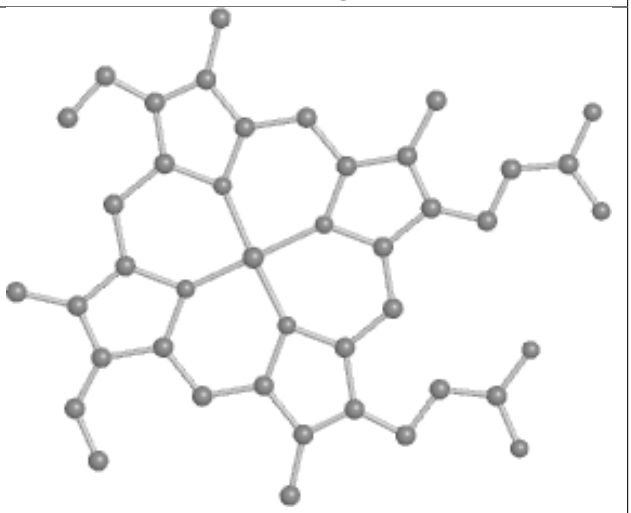
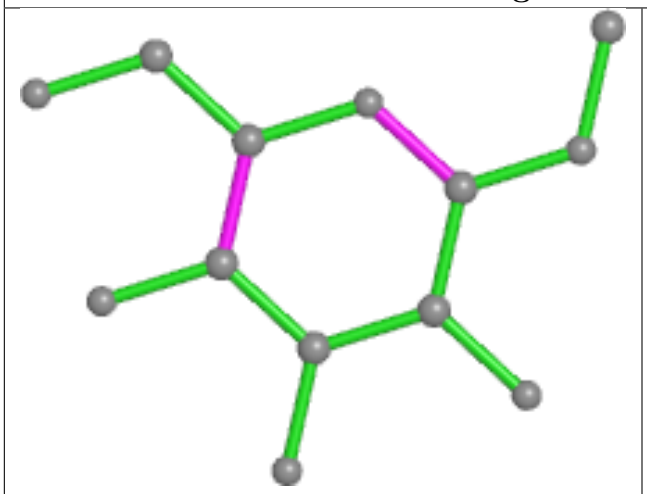


Rings

Ligand BOG Q 3091



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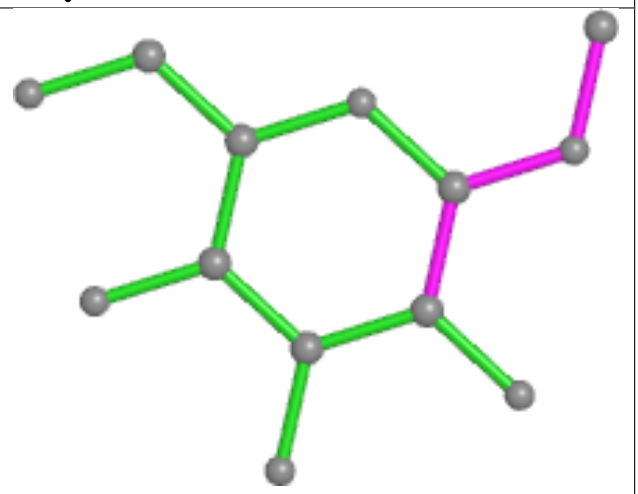

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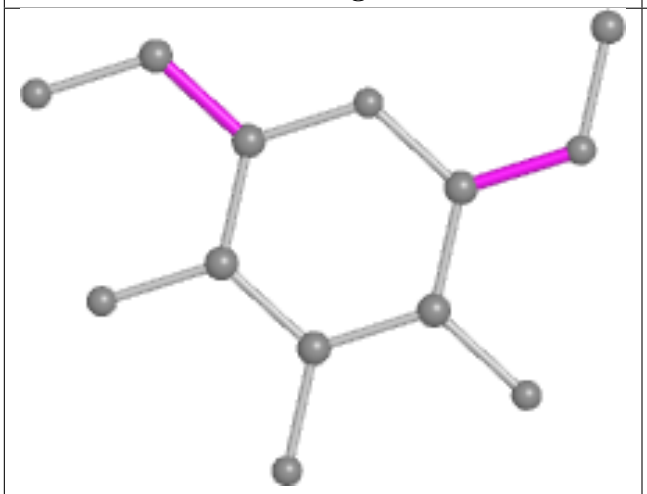

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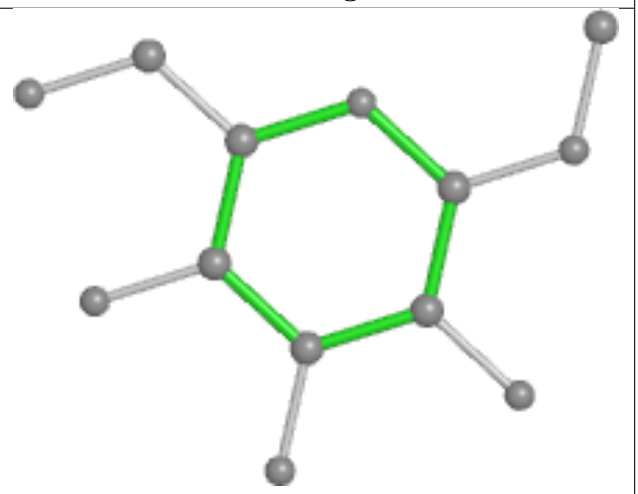
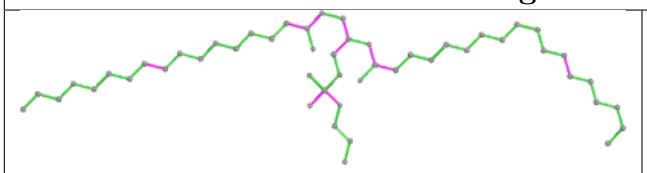


Rings

Ligand PEE E 2005



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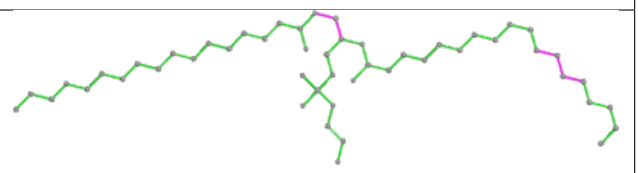

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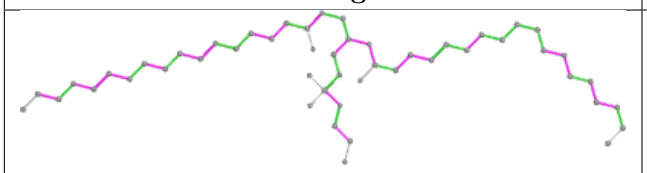

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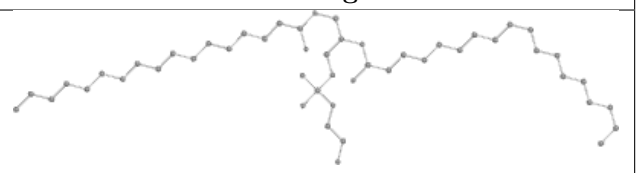
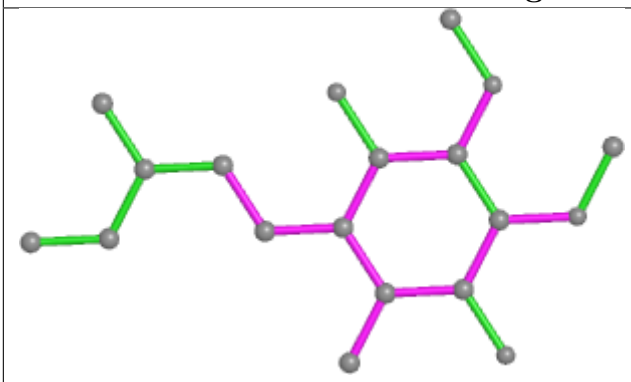


Rings

Ligand UQ C 2002



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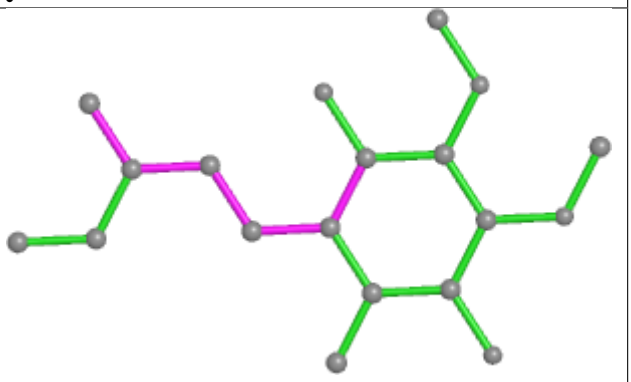

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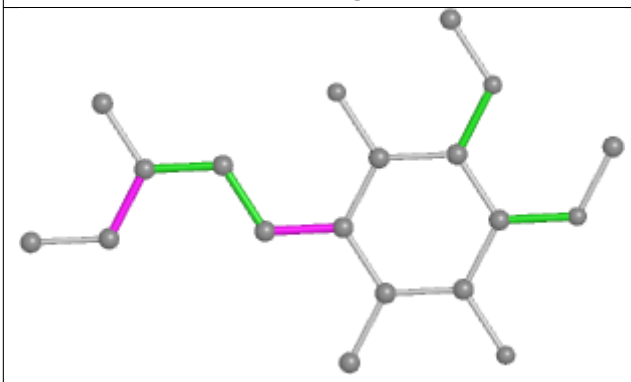
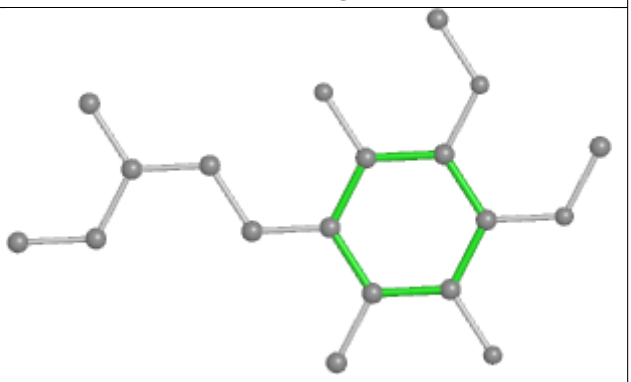
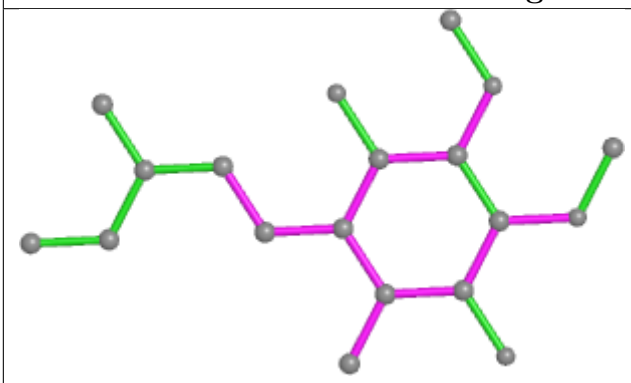


Torsions



Rings

Ligand UQ P 3002



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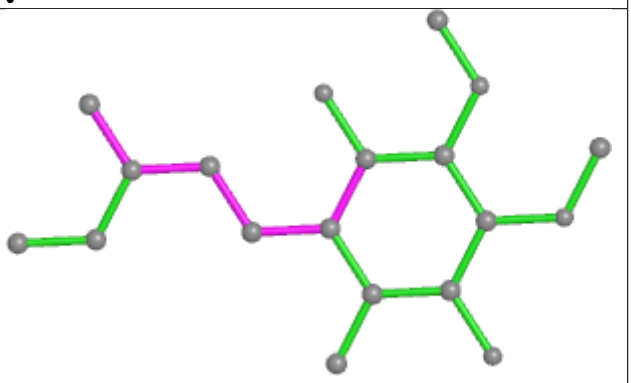

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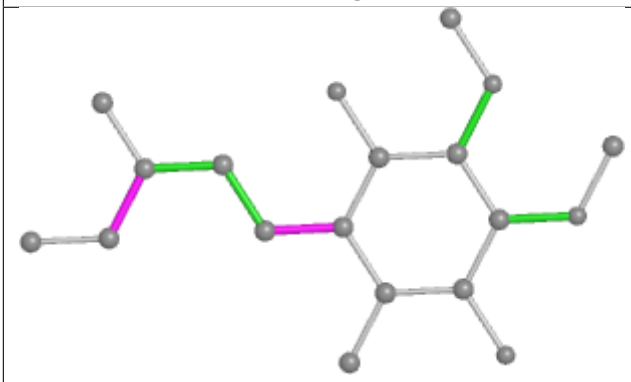
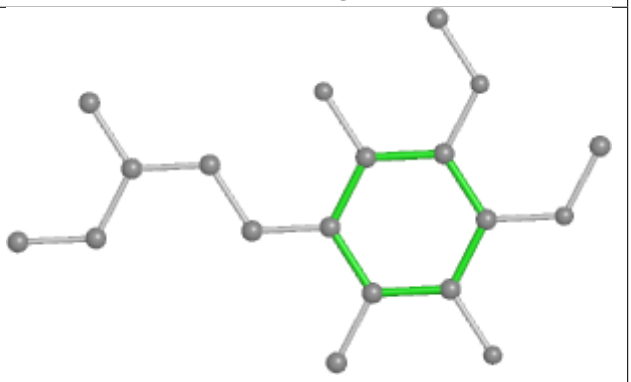
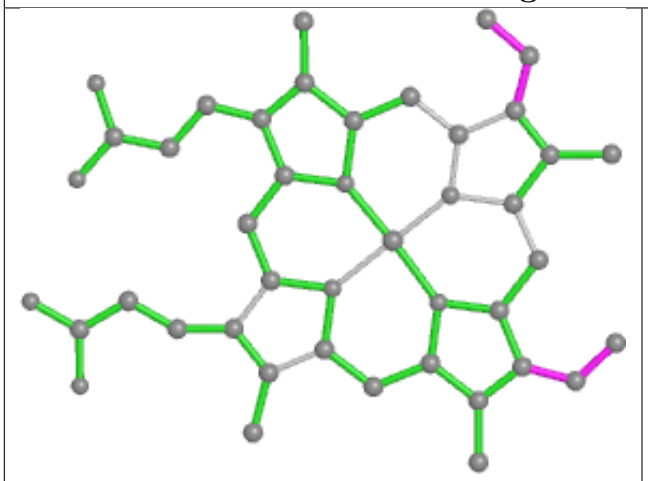


Torsions



Rings

Ligand HEM C 501



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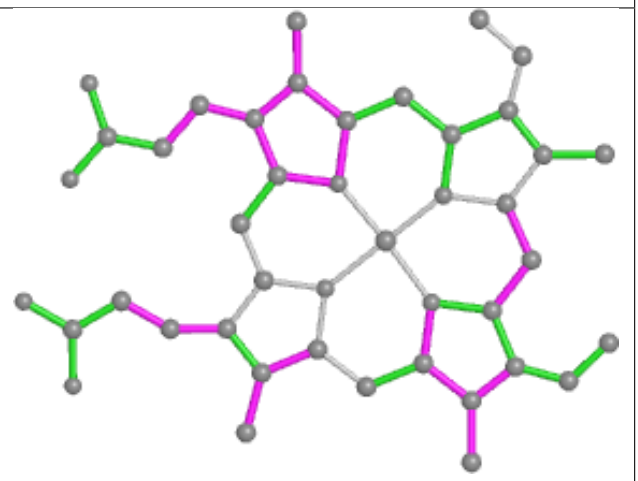

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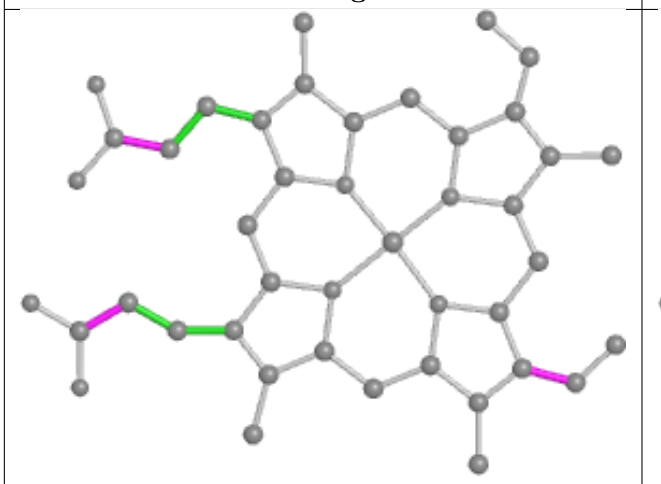

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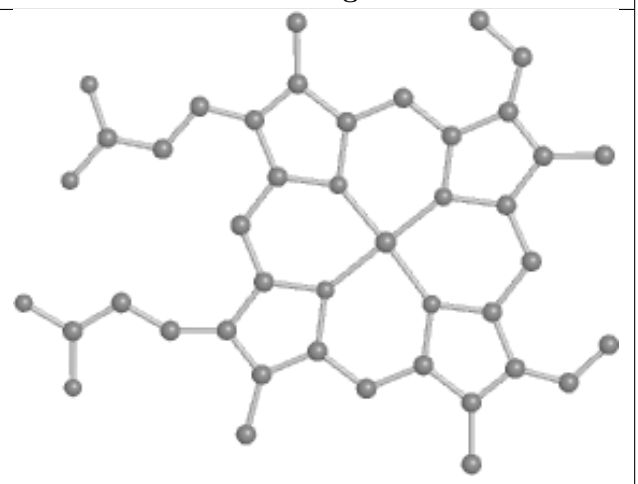

Rings

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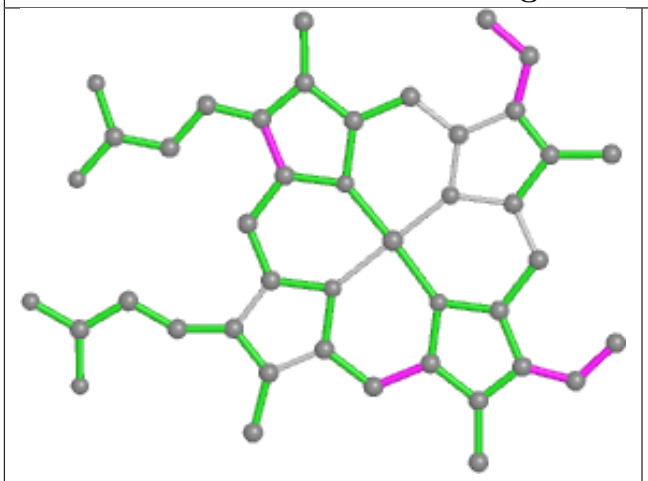

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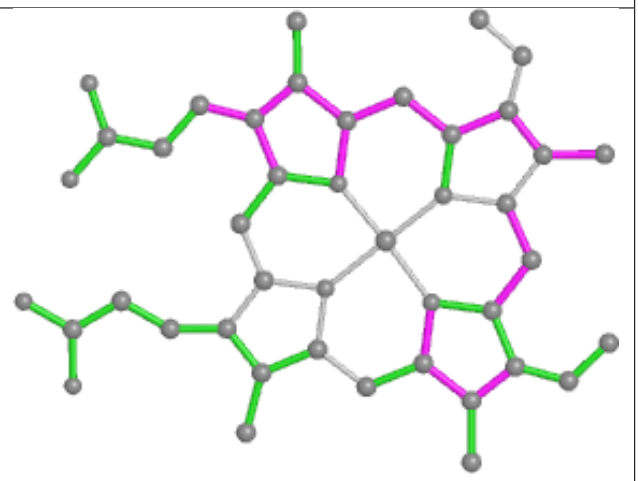

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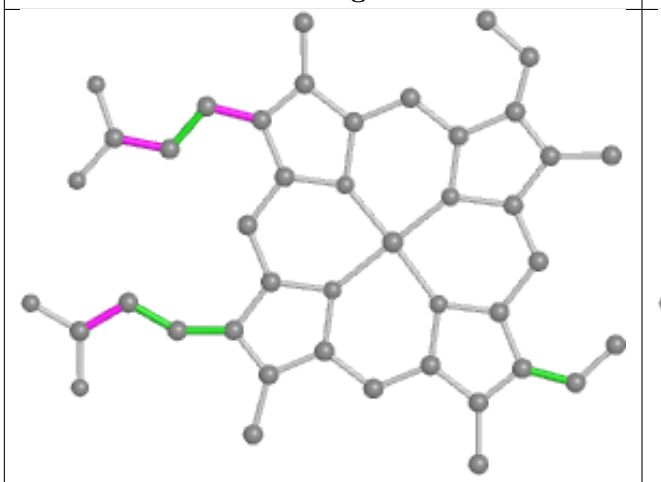

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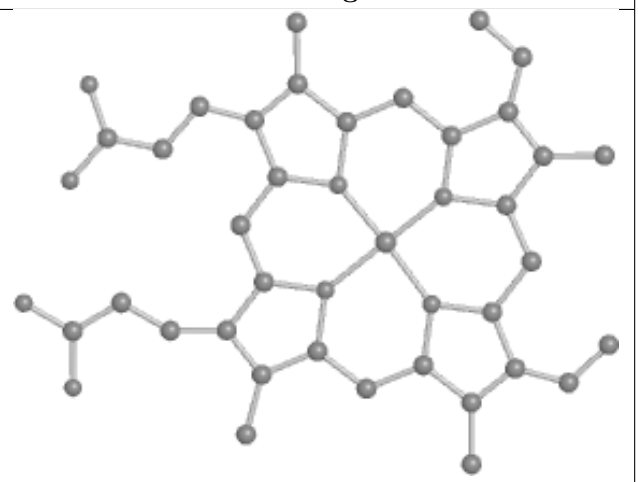

Rings

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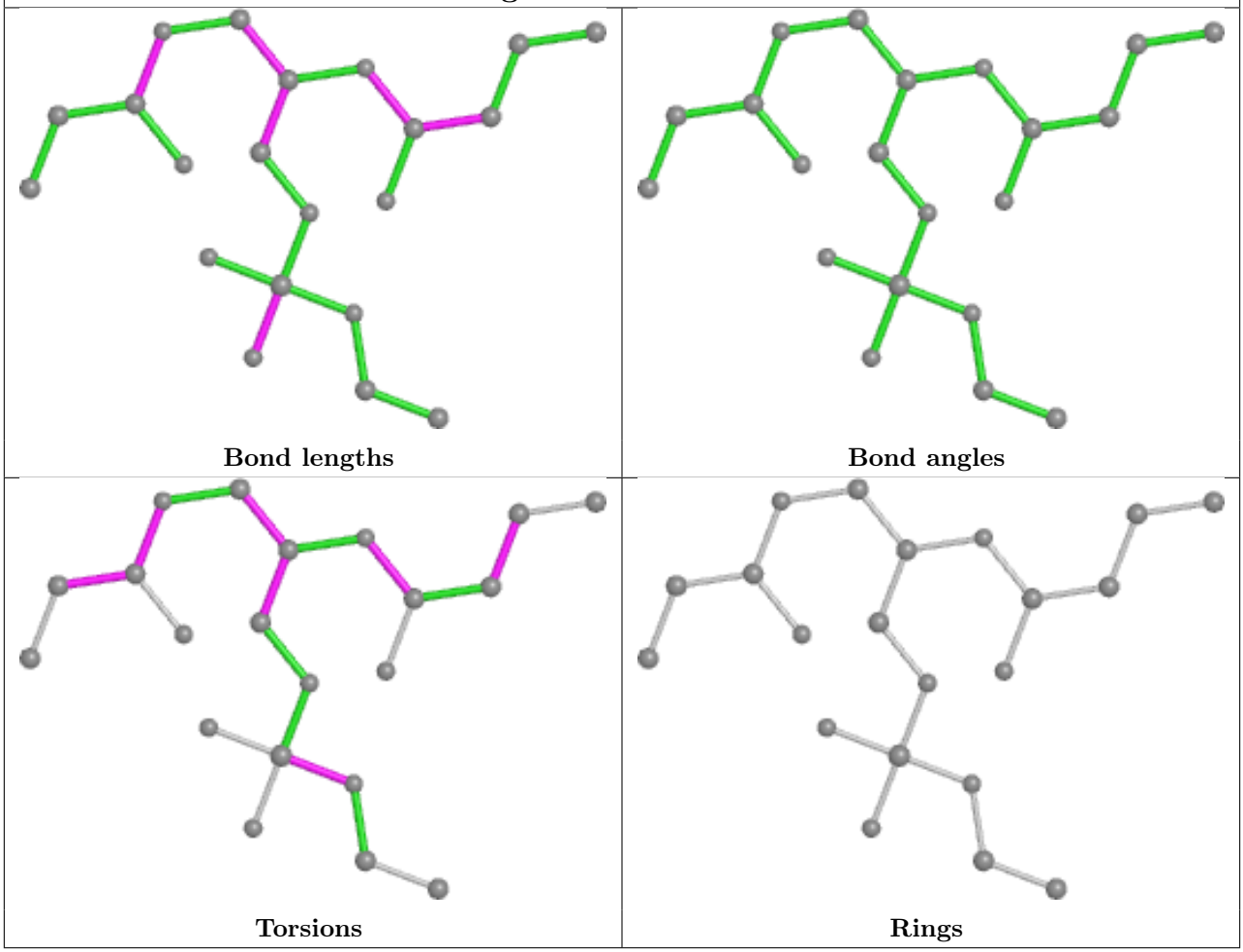
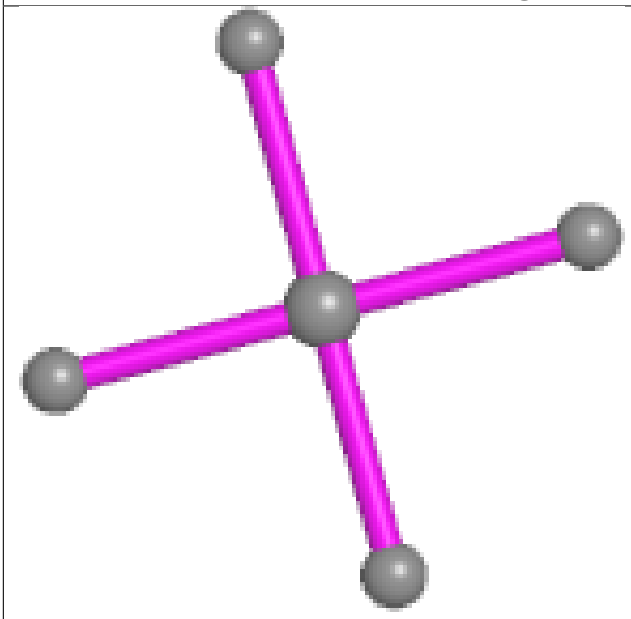


Ligand PEE N 3008



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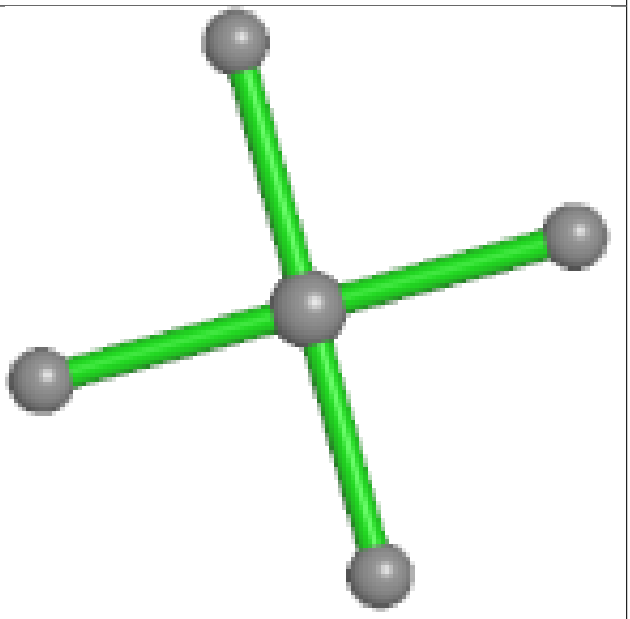
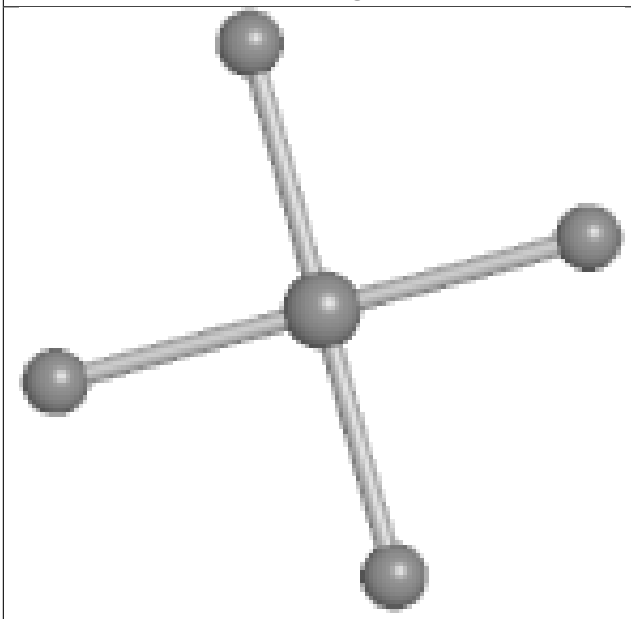
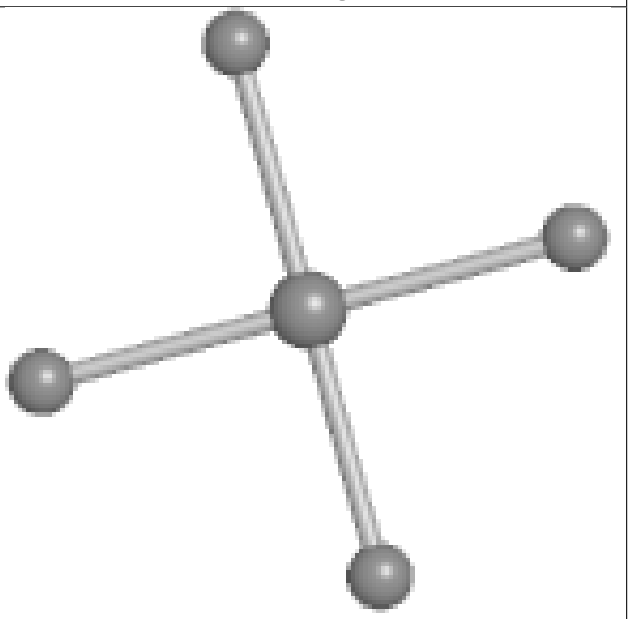


Bond angles

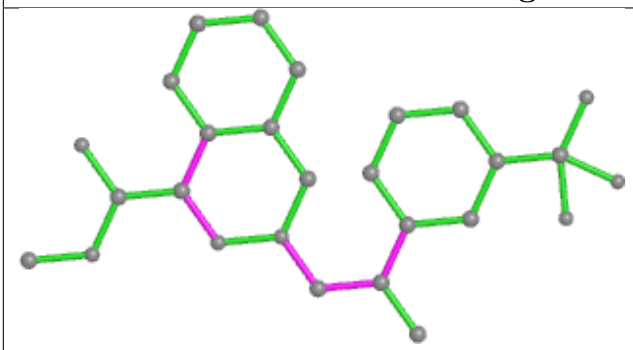


Torsions



Rings

Ligand JZV C 2001



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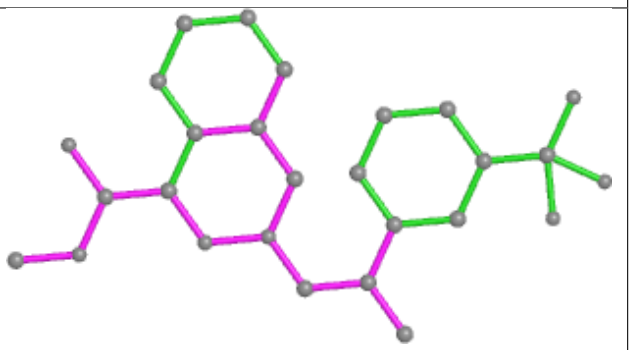

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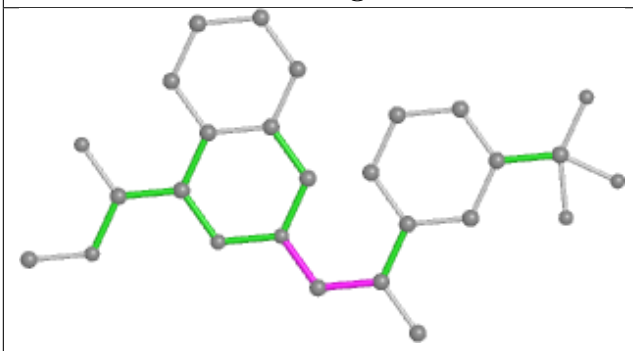
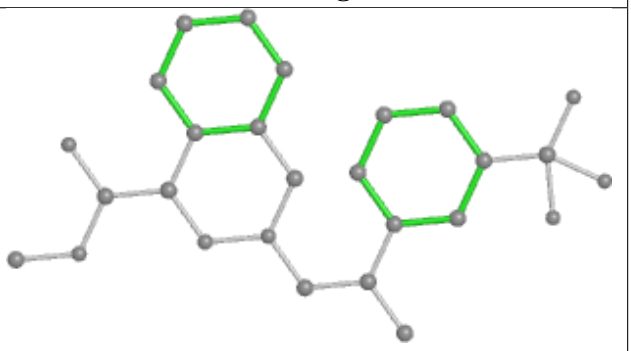
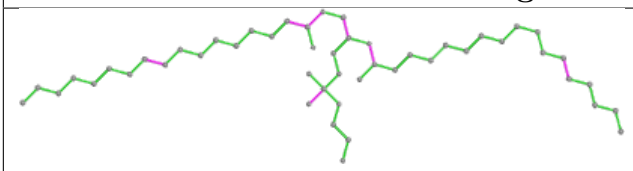


Torsions

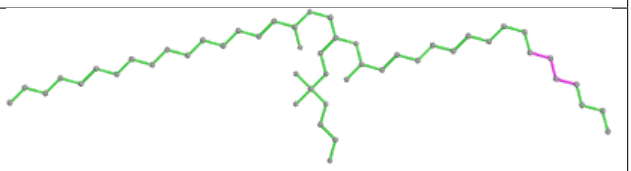


Rings

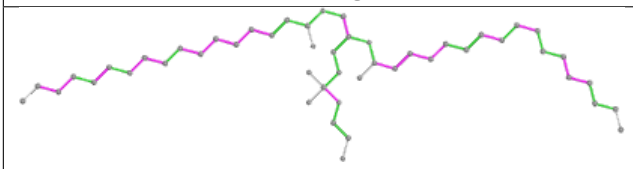
Ligand PEE C 2007



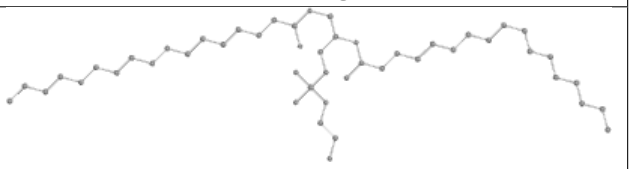
Bond lengths



Bond angles

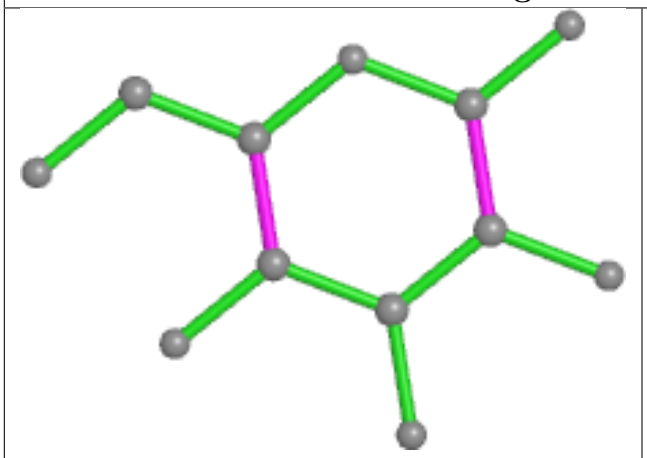


Torsions



Rings

Ligand BOG P 2010



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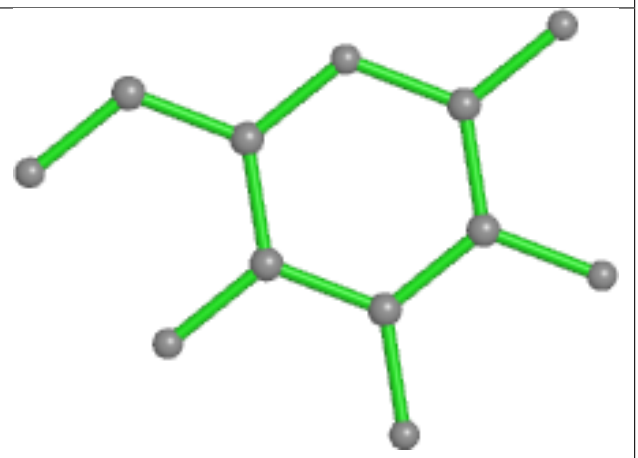
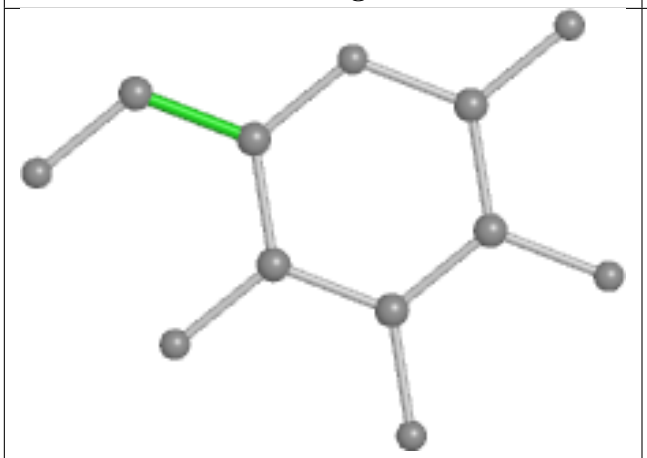
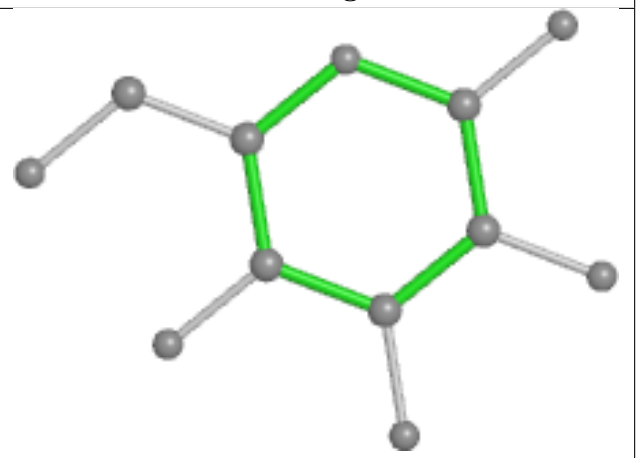


Bond angles

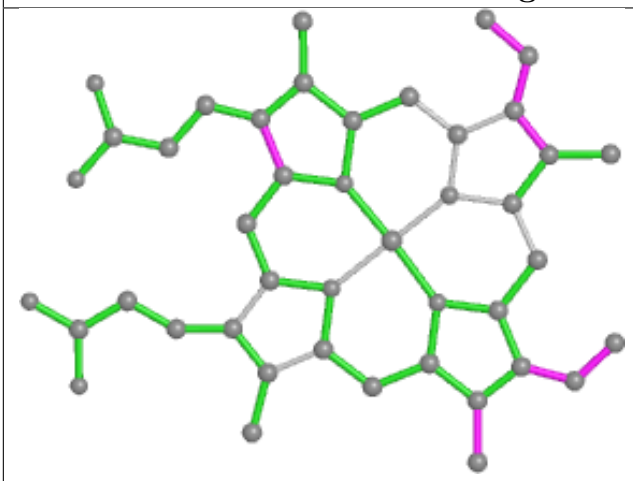


Torsions

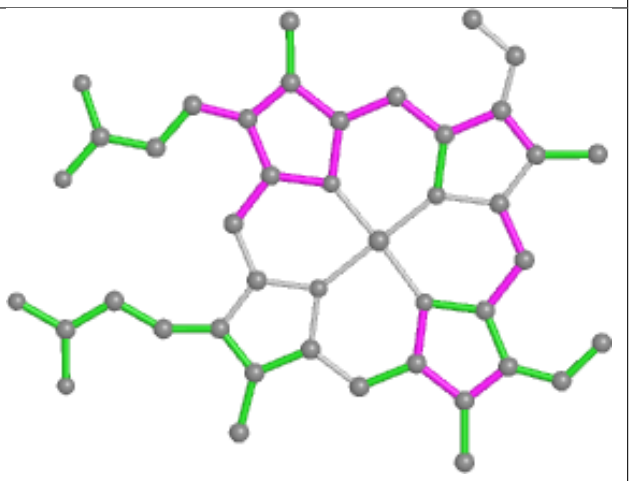


Rings

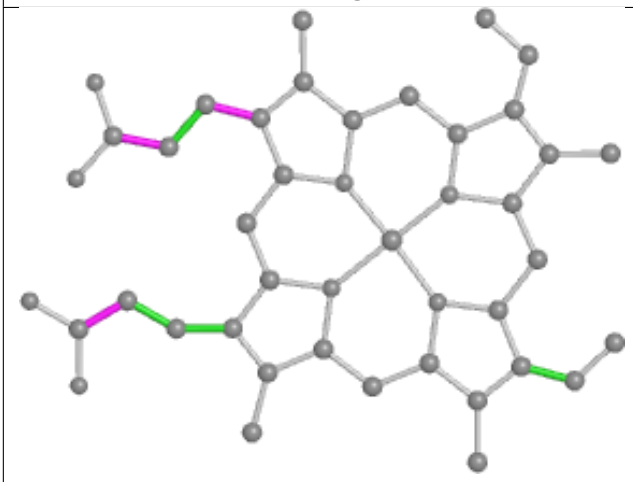
Ligand HEM C 502



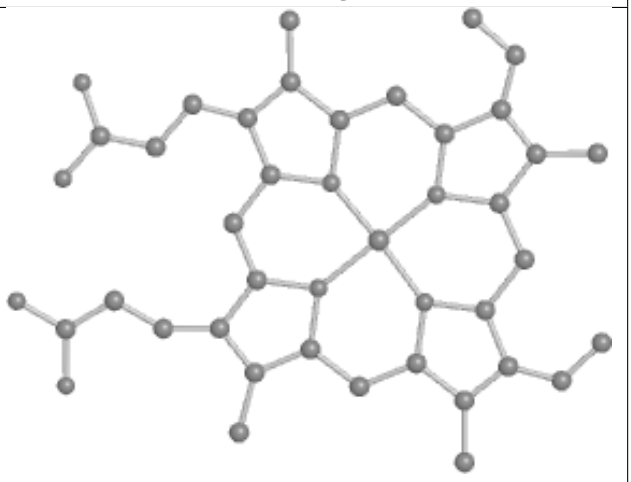
Bond lengths



Bond angles

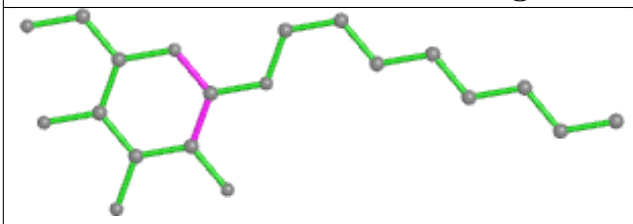


Torsions

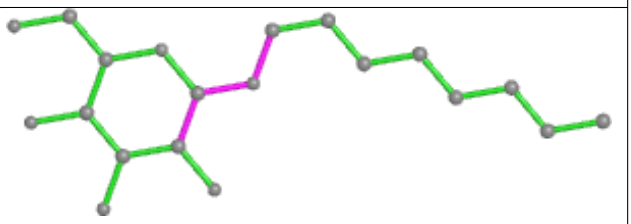


Rings

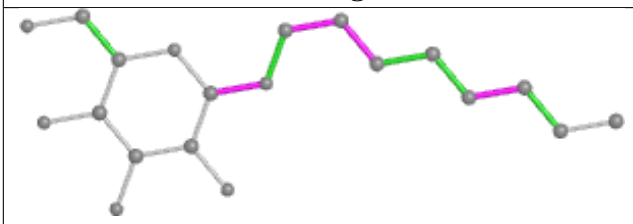
Ligand BOG D 2009



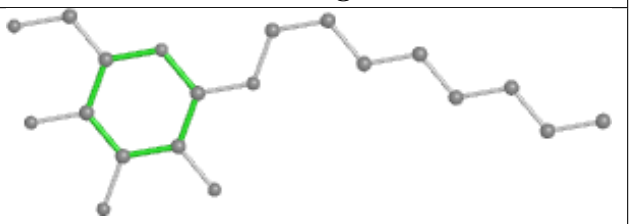
Bond lengths



Bond angles

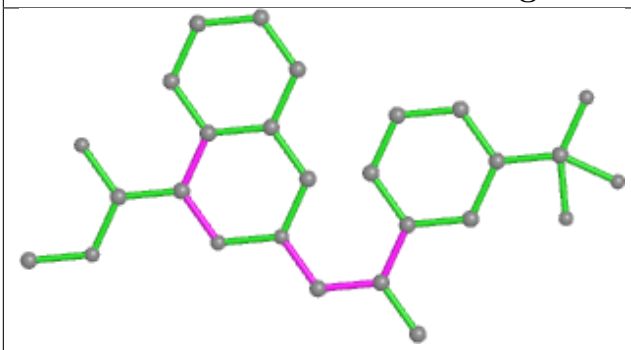


Torsions

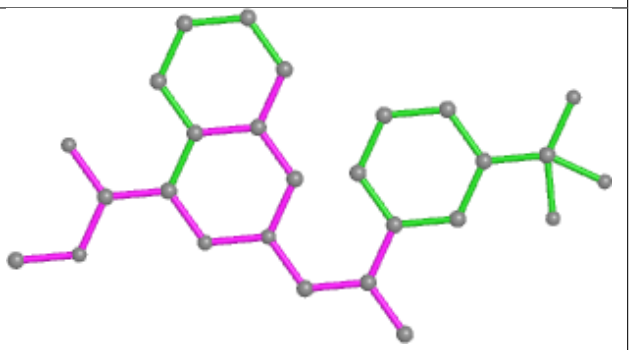


Rings

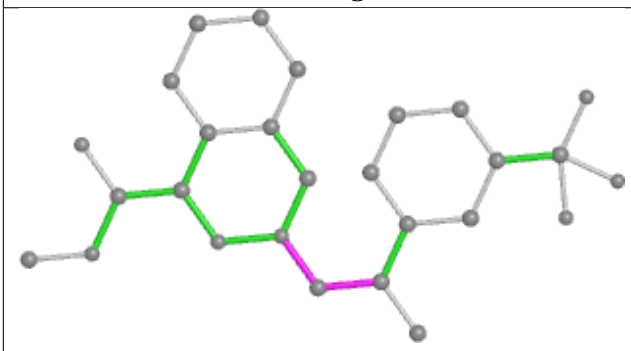
Ligand JZV P 3001



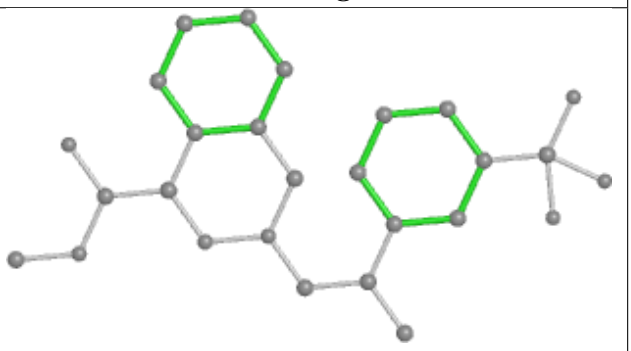
Bond lengths



Bond angles

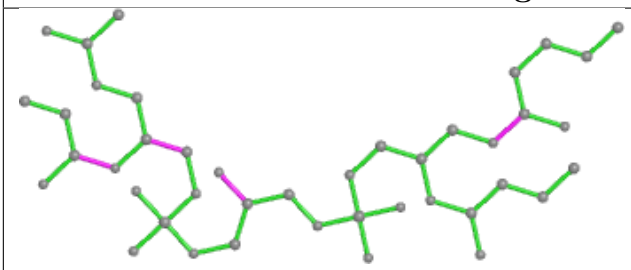


Torsions

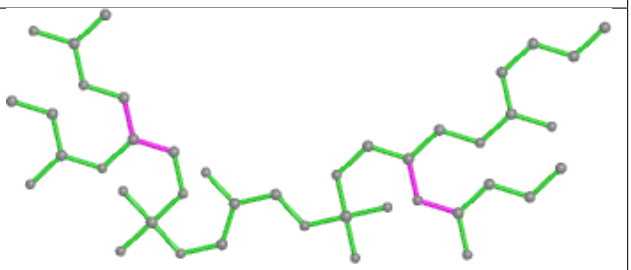


Rings

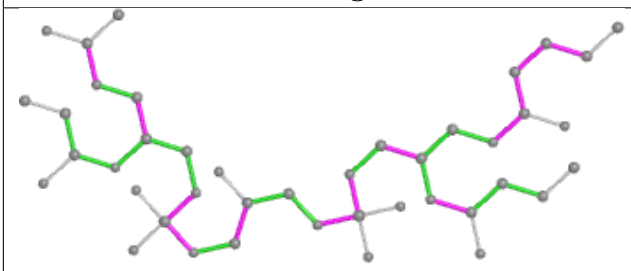
Ligand CDL D 2003



Bond lengths



Bond angles



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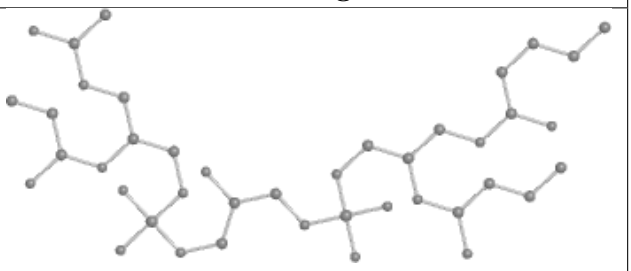
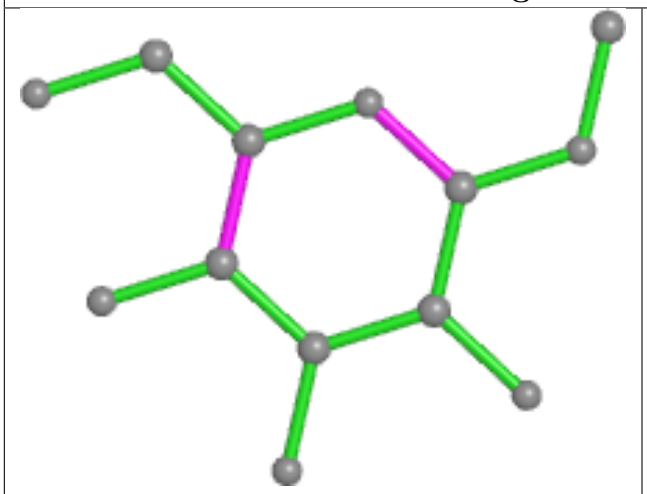


Rings

Ligand BOG D 2091



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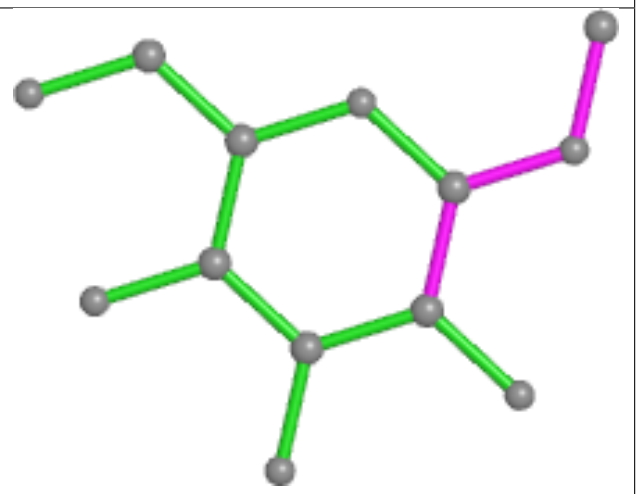
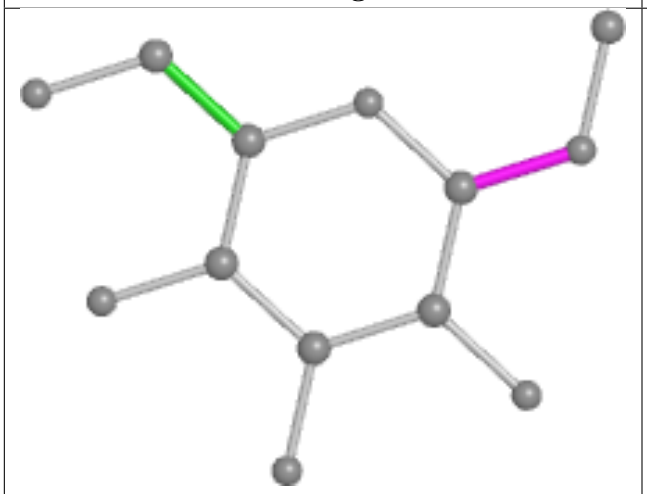
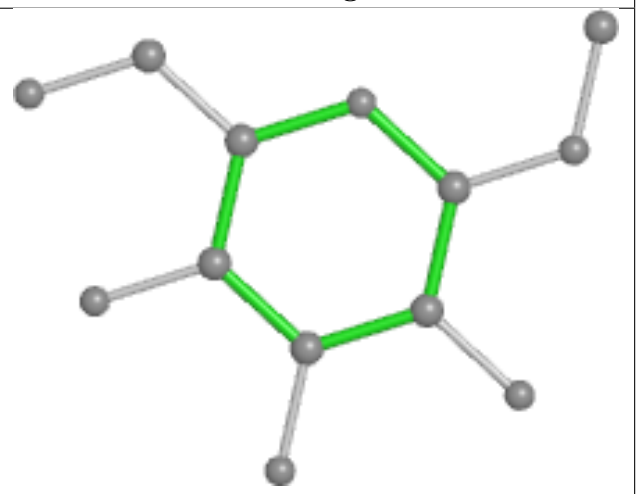


Bond angles

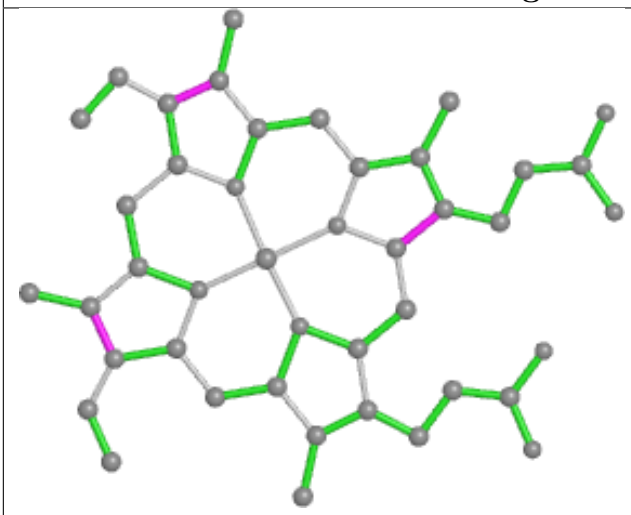


Torsions

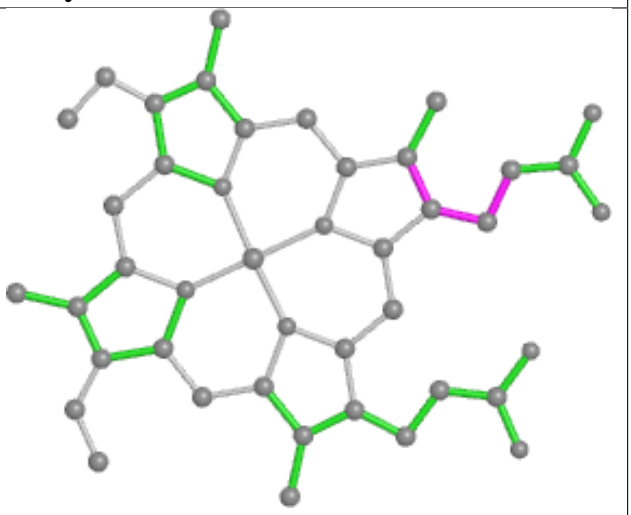


Rings

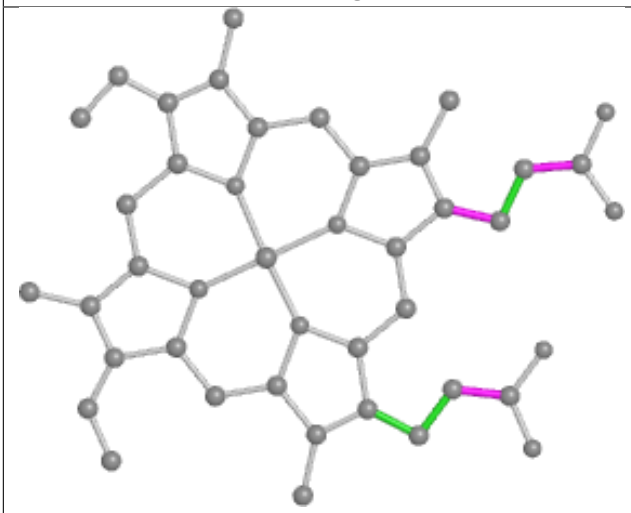
Ligand HEC Q 501



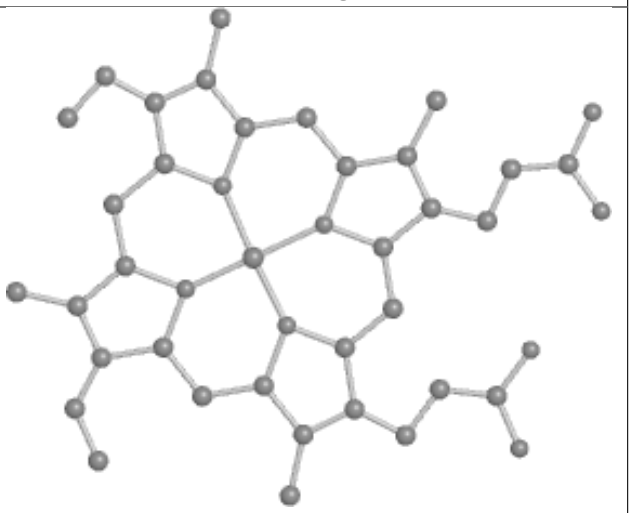
Bond lengths



Bond angles

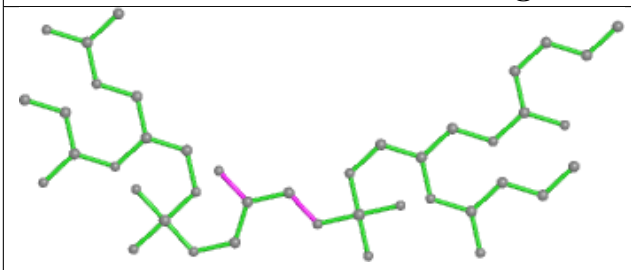


Torsions

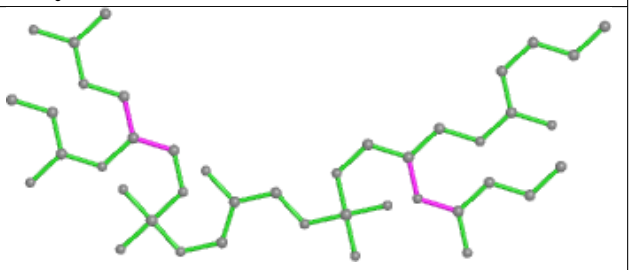


Rings

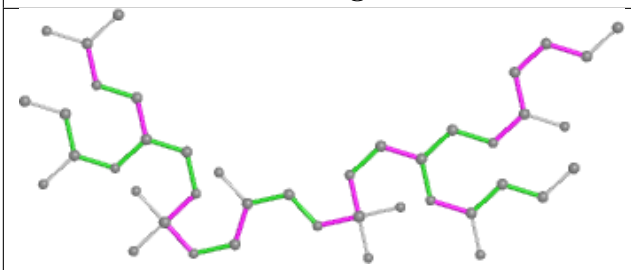
Ligand CDL Q 3003



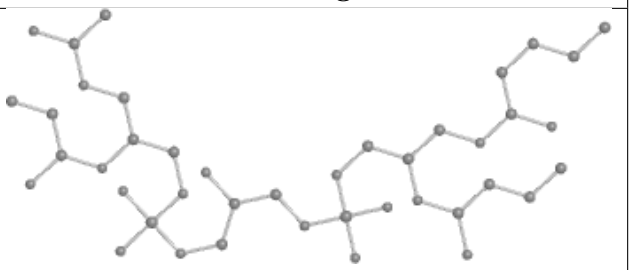
Bond lengths



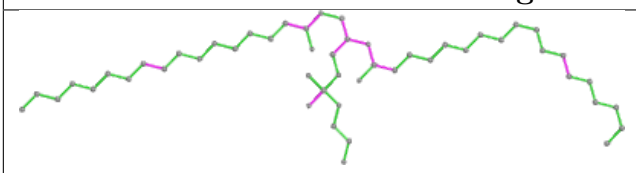
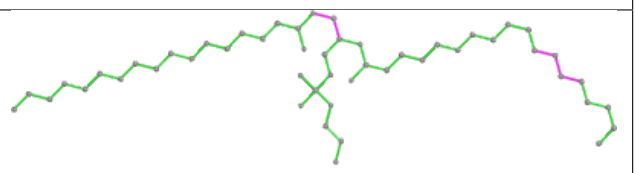
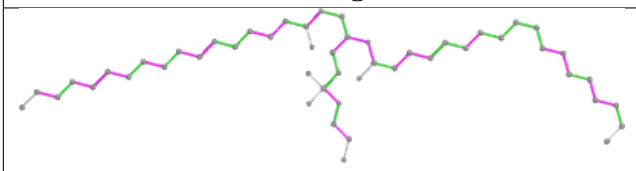
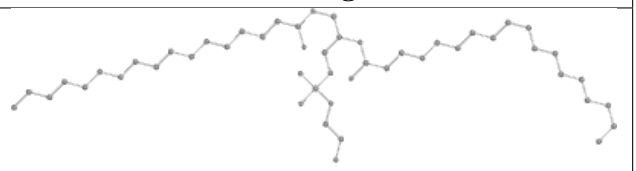
Bond angles



Torsions



Rings

Ligand PEE R 3005	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	444/446 (99%)	0.03	11 (2%) 57 66	32, 58, 86, 100	0
1	N	442/446 (99%)	0.14	8 (1%) 68 76	41, 68, 93, 100	0
2	B	420/441 (95%)	0.25	17 (4%) 38 45	48, 76, 111, 133	0
2	O	422/441 (95%)	0.34	16 (3%) 40 48	39, 74, 103, 122	0
3	C	380/380 (100%)	0.04	5 (1%) 77 84	21, 39, 83, 123	0
3	P	379/380 (99%)	0.19	9 (2%) 59 68	29, 58, 88, 125	0
4	D	241/241 (100%)	-0.09	3 (1%) 79 85	29, 41, 81, 103	0
4	Q	241/241 (100%)	0.17	13 (5%) 25 31	46, 67, 97, 120	0
5	E	196/196 (100%)	1.71	75 (38%) 0 0	34, 135, 167, 175	0
5	R	196/196 (100%)	0.58	25 (12%) 3 4	40, 86, 132, 147	0
6	F	101/110 (91%)	-0.33	0 100 100	26, 43, 61, 94	0
6	S	101/110 (91%)	0.00	4 (3%) 38 45	50, 65, 102, 121	0
7	G	80/81 (98%)	0.10	2 (2%) 57 66	33, 52, 97, 111	0
7	T	79/81 (97%)	0.93	12 (15%) 2 2	46, 78, 139, 149	0
8	H	70/77 (90%)	-0.05	2 (2%) 51 61	34, 58, 80, 119	0
8	U	67/77 (87%)	0.99	13 (19%) 1 1	82, 108, 128, 130	0
9	I	31/47 (65%)	2.17	12 (38%) 0 0	72, 107, 133, 134	0
9	V	31/47 (65%)	2.21	17 (54%) 0 0	66, 107, 132, 136	0
10	J	61/61 (100%)	0.23	4 (6%) 18 21	43, 54, 95, 139	0
10	W	60/61 (98%)	0.53	3 (5%) 28 35	55, 68, 99, 107	0
All	All	4042/4160 (97%)	0.29	251 (6%) 20 25	21, 64, 121, 175	0

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	11.3
5	E	98	VAL	10.0
5	E	188	VAL	8.7
7	T	2	ILE	7.3
5	E	87	VAL	7.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
18	BOG	Q	3091	13/20	0.24	0.61	183,186,187,187	0
18	BOG	D	2091	13/20	0.26	0.62	200,201,201,201	0
18	BOG	P	2010	12/20	0.46	0.35	135,137,138,138	0
11	PEE	A	2008	21/51	0.54	0.39	129,133,134,135	0
11	PEE	R	3005	50/51	0.71	0.42	80,98,108,110	0
15	CDL	Q	3003	42/100	0.73	0.29	109,121,139,139	0
14	UQ	P	3002	19/63	0.76	0.38	119,124,125,126	0
16	GOL	P	3011	6/6	0.80	0.40	73,75,76,77	0
15	CDL	D	2003	42/100	0.81	0.29	82,92,106,108	0
11	PEE	E	2005	50/51	0.82	0.35	68,89,95,97	0
11	PEE	N	3008	5/51	0.83	0.20	110,111,112,112	0
11	PEE	P	3007	49/51	0.83	0.33	53,79,93,94	0
14	UQ	C	2002	19/63	0.84	0.30	88,90,90,91	0
16	GOL	C	2011	6/6	0.85	0.34	67,70,72,72	0
11	PEE	C	2007	49/51	0.86	0.30	43,58,70,73	0
15	CDL	P	3004	40/100	0.86	0.21	96,102,111,111	0
18	BOG	Q	3009	20/20	0.89	0.23	62,75,77,78	0
13	JZV	P	3001	29/29	0.89	0.24	59,66,104,106	0
15	CDL	C	2004	40/100	0.91	0.22	66,80,91,93	0

Continued on next page...

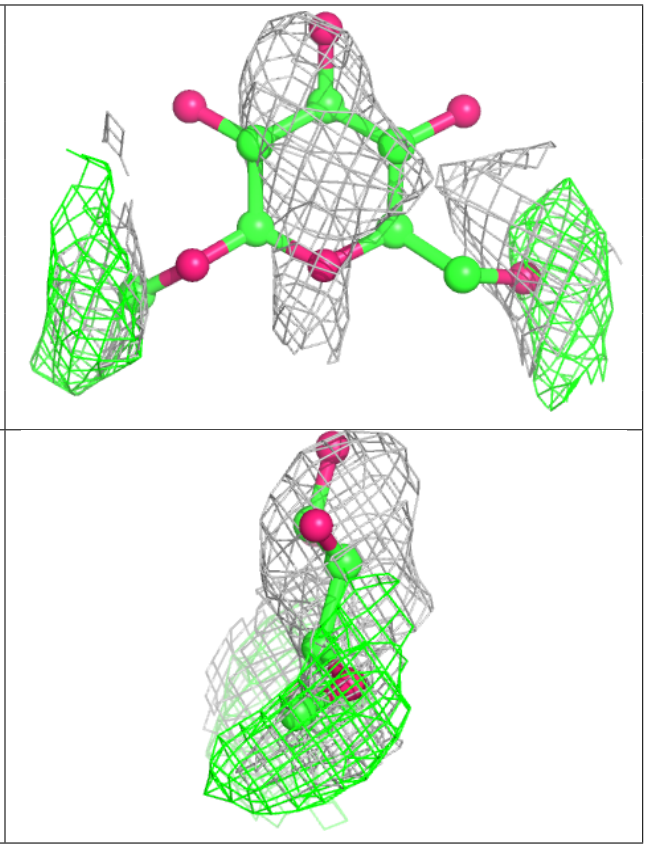
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	JZV	C	2001	29/29	0.93	0.23	38,46,86,87	0
18	BOG	D	2009	20/20	0.93	0.17	53,59,62,64	0
19	FES	E	501	4/4	0.93	0.11	144,144,145,145	0
17	HEC	Q	501	43/43	0.96	0.18	52,56,64,65	0
12	HEM	P	501	43/43	0.97	0.22	33,40,48,54	0
17	HEC	D	501	43/43	0.98	0.17	21,29,34,35	0
12	HEM	C	501	43/43	0.98	0.21	23,30,37,42	0
12	HEM	P	502	43/43	0.98	0.17	29,41,54,59	0
12	HEM	C	502	43/43	0.98	0.17	24,27,35,41	0
19	FES	R	501	4/4	0.98	0.06	74,76,77,78	0

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

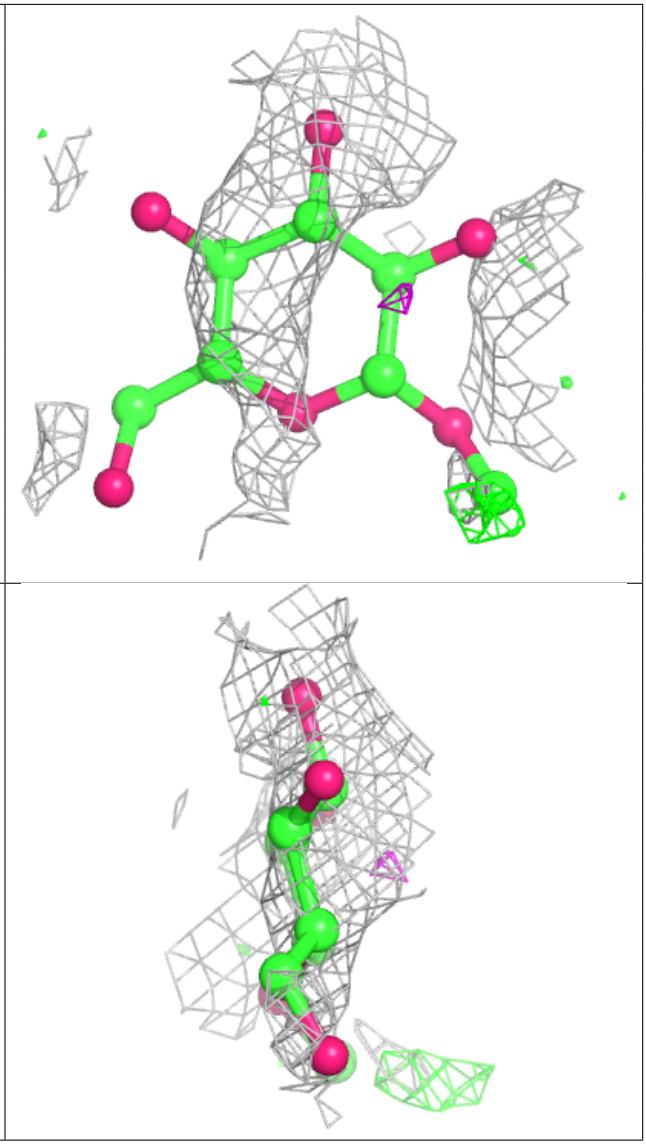
Electron density around BOG Q 3091:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BOG 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 BOG P 2010:

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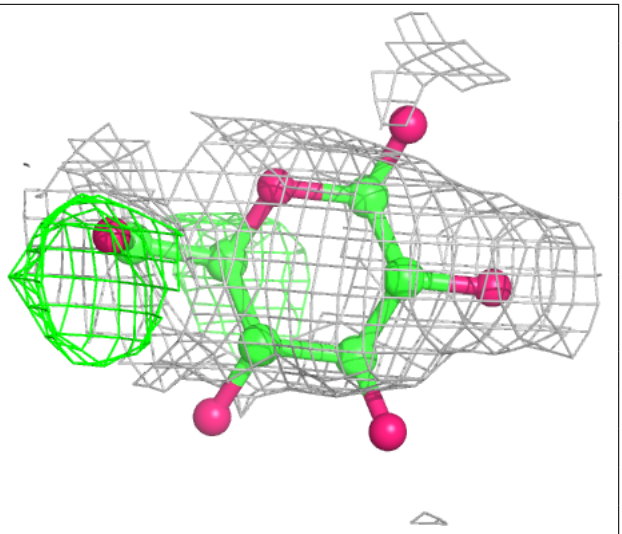
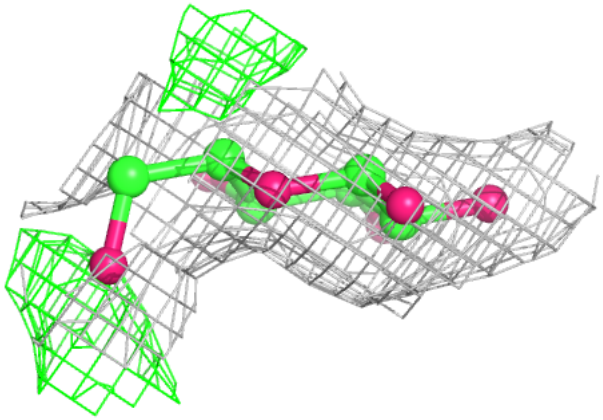
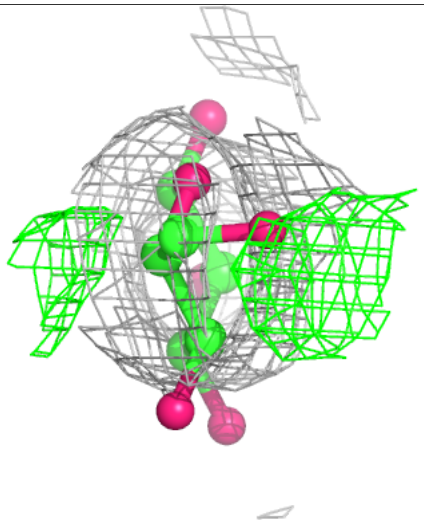
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around PEE A 2008:

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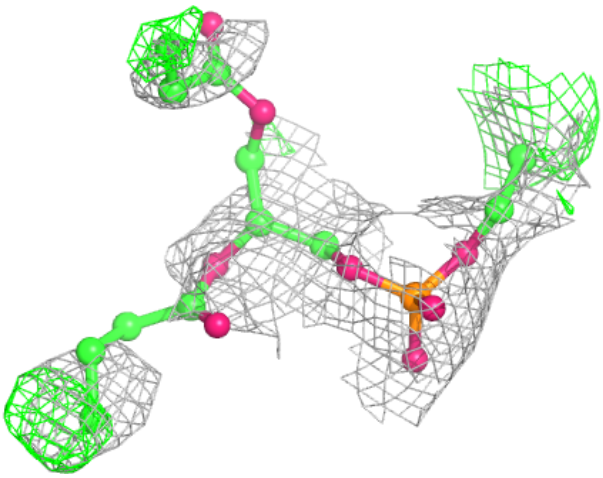
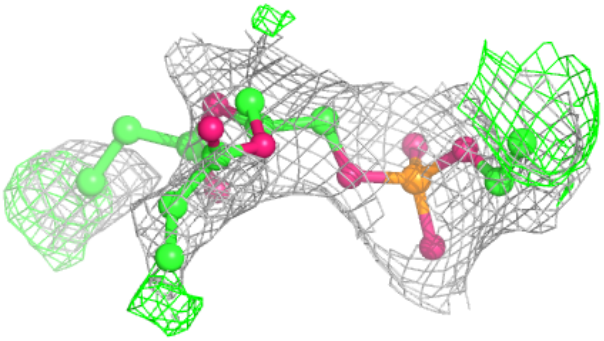
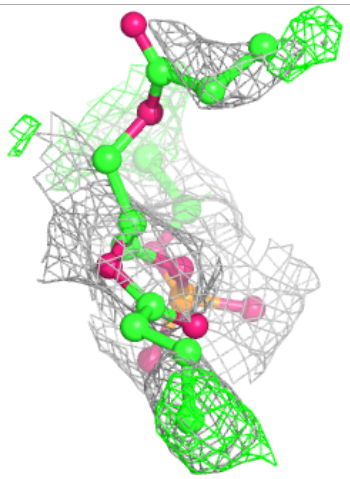
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

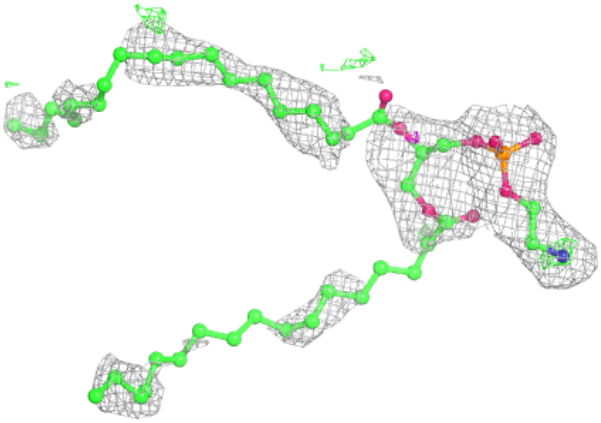


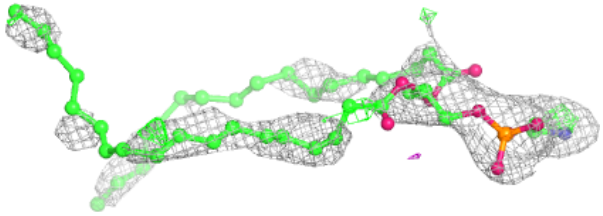


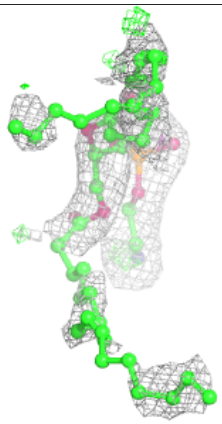


Electron density around PEE R 3005:

$2mF_o$-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 Q 3003:

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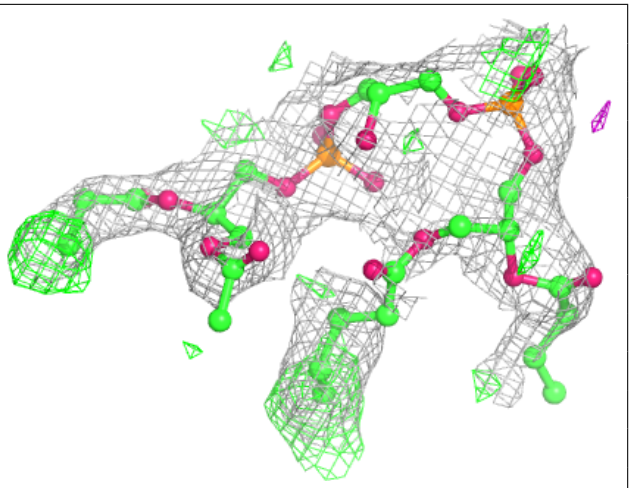
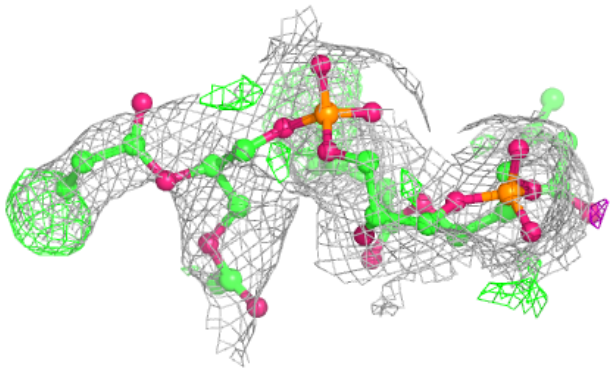
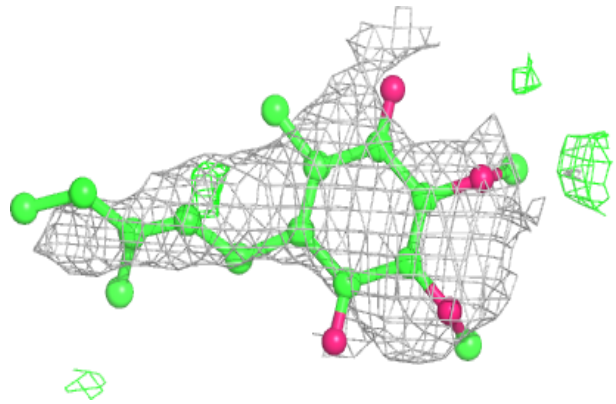
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

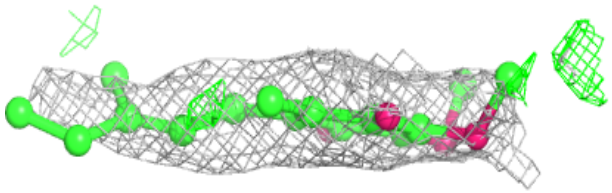


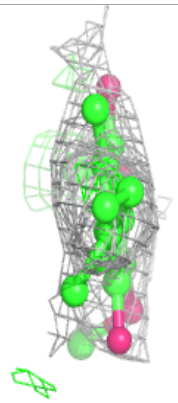


Electron density around UQ P 3002:

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

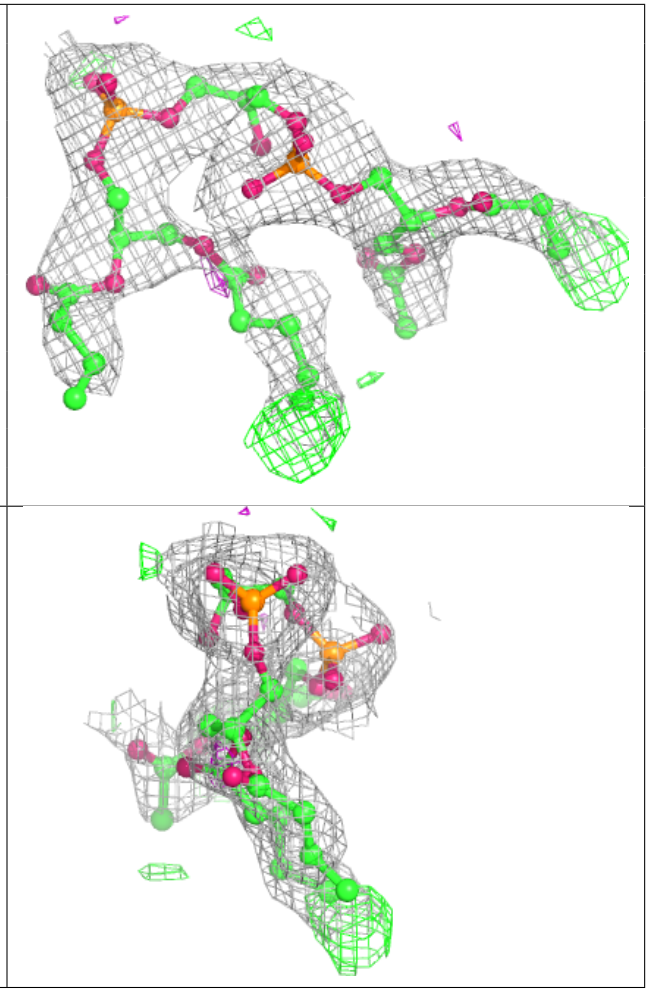






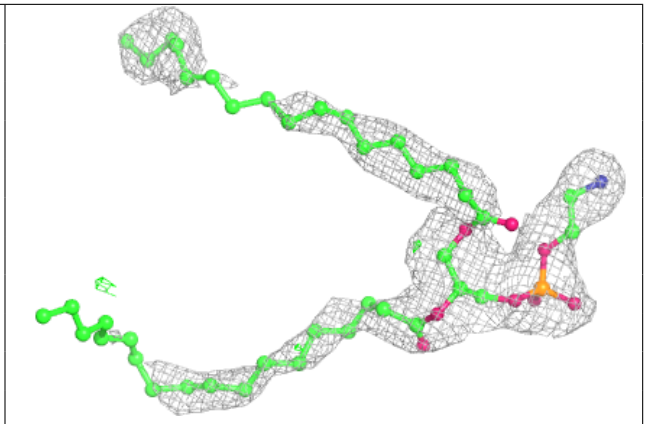
Electron density around CDL D 2003:

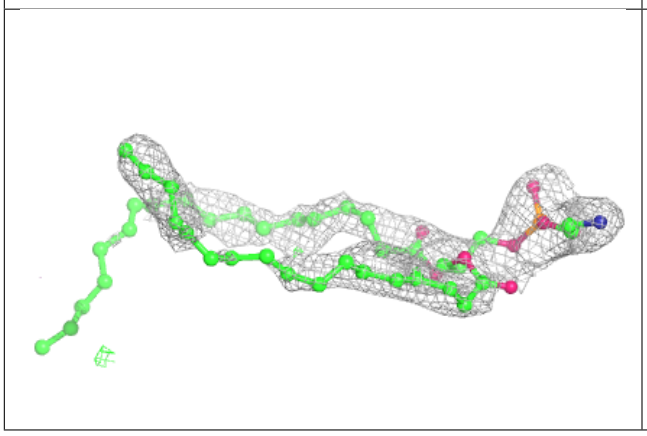
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

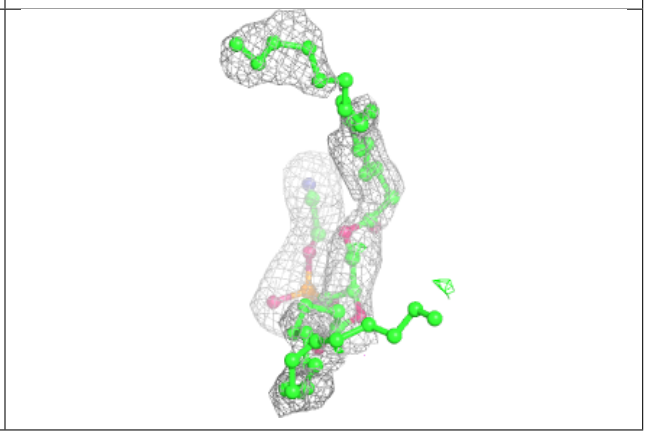


Electron density around PEE E 2005:

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

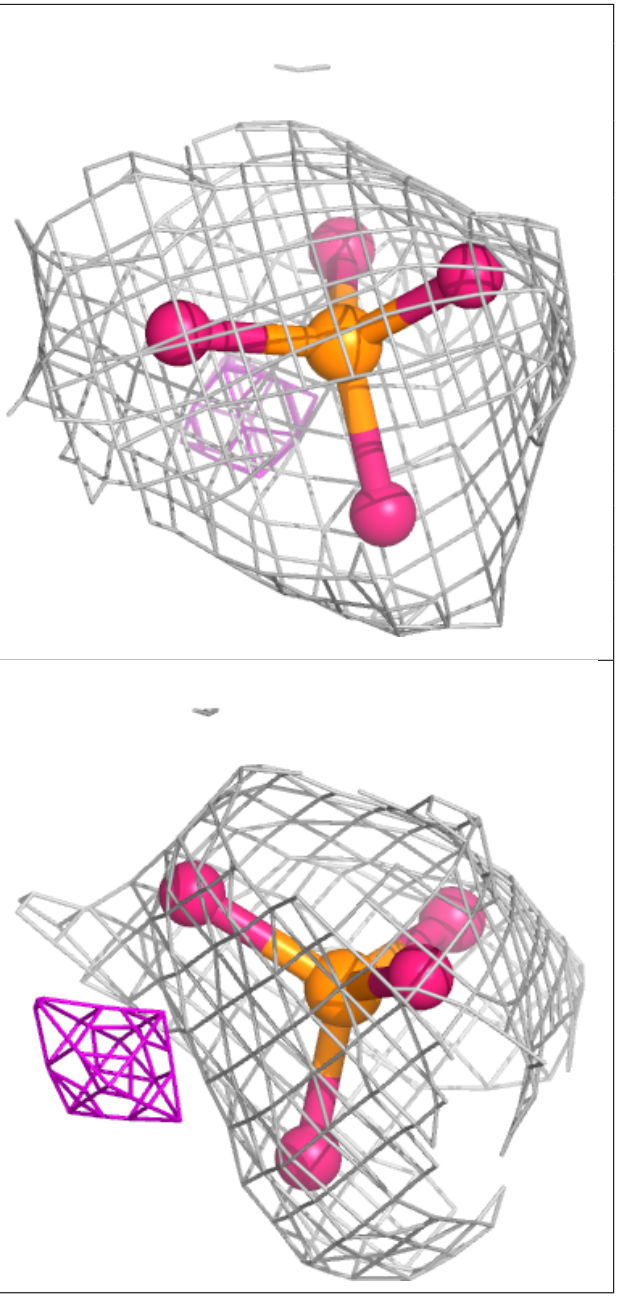






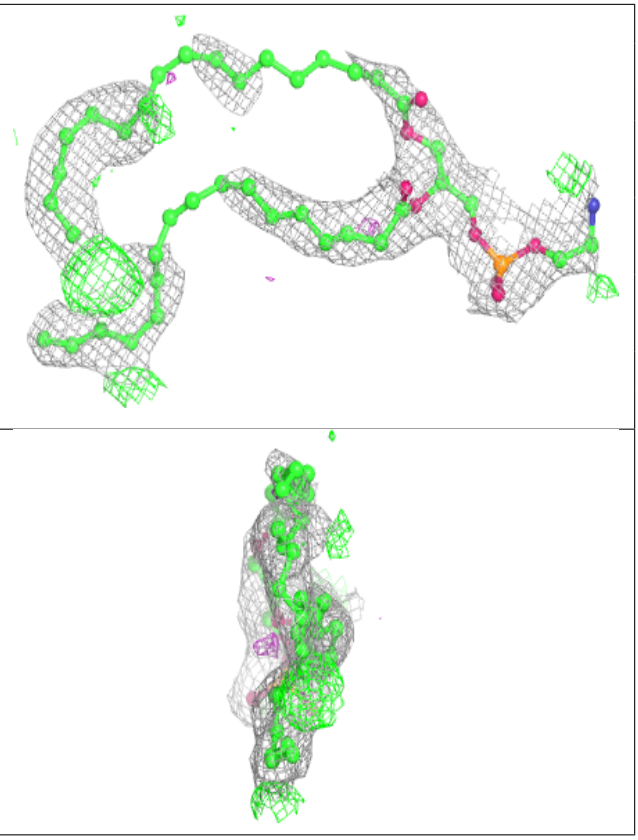
Electron density around PEE N 3008:

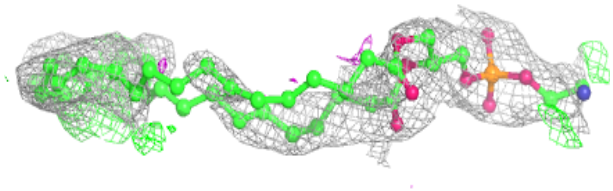
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEE P 3007:

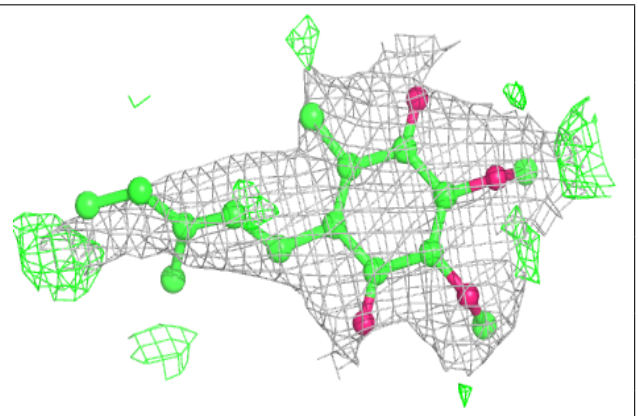
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

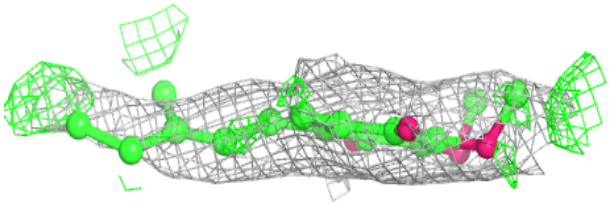


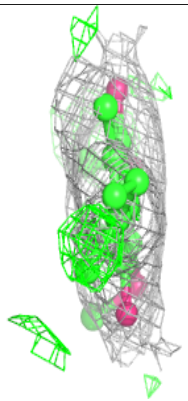


Electron density around UQ C 2002:

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

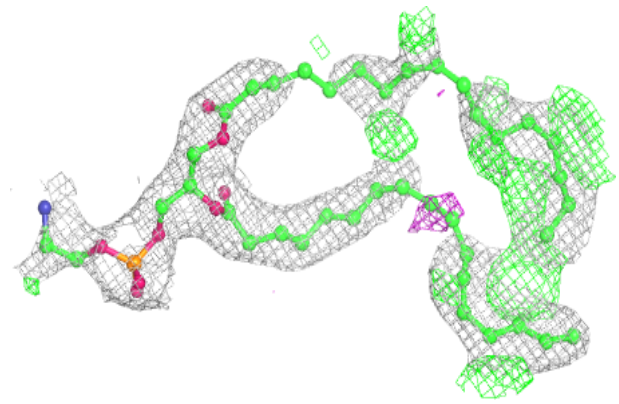


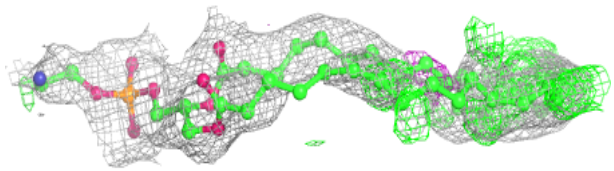


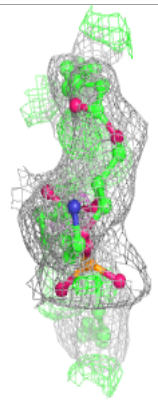


Electron density around PEE C 2007:

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

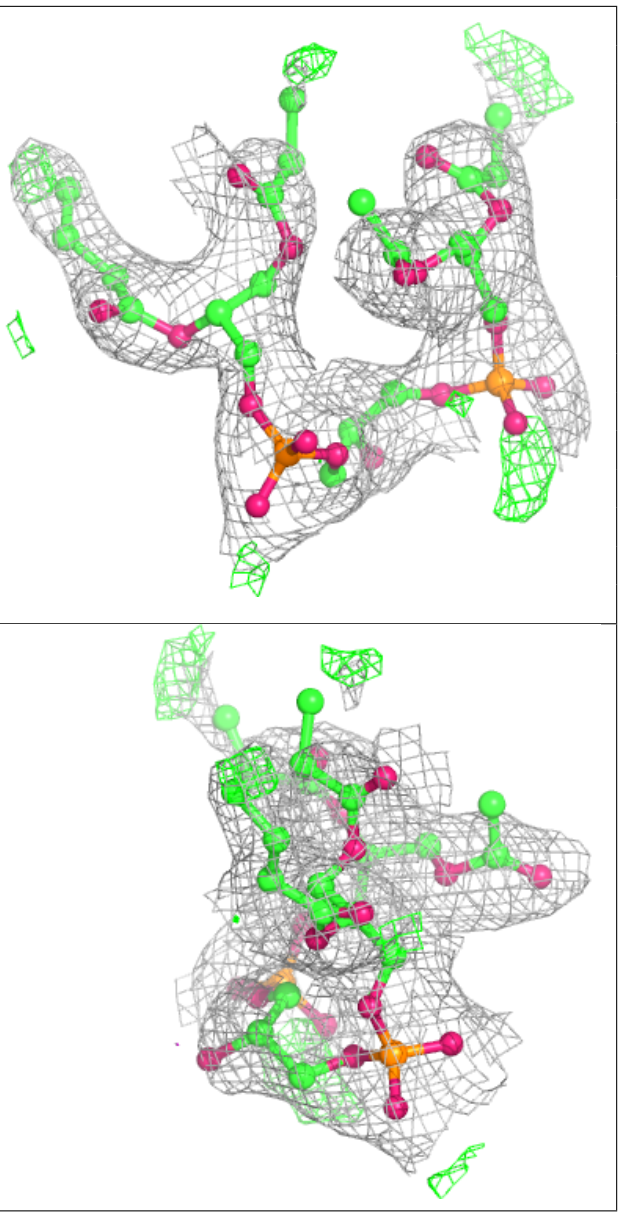


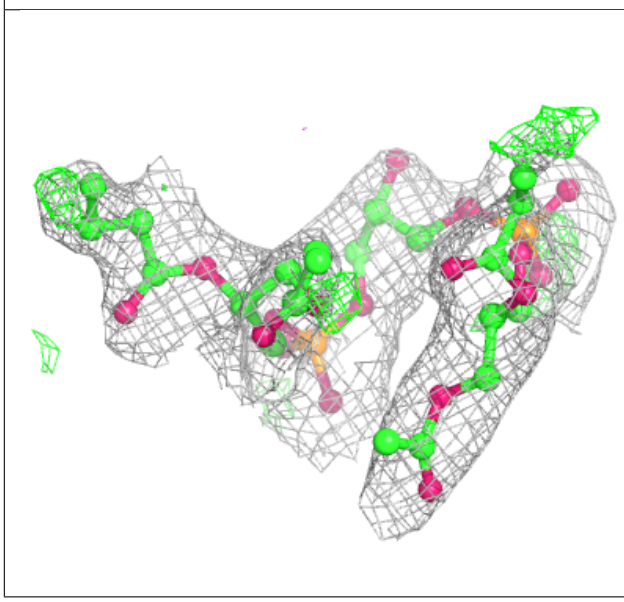




Electron density around CDL P 3004:

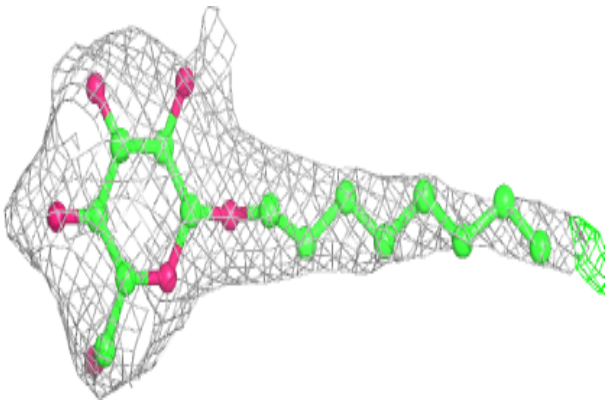
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

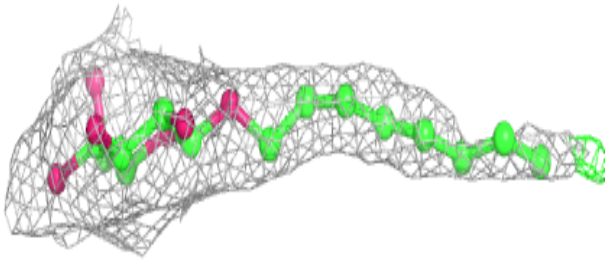


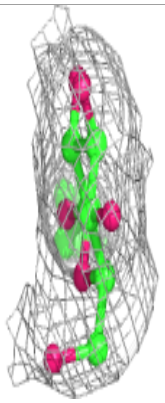


Electron density around BOG Q 3009:

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

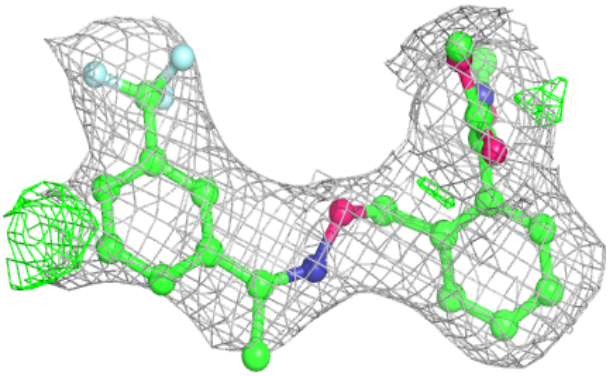


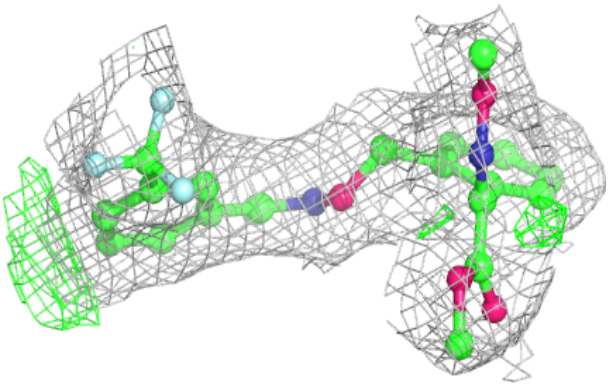


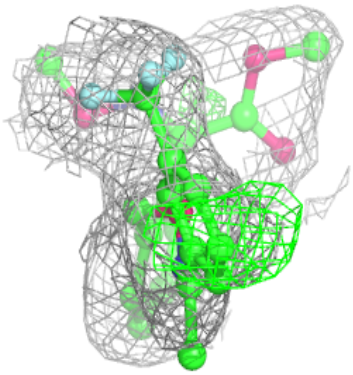


Electron density around JZV P 3001:

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

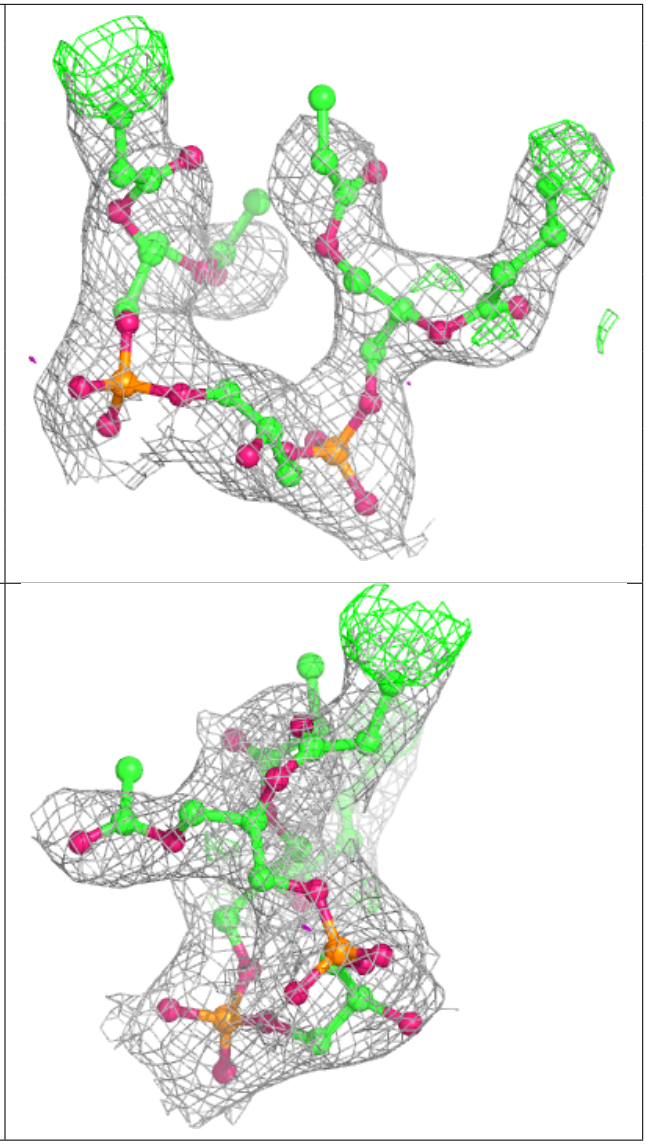






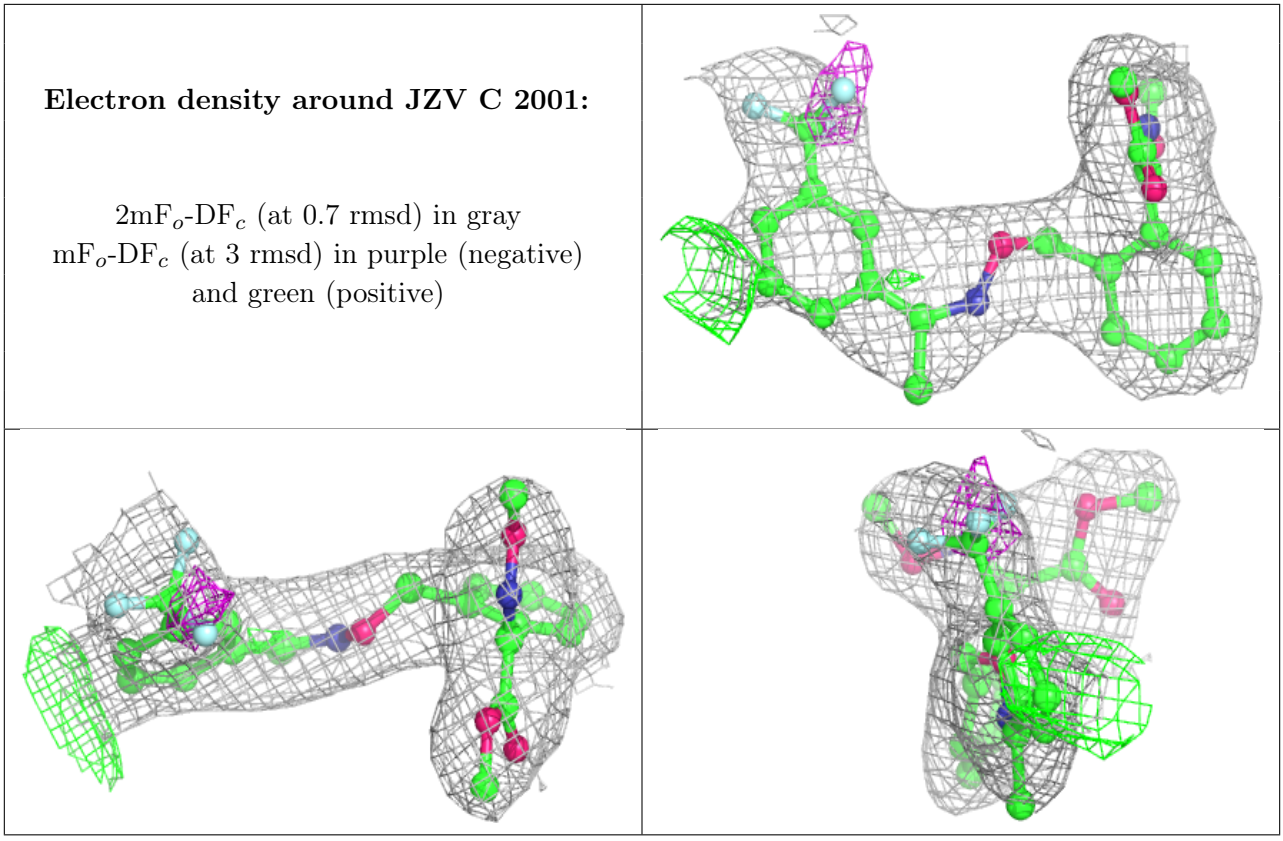
Electron density around CDL C 2004:

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



Electron density around JZV 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 BOG D 2009:

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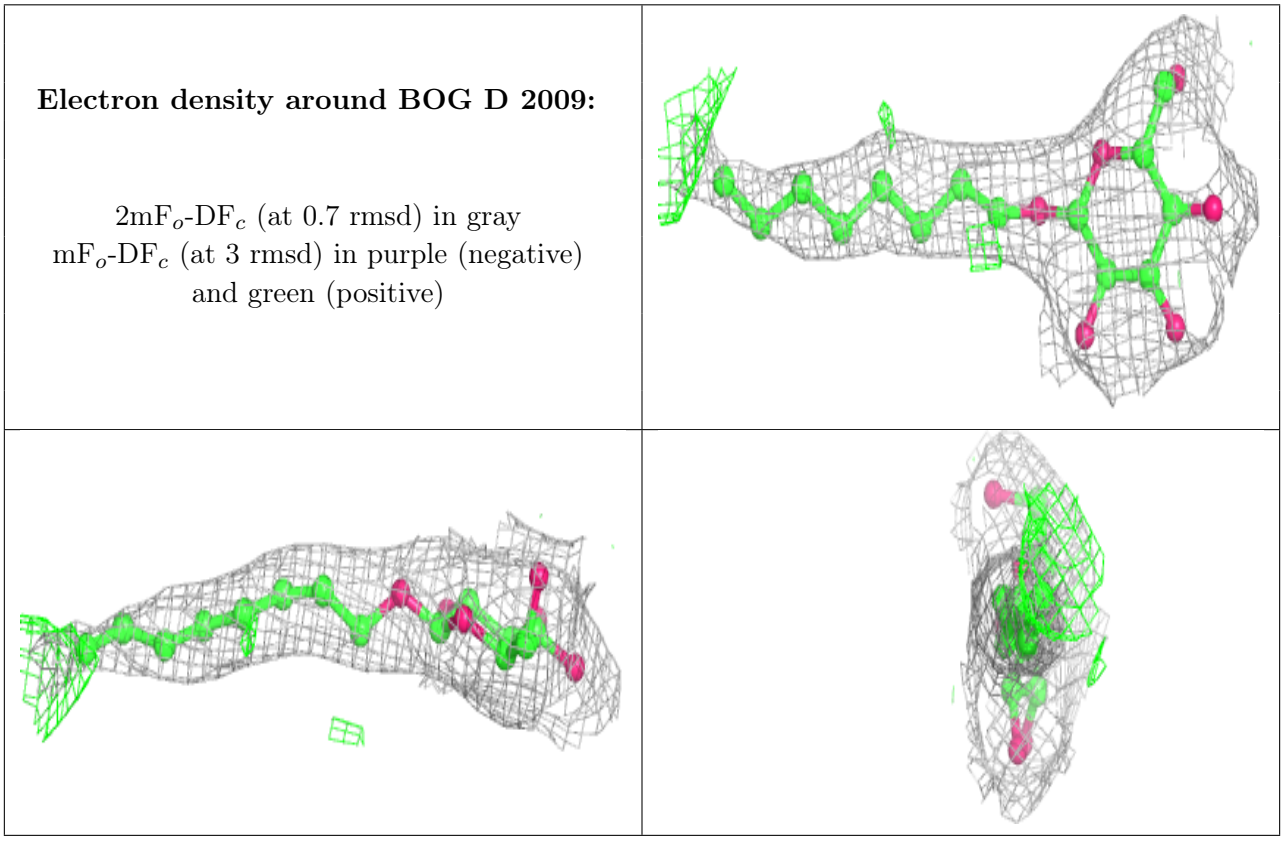
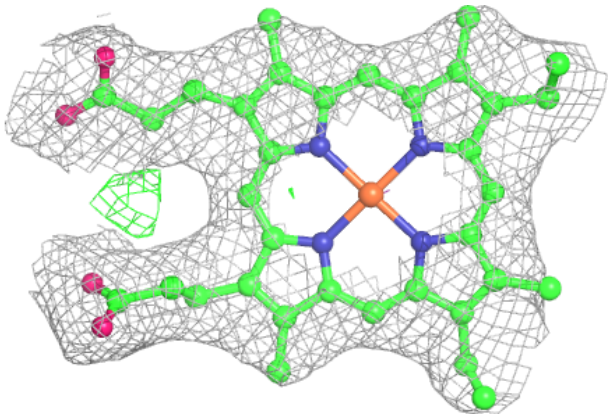
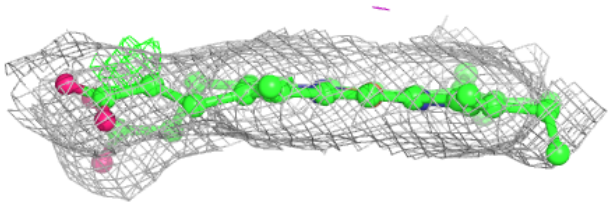
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

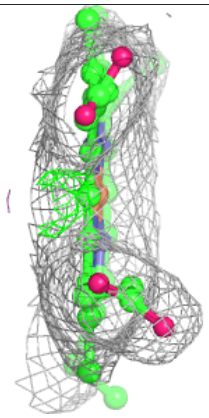


Electron density around HEC Q 501:

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

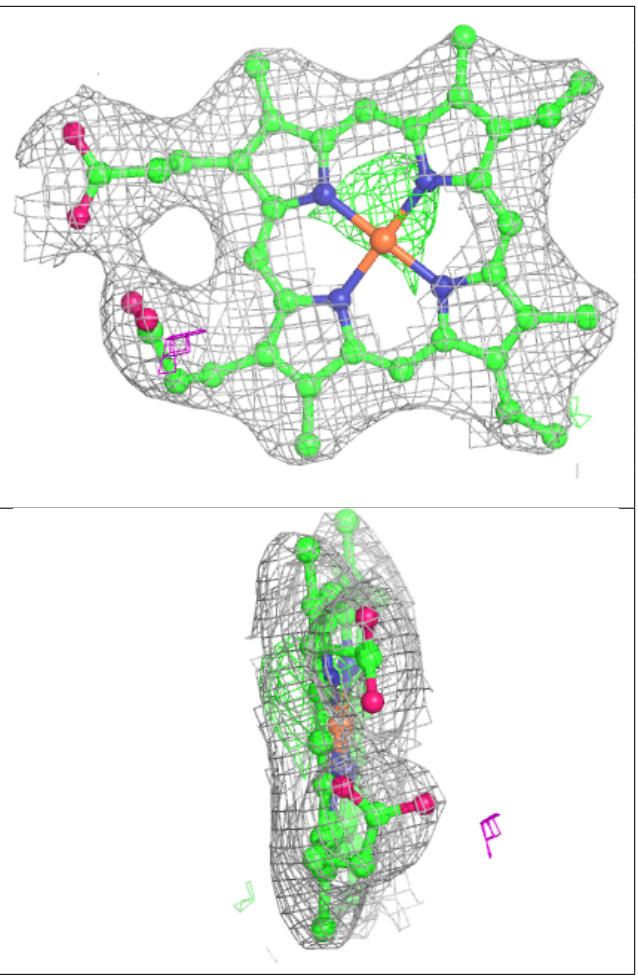






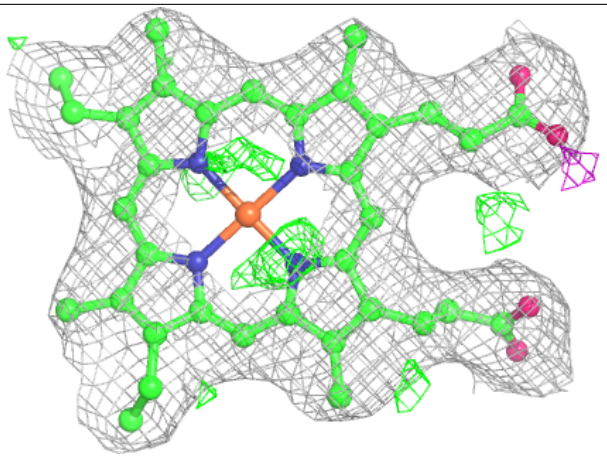
Electron density around HEM P 501:

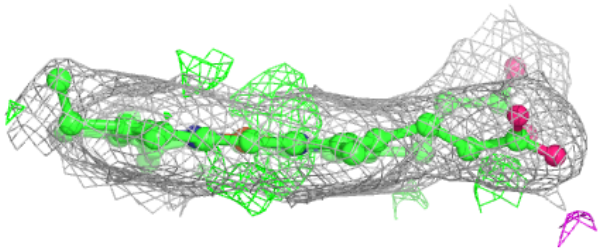
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

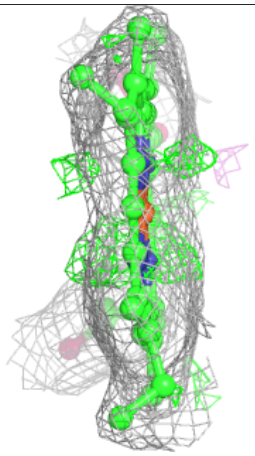


Electron density around HEC D 501:

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

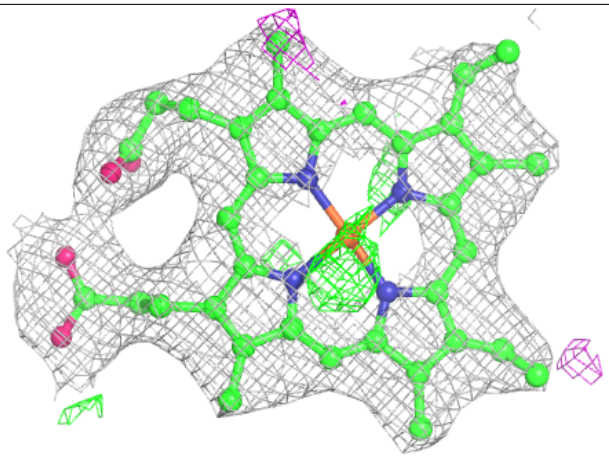


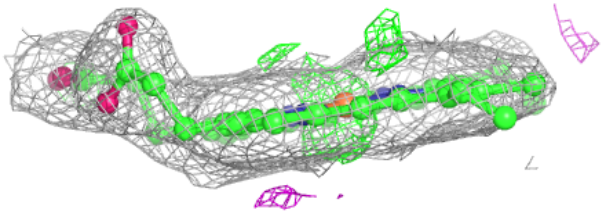


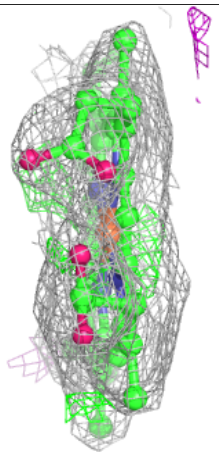


Electron density around HEM C 501:

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

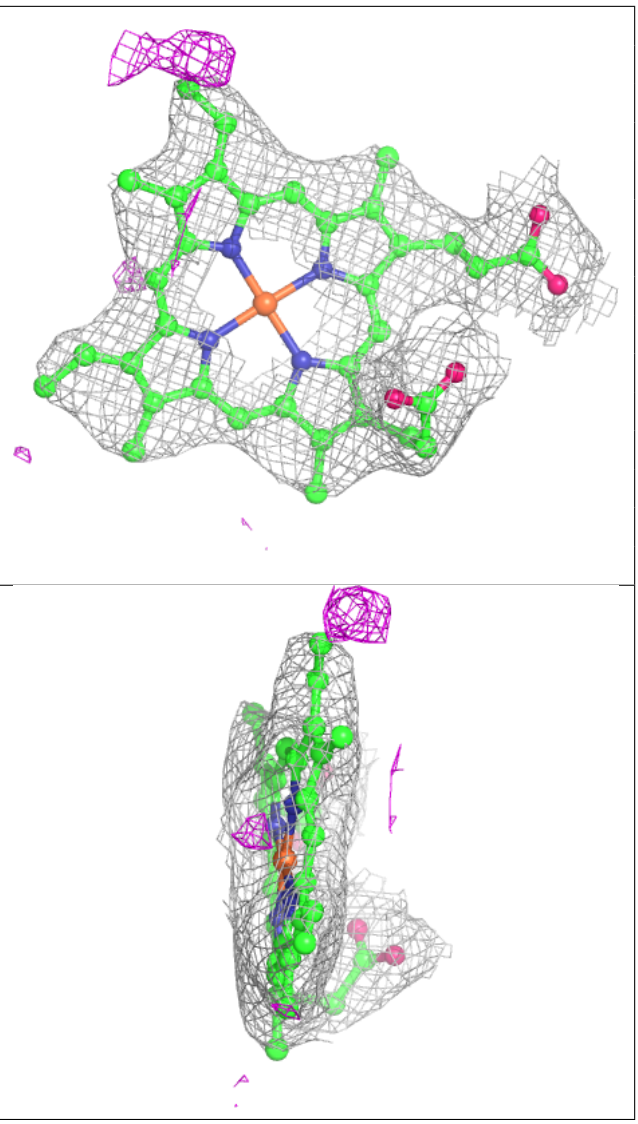






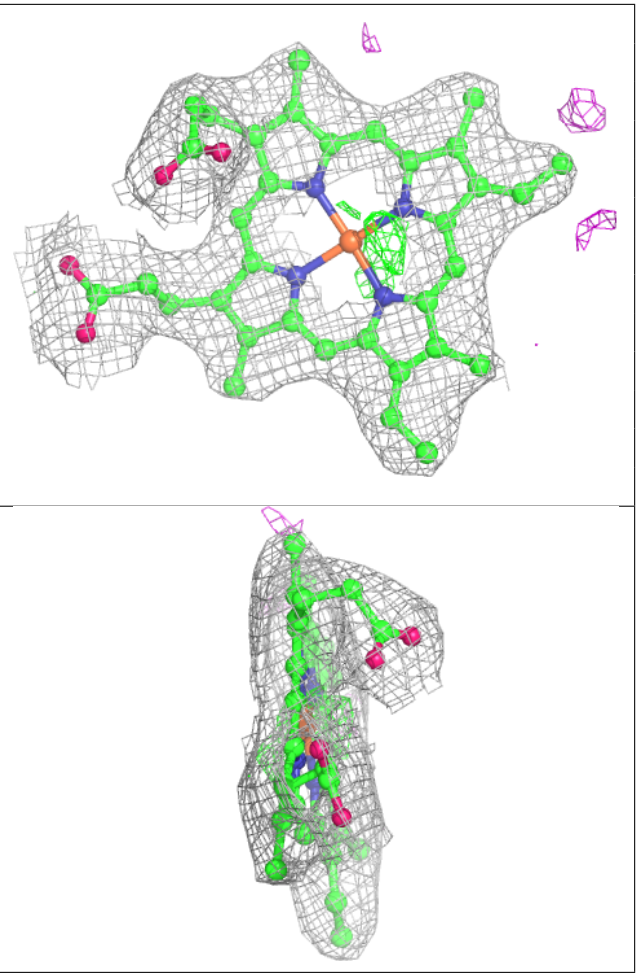
Electron density around HEM P 502:

$2mF_o$-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 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.