wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 09:18 PM EDT

PDB ID	:	3L71 / pdb_00003l71
Title	:	Cytochrome BC1 complex from chicken with azoxystrobin bound
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-27
Resolution	:	2.84 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:

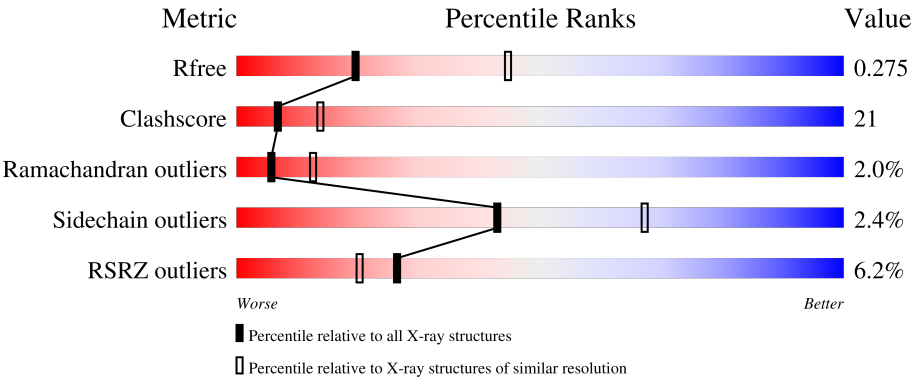
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	3% 60% 36% .
1	N	446	4% 57% 38% . .
2	B	441	4% 50% 40% 5% 5%
2	O	441	5% 52% 38% 5% .
3	C	380	3% 73% 24% .

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Mol	Chain	Length	Quality of chain
3	P	380	2% 71% 27%
4	D	241	68% 28%
4	Q	241	% 64% 33%
5	E	196	38% 46% 47% 7%
5	R	196	12% 51% 45%
6	F	110	66% 23% 8%
6	S	110	3% 55% 33% 8%
7	G	81	5% 63% 33%
7	T	81	6% 63% 32%
8	H	77	% 57% 32% 9%
8	U	77	12% 51% 34% 13%
9	I	47	34% 43% 51%
9	V	47	38% 32% 53% 6% 9%
10	J	61	70% 26%
10	W	61	3% 70% 26%

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	-	-
16	HEC	D	501	X	-	-	-
16	HEC	Q	501	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 32655 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3447	2160	607	659	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3133	1968	544	612	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

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

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

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

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	28	UNK	-	insertion	UNP Q5ZLR5

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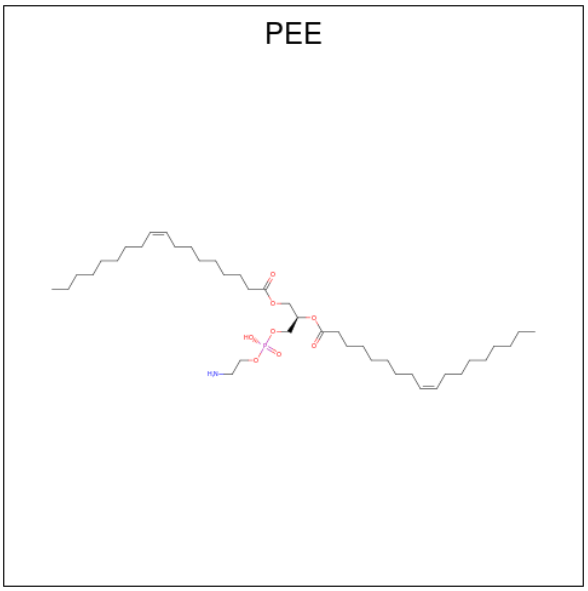
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Chain	Residue	Modelled	Actual	Comment	Reference
I	29	UNK	-	insertion	UNP Q5ZLR5
I	30	UNK	-	insertion	UNP Q5ZLR5
I	31	UNK	-	insertion	UNP Q5ZLR5
I	32	UNK	-	insertion	UNP Q5ZLR5
I	33	UNK	-	insertion	UNP Q5ZLR5
I	34	UNK	-	insertion	UNP Q5ZLR5
I	35	UNK	-	insertion	UNP Q5ZLR5
I	36	UNK	-	insertion	UNP Q5ZLR5
I	37	UNK	-	insertion	UNP Q5ZLR5
I	38	UNK	-	insertion	UNP Q5ZLR5
I	39	UNK	-	insertion	UNP Q5ZLR5
I	40	UNK	-	insertion	UNP Q5ZLR5
I	41	UNK	-	insertion	UNP Q5ZLR5
I	42	UNK	-	insertion	UNP Q5ZLR5
V	25	UNK	-	insertion	UNP Q5ZLR5
V	26	UNK	-	insertion	UNP Q5ZLR5
V	27	UNK	-	insertion	UNP Q5ZLR5
V	28	UNK	-	insertion	UNP Q5ZLR5
V	29	UNK	-	insertion	UNP Q5ZLR5
V	30	UNK	-	insertion	UNP Q5ZLR5
V	31	UNK	-	insertion	UNP Q5ZLR5
V	32	UNK	-	insertion	UNP Q5ZLR5
V	33	UNK	-	insertion	UNP Q5ZLR5
V	35	UNK	-	insertion	UNP Q5ZLR5
V	36	UNK	-	insertion	UNP Q5ZLR5
V	37	UNK	-	insertion	UNP Q5ZLR5
V	38	UNK	-	insertion	UNP Q5ZLR5
V	39	UNK	-	insertion	UNP Q5ZLR5
V	40	UNK	-	insertion	UNP Q5ZLR5

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

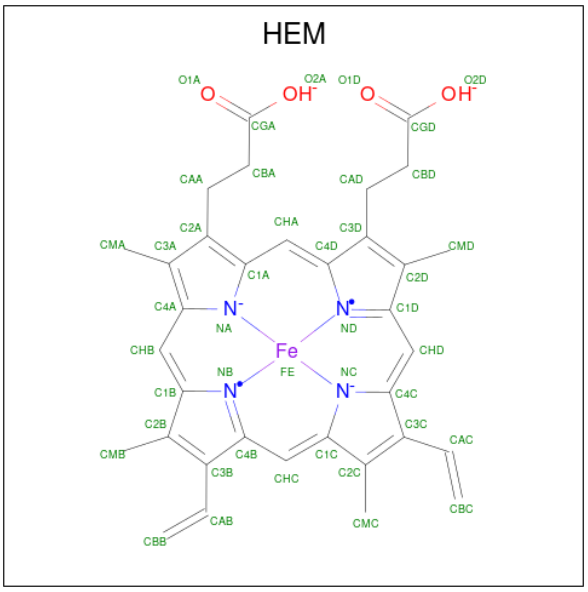
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

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



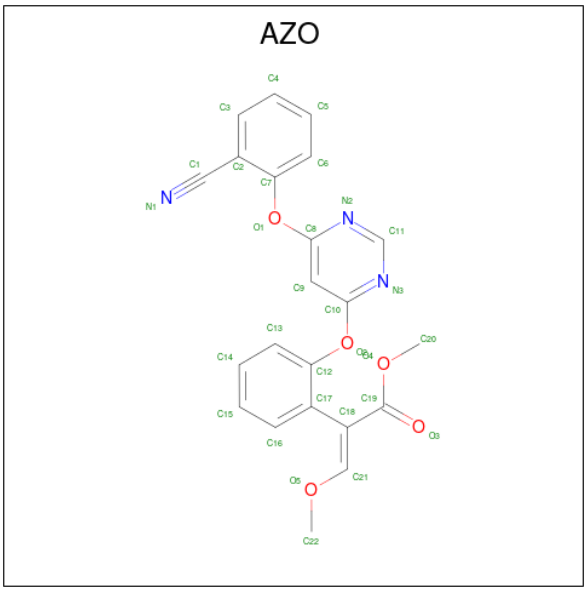
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O P 50 40 1 8 1	0	0
11	A	1	Total C O P 21 12 8 1	0	0
11	C	1	Total C N O P 49 39 1 8 1	0	0
11	N	1	Total O P 5 4 1	0	0
11	P	1	Total C N O P 50 40 1 8 1	0	0
11	P	1	Total C N O P 49 39 1 8 1	0	0

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



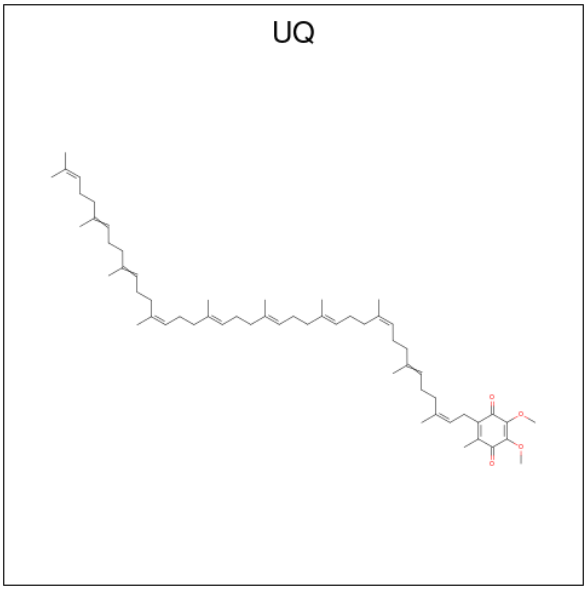
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (CCD ID: AZO) (formula: $C_{22}H_{17}N_3O_5$).



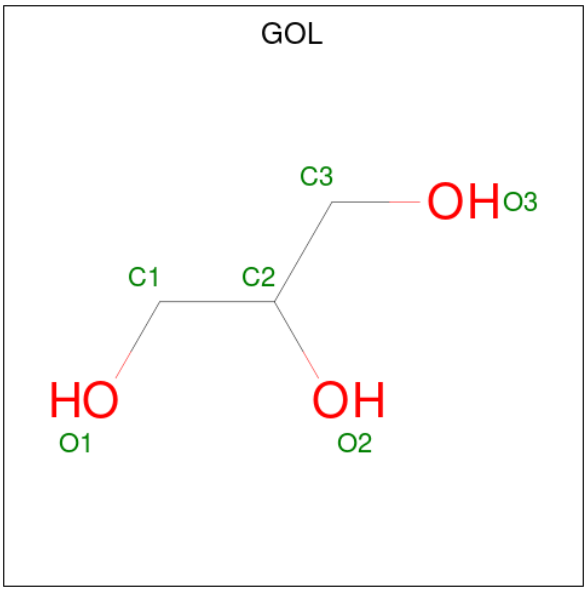
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C N O 30 22 3 5	0	0
13	P	1	Total C N O 30 22 3 5	0	0

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



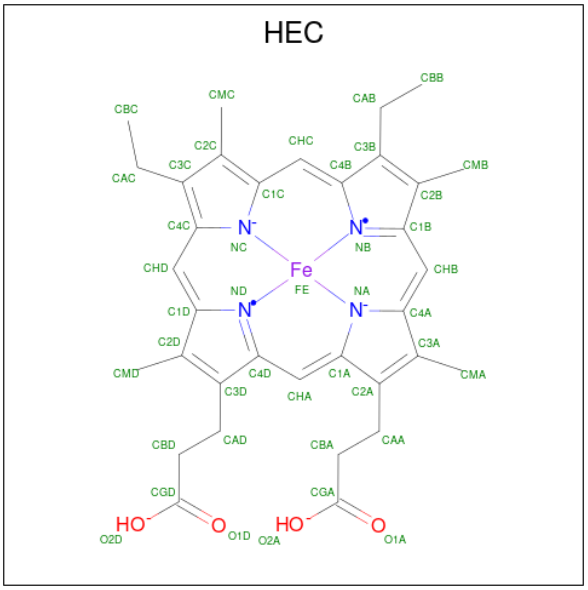
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total C O 19 15 4	0	0
14	P	1	Total C O 19 15 4	0	0

- Molecule 15 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



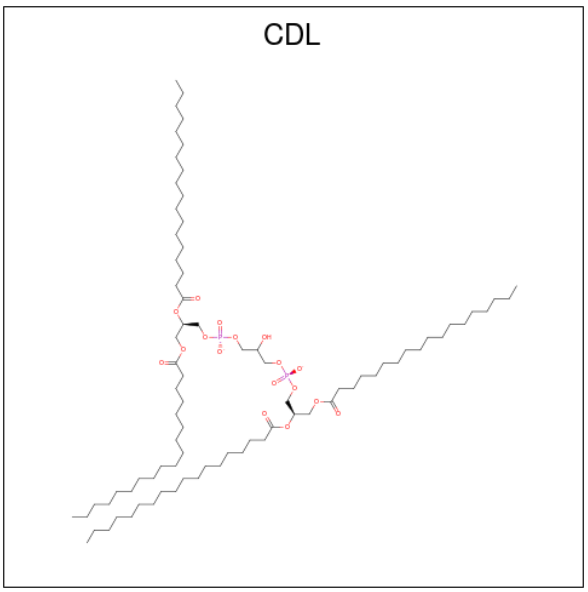
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C O 6 3 3	0	0
15	P	1	Total C O 6 3 3	0	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



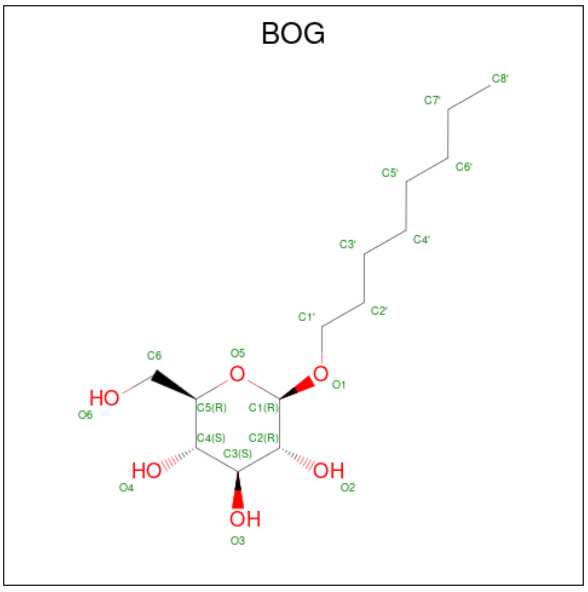
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	D	1	Total C Fe N O 43 34 1 4 4	0	0
16	Q	1	Total C Fe N O 43 34 1 4 4	0	0

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



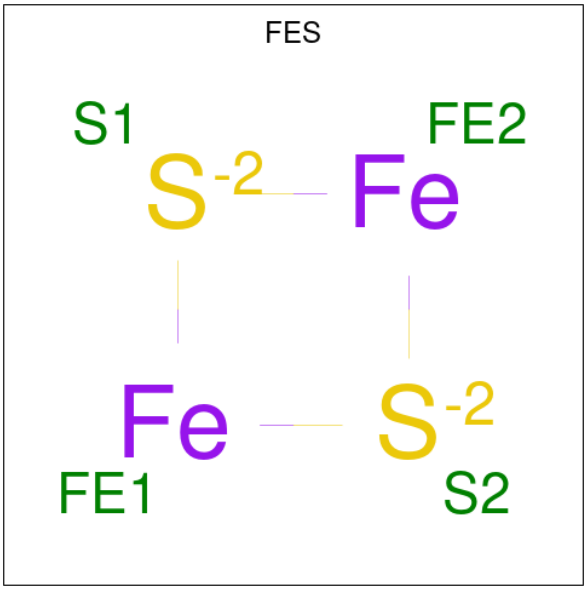
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			42	23	17	2		
17	G	1	Total	C	O	P	0	0
			40	21	17	2		
17	Q	1	Total	C	O	P	0	0
			42	23	17	2		
17	T	1	Total	C	O	P	0	0
			40	21	17	2		

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



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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 20 is water.

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

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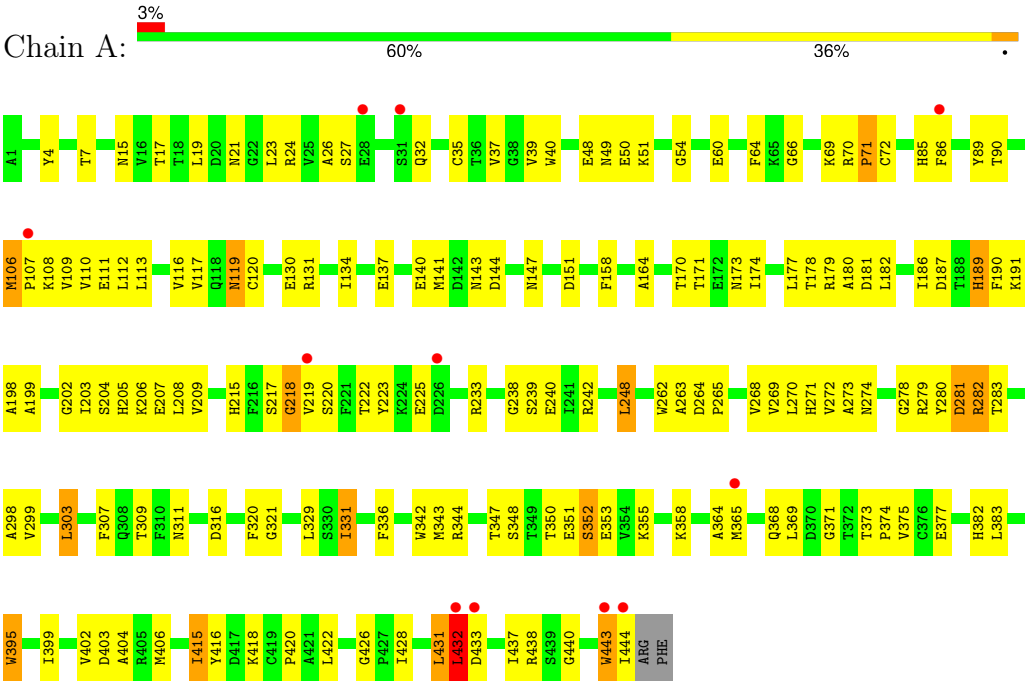
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	R	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

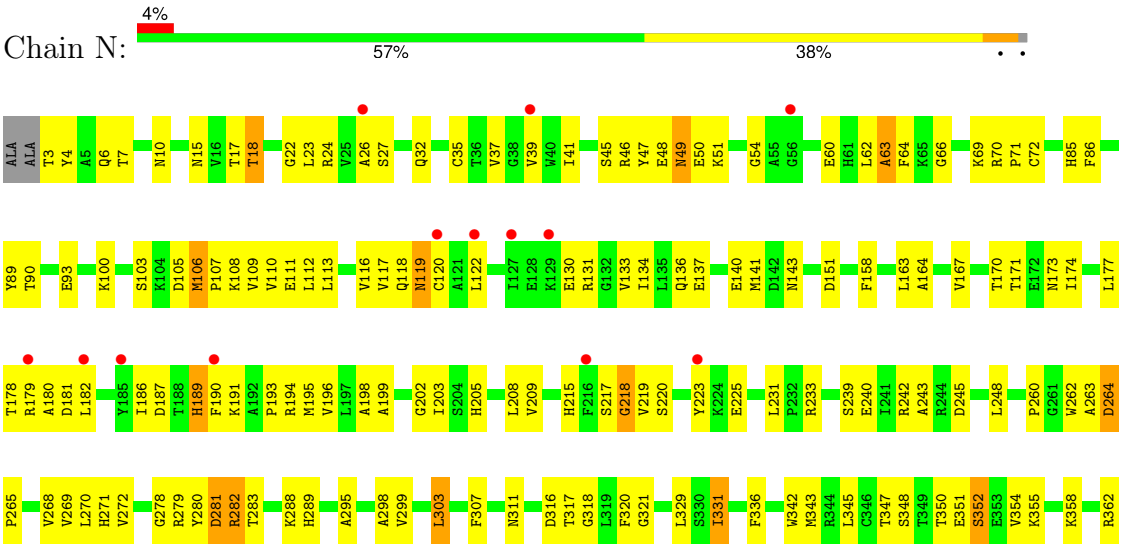
• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

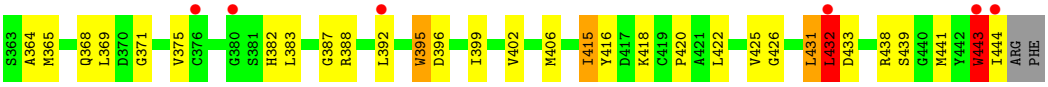
Chain A:



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

Chain N:

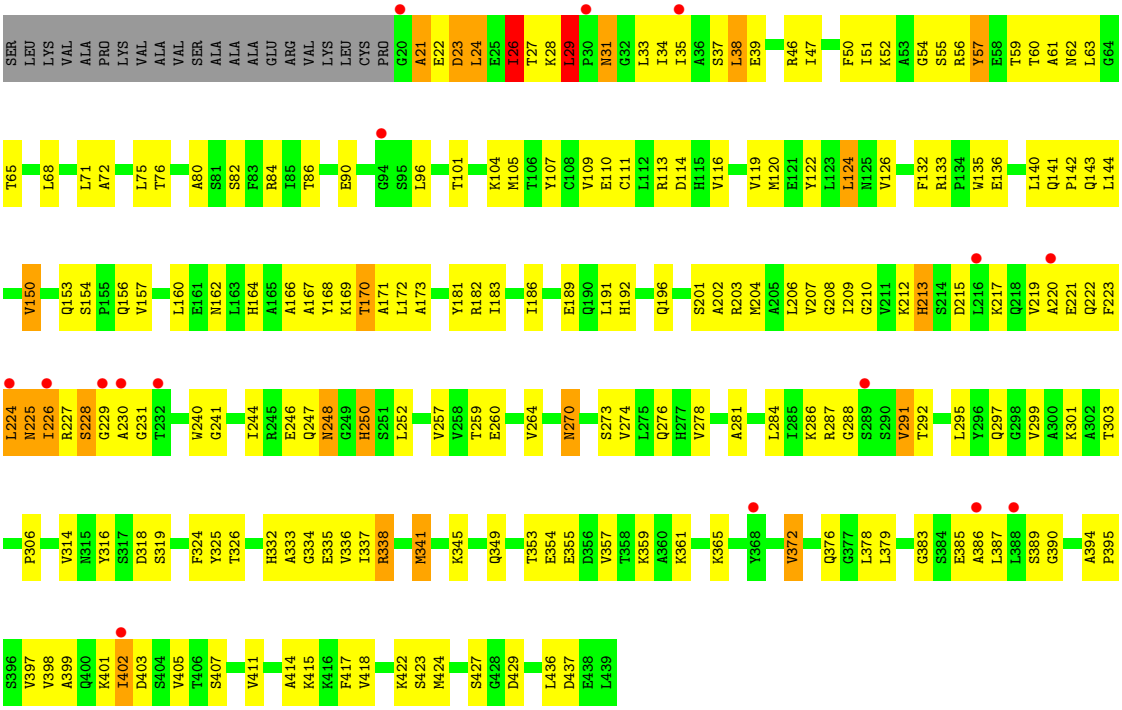




• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain B:

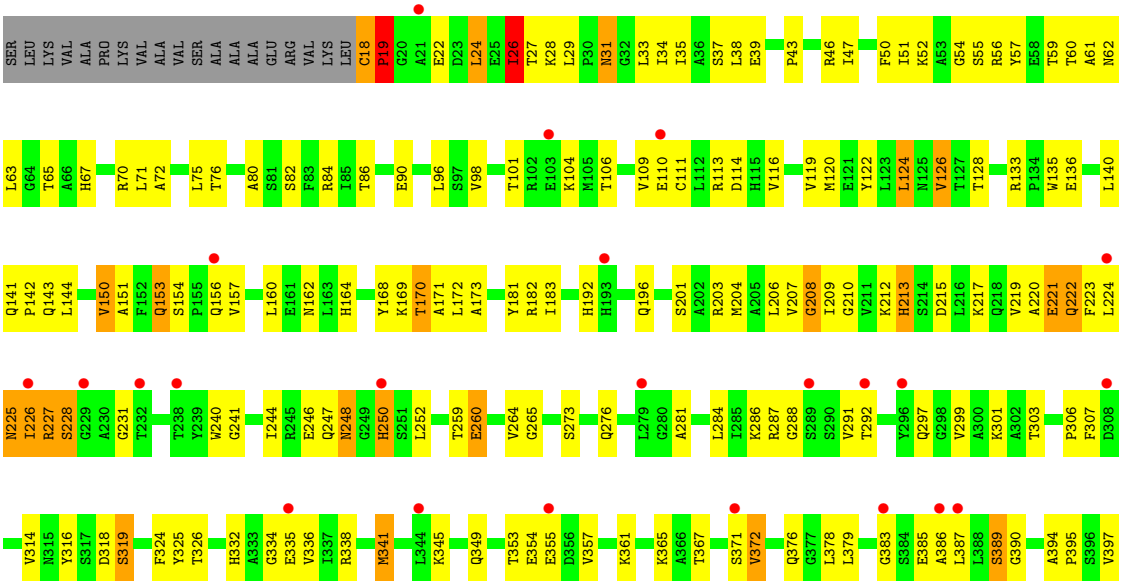




• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain O:

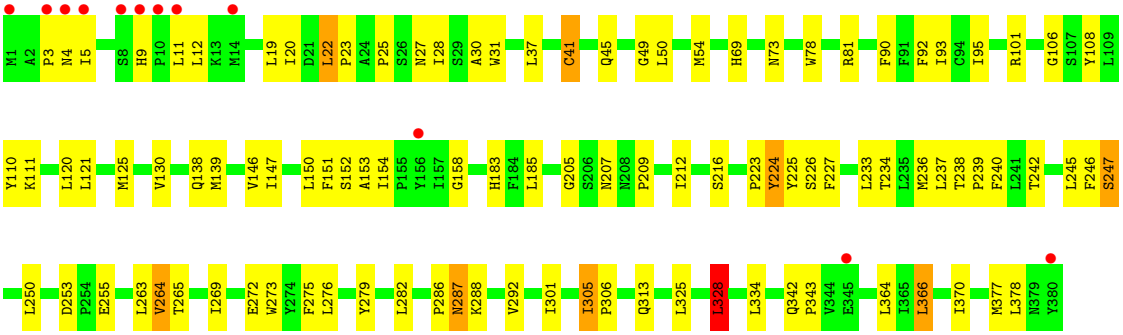






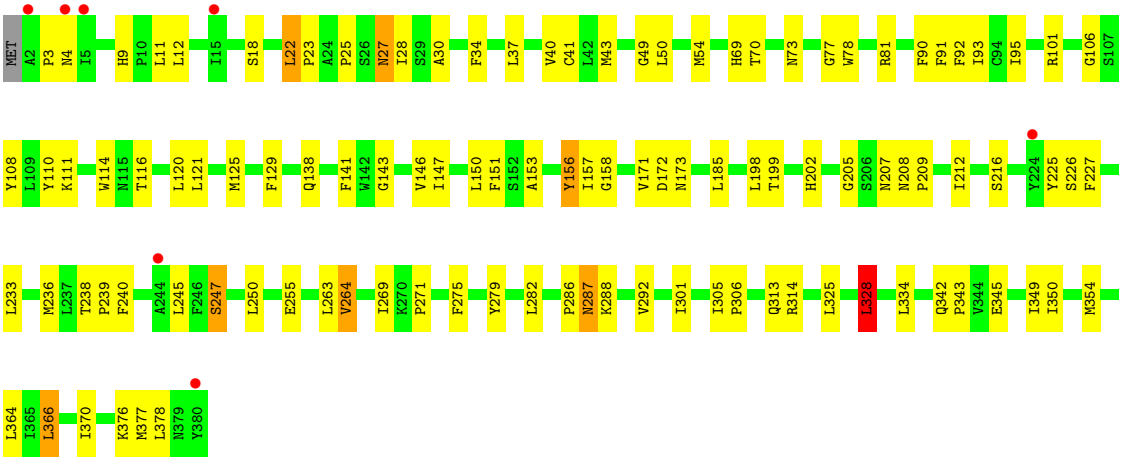
• Molecule 3: Cytochrome b





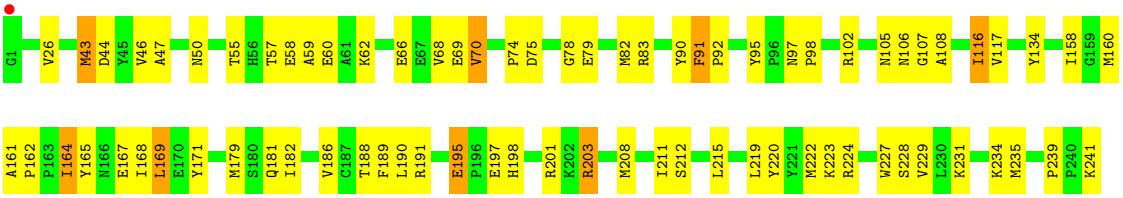
• Molecule 3: Cytochrome b





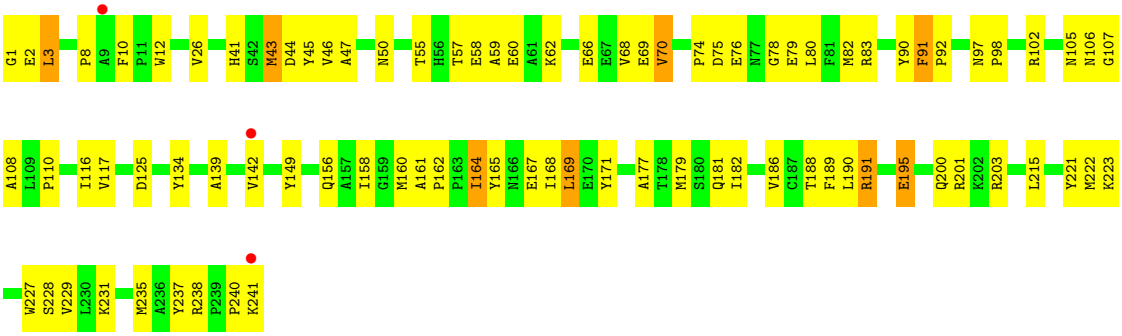
• Molecule 4: Mitochondrial cytochrome c1, heme protein



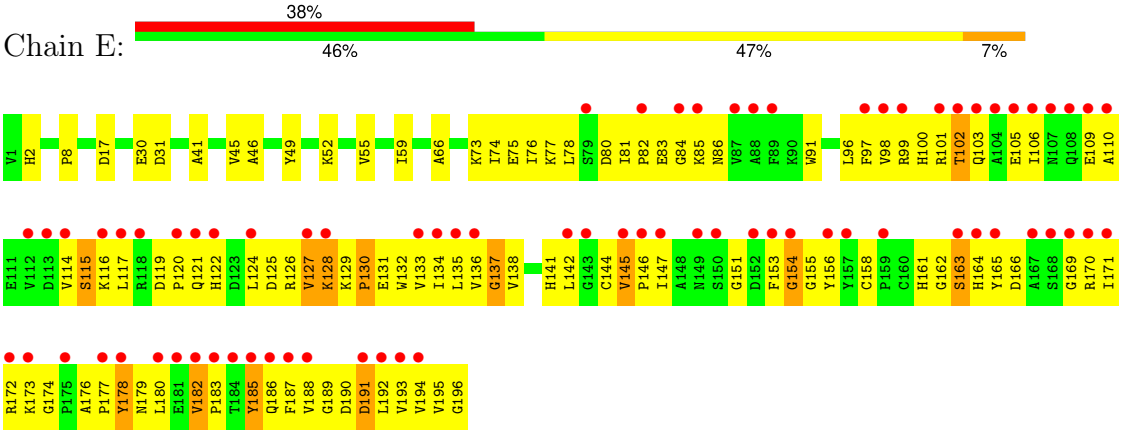


• Molecule 4: Mitochondrial cytochrome c1, heme protein

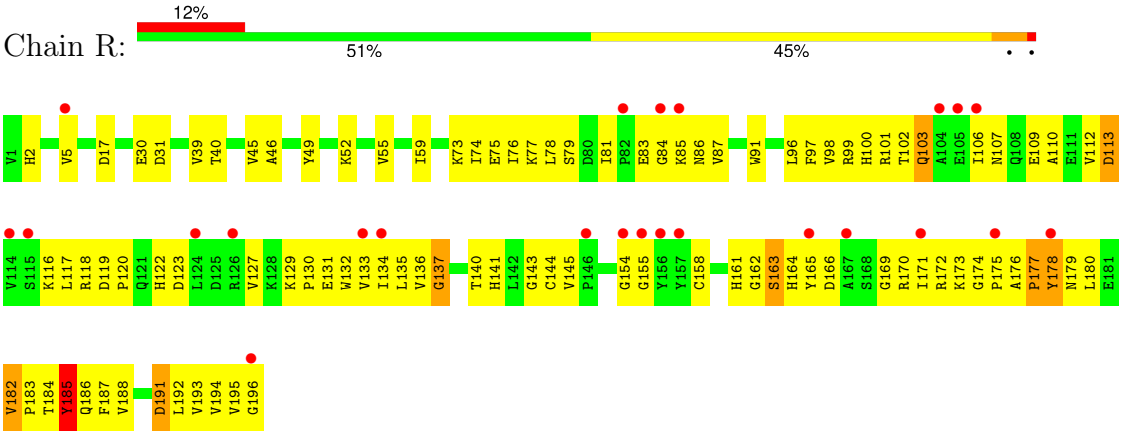




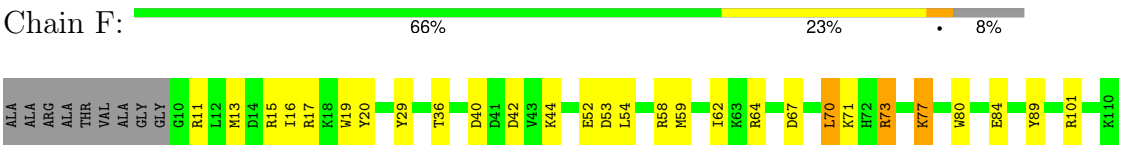
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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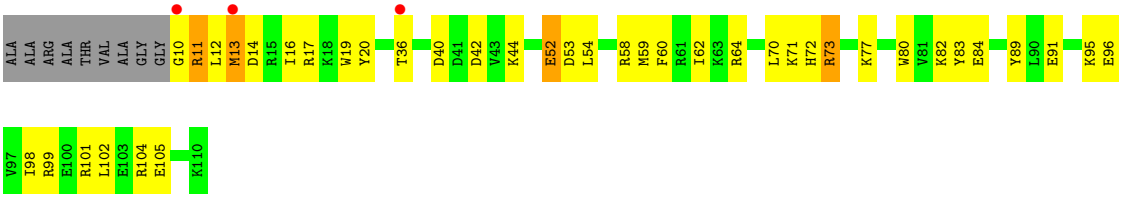


• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



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





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

Chain G:

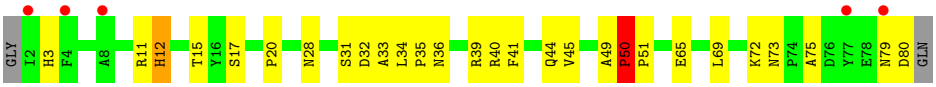




• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain T:

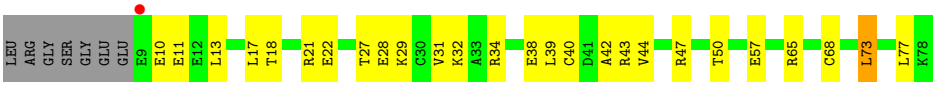




• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain H:

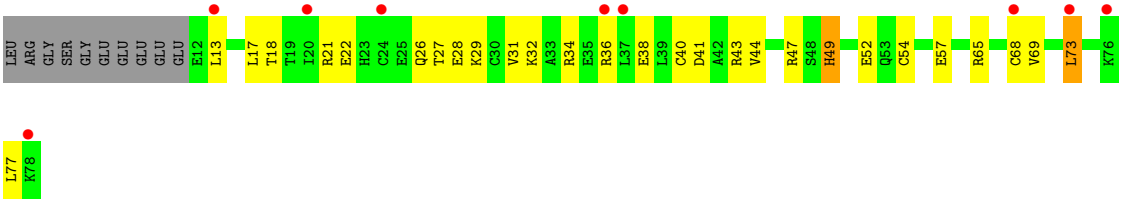




• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain U:

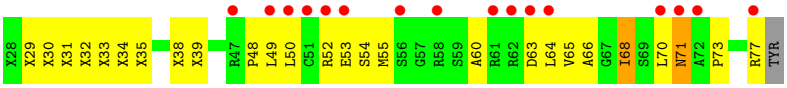




• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

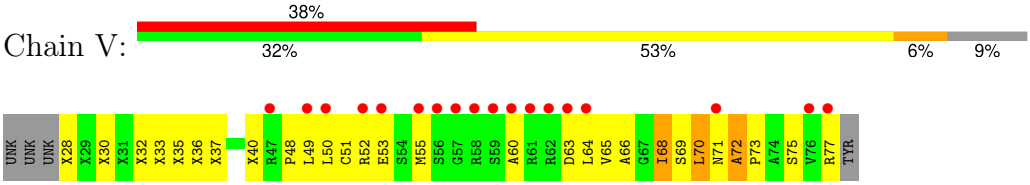
Chain I:





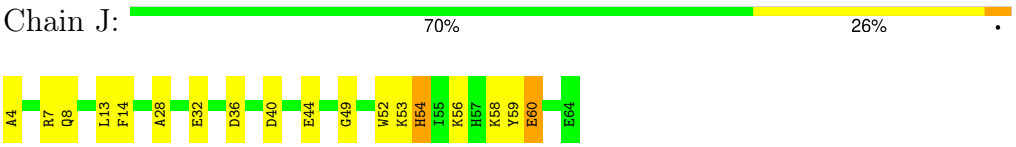
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



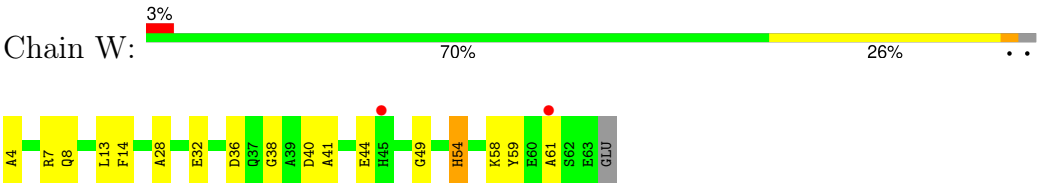
• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain J:



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

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	170.15Å 181.31Å 240.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.84 24.94 – 2.84	Depositor EDS
% Data completeness (in resolution range)	94.5 (24.94-2.84) 94.3 (24.94-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.82Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.281 0.245 , 0.275	Depositor DCC
R_{free} test set	3351 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32655	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: BOG, HEC, AZO, FES, CDL, PEE, GOL, HEM, UQ

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	0.54	0/3518	1.01	22/4767 (0.5%)
1	N	0.49	0/3508	1.00	19/4753 (0.4%)
2	B	0.47	0/3187	0.96	6/4321 (0.1%)
2	O	0.49	0/3202	0.97	8/4343 (0.2%)
3	C	0.65	0/3119	1.03	21/4270 (0.5%)
3	P	0.55	0/3114	1.02	17/4263 (0.4%)
4	D	0.59	0/1956	1.04	9/2658 (0.3%)
4	Q	0.48	0/1956	1.00	10/2658 (0.4%)
5	E	0.47	0/1547	0.91	5/2103 (0.2%)
5	R	0.45	0/1543	0.96	5/2098 (0.2%)
6	F	0.60	0/911	0.92	0/1219
6	S	0.48	0/911	0.90	0/1219
7	G	0.55	0/694	1.00	2/941 (0.2%)
7	T	0.44	0/684	0.97	2/929 (0.2%)
8	H	0.49	0/582	0.94	1/779 (0.1%)
8	U	0.39	0/561	0.91	1/751 (0.1%)
9	I	0.58	0/218	0.96	0/293
9	V	0.56	0/218	1.04	3/293 (1.0%)
10	J	0.51	0/508	0.93	3/682 (0.4%)
10	W	0.47	0/490	0.92	3/660 (0.5%)
All	All	0.52	0/32427	0.99	137/44000 (0.3%)

There are no bond length outliers.

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	227	ARG	N-CA-C	8.41	119.03	108.19
5	R	143	GLY	N-CA-C	8.23	127.15	115.30
1	A	32	GLN	CA-C-N	8.19	127.92	119.56
1	A	32	GLN	C-N-CA	8.19	127.92	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	32	GLN	CA-C-N	8.08	127.74	119.82

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	138	0
1	N	3437	0	3349	156	0
2	B	3133	0	3130	201	0
2	O	3147	0	3146	201	0
3	C	3017	0	3063	80	0
3	P	3012	0	3058	97	0
4	D	1898	0	1846	64	0
4	Q	1898	0	1846	79	0
5	E	1513	0	1478	117	0
5	R	1509	0	1474	102	0
6	F	891	0	893	27	0
6	S	891	0	893	38	0
7	G	672	0	653	30	0
7	T	662	0	645	35	0
8	H	574	0	548	21	0
8	U	553	0	535	27	0
9	I	287	0	250	39	0
9	V	277	0	249	39	0
10	J	497	0	490	17	0
10	W	479	0	478	16	0
11	A	71	0	90	0	0
11	C	49	0	72	5	0
11	N	5	0	0	0	0
11	P	99	0	149	3	0
12	C	86	0	60	5	0
12	P	86	0	60	4	0
13	C	30	0	17	0	0
13	P	30	0	17	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	19	0	17	2	0
14	P	19	0	17	3	0
15	C	6	0	8	1	0
15	P	6	0	8	0	0
16	D	43	0	30	1	0
16	Q	43	0	30	1	0
17	D	42	0	28	4	0
17	G	40	0	24	4	0
17	Q	42	0	28	3	0
17	T	40	0	24	3	0
18	D	33	0	39	1	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	0	0
20	E	1	0	0	0	0
20	P	9	0	0	1	0
20	R	1	0	0	0	0
All	All	32655	0	32154	1386	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 1386 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)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.14	1.11
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.12	1.09
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07
2:O:353:THR:HG22	2:O:355:GLU:H	1.14	1.07
2:B:353:THR:HG22	2:B:355:GLU:H	1.17	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%)	411 (93%)	25 (6%)	6 (1%)	9 18
1	N	440/446 (99%)	408 (93%)	25 (6%)	7 (2%)	7 16
2	B	418/441 (95%)	353 (84%)	50 (12%)	15 (4%)	2 5
2	O	420/441 (95%)	364 (87%)	42 (10%)	14 (3%)	3 6
3	C	378/380 (100%)	360 (95%)	14 (4%)	4 (1%)	11 23
3	P	377/380 (99%)	353 (94%)	19 (5%)	5 (1%)	9 20
4	D	239/241 (99%)	223 (93%)	16 (7%)	0	100 100
4	Q	239/241 (99%)	221 (92%)	16 (7%)	2 (1%)	16 31
5	E	194/196 (99%)	148 (76%)	34 (18%)	12 (6%)	1 1
5	R	194/196 (99%)	162 (84%)	23 (12%)	9 (5%)	2 3
6	F	99/110 (90%)	96 (97%)	2 (2%)	1 (1%)	12 24
6	S	99/110 (90%)	90 (91%)	8 (8%)	1 (1%)	12 24
7	G	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	9 20
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	4 9
8	H	68/77 (88%)	65 (96%)	3 (4%)	0	100 100
8	U	65/77 (84%)	61 (94%)	2 (3%)	2 (3%)	3 7
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%)	56 (95%)	3 (5%)	0	100 100
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7 15
All	All	4002/4160 (96%)	3619 (90%)	301 (8%)	82 (2%)	6 12

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ALA

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Mol	Chain	Res	Type
2	B	24	LEU
2	B	29	LEU
2	B	171	ALA
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%)	356 (98%)	9 (2%)	42	66
1	N	365/368 (99%)	354 (97%)	11 (3%)	36	60
2	B	331/347 (95%)	316 (96%)	15 (4%)	24	48
2	O	333/347 (96%)	320 (96%)	13 (4%)	28	53
3	C	328/329 (100%)	324 (99%)	4 (1%)	63	80
3	P	328/329 (100%)	326 (99%)	2 (1%)	78	89
4	D	200/200 (100%)	196 (98%)	4 (2%)	48	72
4	Q	200/200 (100%)	196 (98%)	4 (2%)	48	72
5	E	166/166 (100%)	164 (99%)	2 (1%)	63	80
5	R	165/166 (99%)	163 (99%)	2 (1%)	63	80
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	50
6	S	93/96 (97%)	88 (95%)	5 (5%)	20	42
7	G	71/71 (100%)	70 (99%)	1 (1%)	59	78
7	T	70/71 (99%)	70 (100%)	0	100	100
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	76
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	21
9	V	23/26 (88%)	21 (91%)	2 (9%)	9	21
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	72
10	W	47/49 (96%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3378/3446 (98%)	3296 (98%)	82 (2%)	43 67

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	124	LEU
4	Q	203	ARG
2	O	248	ASN
2	O	402	ILE
6	S	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	49	ASN
2	O	196	GLN
5	R	121	GLN
1	N	118	GLN
1	N	311	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
17	CDL	T	3004	-	39,39,99	1.22	2 (5%)	45,51,111	1.12	4 (8%)
17	CDL	G	2004	-	39,39,99	1.22	1 (2%)	45,51,111	1.11	3 (6%)
13	AZO	P	3001	-	32,32,32	3.30	17 (53%)	42,42,42	3.03	13 (30%)
15	GOL	P	3011	-	5,5,5	1.43	0	5,5,5	0.66	0
16	HEC	D	501	4	50,50,50	1.49	10 (20%)	68,82,82	1.90	21 (30%)
16	HEC	Q	501	4	50,50,50	1.23	6 (12%)	68,82,82	1.56	9 (13%)
11	PEE	C	2007	-	48,48,50	1.42	7 (14%)	51,53,55	0.83	2 (3%)
12	HEM	C	502	3	50,50,50	1.54	7 (14%)	67,82,82	1.50	12 (17%)
12	HEM	P	502	3	50,50,50	1.50	6 (12%)	67,82,82	1.32	8 (11%)
17	CDL	Q	3003	-	41,41,99	1.20	1 (2%)	47,53,111	1.06	3 (6%)
11	PEE	P	3007	-	48,48,50	1.36	6 (12%)	51,53,55	0.78	2 (3%)
19	FES	E	501	5	0,4,4	-	-	-		
11	PEE	A	2008	-	20,20,50	1.83	6 (30%)	23,25,55	0.70	0
18	BOG	P	2010	-	12,12,20	1.31	2 (16%)	17,17,25	0.60	0
13	AZO	C	2001	-	32,32,32	3.12	16 (50%)	42,42,42	3.00	13 (30%)
11	PEE	N	3008	-	4,4,50	3.73	4 (100%)	6,6,55	0.65	0
19	FES	R	501	5	0,4,4	-	-	-		
11	PEE	P	3005	-	49,49,50	1.52	10 (20%)	52,54,55	0.85	3 (5%)
18	BOG	Q	3009	-	20,20,20	0.98	1 (5%)	25,25,25	0.83	1 (4%)
15	GOL	C	2011	-	5,5,5	1.42	0	5,5,5	0.64	0
17	CDL	D	2003	-	41,41,99	1.19	1 (2%)	47,53,111	1.05	2 (4%)
18	BOG	Q	3091	-	13,13,20	1.35	2 (15%)	18,18,25	1.15	2 (11%)
14	UQ	P	3002	-	19,19,63	2.65	10 (52%)	24,26,79	1.33	3 (12%)
11	PEE	A	2005	-	49,49,50	1.54	10 (20%)	52,54,55	0.86	3 (5%)
14	UQ	C	2002	-	19,19,63	2.68	10 (52%)	24,26,79	1.37	3 (12%)
12	HEM	C	501	3	50,50,50	1.51	8 (16%)	67,82,82	1.34	8 (11%)
18	BOG	D	2091	-	13,13,20	1.29	2 (15%)	18,18,25	1.13	2 (11%)
18	BOG	D	2009	-	20,20,20	1.03	1 (5%)	25,25,25	0.87	2 (8%)
12	HEM	P	501	3	50,50,50	1.37	4 (8%)	67,82,82	1.33	9 (13%)

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
17	CDL	T	3004	-	-	21/49/49/110	-
17	CDL	G	2004	-	-	21/49/49/110	-
16	HEC	D	501	4	1/1/3/7	9/14/54/54	-
16	HEC	Q	501	4	1/1/3/7	9/14/54/54	-
13	AZO	P	3001	-	-	1/23/23/23	0/3/3/3
15	GOL	P	3011	-	-	2/4/4/4	-
11	PEE	C	2007	-	-	20/52/52/54	-
12	HEM	C	502	3	-	5/14/54/54	-
12	HEM	P	502	3	-	5/14/54/54	-
17	CDL	Q	3003	-	-	23/51/51/110	-
11	PEE	P	3007	-	-	23/52/52/54	-
19	FES	E	501	5	-	-	0/1/1/1
11	PEE	A	2008	-	-	11/24/24/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
13	AZO	C	2001	-	-	1/23/23/23	0/3/3/3
19	FES	R	501	5	-	-	0/1/1/1
11	PEE	P	3005	-	-	26/53/53/54	-
18	BOG	Q	3009	-	-	4/11/31/31	0/1/1/1
15	GOL	C	2011	-	-	4/4/4/4	-
17	CDL	D	2003	-	-	23/51/51/110	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
14	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
11	PEE	A	2005	-	-	25/53/53/54	-
14	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
12	HEM	C	501	3	-	8/14/54/54	-
18	BOG	D	2091	-	-	2/4/24/31	0/1/1/1
18	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
12	HEM	P	501	3	-	6/14/54/54	-

The worst 5 of 150 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	AZO	C21-C18	8.42	1.51	1.34
13	C	2001	AZO	C21-C18	8.04	1.50	1.34
13	P	3001	AZO	C18-C19	-6.54	1.32	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	AZO	C2-C7	6.30	1.53	1.40
13	C	2001	AZO	C18-C19	-6.24	1.33	1.48

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	2001	AZO	C11-N3-C10	10.06	122.16	114.50
13	P	3001	AZO	C11-N3-C10	9.85	122.00	114.50
13	P	3001	AZO	C11-N2-C8	9.68	121.88	114.50
13	C	2001	AZO	C11-N2-C8	9.57	121.79	114.50
13	C	2001	AZO	N2-C11-N3	-6.66	118.50	128.58

All (2) chirality outliers are listed below:

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

5 of 265 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2005	PEE	C11-C10-O2-C2
11	A	2005	PEE	C4-O4P-P-O3P
11	A	2005	PEE	C4-O4P-P-O2P
11	A	2005	PEE	C4-O4P-P-O1P
11	A	2005	PEE	O4P-C4-C5-N

There are no ring outliers.

21 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	3004	CDL	3	0
17	G	2004	CDL	4	0
13	P	3001	AZO	2	0
16	D	501	HEC	1	0
16	Q	501	HEC	1	0
11	C	2007	PEE	5	0
12	C	502	HEM	2	0
12	P	502	HEM	2	0
17	Q	3003	CDL	3	0
11	P	3007	PEE	3	0

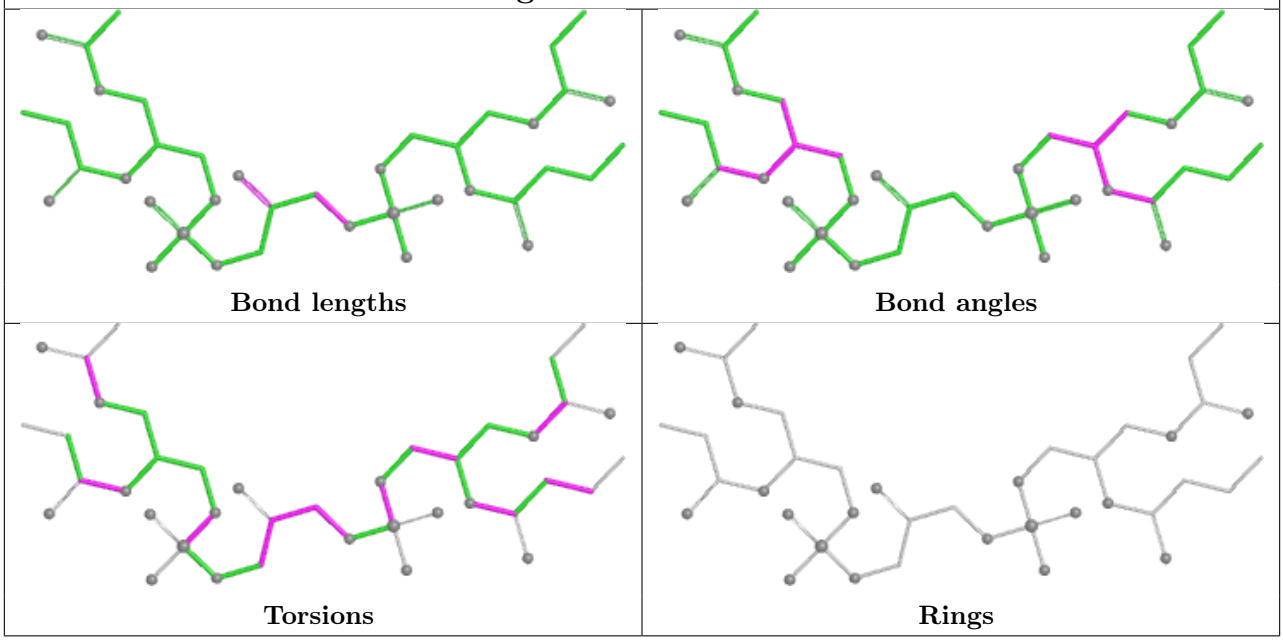
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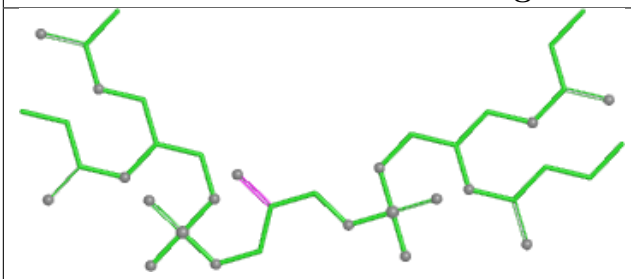
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	E	501	FES	2	0
18	P	2010	BOG	1	0
19	R	501	FES	2	0
15	C	2011	GOL	1	0
17	D	2003	CDL	4	0
18	Q	3091	BOG	1	0
14	P	3002	UQ	3	0
14	C	2002	UQ	2	0
12	C	501	HEM	3	0
18	D	2091	BOG	1	0
12	P	501	HEM	2	0

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.

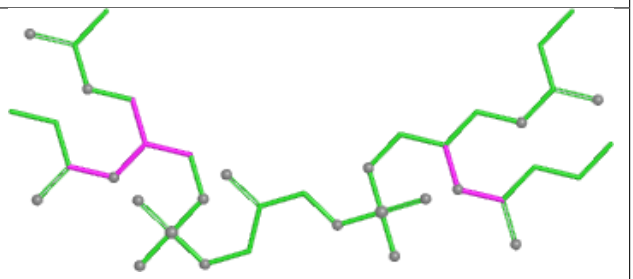
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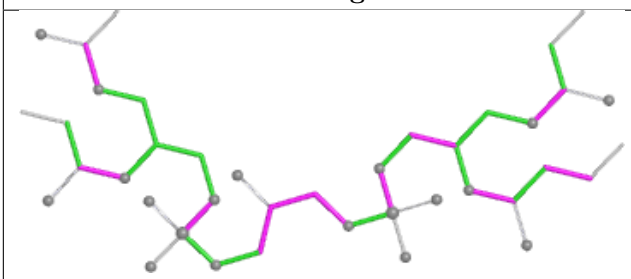
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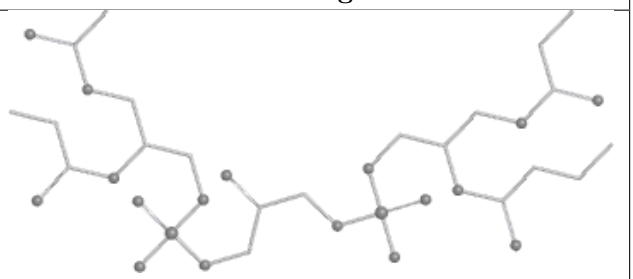
Bond lengths



Bond angles

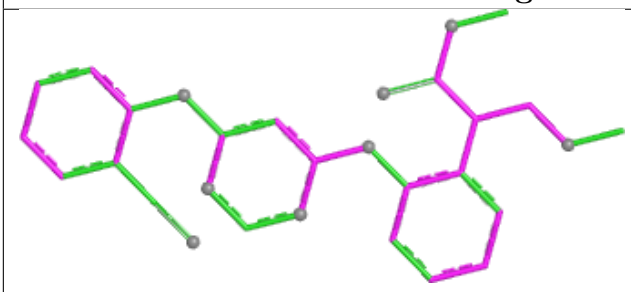


Torsions

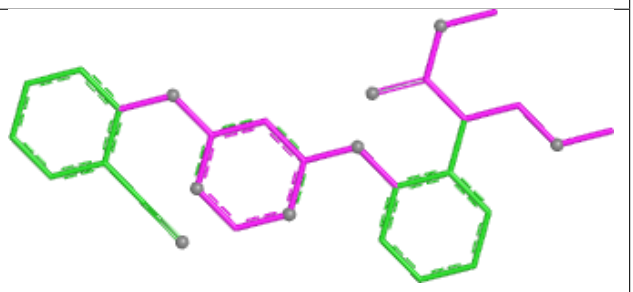


Rings

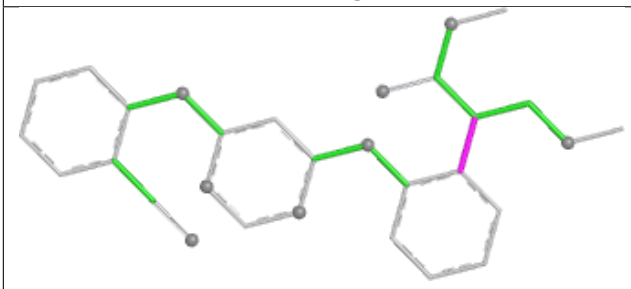
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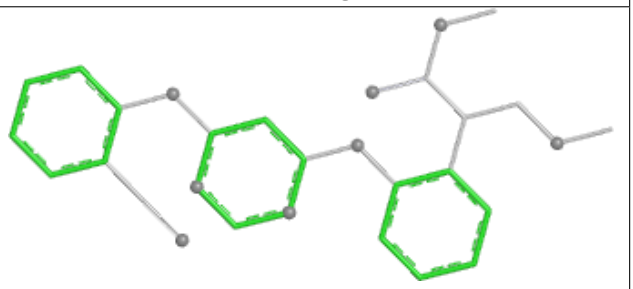
Bond lengths



Bond angles

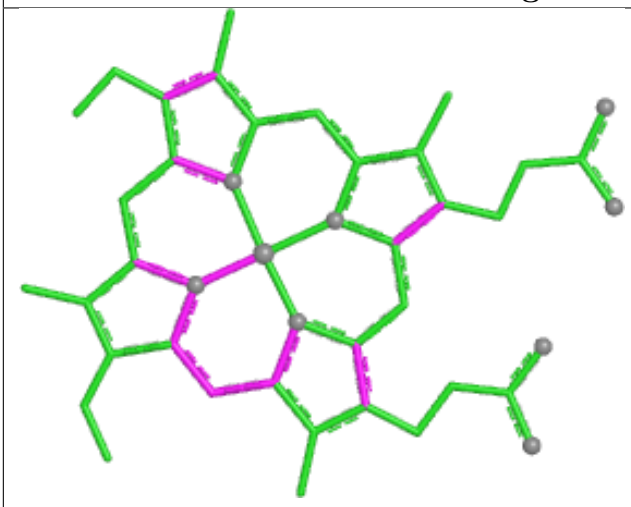


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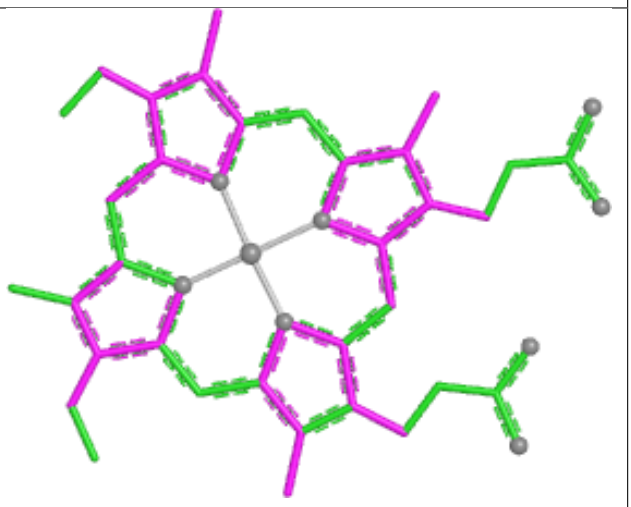


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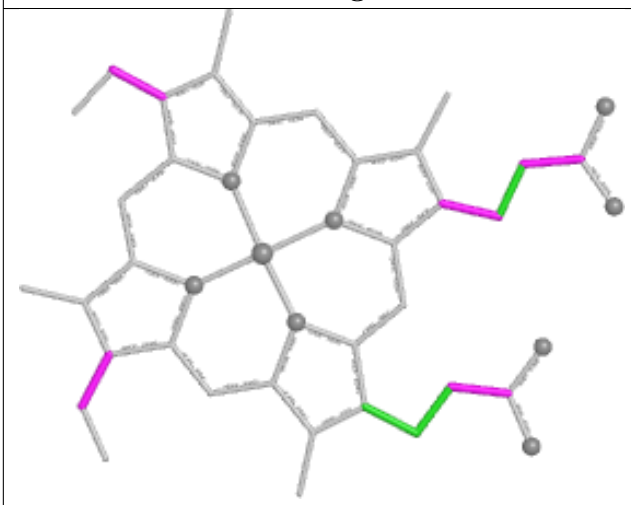
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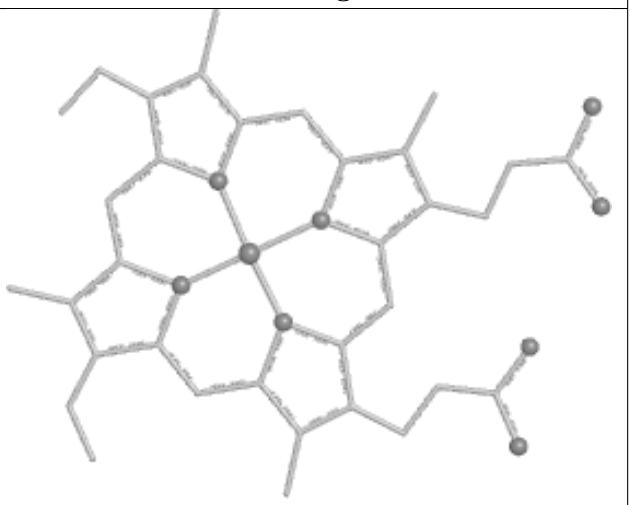
Bond lengths



Bond angles

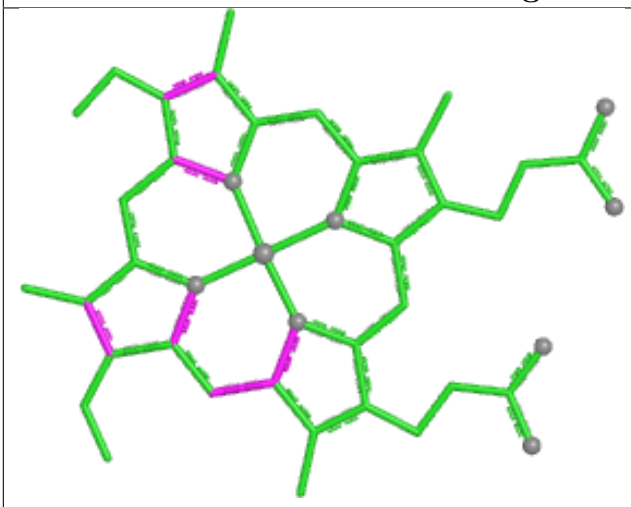


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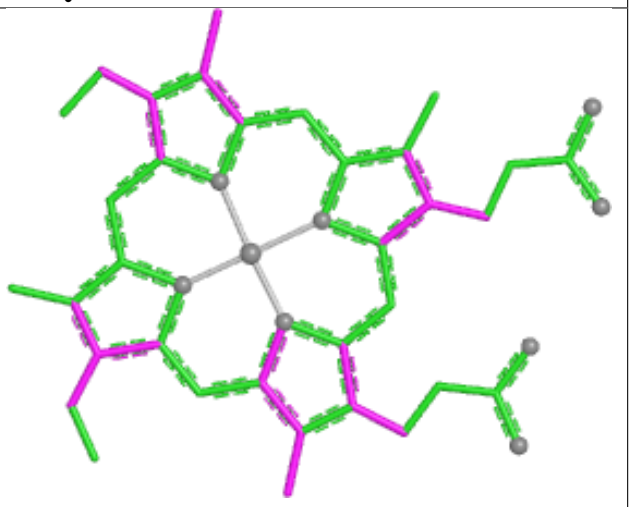


Rings

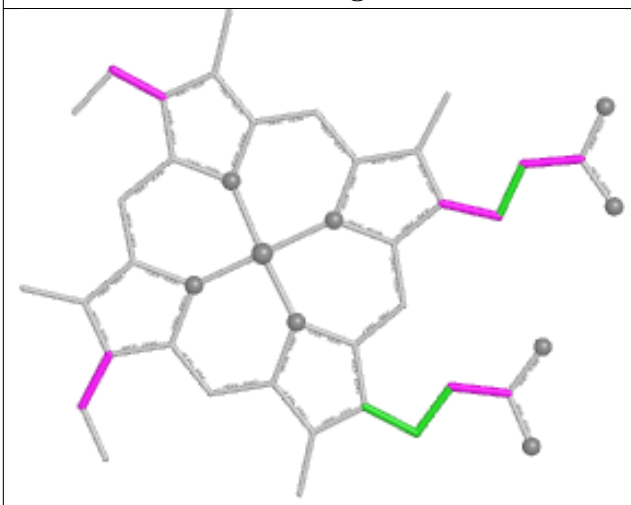
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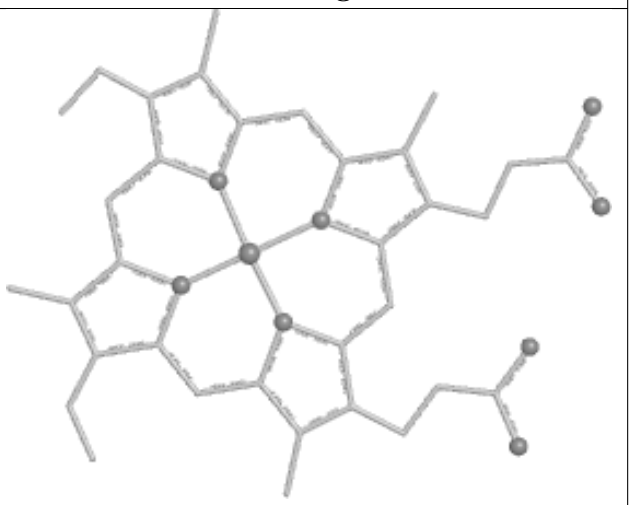
Bond lengths



Bond angles

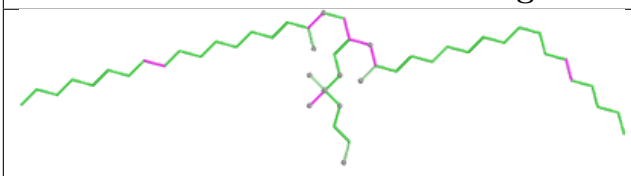


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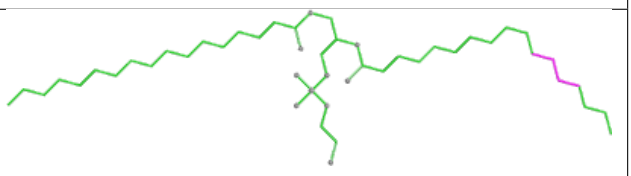


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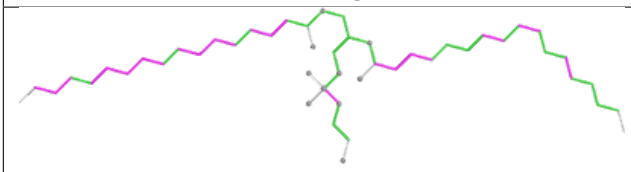
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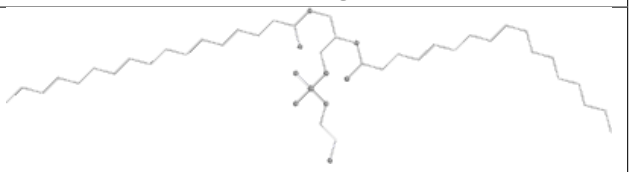
Bond lengths



Bond angles

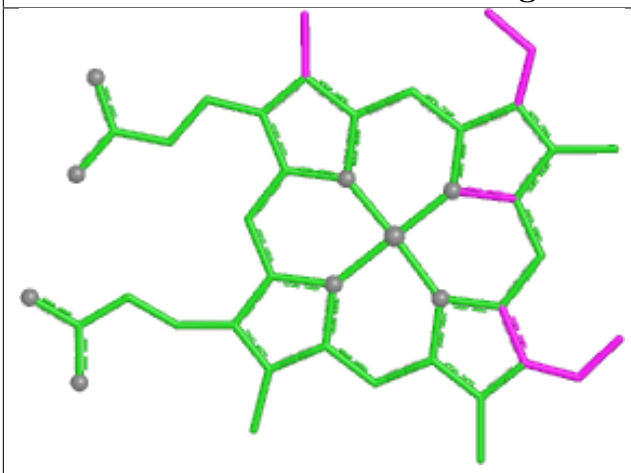


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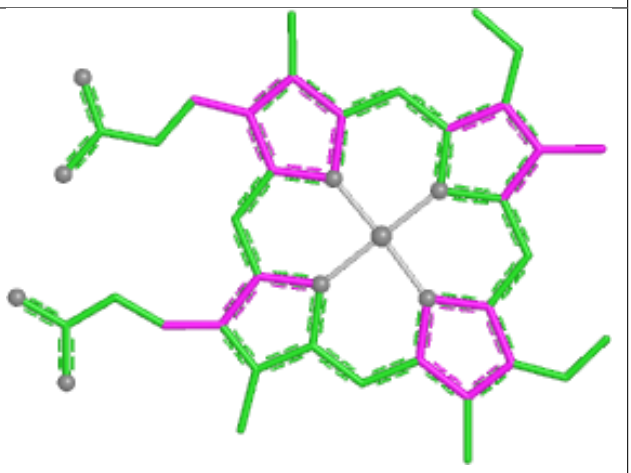


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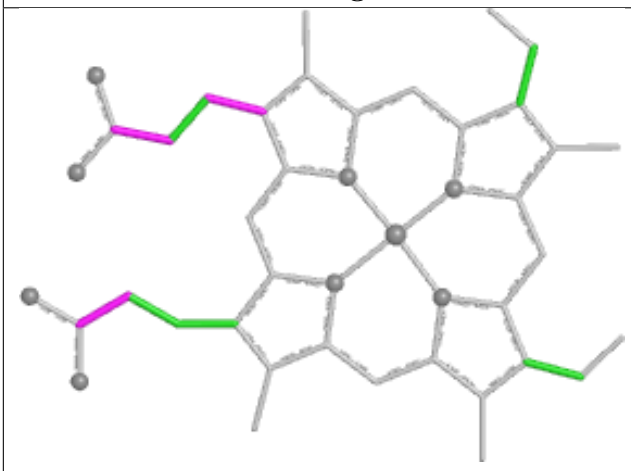
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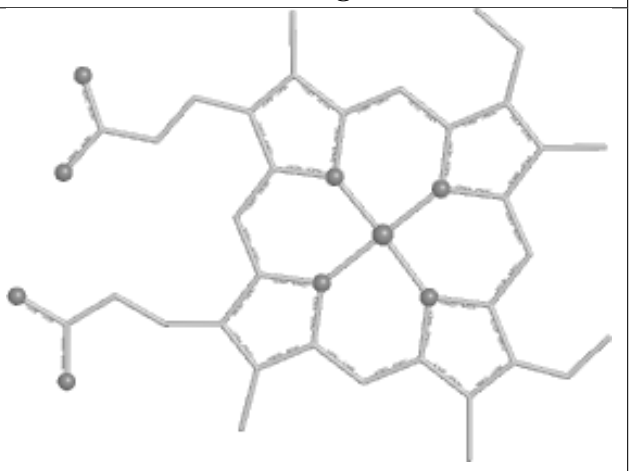
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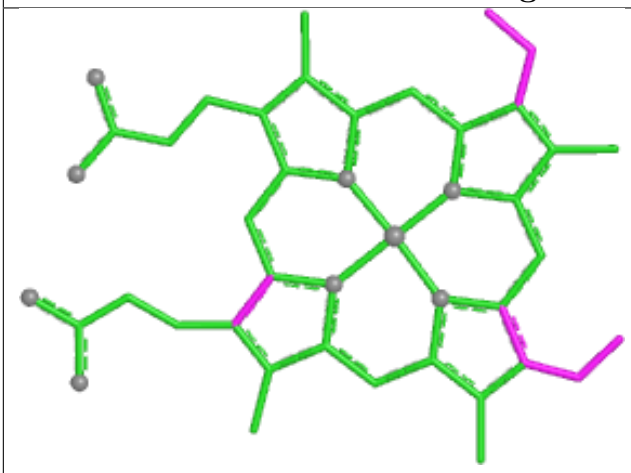


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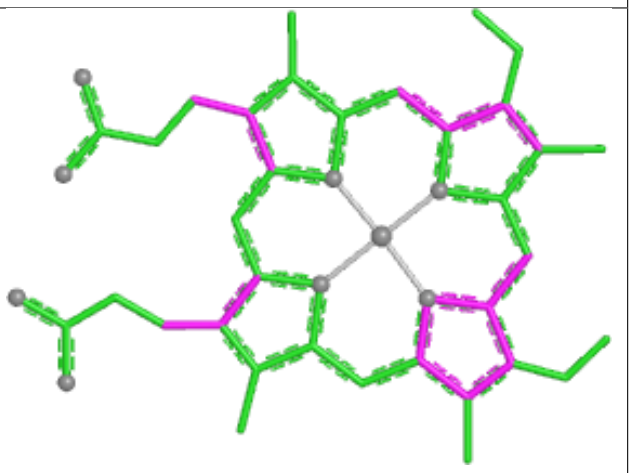


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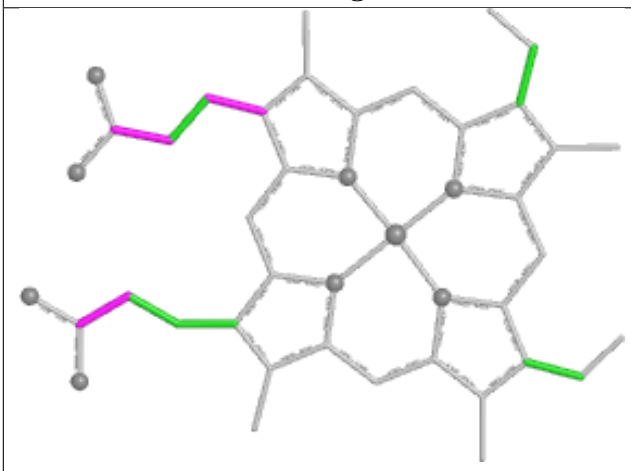
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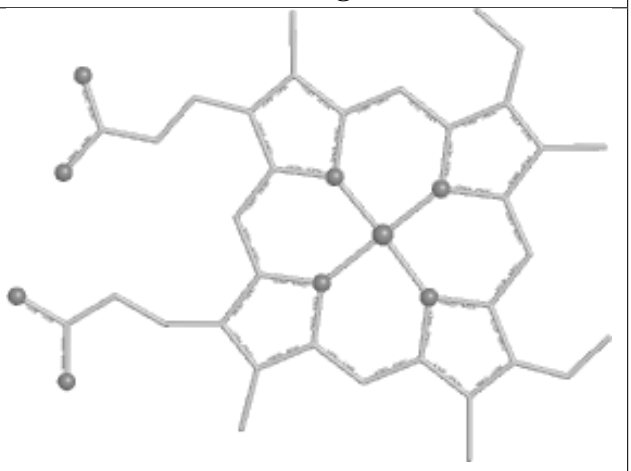
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Bond angles

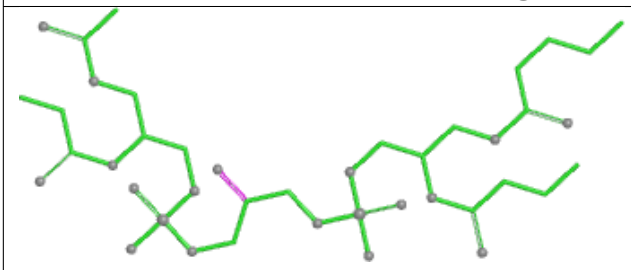


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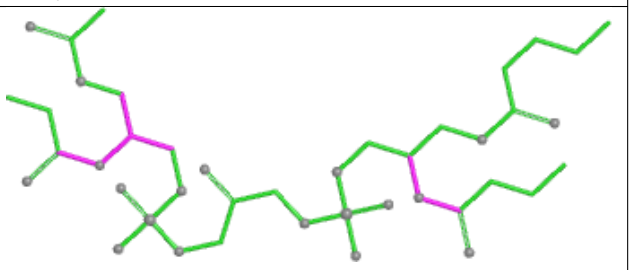


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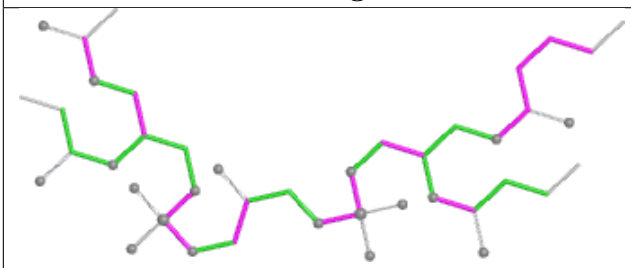
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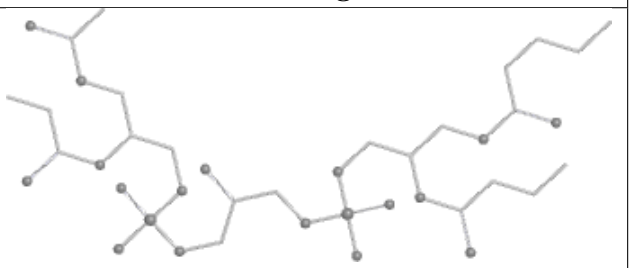
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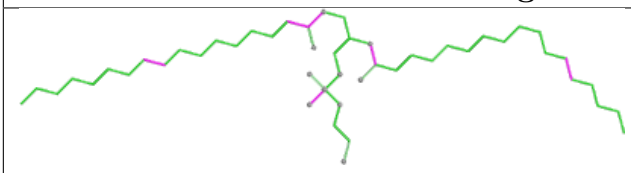


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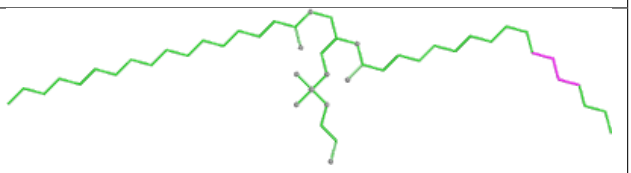


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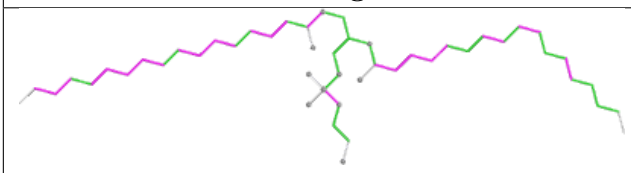
Ligand PEE P 3007



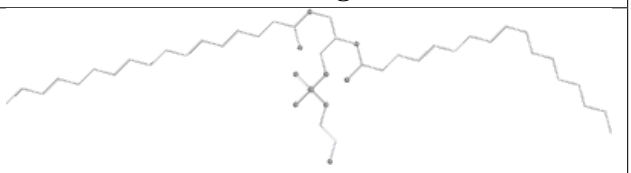
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Bond angles

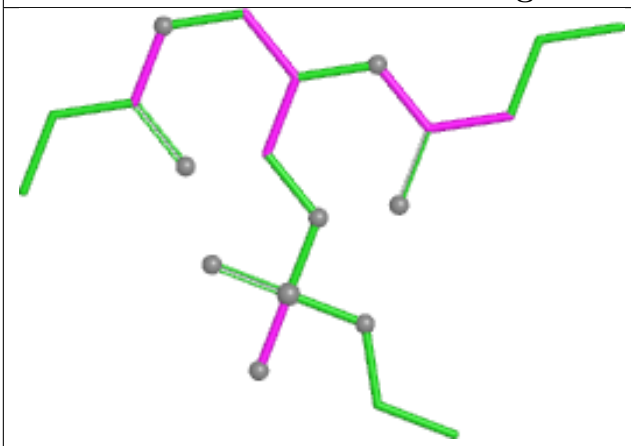


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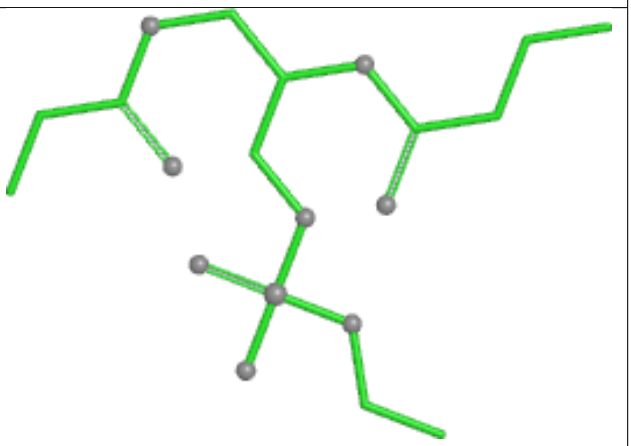


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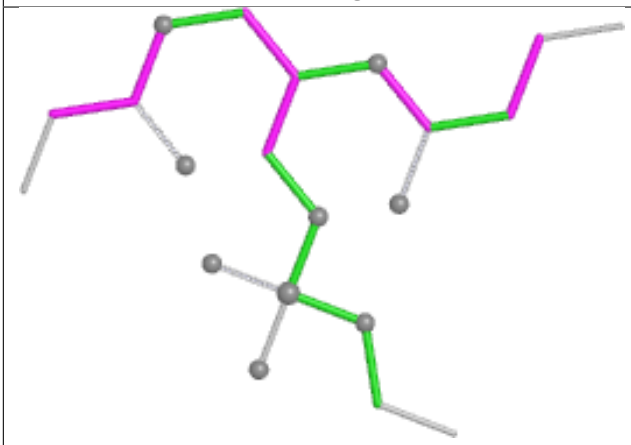
Ligand PEE A 2008



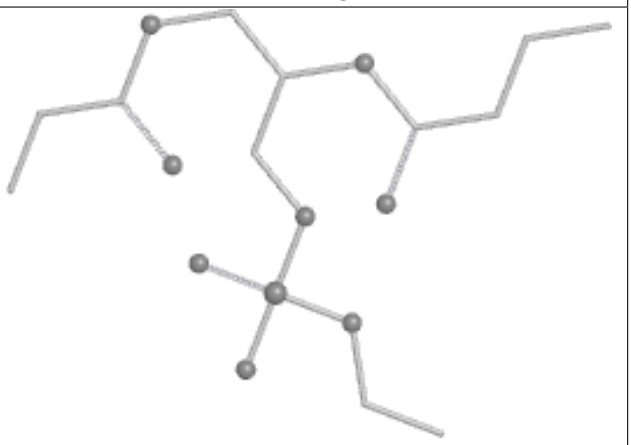
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Bond angles

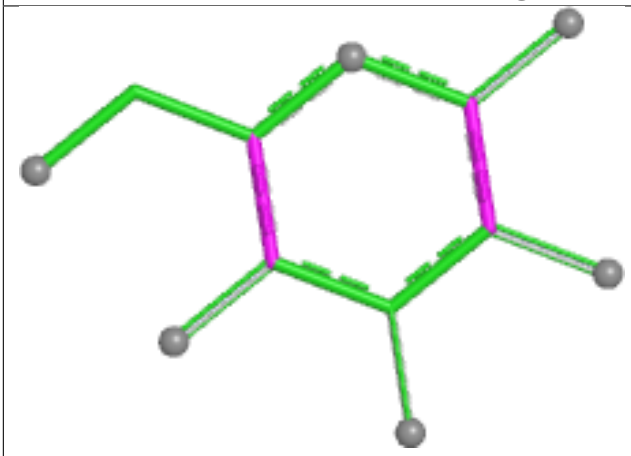


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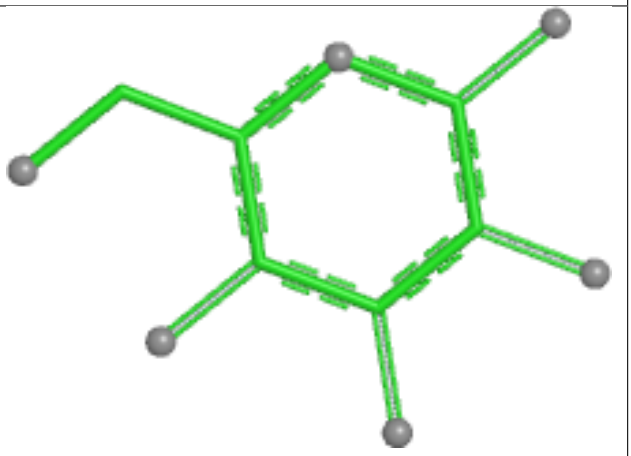


Rings

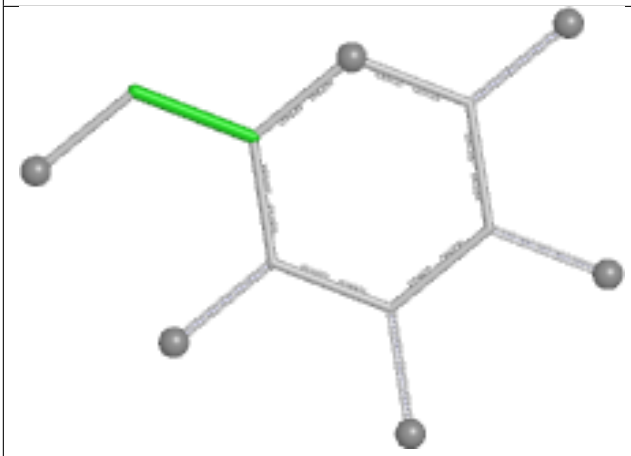
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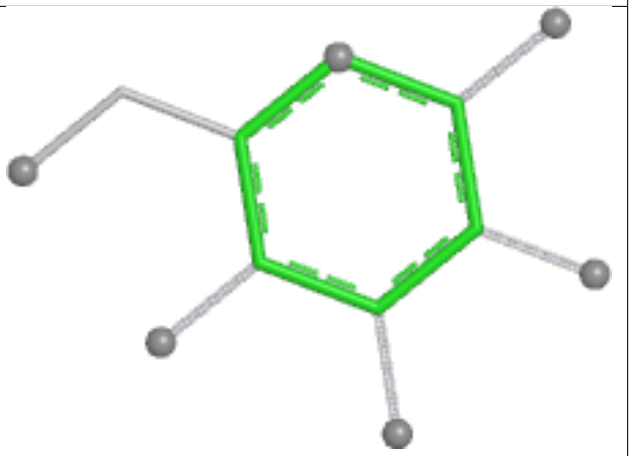
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Bond angles

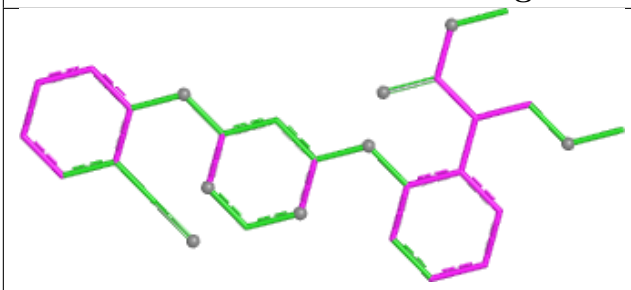


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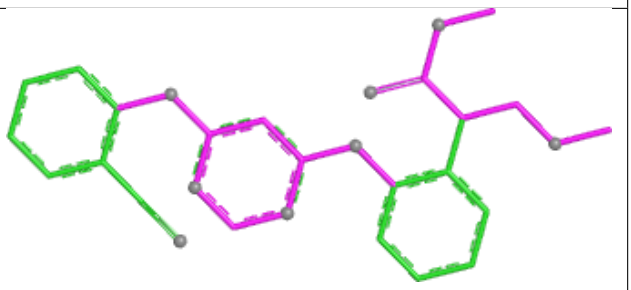


Rings

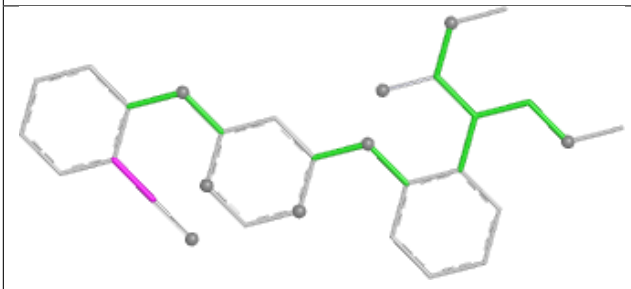
Ligand AZO C 2001



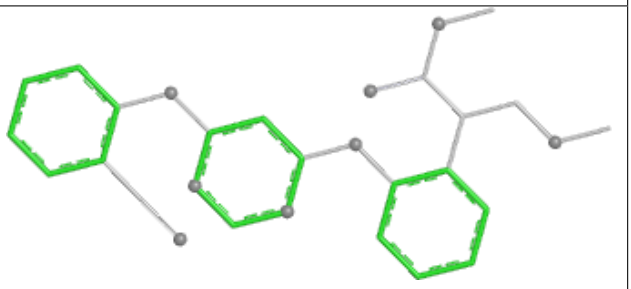
Bond lengths



Bond angles

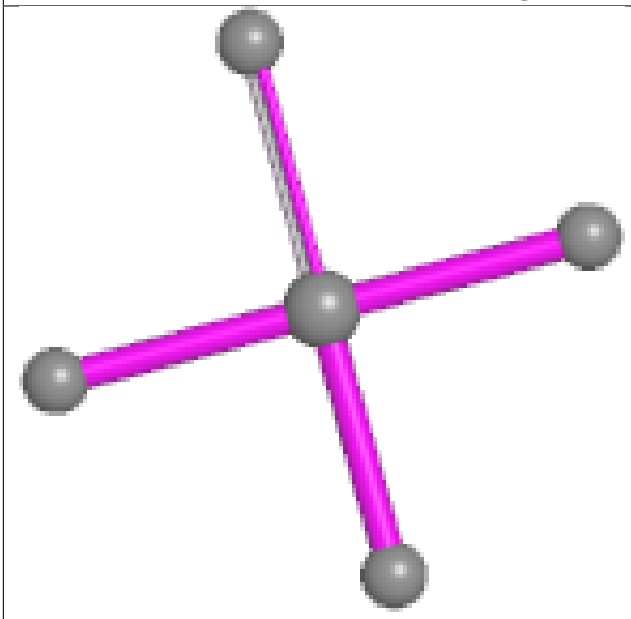


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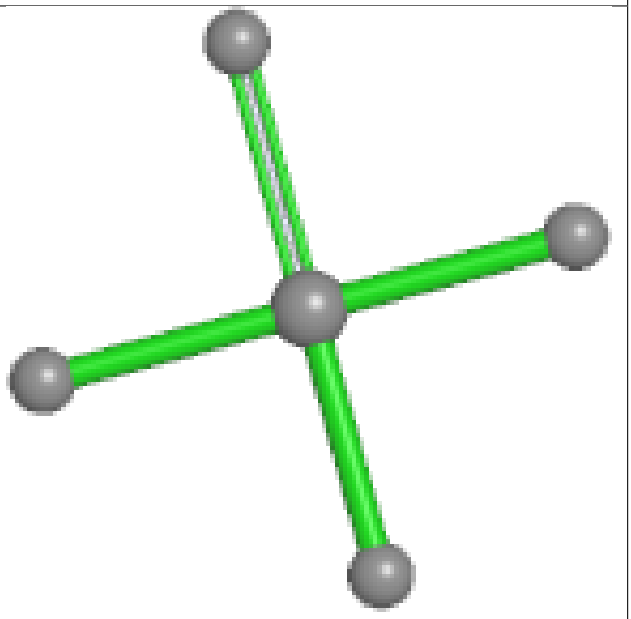


Rings

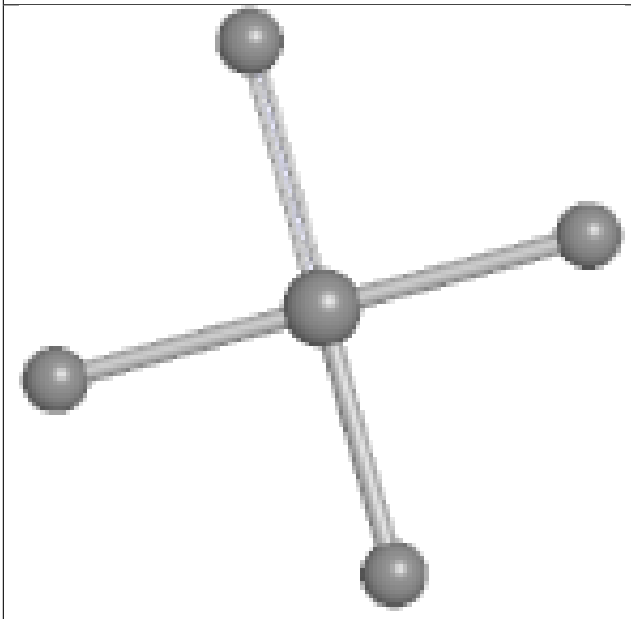
Ligand PEE N 3008



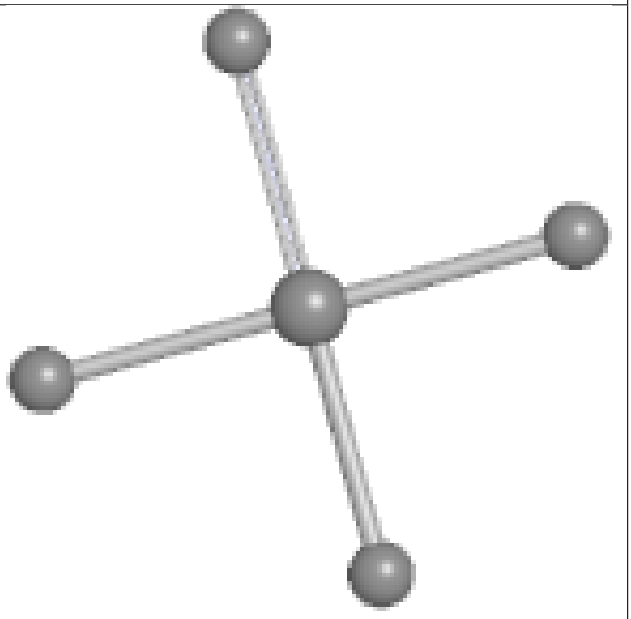
Bond lengths



Bond angles

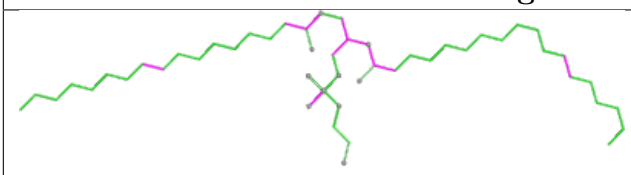


Torsions

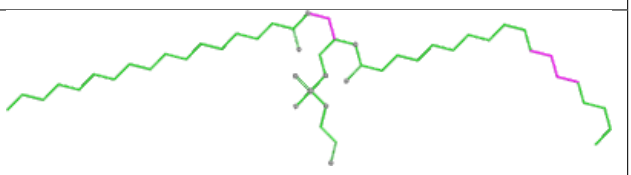


Rings

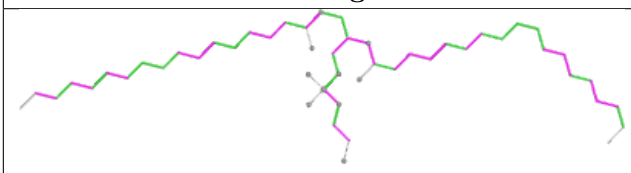
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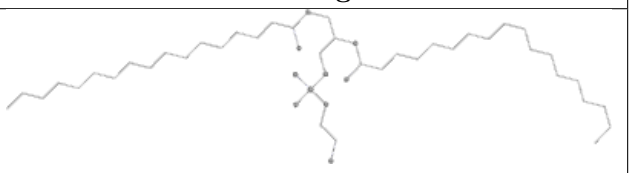
Bond lengths



Bond angles

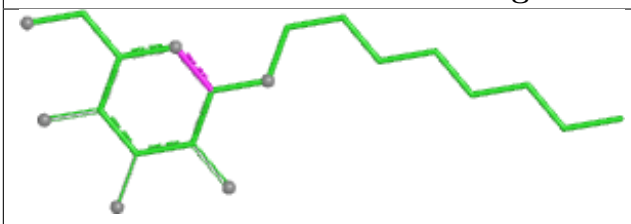


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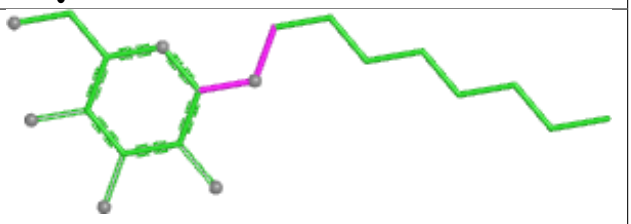


Rings

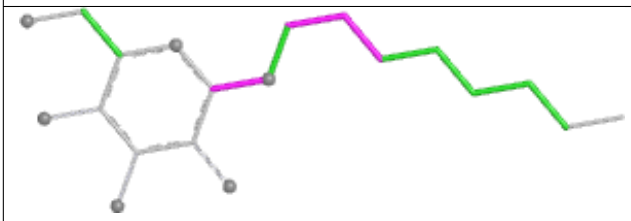
Ligand BOG Q 3009



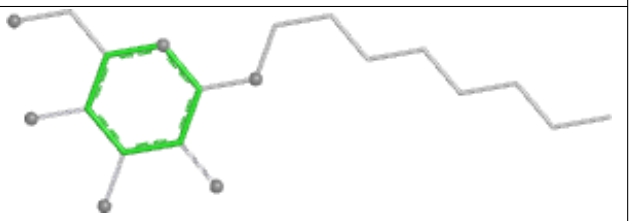
Bond lengths



Bond angles

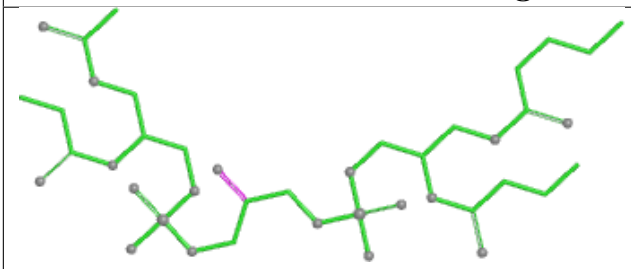


Torsions

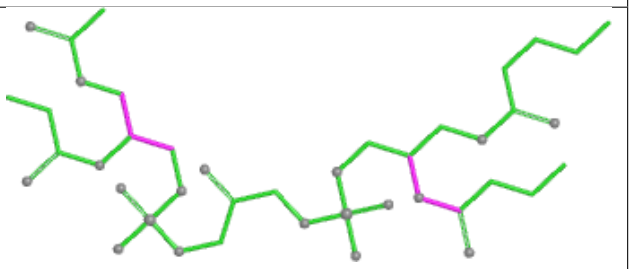


Rings

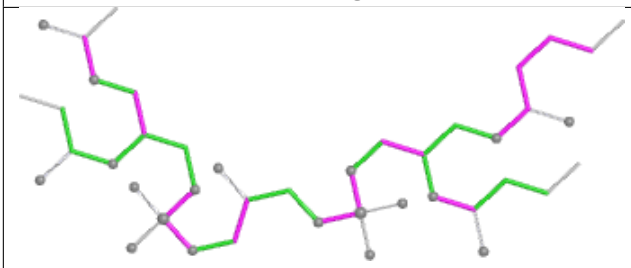
Ligand CDL D 2003



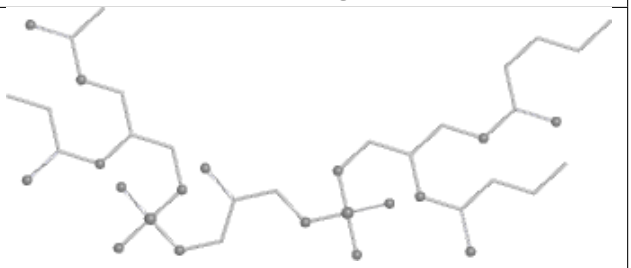
Bond lengths



Bond angles

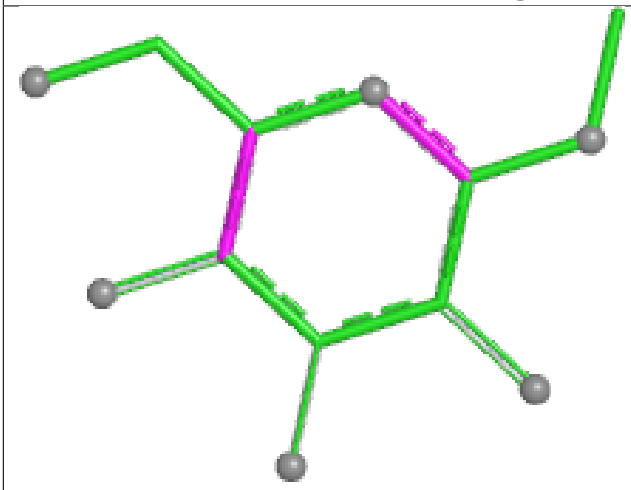


Torsions

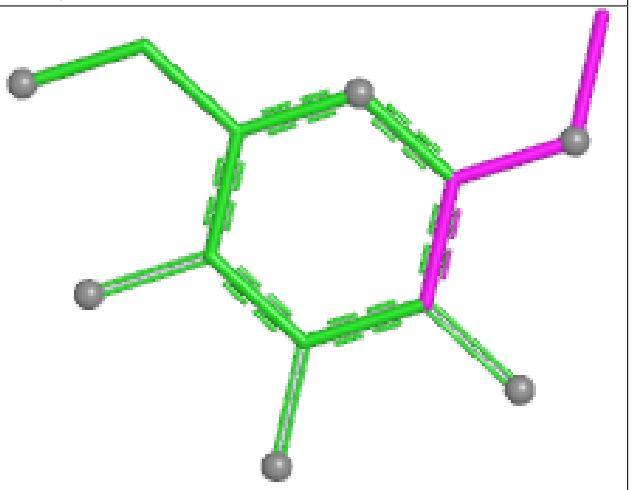


Rings

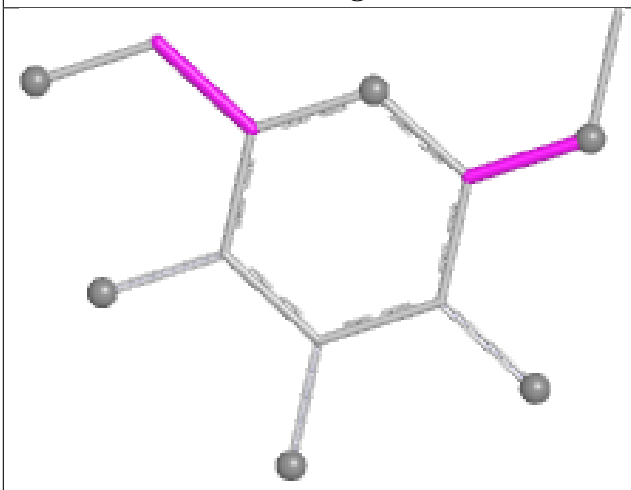
Ligand BOG Q 3091



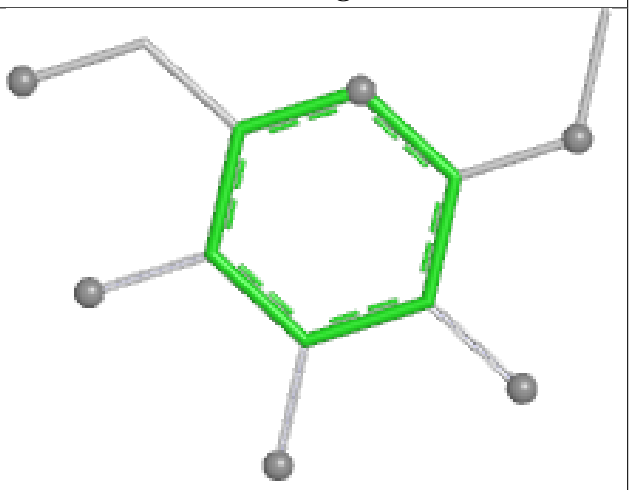
Bond lengths



Bond angles

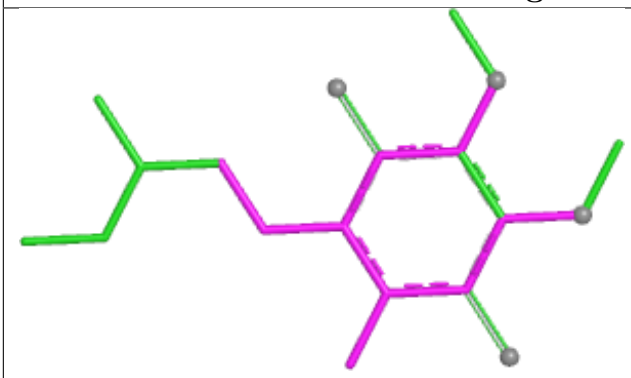


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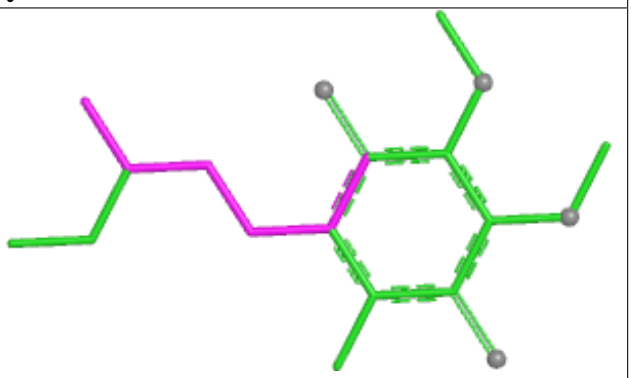


Rings

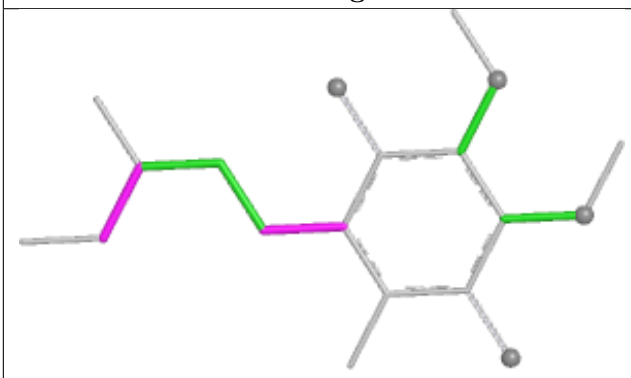
Ligand UQ P 3002



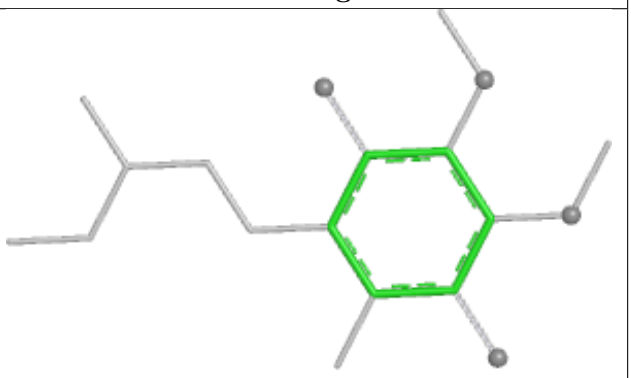
Bond lengths



Bond angles

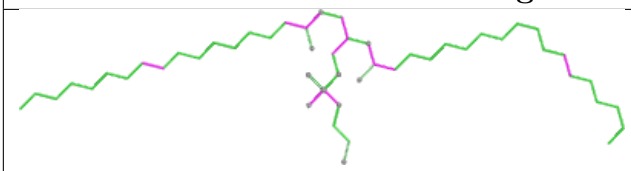


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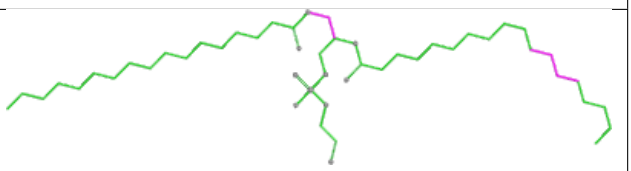


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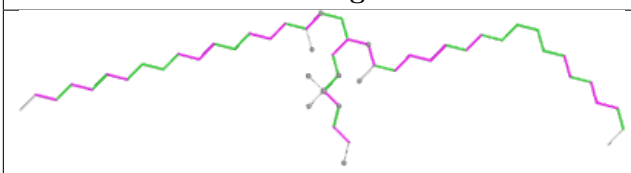
Ligand PEE A 2005



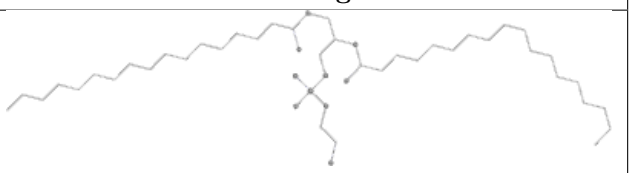
Bond lengths



Bond angles

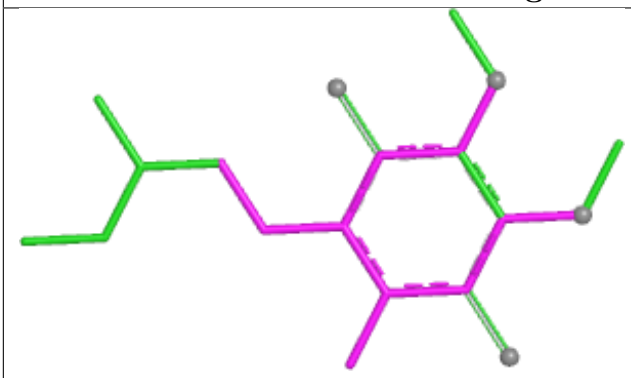


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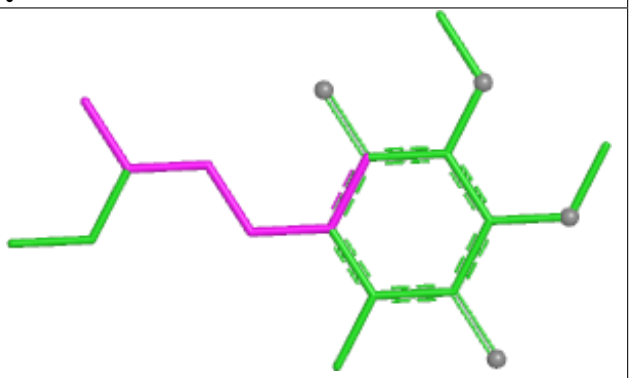


Rings

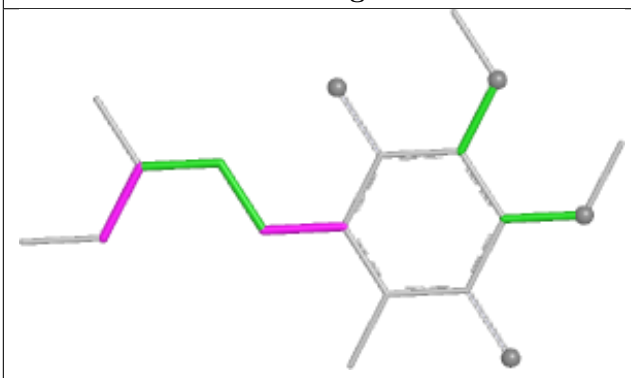
Ligand UQ C 2002



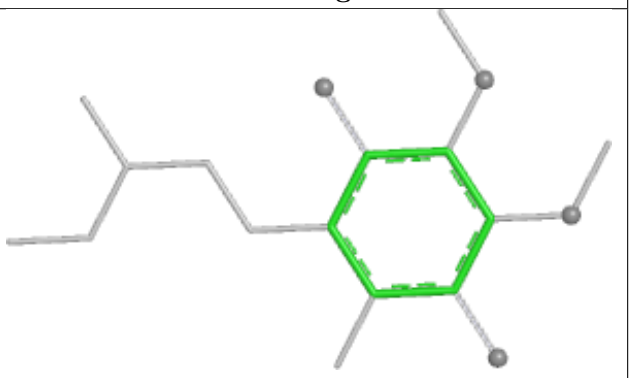
Bond lengths



Bond angles

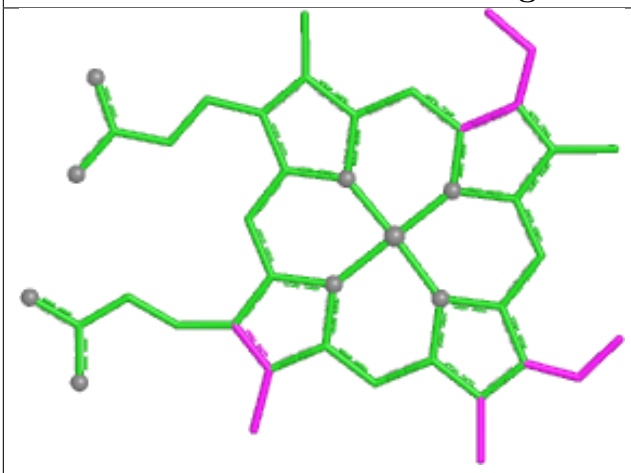


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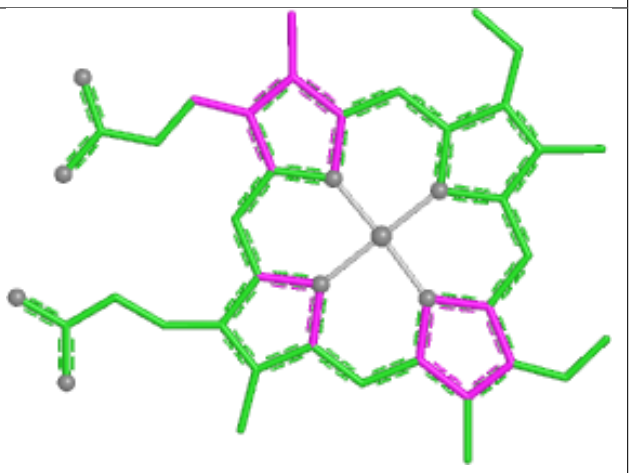


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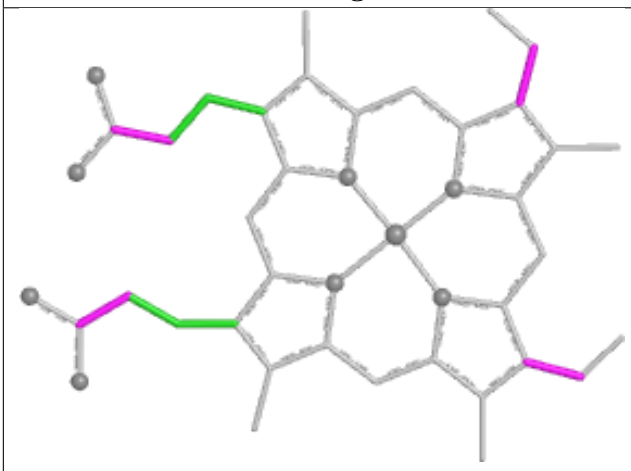
Ligand HEM C 501



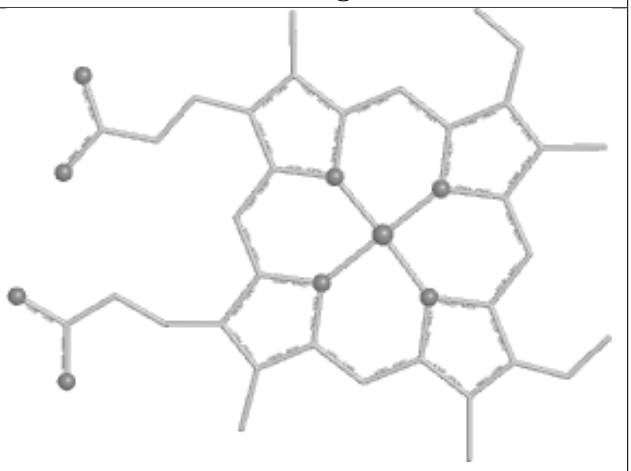
Bond lengths



Bond angles

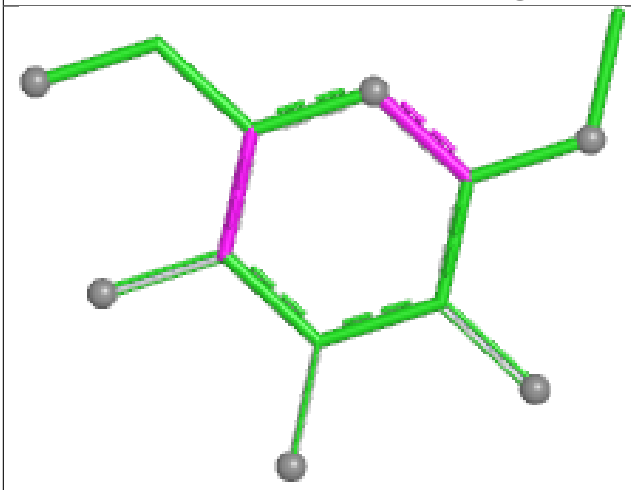


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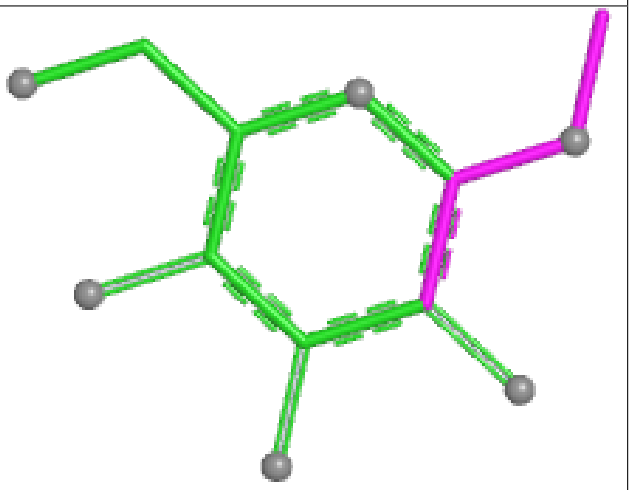


Rings

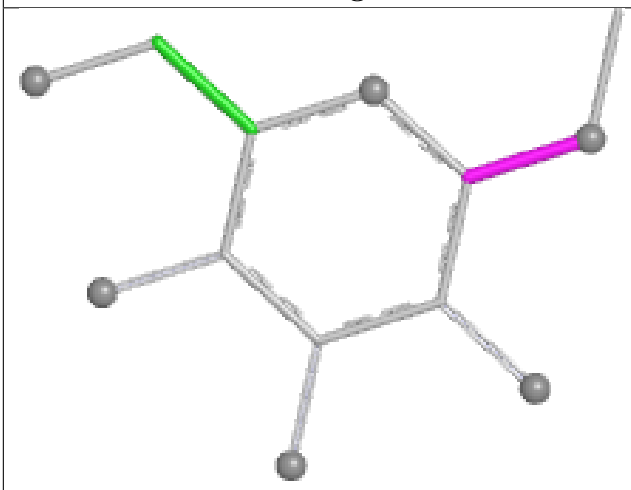
Ligand BOG D 2091



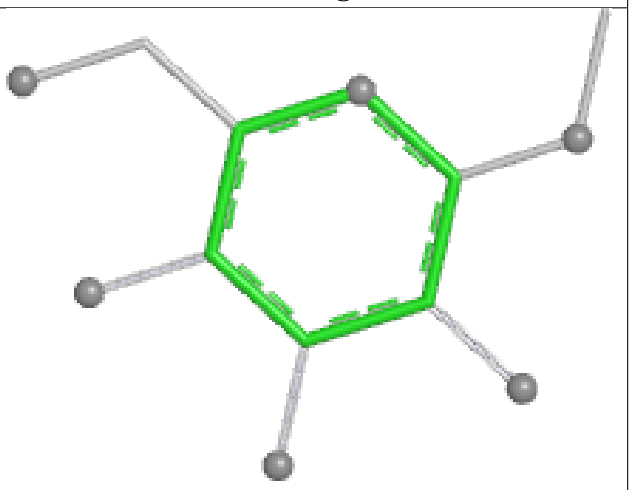
Bond lengths



Bond angles

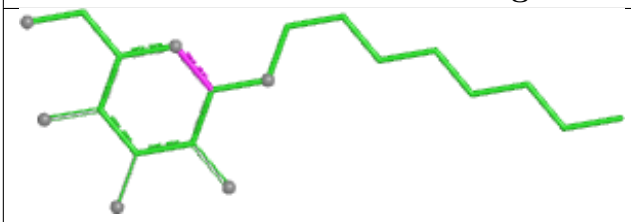


Torsions

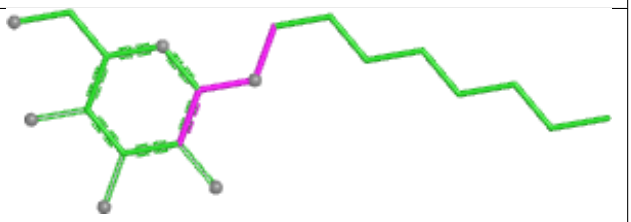


Rings

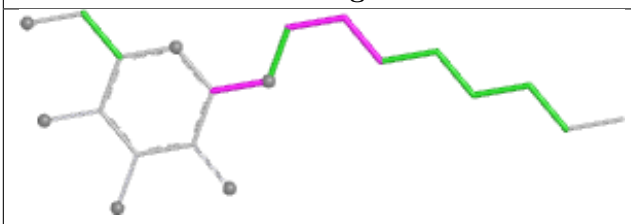
Ligand BOG D 2009



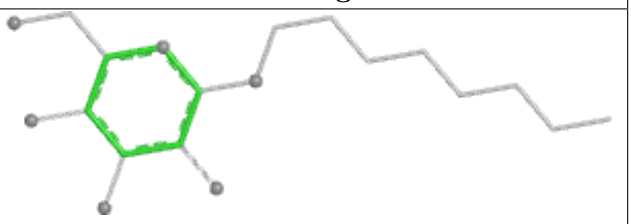
Bond lengths



Bond angles

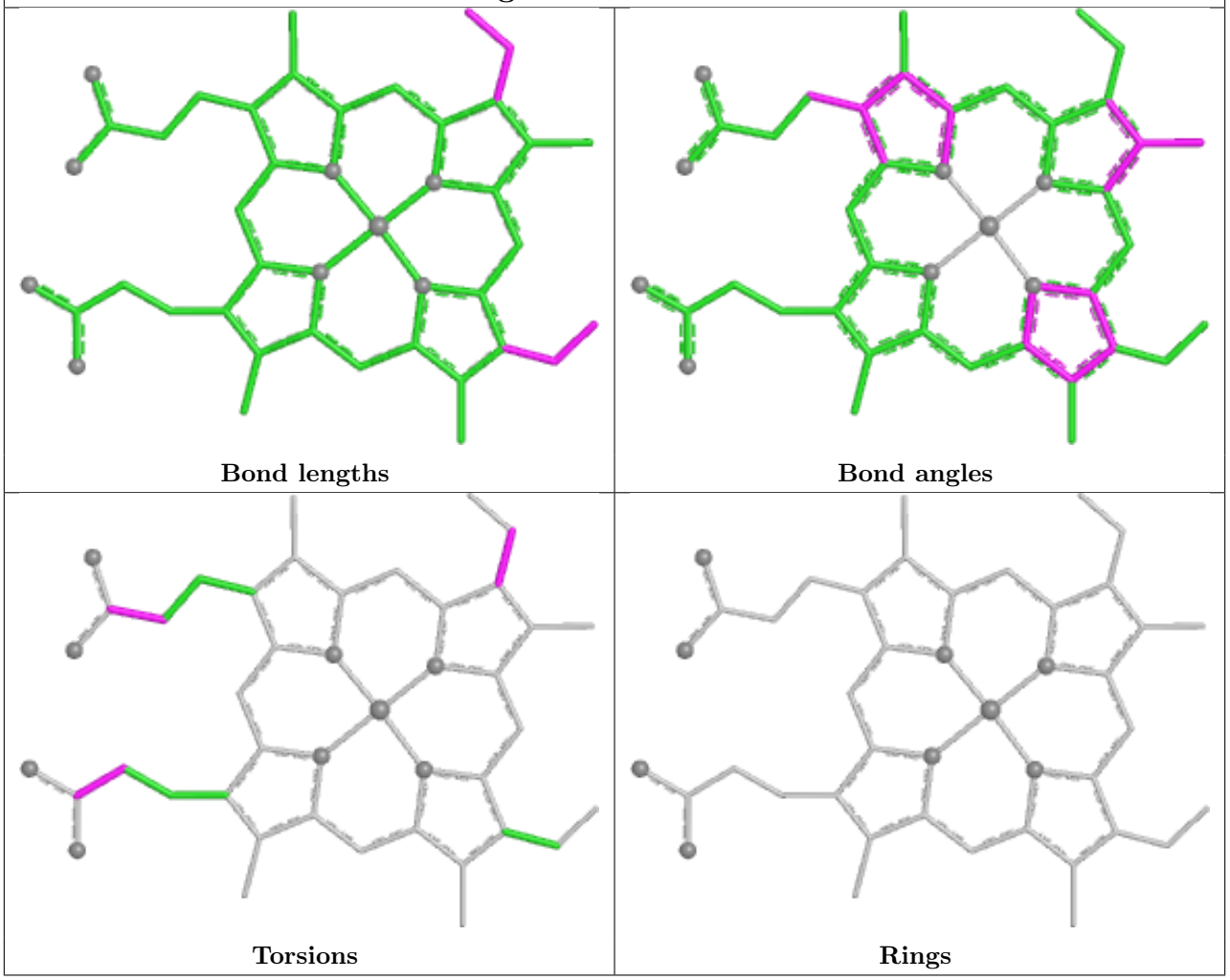


Torsions



Rings

Ligand HEM P 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	444/446 (99%)	0.22	12 (2%) 56 47	41, 68, 96, 110	0
1	N	442/446 (99%)	0.55	19 (4%) 40 31	48, 80, 103, 110	0
2	B	420/441 (95%)	0.66	16 (3%) 44 35	57, 87, 120, 142	0
2	O	422/441 (95%)	0.63	24 (5%) 29 22	49, 85, 113, 129	0
3	C	380/380 (100%)	-0.23	12 (3%) 50 40	30, 48, 88, 132	0
3	P	379/380 (99%)	0.12	7 (1%) 67 60	33, 63, 94, 132	0
4	D	241/241 (100%)	-0.27	1 (0%) 88 87	36, 51, 88, 109	0
4	Q	241/241 (100%)	0.33	3 (1%) 76 71	56, 76, 106, 127	0
5	E	196/196 (100%)	1.39	75 (38%) 1 0	41, 131, 160, 168	0
5	R	196/196 (100%)	0.89	24 (12%) 8 6	51, 95, 141, 153	0
6	F	101/110 (91%)	-0.31	0 100 100	38, 52, 70, 104	0
6	S	101/110 (91%)	0.37	3 (2%) 52 43	60, 74, 107, 131	0
7	G	80/81 (98%)	0.22	4 (5%) 34 27	42, 61, 106, 117	0
7	T	79/81 (97%)	0.68	5 (6%) 26 20	56, 85, 150, 159	0
8	H	70/77 (90%)	0.35	1 (1%) 73 67	45, 68, 91, 128	0
8	U	67/77 (87%)	1.22	9 (13%) 7 4	90, 117, 137, 141	0
9	I	31/47 (65%)	2.35	16 (51%) 0 0	80, 115, 142, 143	0
9	V	31/47 (65%)	2.65	18 (58%) 0 0	78, 115, 140, 145	0
10	J	61/61 (100%)	0.00	0 100 100	52, 65, 103, 147	0
10	W	60/61 (98%)	0.18	2 (3%) 49 39	63, 79, 109, 119	0
All	All	4042/4160 (97%)	0.41	251 (6%) 26 20	30, 73, 129, 168	0

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	7.9
9	V	56	SER	7.6
5	E	106	ILE	6.2
5	E	147	ILE	6.0
9	V	59	SER	5.9

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	BOG	Q	3091	13/20	0.36	0.34	192,194,195,195	0
11	PEE	A	2008	21/51	0.46	0.30	132,136,139,140	0
18	BOG	P	2010	12/20	0.61	0.29	140,143,144,145	0
18	BOG	D	2091	13/20	0.70	0.35	207,208,208,208	0
11	PEE	N	3008	5/51	0.72	0.14	110,111,112,112	0
17	CDL	Q	3003	42/100	0.82	0.24	117,129,145,145	0
17	CDL	T	3004	40/100	0.83	0.18	97,104,113,114	0
14	UQ	P	3002	19/63	0.83	0.37	126,136,137,137	0
11	PEE	P	3005	50/51	0.84	0.28	92,105,114,115	0
17	CDL	D	2003	42/100	0.85	0.20	92,101,111,114	0
14	UQ	C	2002	19/63	0.86	0.27	91,92,94,95	0
11	PEE	A	2005	50/51	0.88	0.23	79,96,106,107	0
15	GOL	C	2011	6/6	0.88	0.27	80,84,85,86	0
17	CDL	G	2004	40/100	0.89	0.15	73,85,100,101	0
15	GOL	P	3011	6/6	0.90	0.22	84,86,87,88	0
18	BOG	Q	3009	20/20	0.90	0.17	74,89,91,93	0
11	PEE	P	3007	49/51	0.90	0.20	74,88,100,101	0
19	FES	E	501	4/4	0.90	0.10	153,153,154,154	0
18	BOG	D	2009	20/20	0.93	0.11	60,72,75,76	0

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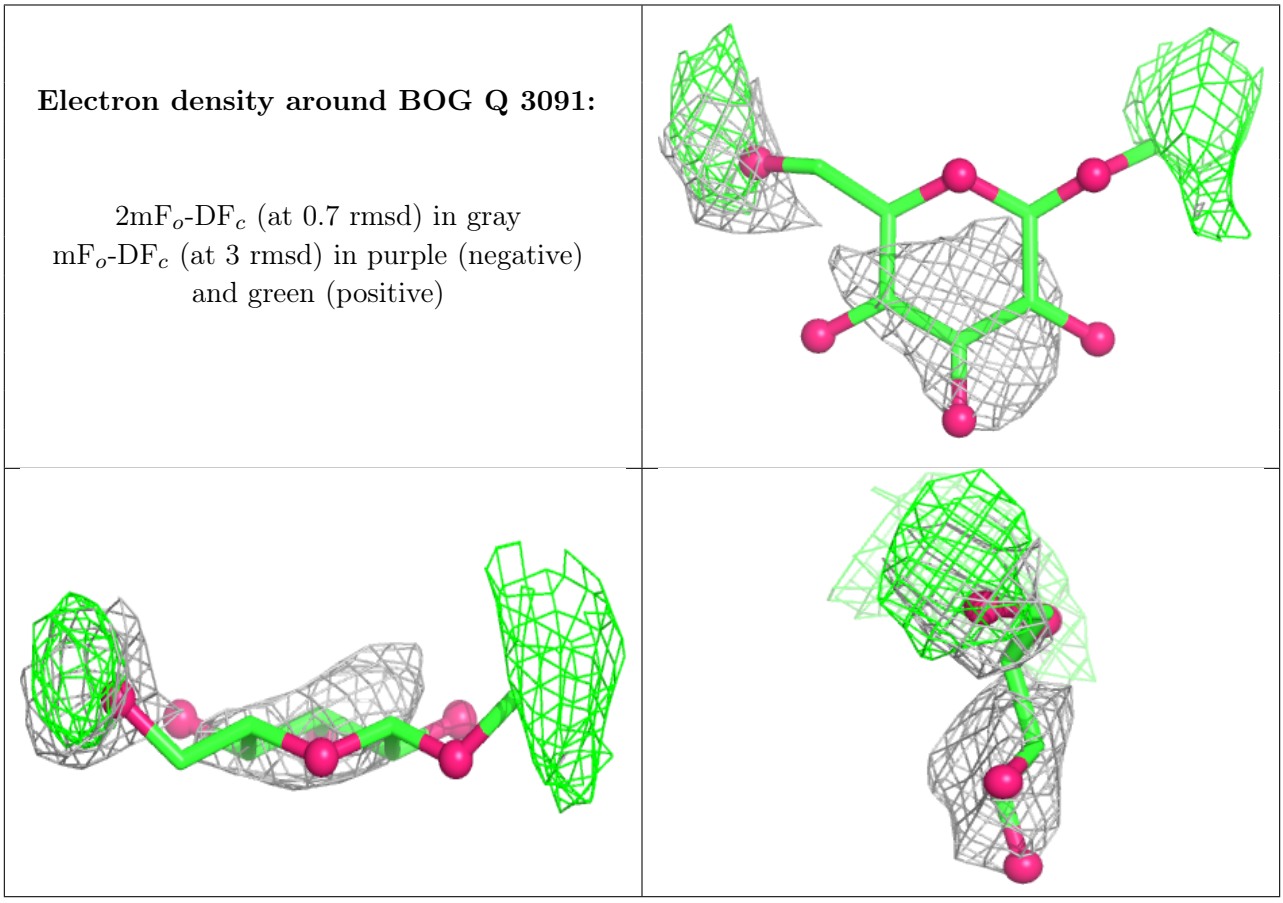
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	AZO	P	3001	30/30	0.93	0.13	52,60,66,67	0
11	PEE	C	2007	49/51	0.94	0.15	46,67,84,85	0
13	AZO	C	2001	30/30	0.95	0.09	36,39,41,41	0
16	HEC	Q	501	43/43	0.97	0.10	60,65,71,72	0
16	HEC	D	501	43/43	0.98	0.07	31,37,45,48	0
12	HEM	P	501	43/43	0.98	0.09	42,49,60,64	0
12	HEM	P	502	43/43	0.98	0.08	38,47,58,60	0
19	FES	R	501	4/4	0.98	0.04	88,89,90,91	0
12	HEM	C	502	43/43	0.99	0.08	32,37,47,54	0
12	HEM	C	501	43/43	0.99	0.08	35,40,50,55	0

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

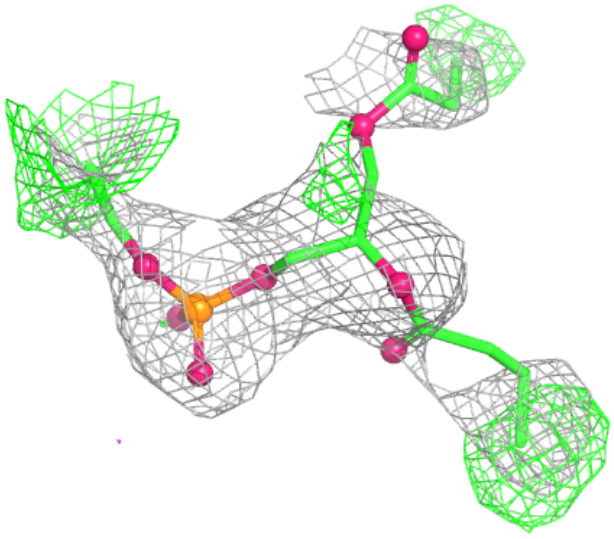
Electron density around BOG Q 3091:

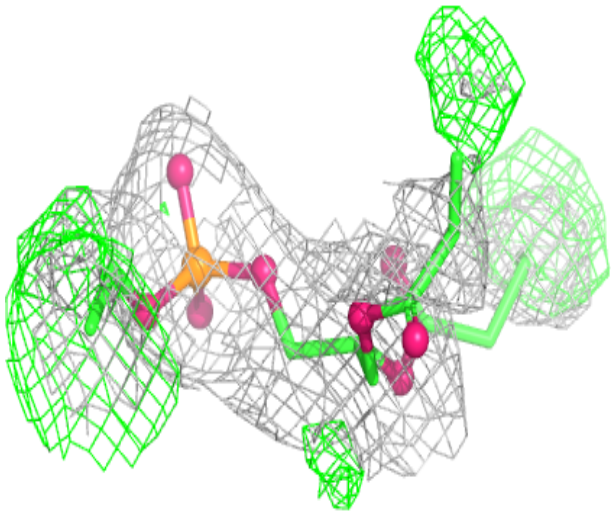
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

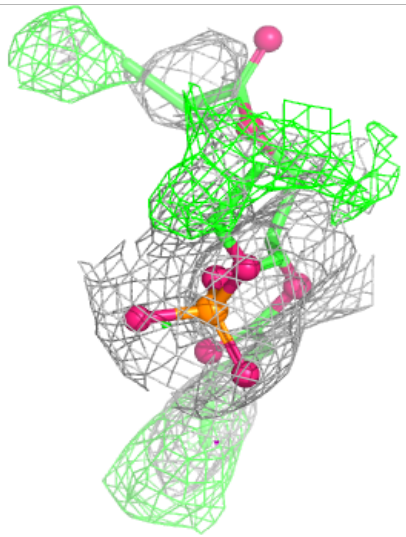


Electron density around PEE A 2008:

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

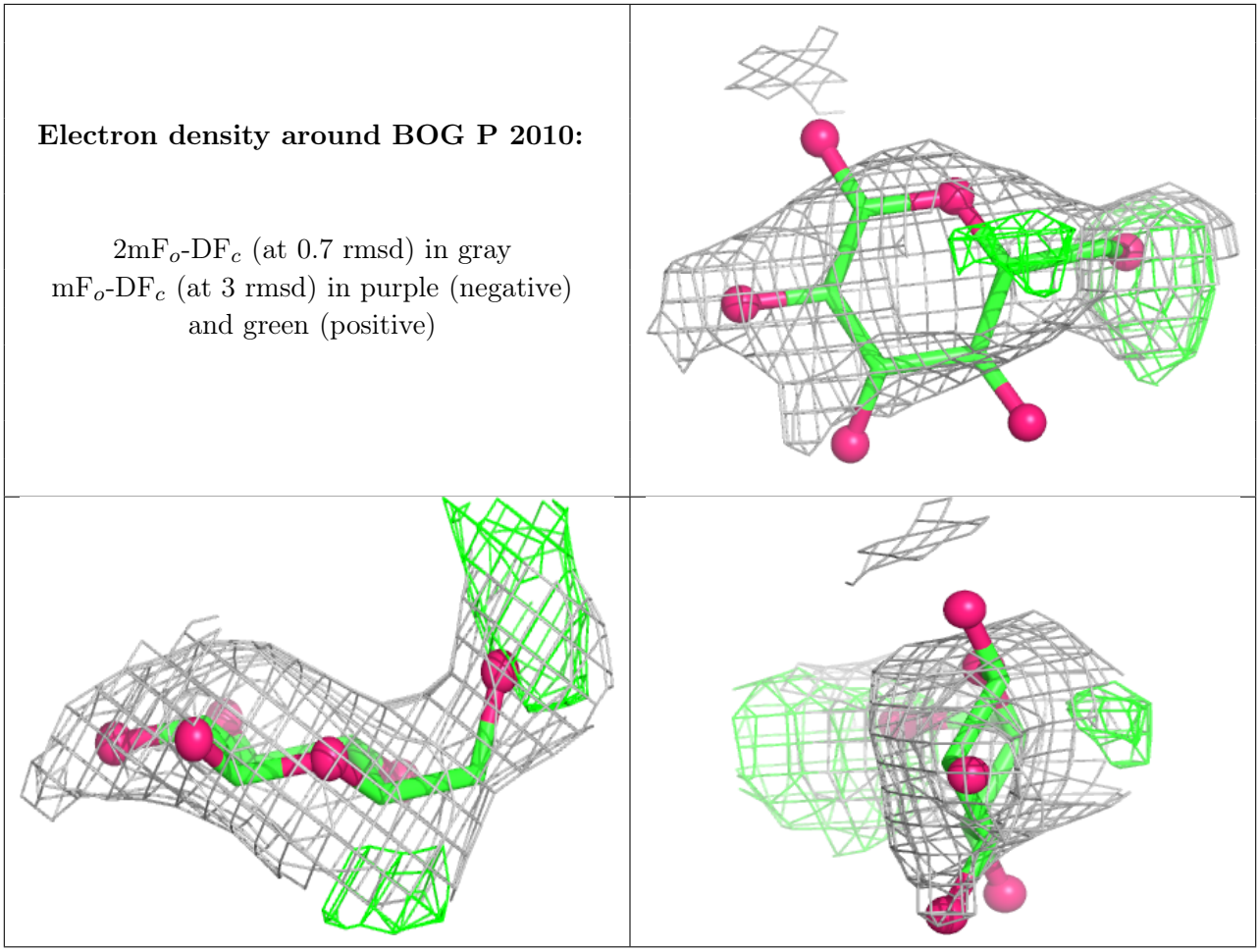






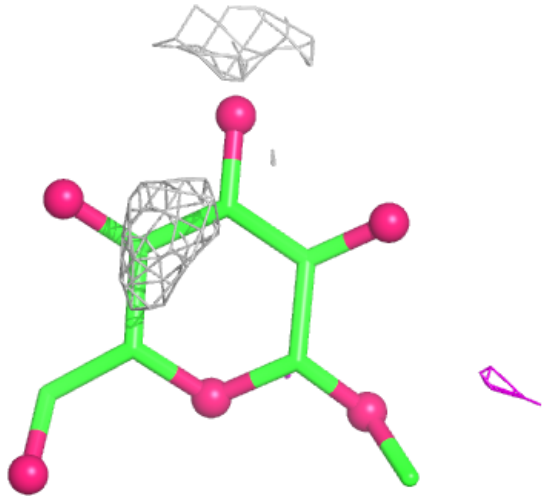
Electron density around BOG P 2010:

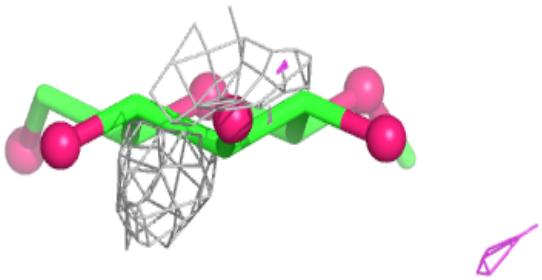
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

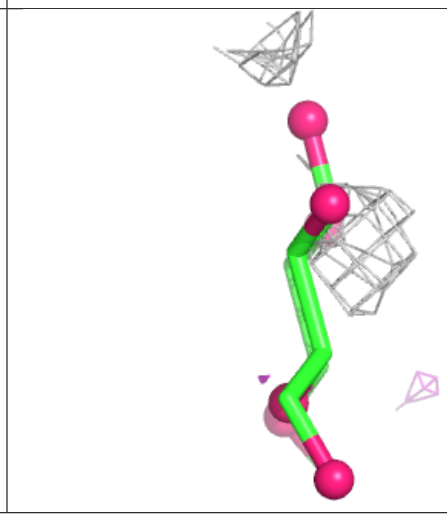


Electron density around BOG D 2091:

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

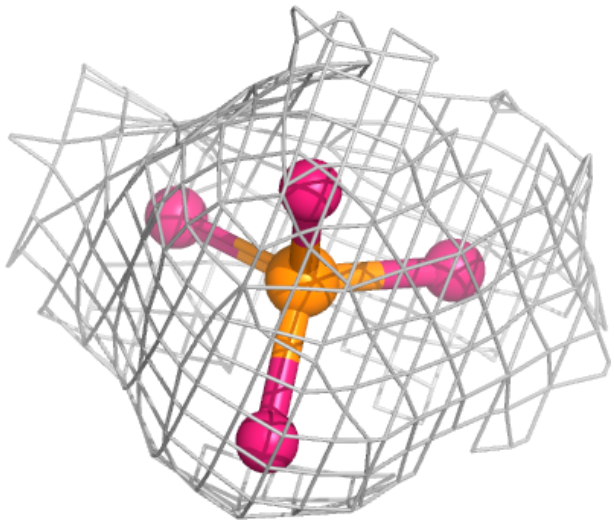


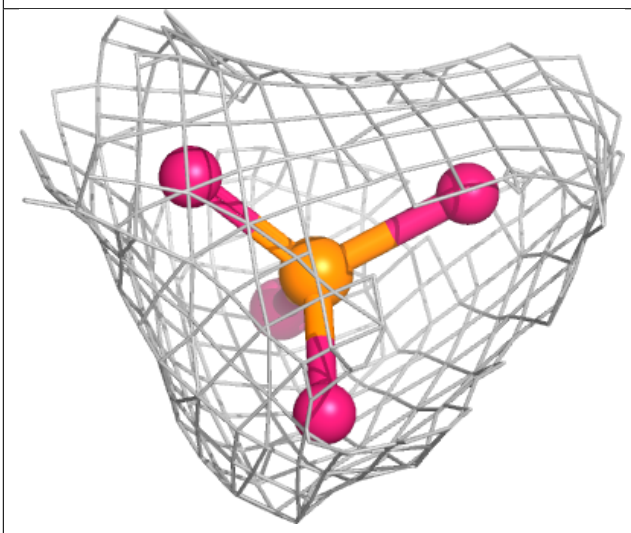


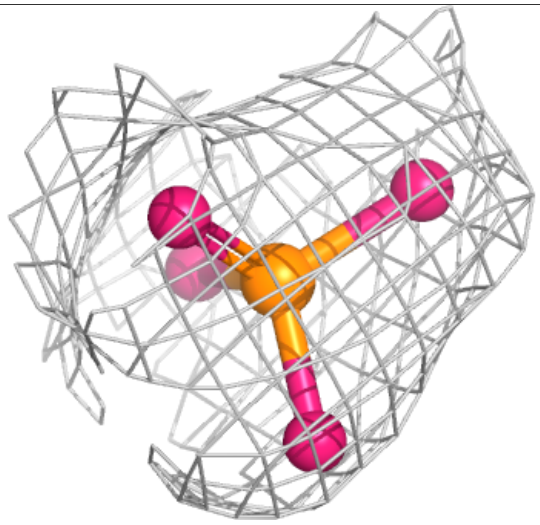


Electron density around PEE N 3008:

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

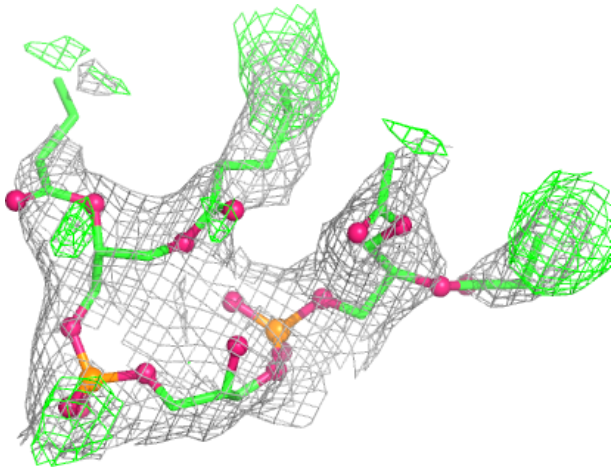


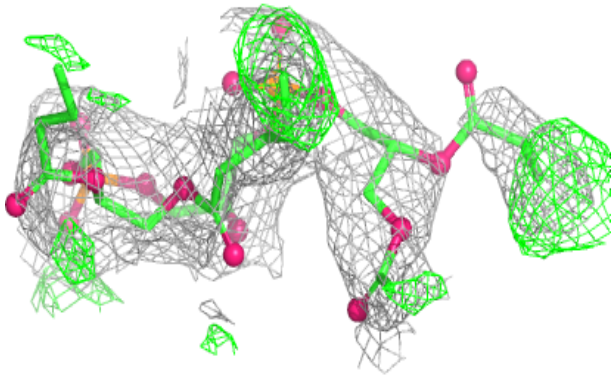




Electron density around CDL Q 3003:

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

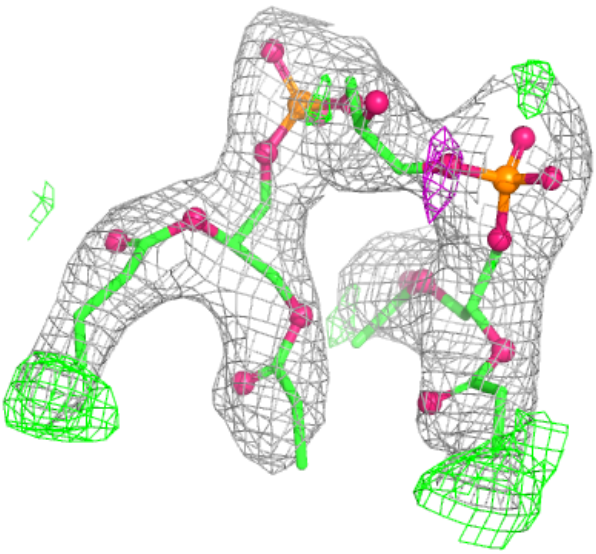


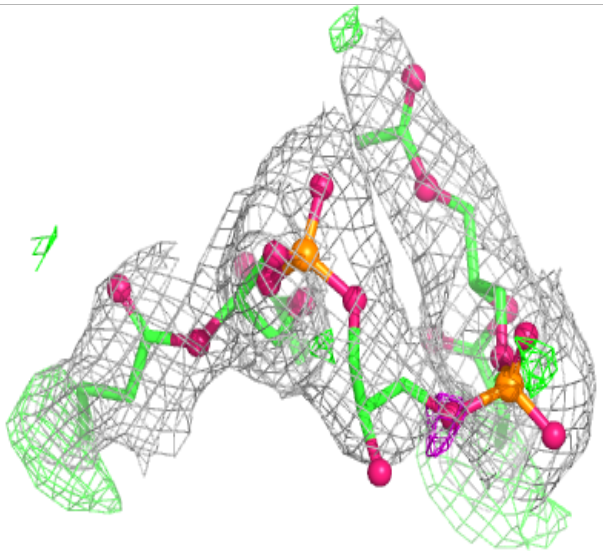


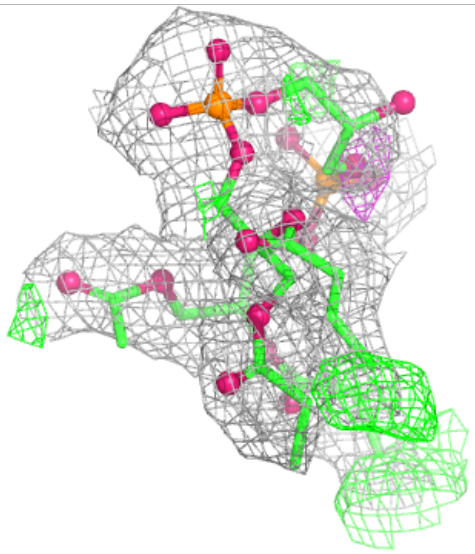


Electron density around CDL T 3004:

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

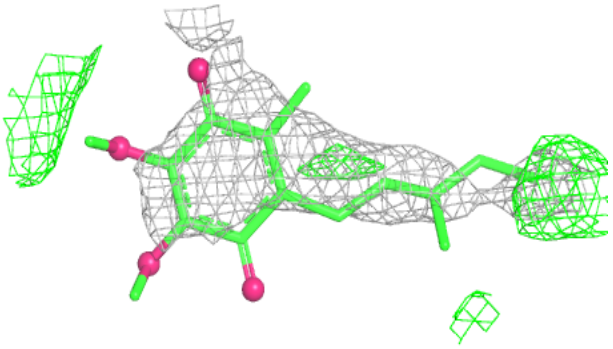


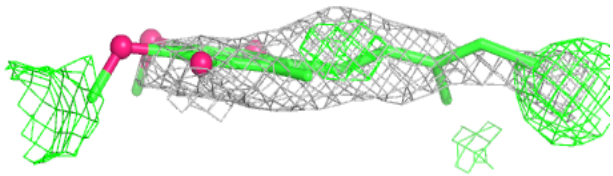


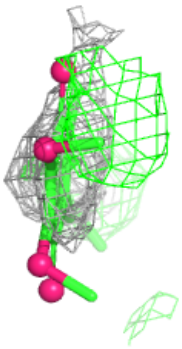


Electron density around UQ P 3002:

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

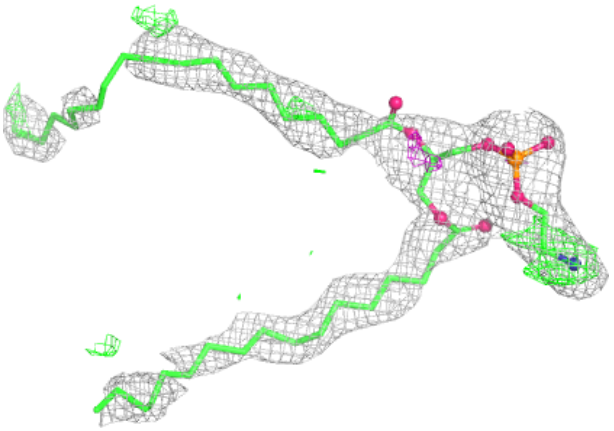


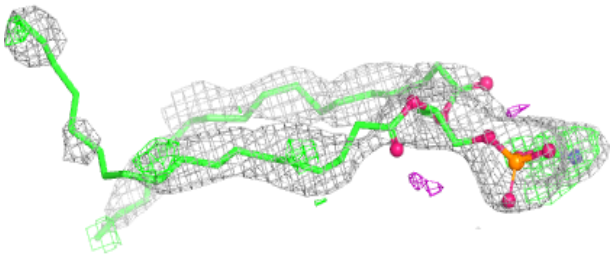




Electron density around PEE P 3005:

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

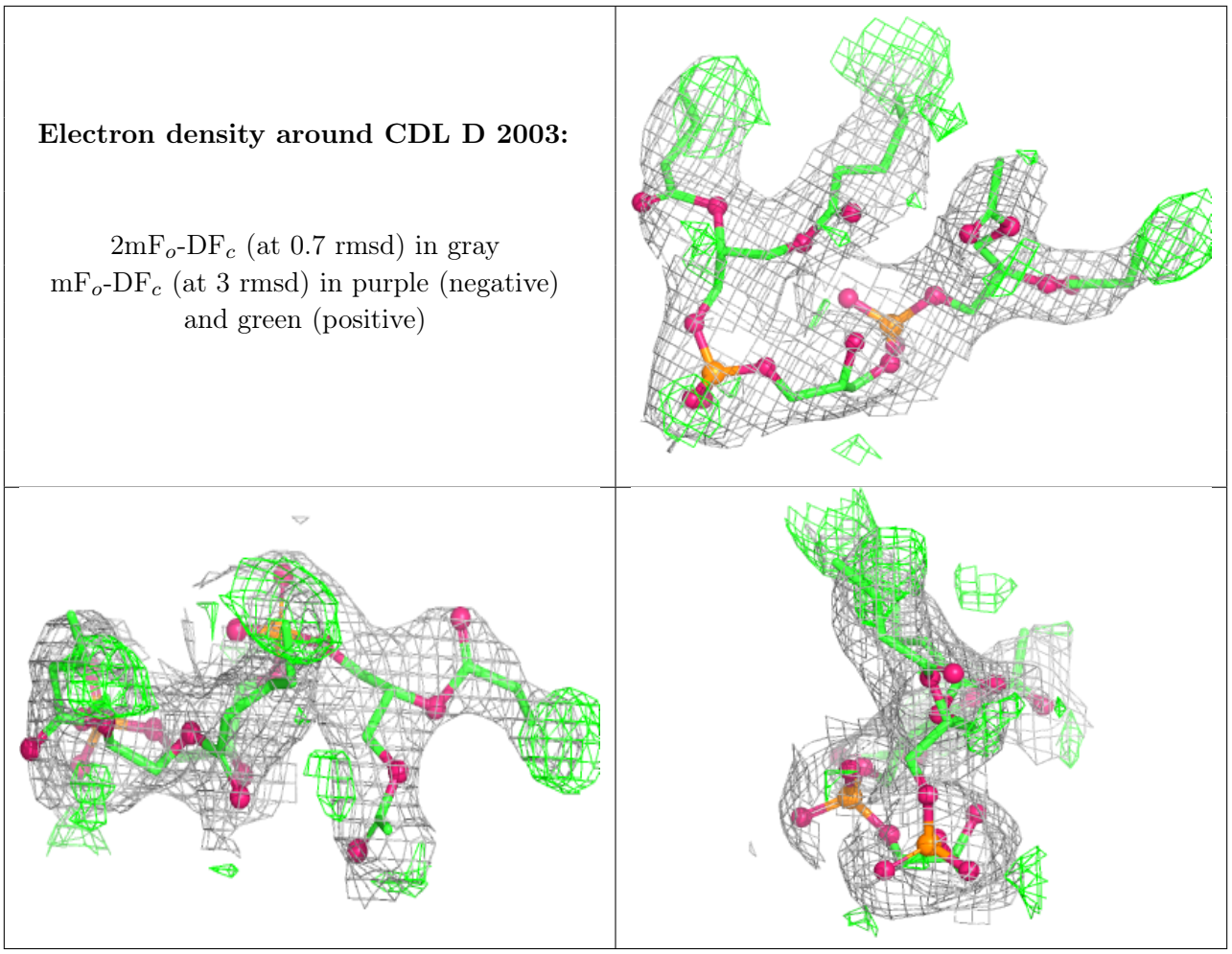






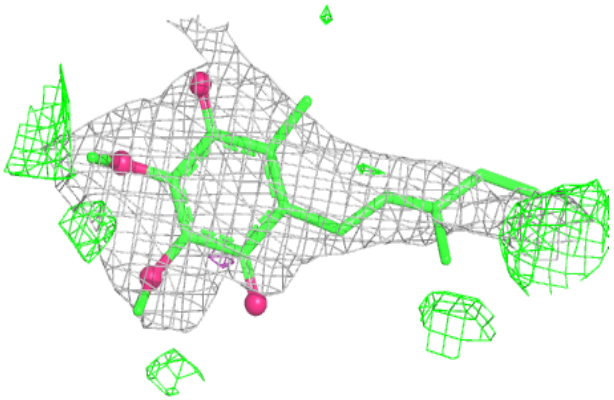
Electron density around CDL D 2003:

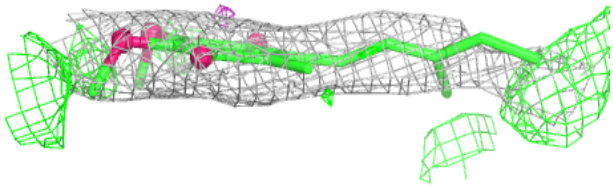
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

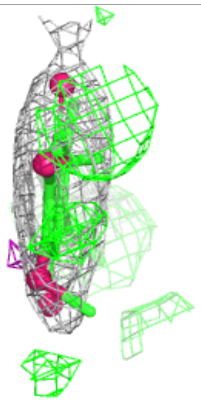


Electron density around UQ C 2002:

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

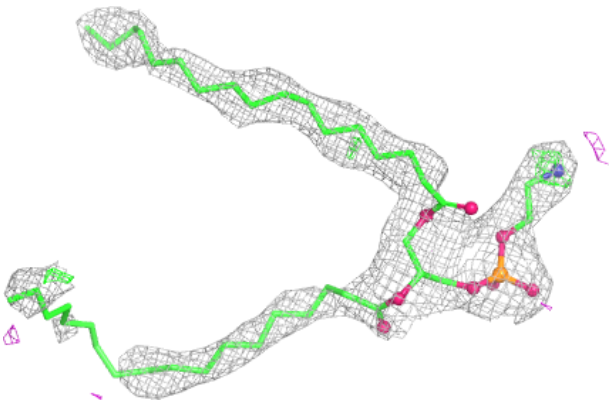


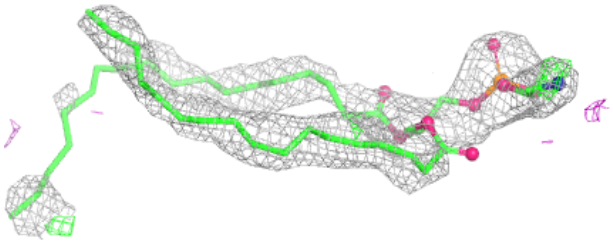




Electron density around PEE A 2005:

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

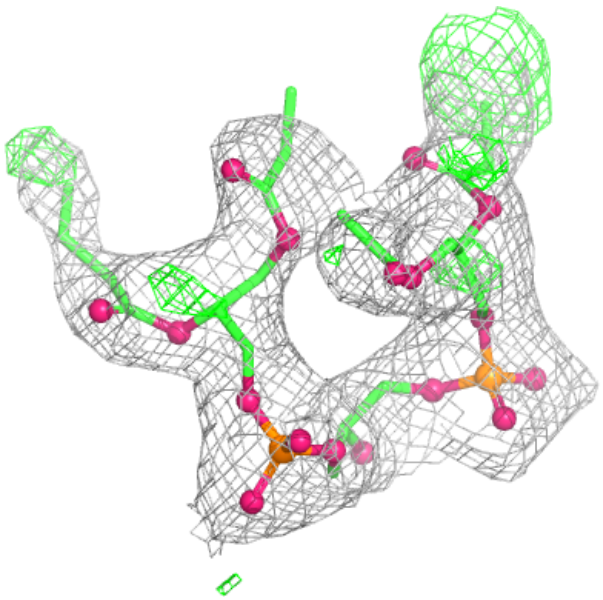


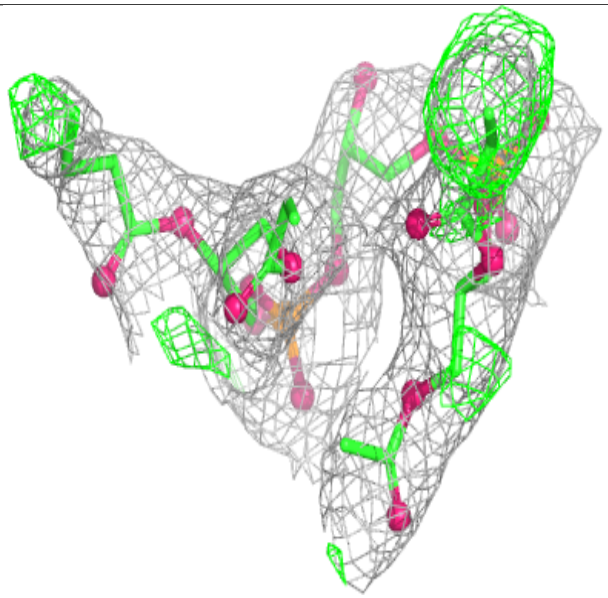


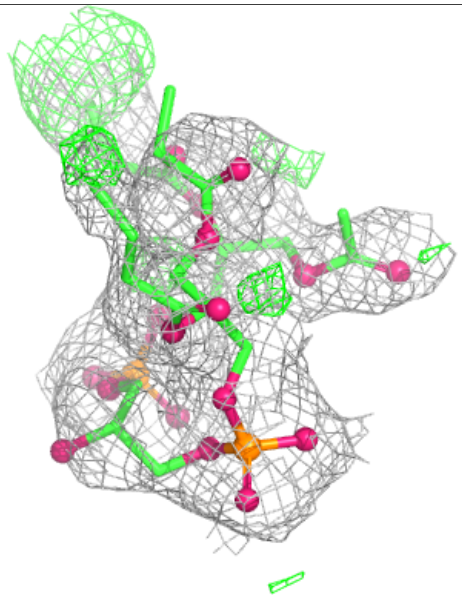


Electron density around CDL G 2004:

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

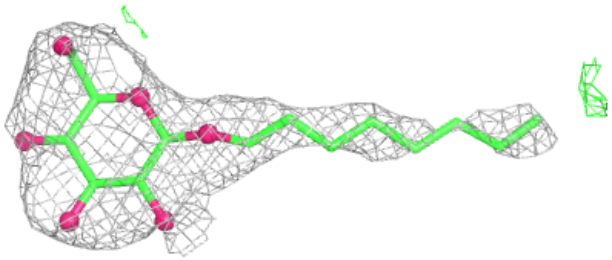


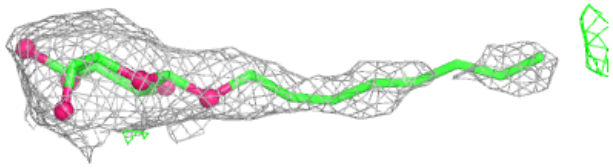


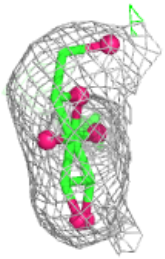


Electron density around BOG Q 3009:

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

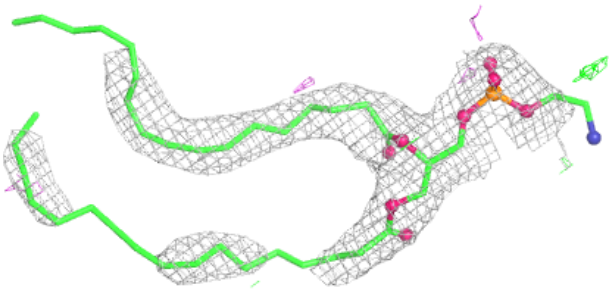


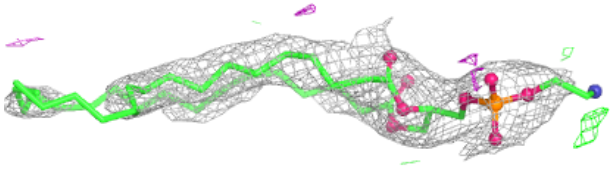


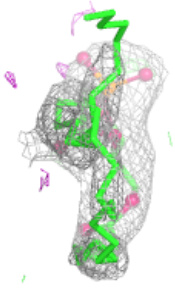


Electron density around PEE P 3007:

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

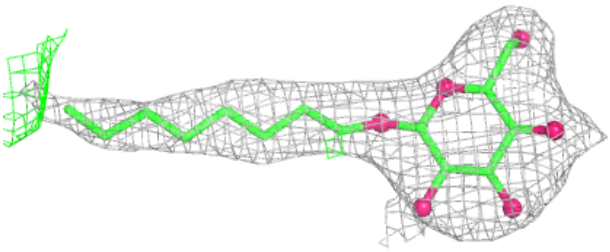


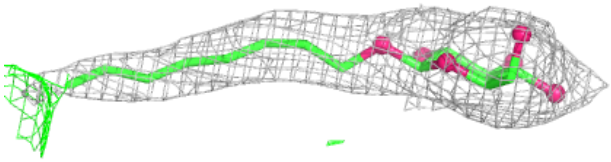


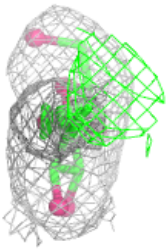


Electron density around BOG D 2009:

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

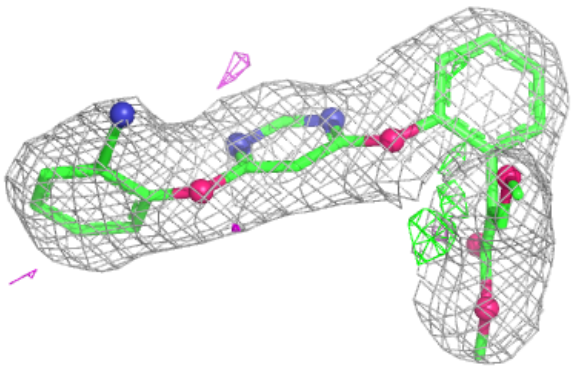


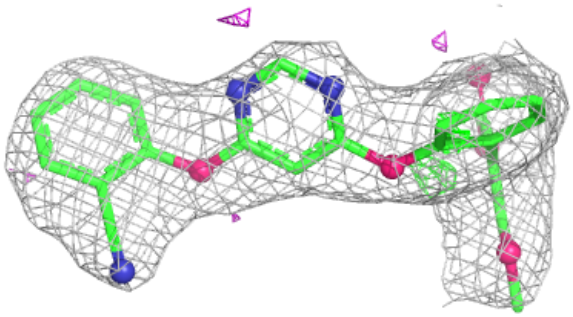


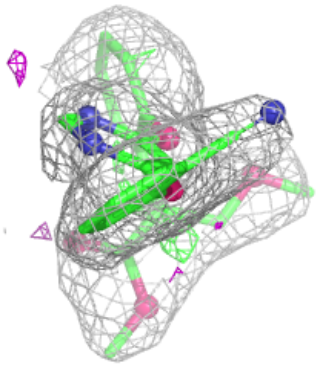


Electron density around AZO P 3001:

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

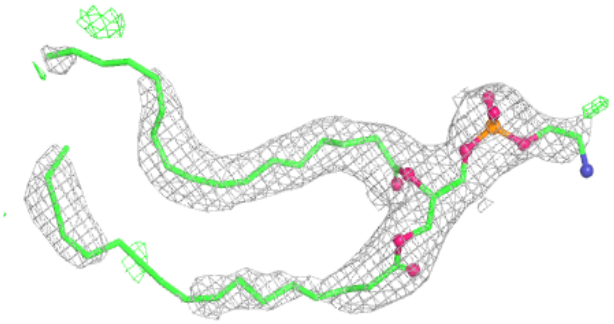


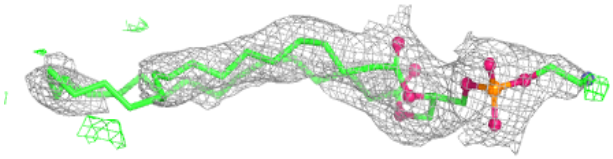


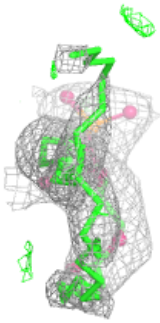


Electron density around PEE C 2007:

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

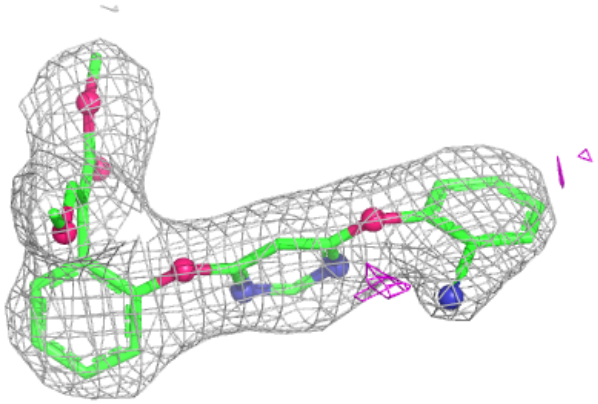


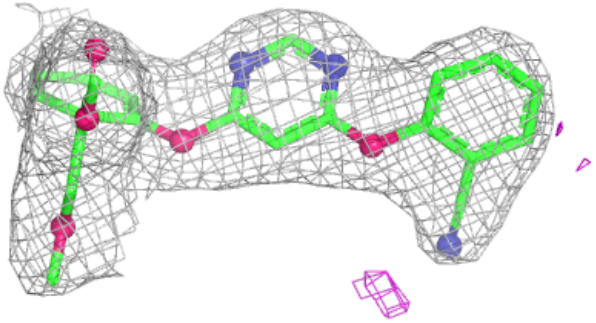


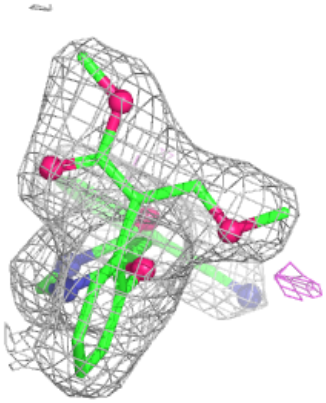


Electron density around AZO C 2001:

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

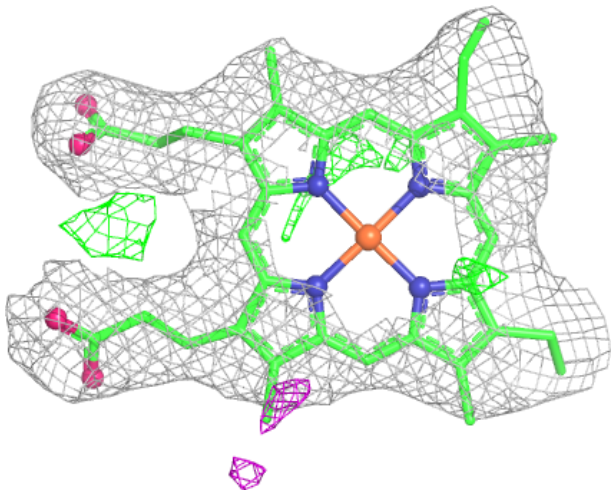


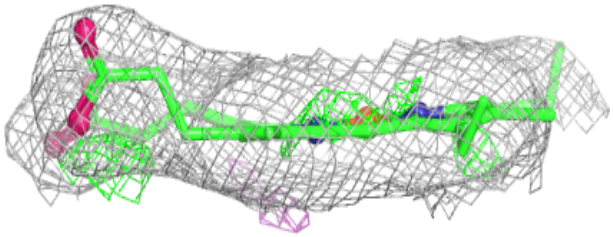


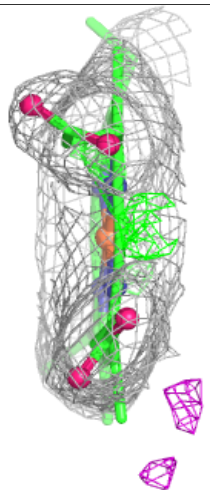


Electron density around HEC Q 501:

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

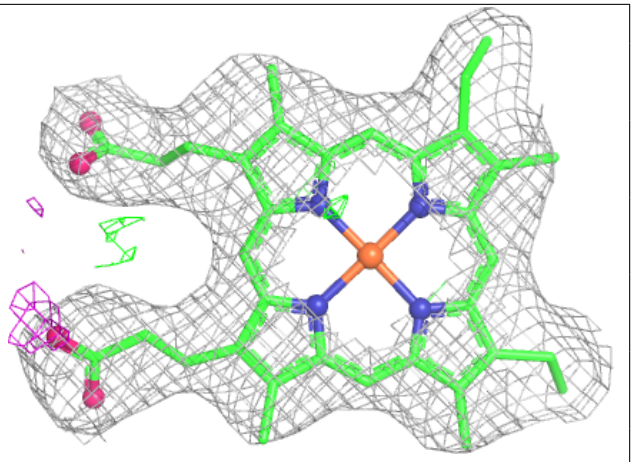


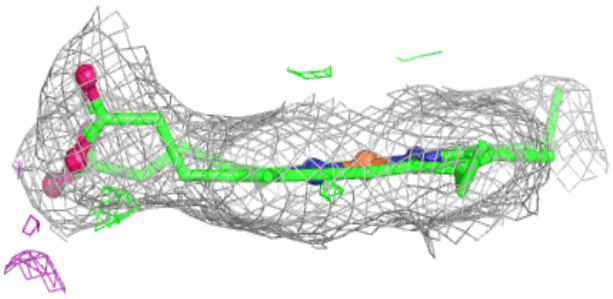


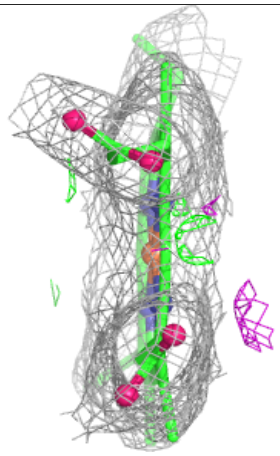


Electron density around HEC D 501:

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

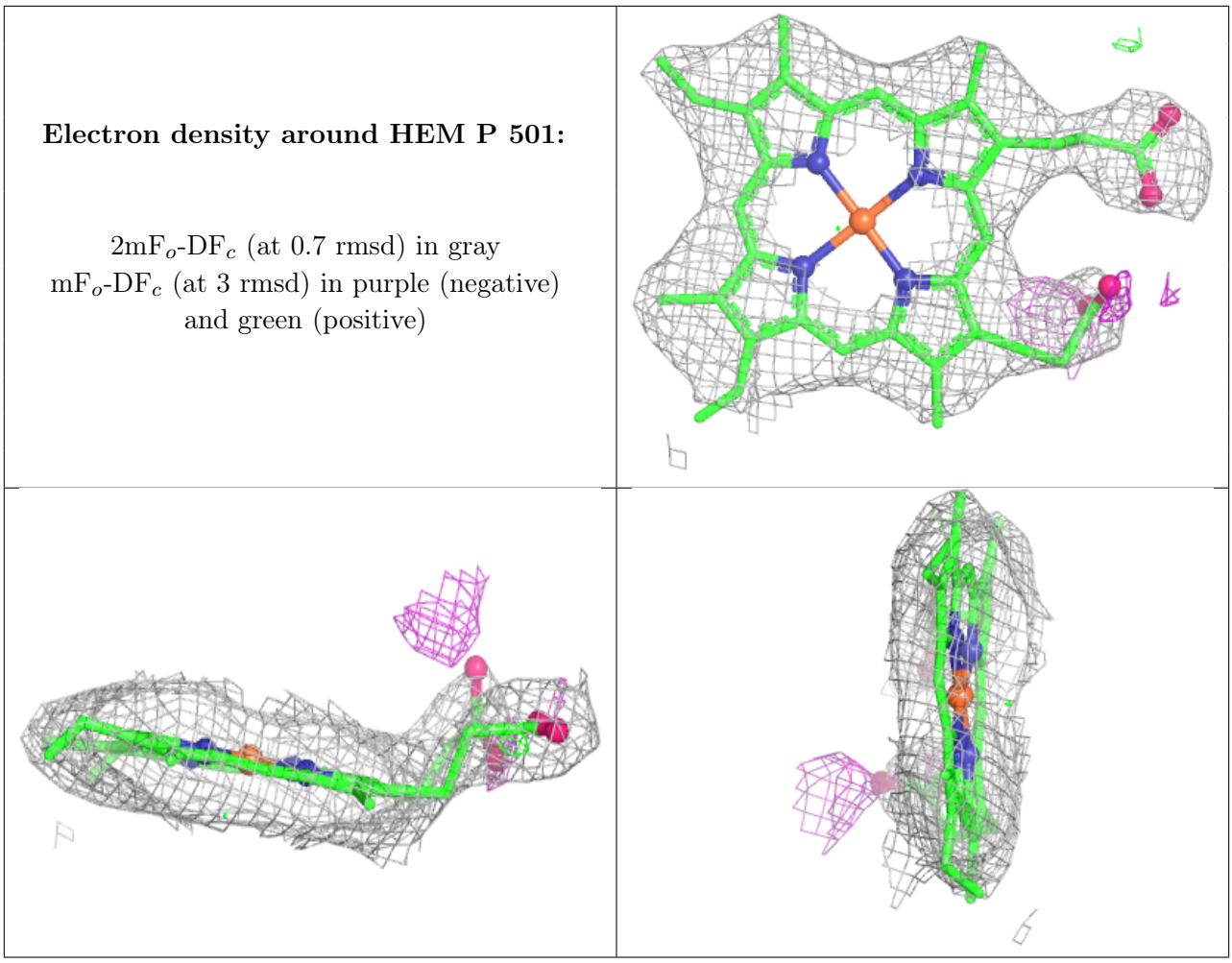






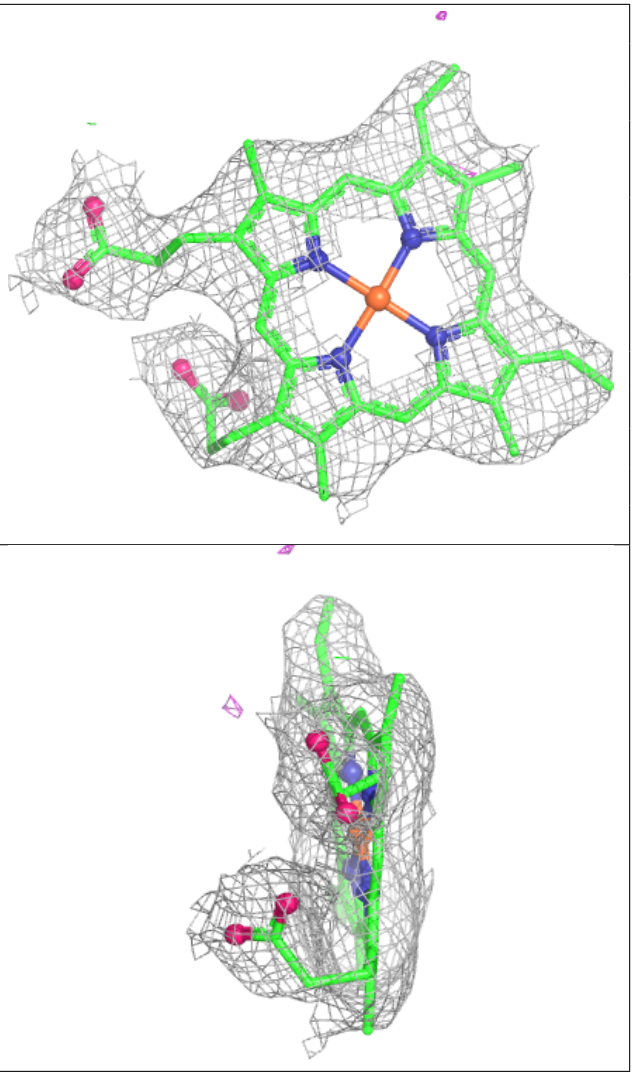
Electron density around HEM P 501:

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



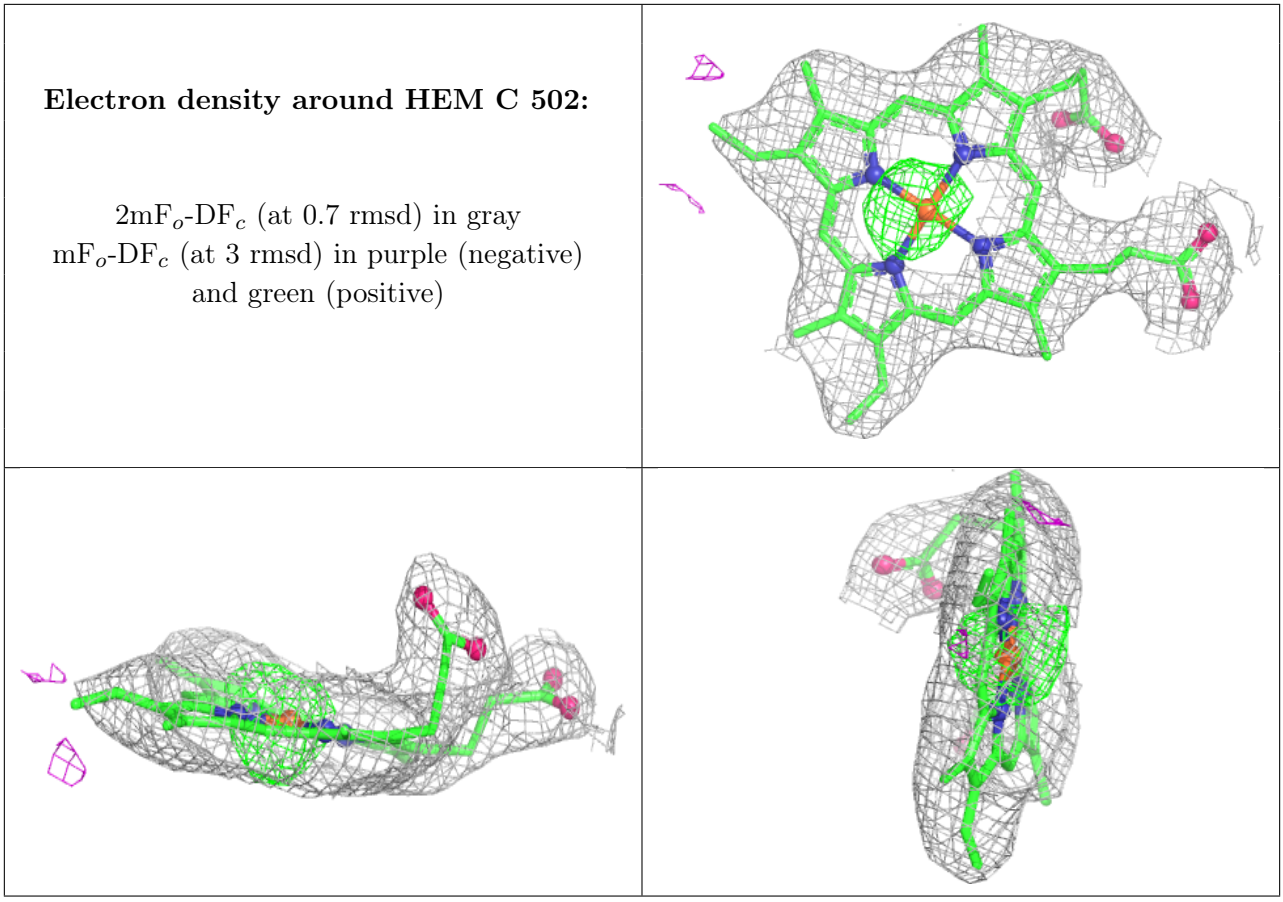
Electron density around HEM P 502:

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



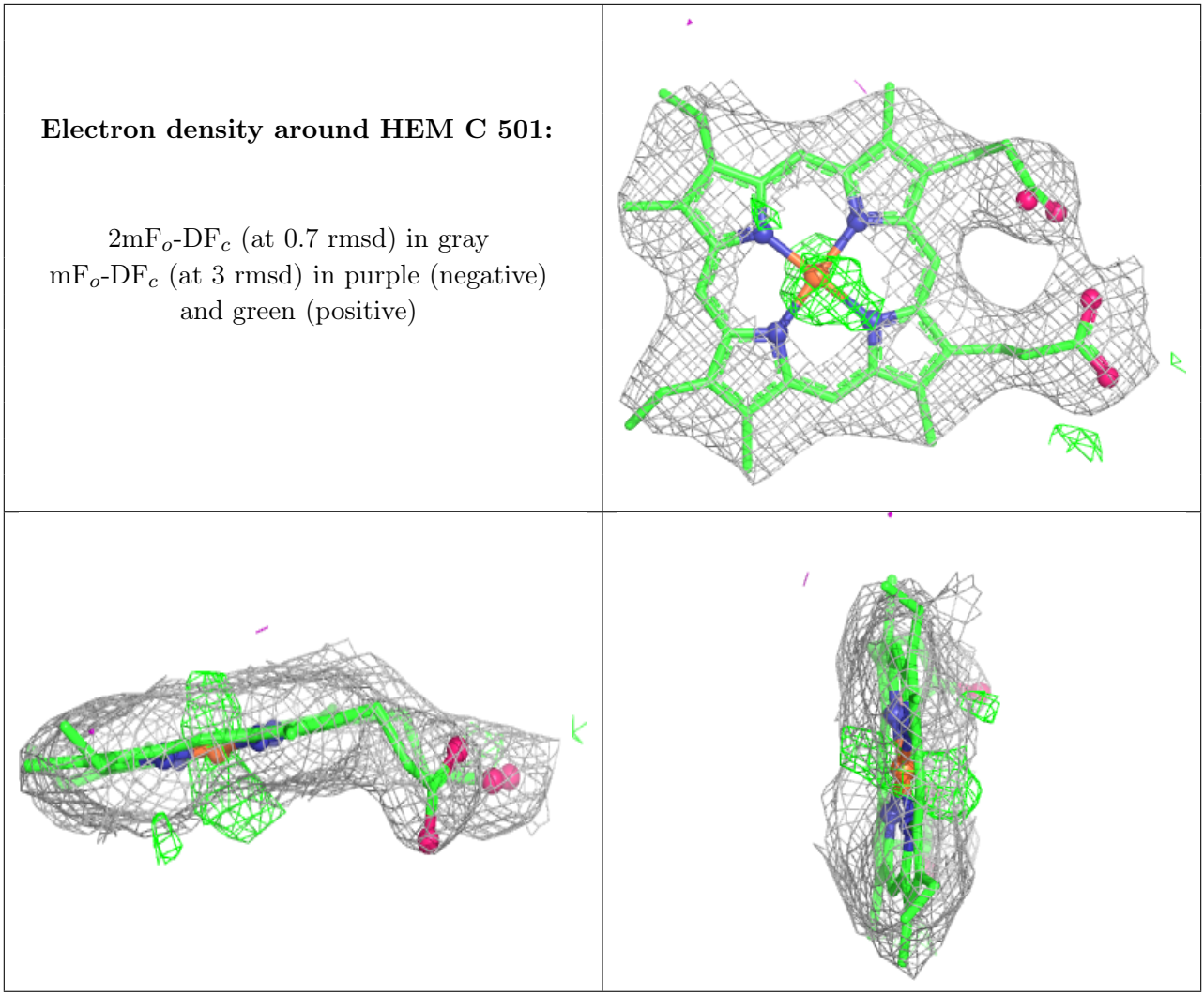
Electron density around HEM C 502:

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



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)



6.5 Other polymers

There are no such residues in this entry.