



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 08:30 AM EDT

PDB ID : 3H1J / pdb_00003h1j
Title : Stigmatellin-bound cytochrome bc1 complex from chicken
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.;
Crofts, A.R.; Berry, E.A.; Kim, S.-H.
Deposited on : 2009-04-12
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) 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

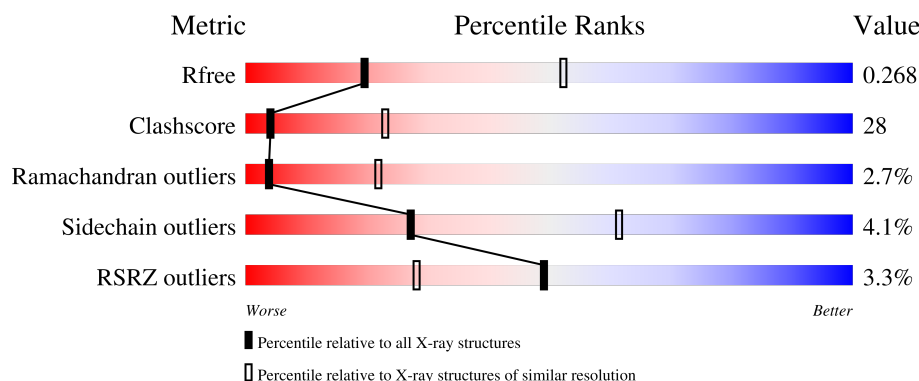
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	
1	N	446	
2	B	441	
2	O	441	
3	C	380	

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PEE	N	3008	-	X	-	-
17	HEC	D	501	X	-	-	-
17	HEC	Q	501	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32679 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

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

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

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

- Molecule 3 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

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

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

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

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

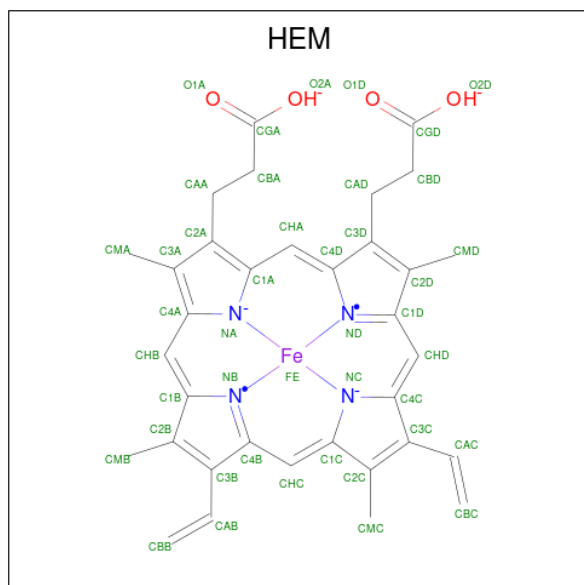
- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	O	0	0
			1	1		
11	C	3	Total	O	0	0
			3	3		
11	E	2	Total	O	0	0
			2	2		
11	P	3	Total	O	0	0
			3	3		
11	R	1	Total	O	0	0
			1	1		

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



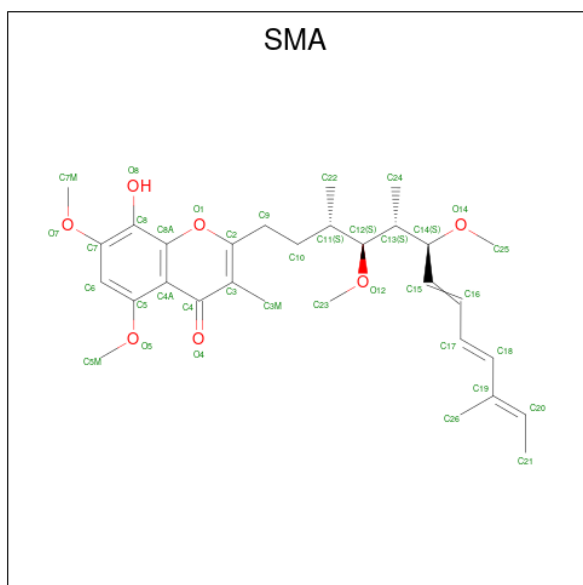
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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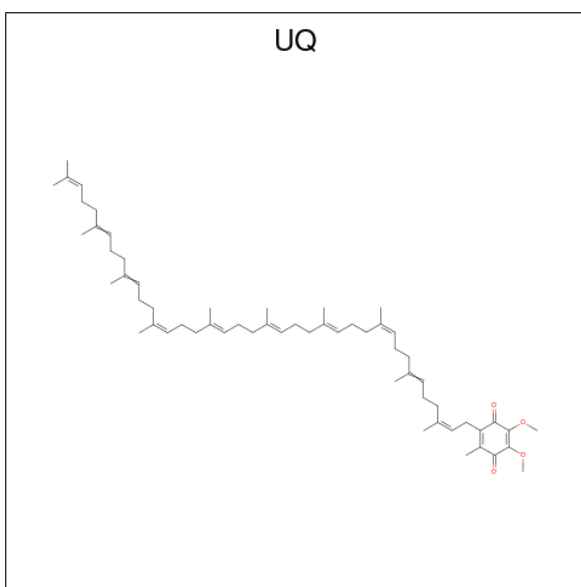
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 13 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



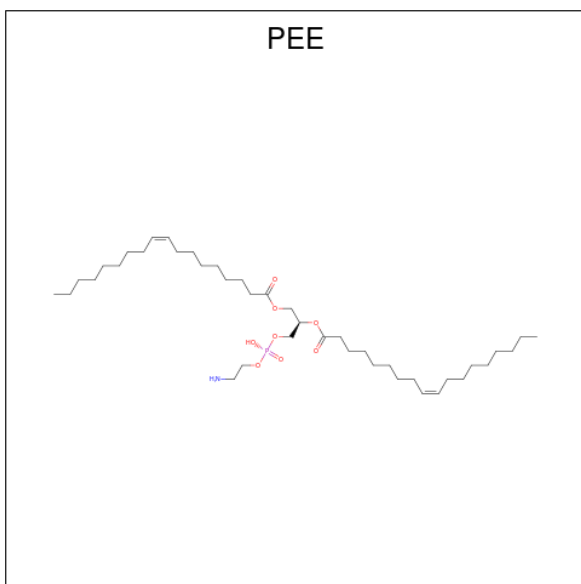
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O		
			37	30	7	0	0
13	P	1	Total	C	O		
			37	30	7	0	0

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

- Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



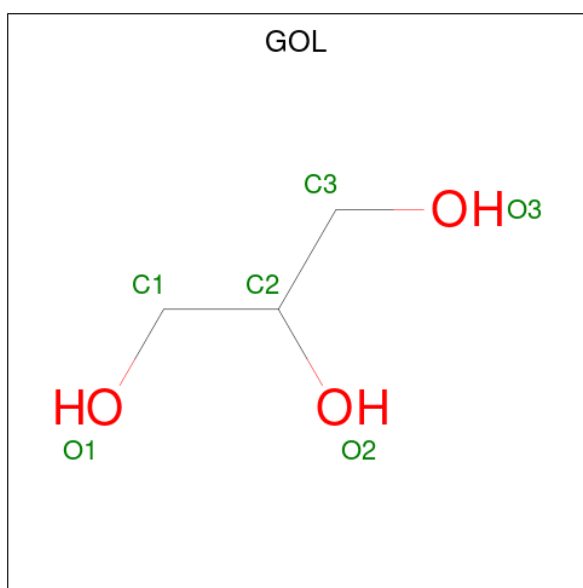
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

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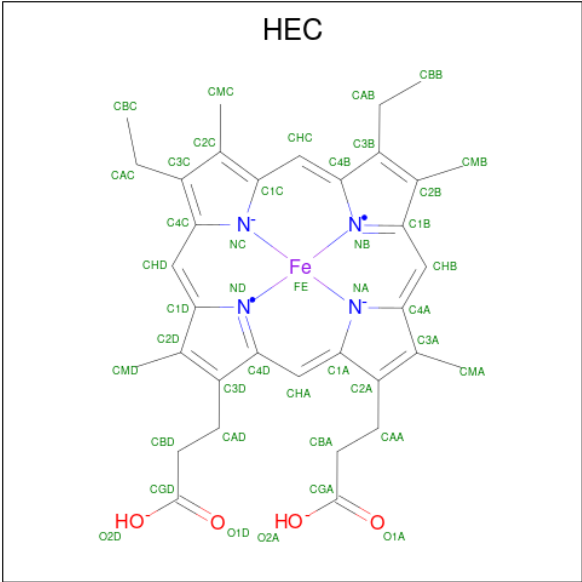
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	O	P		0	0
			21	12	8	1			
15	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
15	N	1	Total	O	P			0	0
			5	4	1				
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	R	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 16 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



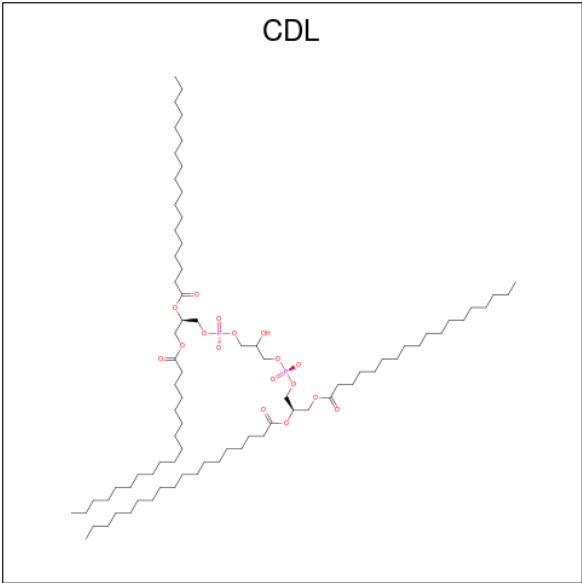
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



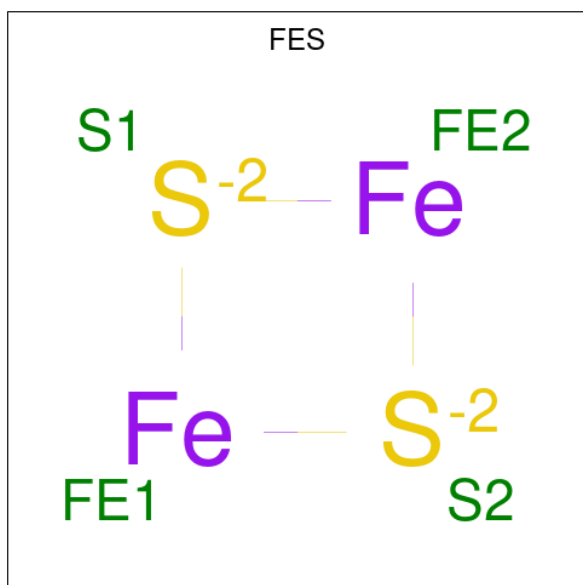
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			50	31	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		

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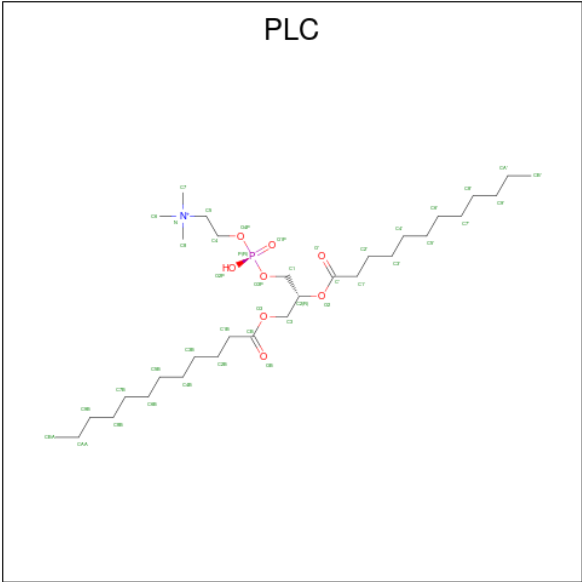
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			40	21	17	2		
18	S	1	Total	C	O	P	0	0
			50	31	17	2		

- 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	0	0
			4	2	2		
19	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $\text{C}_{32}\text{H}_{65}\text{NO}_8\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		
20	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

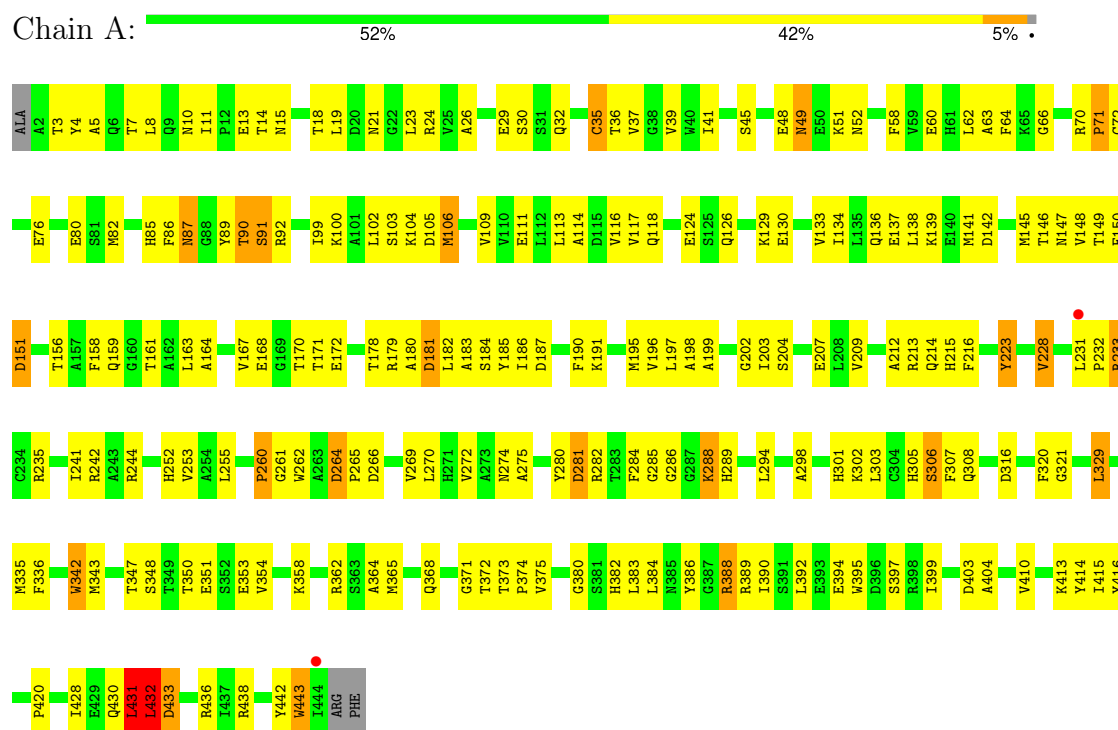
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	O	0	0
			1	1		
21	C	6	Total	O	0	0
			6	6		
21	P	6	Total	O	0	0
			6	6		
21	U	1	Total	O	0	0
			1	1		

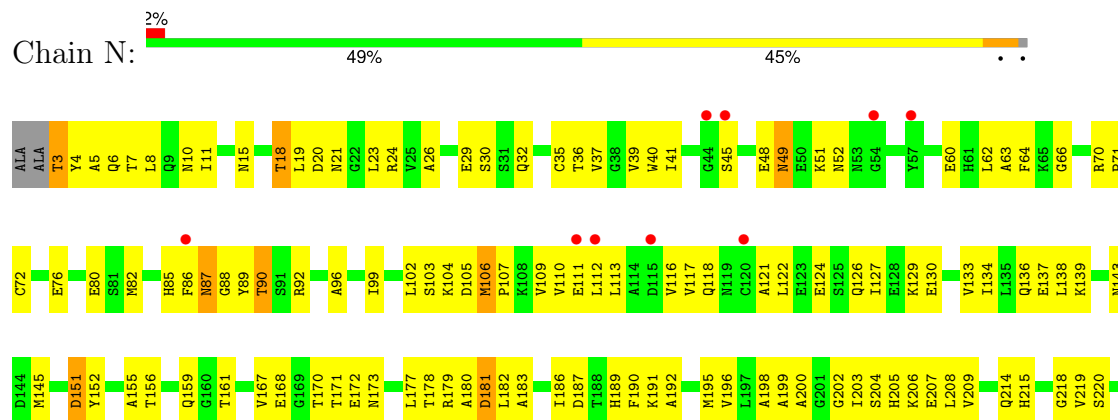
3 Residue-property plots

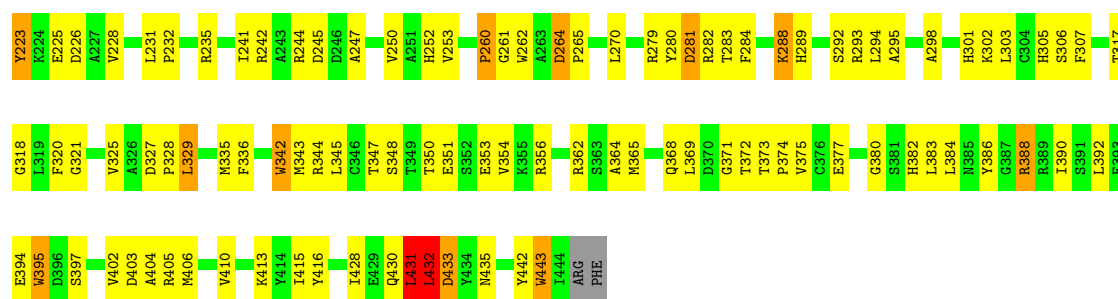
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

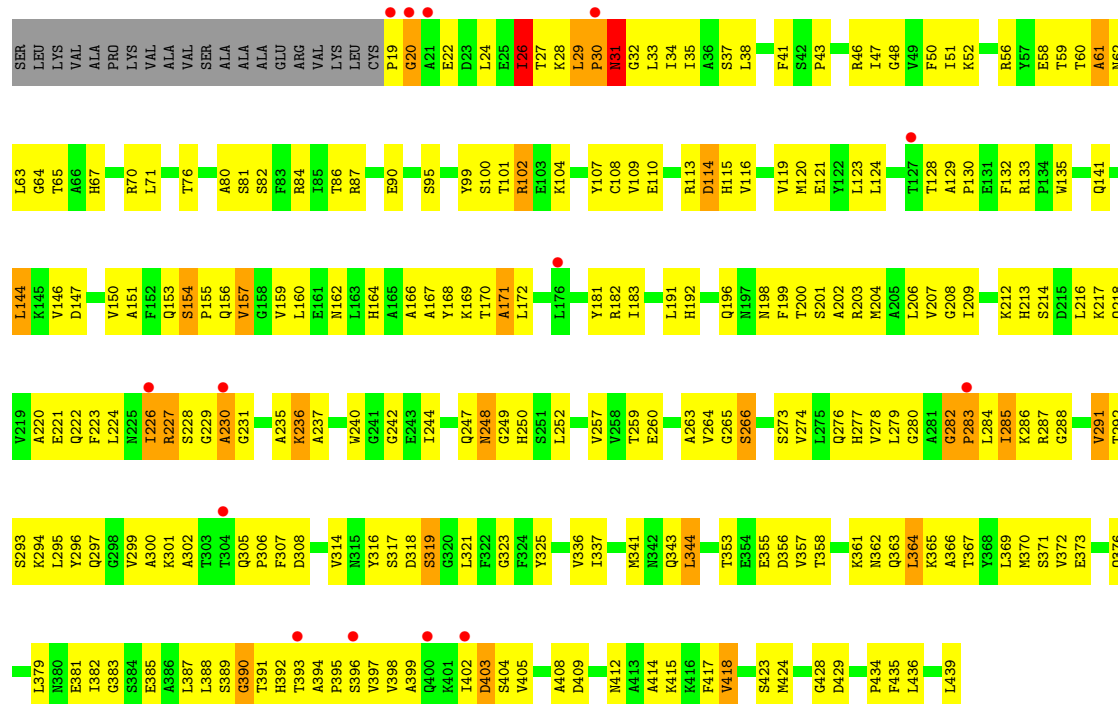


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

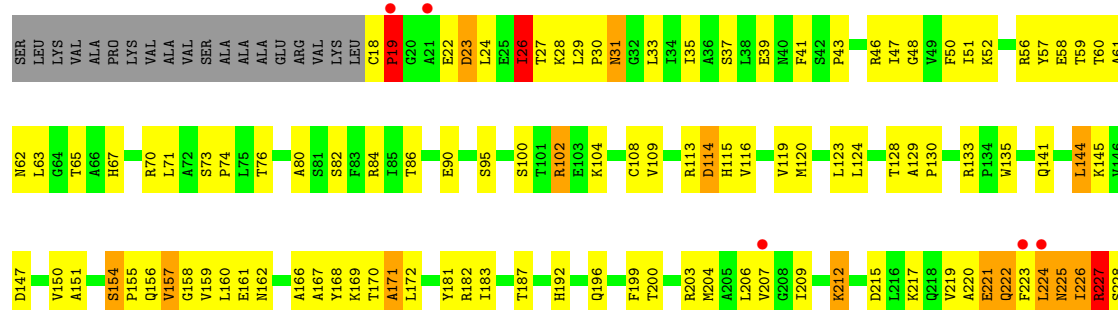
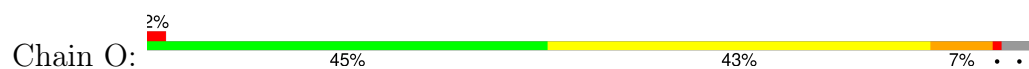




• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

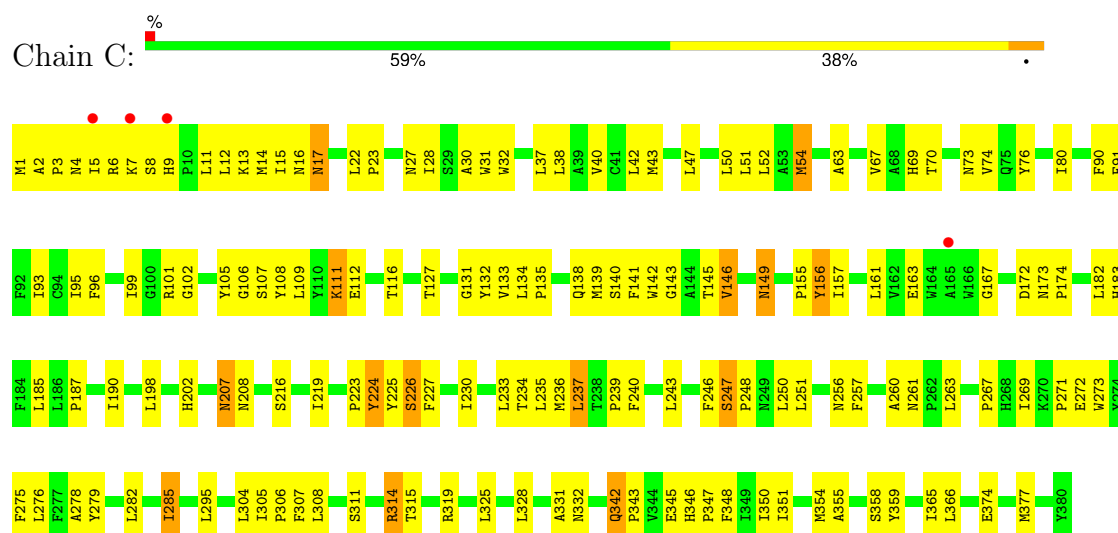


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

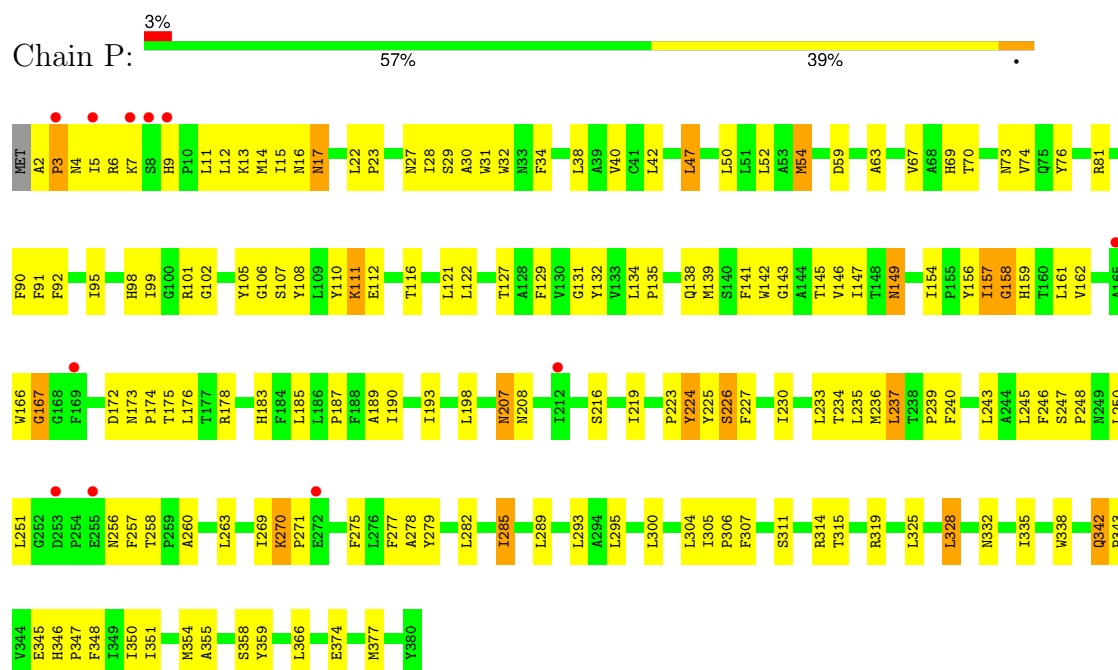




• Molecule 3: Cytochrome b

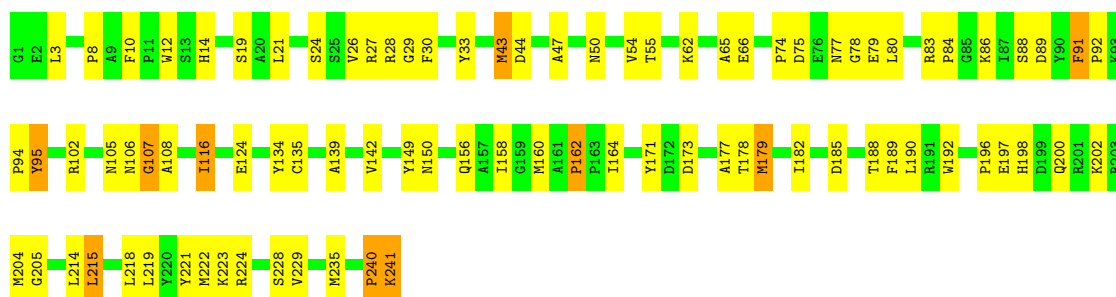


• Molecule 3: Cytochrome b



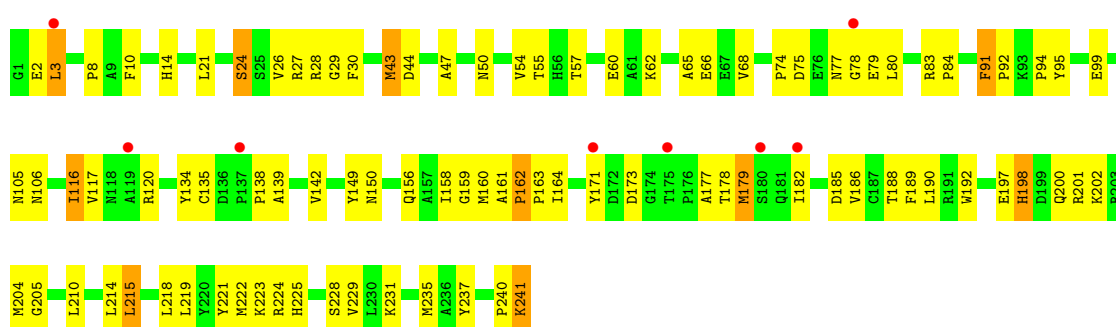
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:  64% 32% .



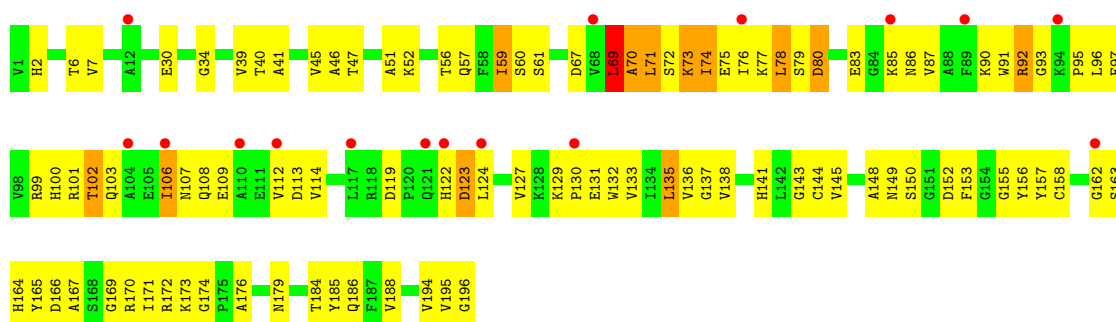
● Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q:  3% 61% 34% .



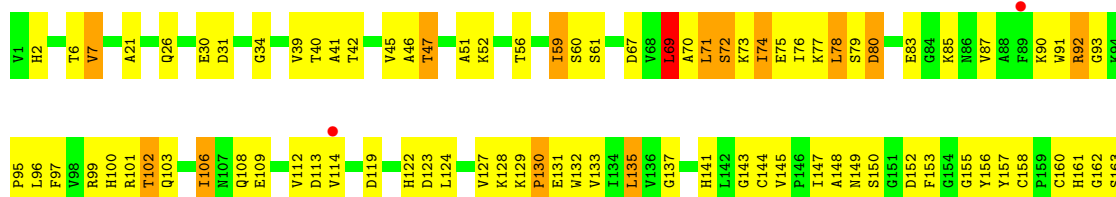
● Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

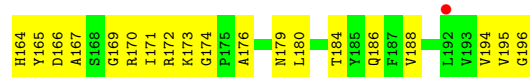
Chain E:  8% 48% 45% 6% .



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

Chain R:  2% 46% 46% 7% .





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



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



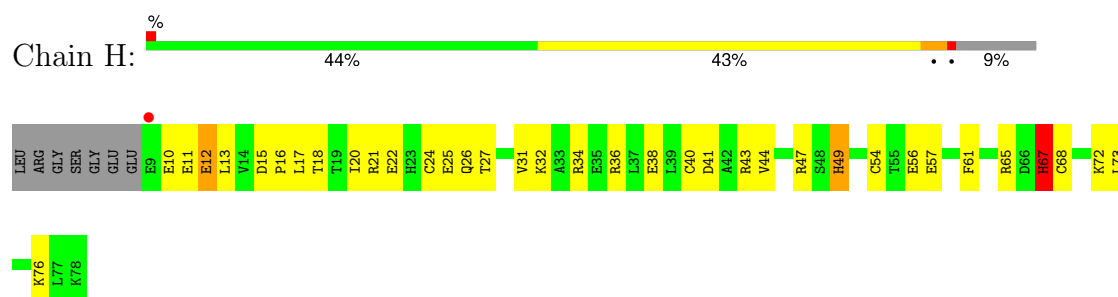
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



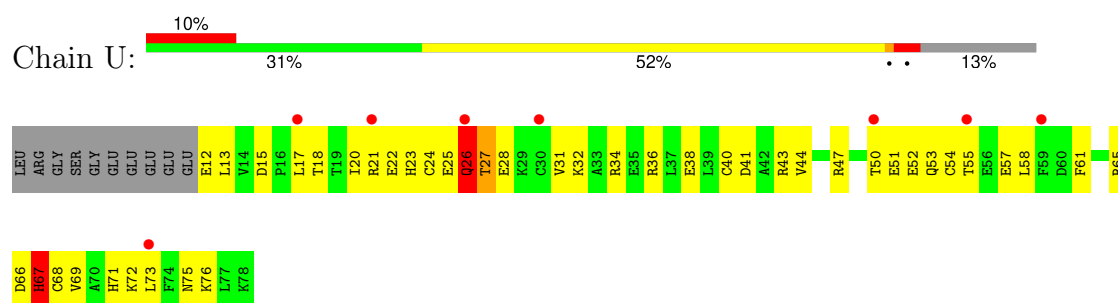
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



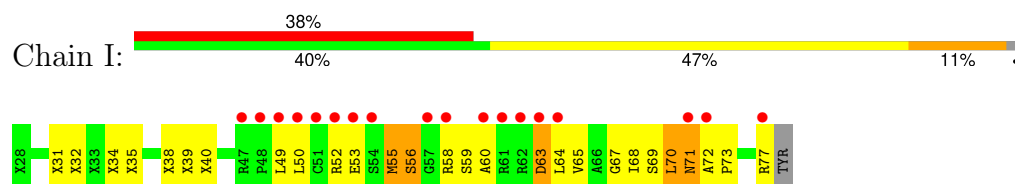
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



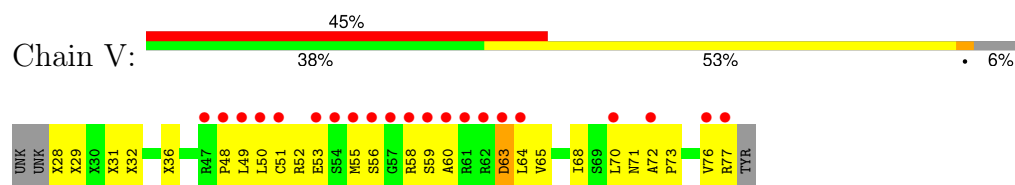
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



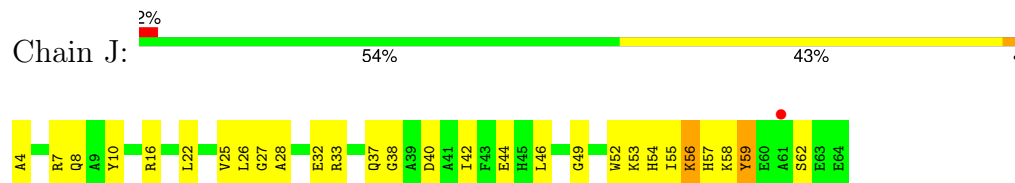
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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

Chain W:

51%

38%

8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 3.00 42.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (42.68-3.00) 92.5 (42.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.277 0.234 , 0.268	Depositor DCC
R_{free} test set	2796 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32679	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/3511	1.01	17/4757 (0.4%)
1	N	0.51	0/3508	1.01	16/4753 (0.3%)
2	B	0.46	0/3196	0.98	8/4334 (0.2%)
2	O	0.51	0/3202	0.98	10/4343 (0.2%)
3	C	0.65	2/3122 (0.1%)	1.04	23/4273 (0.5%)
3	P	0.56	1/3114 (0.0%)	1.02	18/4263 (0.4%)
4	D	0.58	0/1956	1.04	10/2658 (0.4%)
4	Q	0.48	0/1956	1.01	6/2658 (0.2%)
5	E	0.46	0/1547	0.99	6/2103 (0.3%)
5	R	0.47	0/1547	1.05	10/2103 (0.5%)
6	F	0.61	0/911	1.00	4/1219 (0.3%)
6	S	0.50	0/911	0.96	6/1219 (0.5%)
7	G	0.62	0/698	1.03	3/946 (0.3%)
7	T	0.50	0/680	0.99	3/923 (0.3%)
8	H	0.52	0/582	0.88	1/779 (0.1%)
8	U	0.41	0/561	0.92	3/751 (0.4%)
9	I	0.58	0/218	0.99	0/293
9	V	0.63	0/218	1.00	0/293
10	J	0.54	0/508	0.94	1/682 (0.1%)
10	W	0.49	0/489	0.90	1/658 (0.2%)
All	All	0.53	3/32435 (0.0%)	1.00	146/44008 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	P	0	1
4	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	43	MET	SD-CE	6.73	1.96	1.79
3	C	54	MET	SD-CE	5.78	1.94	1.79
3	P	54	MET	SD-CE	5.44	1.93	1.79

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	143	GLY	N-CA-C	10.12	128.82	115.36
5	R	71	LEU	N-CA-C	10.12	125.02	110.14
5	R	143	GLY	N-CA-C	10.11	128.80	115.36
4	Q	116	ILE	N-CA-C	9.22	119.27	110.42
4	Q	91	PHE	CA-C-N	9.10	129.67	119.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	33	TYR	Sidechain
3	P	224	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	189	0
1	N	3437	0	3349	208	0
2	B	3141	0	3142	271	0
2	O	3147	0	3146	251	0
3	C	3020	0	3070	151	0
3	P	3012	0	3058	163	0
4	D	1898	0	1846	70	0
4	Q	1898	0	1846	89	0
5	E	1513	0	1478	95	0
5	R	1513	0	1478	96	0
6	F	891	0	893	41	0
6	S	891	0	893	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	676	0	659	48	0
7	T	658	0	647	48	0
8	H	574	0	548	35	0
8	U	553	0	535	48	0
9	I	285	0	237	53	0
9	V	275	0	238	43	0
10	J	497	0	490	20	0
10	W	478	0	478	31	0
11	A	1	0	0	0	0
11	C	3	0	0	0	0
11	E	2	0	0	0	0
11	P	3	0	0	0	0
11	R	1	0	0	0	0
12	C	86	0	60	11	0
12	P	86	0	60	12	0
13	C	37	0	42	4	0
13	P	37	0	42	4	0
14	C	19	0	17	4	0
14	P	19	0	17	2	0
15	C	70	0	85	1	0
15	E	50	0	77	4	0
15	N	5	0	0	0	0
15	P	49	0	72	1	0
15	R	50	0	77	4	0
16	C	6	0	8	0	0
16	P	6	0	8	1	0
17	D	43	0	30	0	0
17	Q	43	0	30	0	0
18	D	50	0	44	1	0
18	G	40	0	24	1	0
18	P	40	0	24	3	0
18	S	50	0	44	2	0
19	E	4	0	0	0	0
19	R	4	0	0	1	0
20	E	32	0	38	3	0
20	R	32	0	38	2	0
21	B	1	0	0	0	0
21	C	6	0	0	0	0
21	P	6	0	0	1	0
21	U	1	0	0	1	0
All	All	32679	0	32221	1792	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 28.

The worst 5 of 1792 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)
6:F:32:MET:HE2	6:F:87:LYS:HG2	1.25	1.17
2:O:47:ILE:HG12	2:O:120:MET:HE1	1.27	1.13
6:F:32:MET:HE3	6:F:87:LYS:H	1.11	1.12
2:B:47:ILE:HG12	2:B:120:MET:HE1	1.23	1.10
2:B:353:THR:HG22	2:B:355:GLU:H	1.15	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	393 (89%)	40 (9%)	8 (2%)	6	31
1	N	440/446 (99%)	397 (90%)	36 (8%)	7 (2%)	7	34
2	B	419/441 (95%)	339 (81%)	63 (15%)	17 (4%)	2	13
2	O	420/441 (95%)	336 (80%)	66 (16%)	18 (4%)	2	12
3	C	378/380 (100%)	358 (95%)	18 (5%)	2 (0%)	24	60
3	P	377/380 (99%)	349 (93%)	24 (6%)	4 (1%)	11	43
4	D	239/241 (99%)	217 (91%)	20 (8%)	2 (1%)	16	50
4	Q	239/241 (99%)	214 (90%)	22 (9%)	3 (1%)	9	38
5	E	194/196 (99%)	157 (81%)	24 (12%)	13 (7%)	1	5
5	R	194/196 (99%)	161 (83%)	21 (11%)	12 (6%)	1	6
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
6	S	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	12	45
7	G	79/81 (98%)	66 (84%)	9 (11%)	4 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	1	9
8	H	68/77 (88%)	57 (84%)	8 (12%)	3 (4%)	2	12
8	U	65/77 (84%)	48 (74%)	16 (25%)	1 (2%)	8	35
9	I	29/47 (62%)	19 (66%)	7 (24%)	3 (10%)	0	2
9	V	29/47 (62%)	20 (69%)	7 (24%)	2 (7%)	1	5
10	J	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	7	32
10	W	57/61 (93%)	45 (79%)	8 (14%)	4 (7%)	1	4
All	All	4002/4160 (96%)	3475 (87%)	418 (10%)	109 (3%)	4	22

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	114	ASP
2	B	171	ALA

5.3.2 Protein sidechains ⓘ

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%)	349 (96%)	16 (4%)	25	60
1	N	365/368 (99%)	346 (95%)	19 (5%)	21	55
2	B	332/347 (96%)	319 (96%)	13 (4%)	28	62
2	O	333/347 (96%)	315 (95%)	18 (5%)	20	53
3	C	329/329 (100%)	323 (98%)	6 (2%)	51	77
3	P	328/329 (100%)	323 (98%)	5 (2%)	57	80
4	D	200/200 (100%)	194 (97%)	6 (3%)	36	69
4	Q	200/200 (100%)	194 (97%)	6 (3%)	36	69
5	E	166/166 (100%)	158 (95%)	8 (5%)	23	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	166/166 (100%)	157 (95%)	9 (5%)	20	53
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	60
6	S	93/96 (97%)	88 (95%)	5 (5%)	20	53
7	G	71/71 (100%)	68 (96%)	3 (4%)	26	61
7	T	69/71 (97%)	66 (96%)	3 (4%)	26	60
8	H	65/71 (92%)	62 (95%)	3 (5%)	24	58
8	U	63/71 (89%)	60 (95%)	3 (5%)	23	57
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	35
9	V	23/26 (88%)	22 (96%)	1 (4%)	26	60
10	J	49/49 (100%)	45 (92%)	4 (8%)	10	37
10	W	47/49 (96%)	44 (94%)	3 (6%)	16	48
All	All	3380/3446 (98%)	3243 (96%)	137 (4%)	27	61

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	56	THR
5	R	80	ASP
8	U	26	GLN
5	E	184	THR
5	E	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	10	ASN
7	T	64	GLN
1	N	360	HIS
7	T	44	GLN
4	Q	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 10 are unknown - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	PEE	E	2005	-	49,49,50	1.51	10 (20%)	52,54,55	0.86	3 (5%)
19	FES	R	501	5	0,4,4	-	-	-		
18	CDL	P	3004	-	39,39,99	1.25	3 (7%)	45,51,111	1.17	4 (8%)
15	PEE	C	2007	-	48,48,50	1.49	8 (16%)	51,53,55	0.86	3 (5%)
12	HEM	C	502	3	50,50,50	1.51	6 (12%)	67,82,82	1.41	9 (13%)
13	SMA	P	3001	-	38,38,38	1.71	10 (26%)	47,52,52	0.91	2 (4%)
17	HEC	Q	501	4	50,50,50	1.09	4 (8%)	68,82,82	1.58	11 (16%)
14	UQ	P	3002	-	19,19,63	2.62	9 (47%)	24,26,79	1.09	2 (8%)
12	HEM	C	501	3	50,50,50	1.53	8 (16%)	67,82,82	1.41	9 (13%)
13	SMA	C	2001	-	38,38,38	1.68	10 (26%)	47,52,52	0.96	3 (6%)
18	CDL	S	3003	-	49,49,99	1.14	2 (4%)	55,61,111	1.03	2 (3%)
15	PEE	R	3005	-	49,49,50	1.53	9 (18%)	52,54,55	0.85	3 (5%)
15	PEE	C	2008	-	20,20,50	1.75	5 (25%)	23,25,55	0.64	0
20	PLC	E	2009	-	31,31,41	1.70	6 (19%)	37,39,49	0.66	0
12	HEM	P	502	3	50,50,50	1.44	6 (12%)	67,82,82	1.26	6 (8%)
14	UQ	C	2002	-	19,19,63	2.66	9 (47%)	24,26,79	1.08	2 (8%)
17	HEC	D	501	4	50,50,50	0.93	0	68,82,82	1.55	10 (14%)
19	FES	E	501	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	HEM	P	501	3	50,50,50	1.44	6 (12%)	67,82,82	1.36	9 (13%)
15	PEE	P	3007	-	48,48,50	1.44	7 (14%)	51,53,55	0.81	2 (3%)
16	GOL	P	3011	-	5,5,5	1.51	1 (20%)	5,5,5	0.70	0
18	CDL	G	2004	-	39,39,99	1.33	5 (12%)	45,51,111	1.16	4 (8%)
20	PLC	R	3009	-	31,31,41	1.63	7 (22%)	37,39,49	0.63	1 (2%)
15	PEE	N	3008	-	4,4,50	3.63	4 (100%)	6,6,55	0.65	0
16	GOL	C	2011	-	5,5,5	1.32	0	5,5,5	0.57	0
18	CDL	D	2003	-	49,49,99	1.16	2 (4%)	55,61,111	1.03	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PEE	E	2005	-	-	27/53/53/54	-
19	FES	R	501	5	-	-	0/1/1/1
18	CDL	P	3004	-	-	22/49/49/110	-
15	PEE	C	2007	-	-	21/52/52/54	-
12	HEM	C	502	3	-	8/14/54/54	-
13	SMA	P	3001	-	-	5/34/34/34	0/2/2/2
17	HEC	Q	501	4	1/1/3/7	8/14/54/54	-
14	UQ	P	3002	-	-	3/11/35/87	0/1/1/1
12	HEM	C	501	3	-	6/14/54/54	-
13	SMA	C	2001	-	-	5/34/34/34	0/2/2/2
18	CDL	S	3003	-	-	24/59/59/110	-
15	PEE	R	3005	-	-	27/53/53/54	-
15	PEE	C	2008	-	-	9/24/24/54	-
20	PLC	E	2009	-	-	13/35/35/45	-
12	HEM	P	502	3	-	8/14/54/54	-
14	UQ	C	2002	-	-	3/11/35/87	0/1/1/1
17	HEC	D	501	4	1/1/3/7	8/14/54/54	-
19	FES	E	501	5	-	-	0/1/1/1
12	HEM	P	501	3	-	6/14/54/54	-
15	PEE	P	3007	-	-	23/52/52/54	-
16	GOL	P	3011	-	-	0/4/4/4	-
18	CDL	G	2004	-	-	21/49/49/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PLC	R	3009	-	-	12/35/35/45	-
16	GOL	C	2011	-	-	2/4/4/4	-
18	CDL	D	2003	-	-	24/59/59/110	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	UQ	C6-C5	5.27	1.44	1.35
14	C	2002	UQ	C6-C5	4.95	1.44	1.35
13	C	2001	SMA	C7-C8	4.88	1.47	1.40
14	P	3002	UQ	C7-C6	4.82	1.60	1.51
15	N	3008	PEE	P-O1P	4.77	1.61	1.50

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CAA-C2A-C3A	-4.58	119.29	127.87
17	D	501	HEC	CAC-C3C-C4C	-4.52	118.69	124.91
17	Q	501	HEC	CAC-C3C-C4C	-4.39	118.88	124.91
17	Q	501	HEC	CAA-C2A-C3A	-4.31	119.80	127.87
12	P	502	HEM	CAD-C3D-C4D	4.20	132.01	124.70

All (2) chirality outliers are listed below:

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

5 of 285 torsion outliers are listed below:

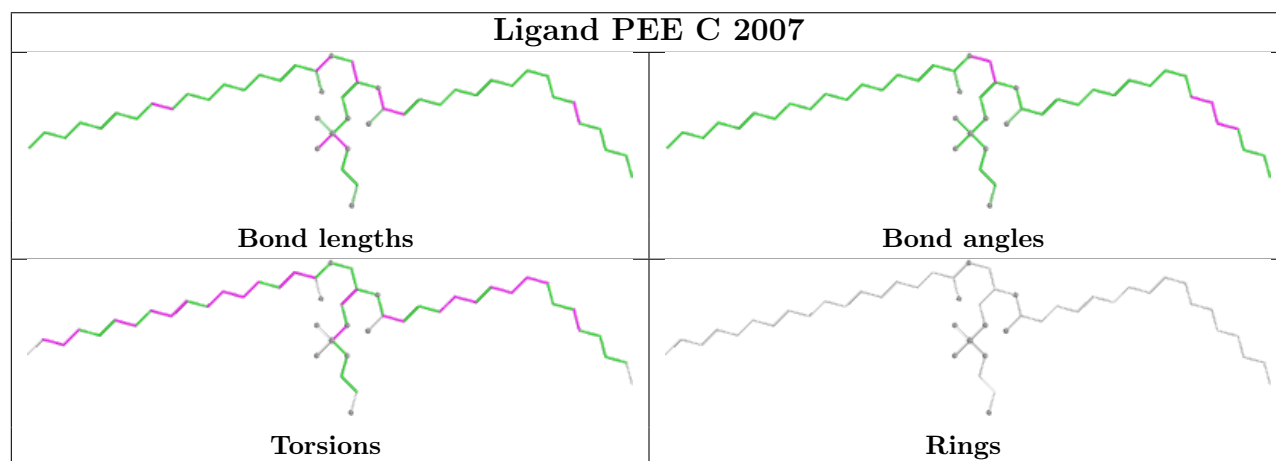
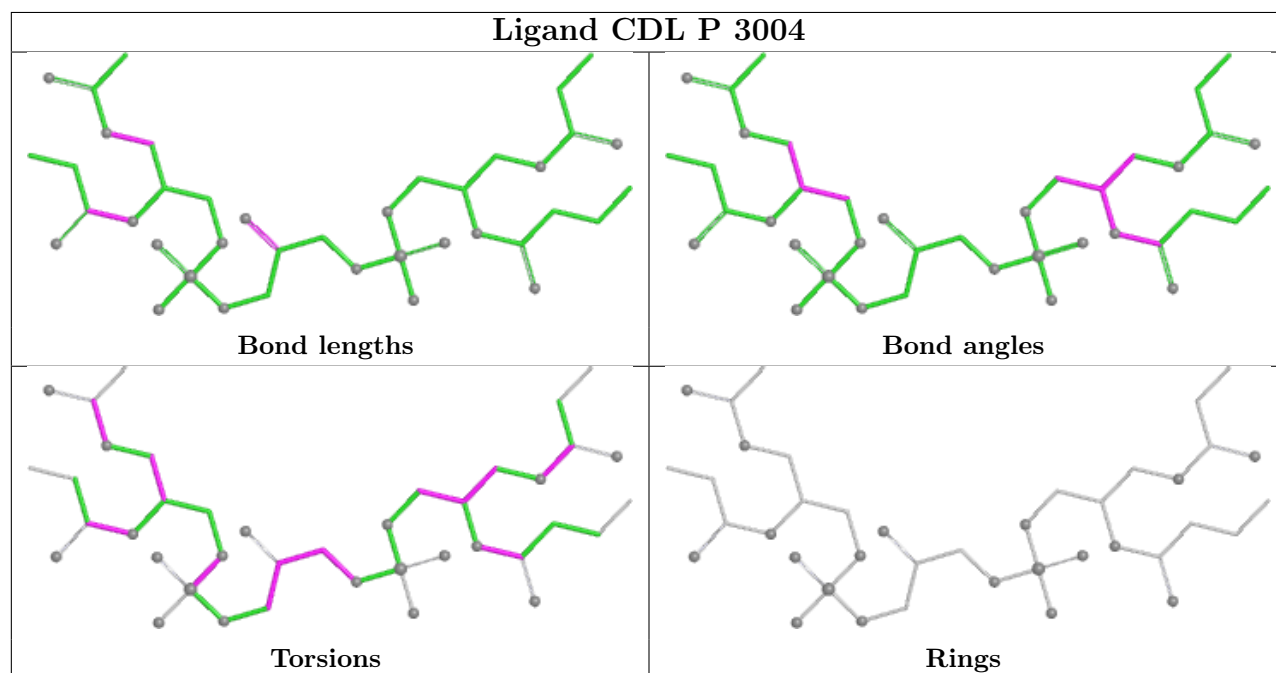
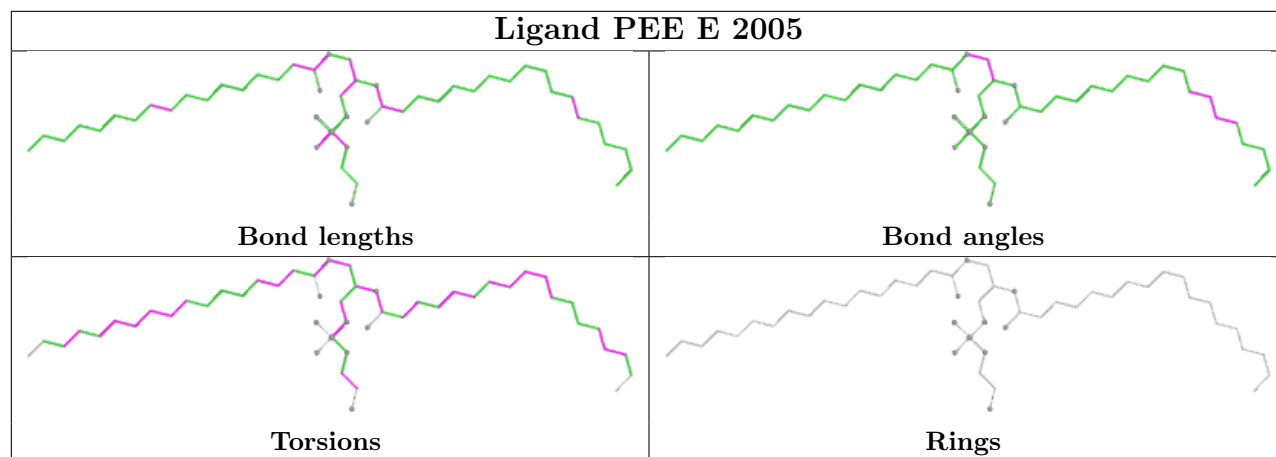
Mol	Chain	Res	Type	Atoms
13	C	2001	SMA	C3-C2-C9-C10
13	C	2001	SMA	O1-C2-C9-C10
13	P	3001	SMA	C3-C2-C9-C10
13	P	3001	SMA	O1-C2-C9-C10
14	C	2002	UQ	C1-C6-C7-C8

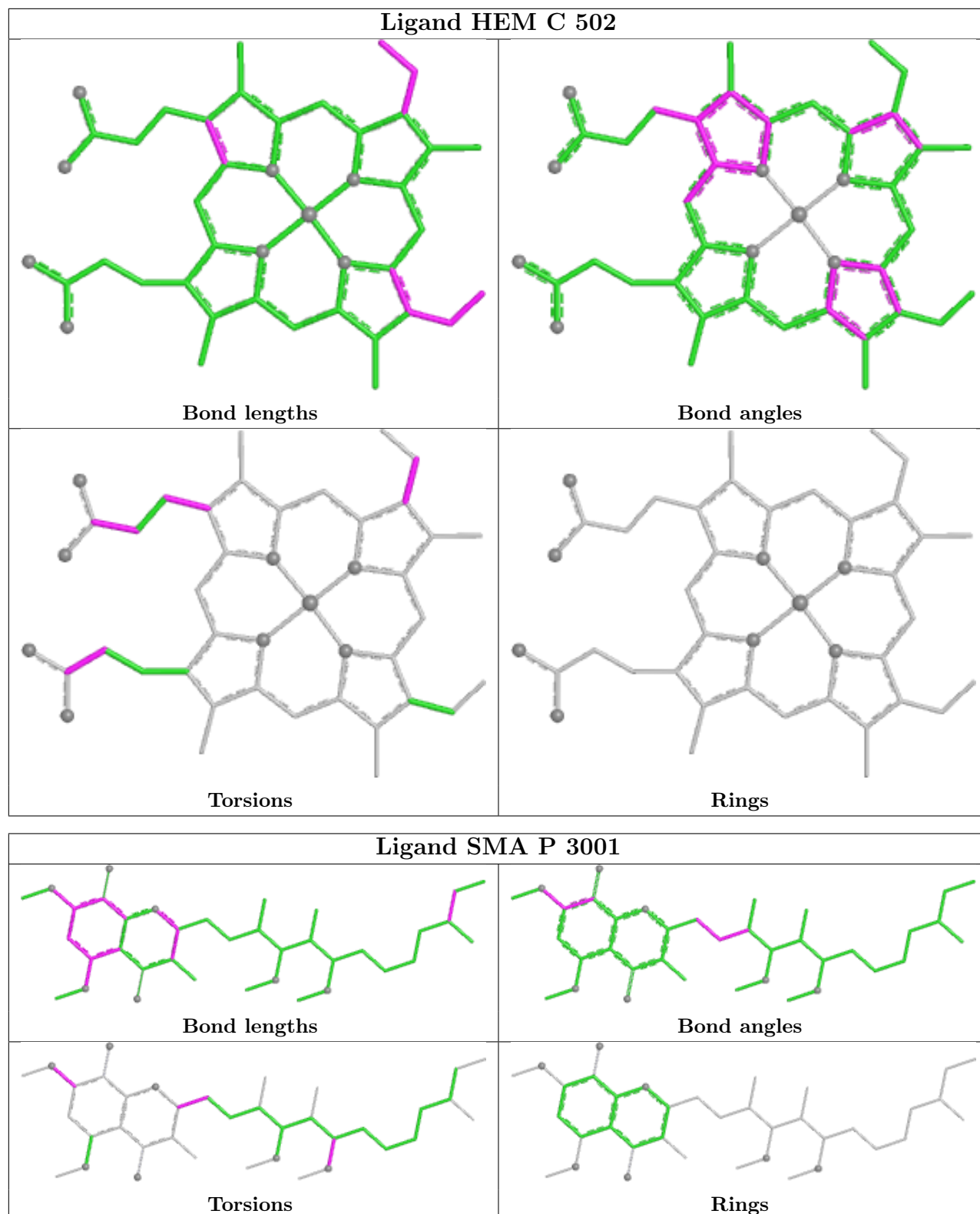
There are no ring outliers.

20 monomers are involved in 61 short contacts:

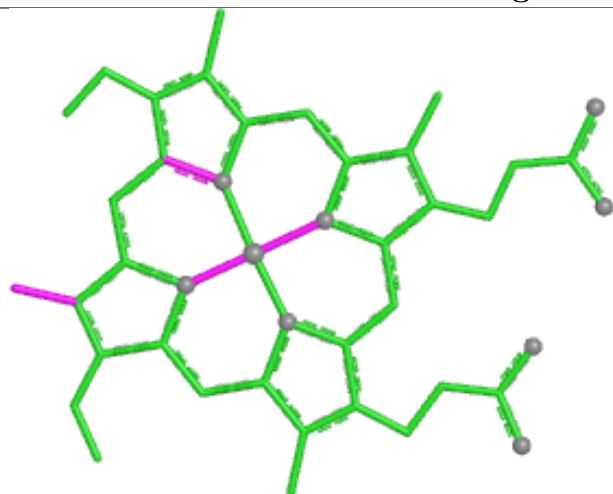
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	2005	PEE	4	0
19	R	501	FES	1	0
18	P	3004	CDL	3	0
15	C	2007	PEE	1	0
12	C	502	HEM	6	0
13	P	3001	SMA	4	0
14	P	3002	UQ	2	0
12	C	501	HEM	5	0
13	C	2001	SMA	4	0
18	S	3003	CDL	2	0
15	R	3005	PEE	4	0
20	E	2009	PLC	3	0
12	P	502	HEM	7	0
14	C	2002	UQ	4	0
12	P	501	HEM	5	0
15	P	3007	PEE	1	0
16	P	3011	GOL	1	0
18	G	2004	CDL	1	0
20	R	3009	PLC	2	0
18	D	2003	CDL	1	0

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

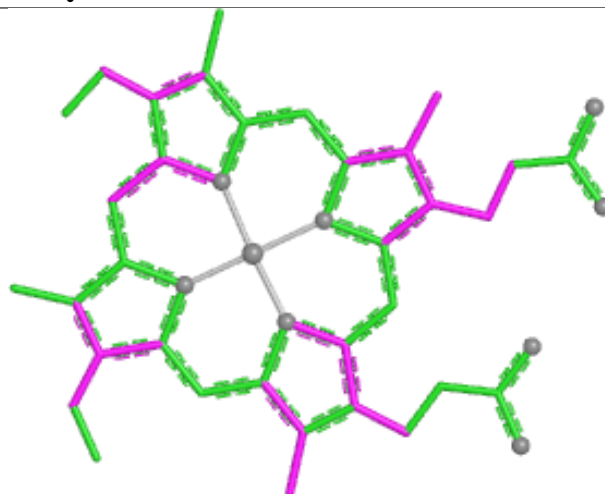




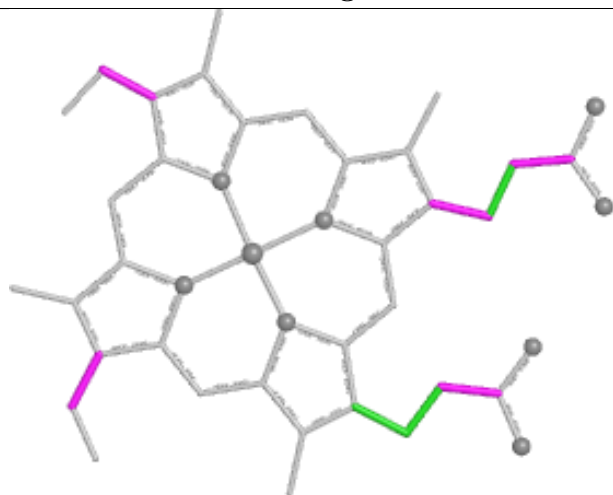
Ligand HEC Q 501



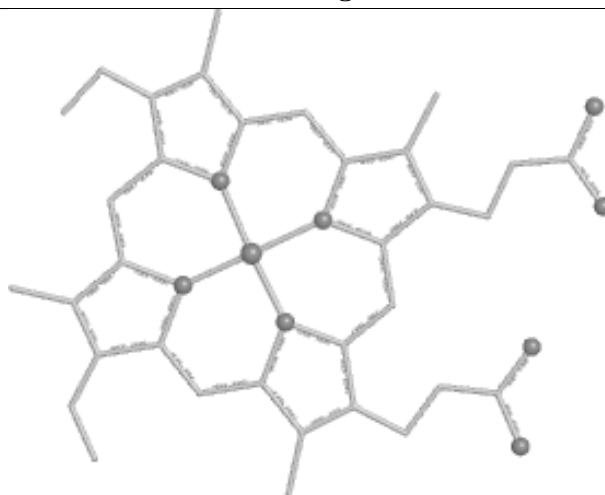
Bond lengths



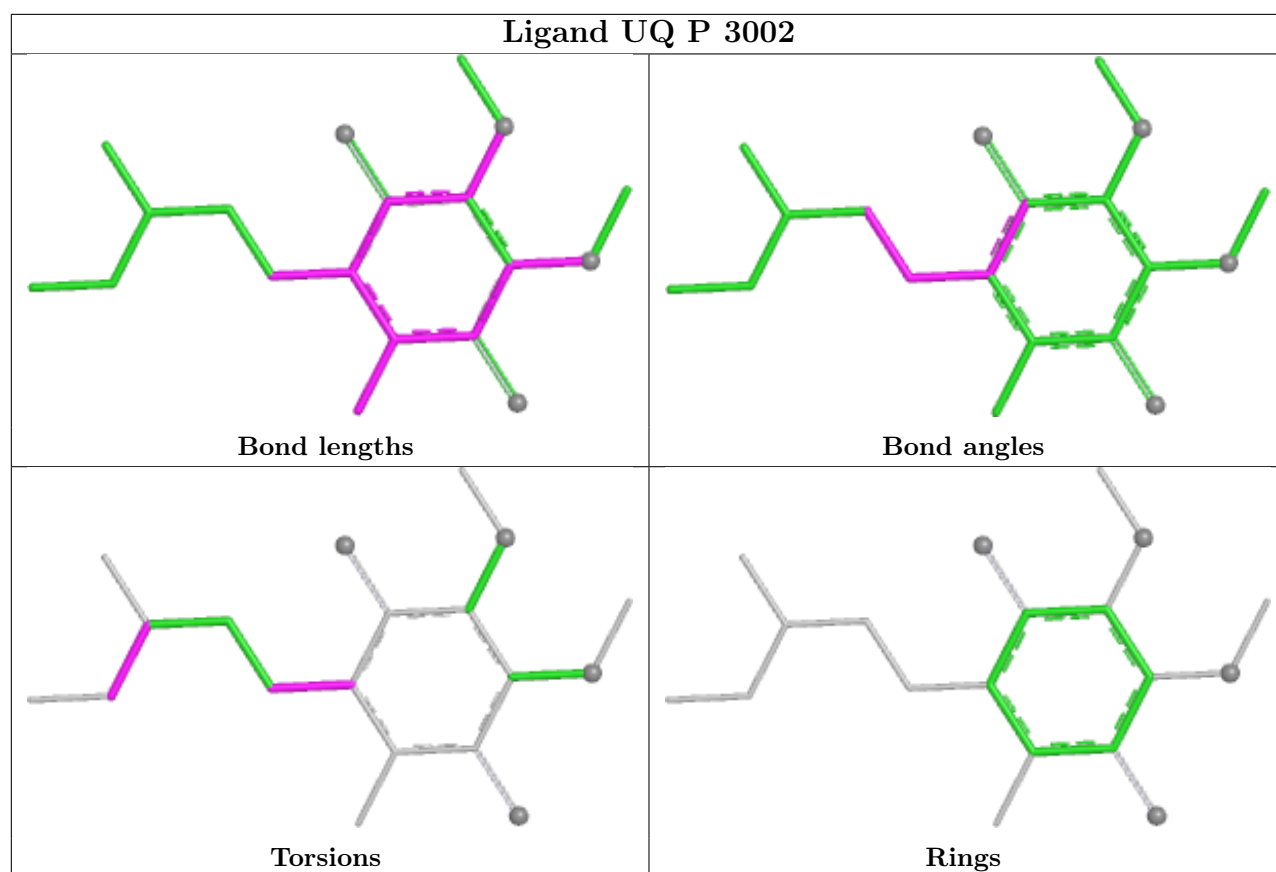
Bond angles

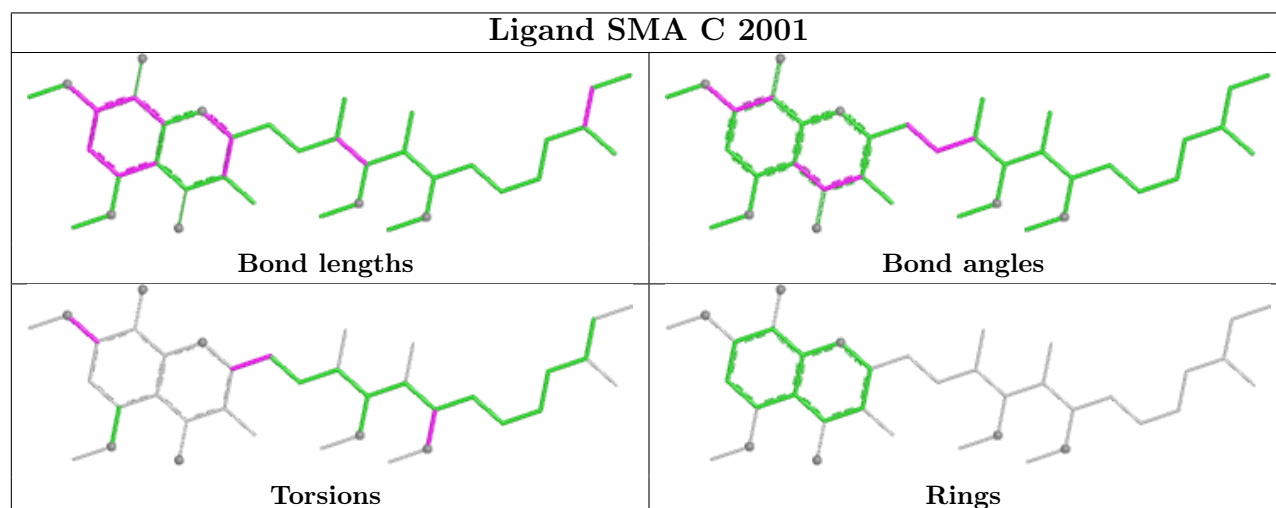
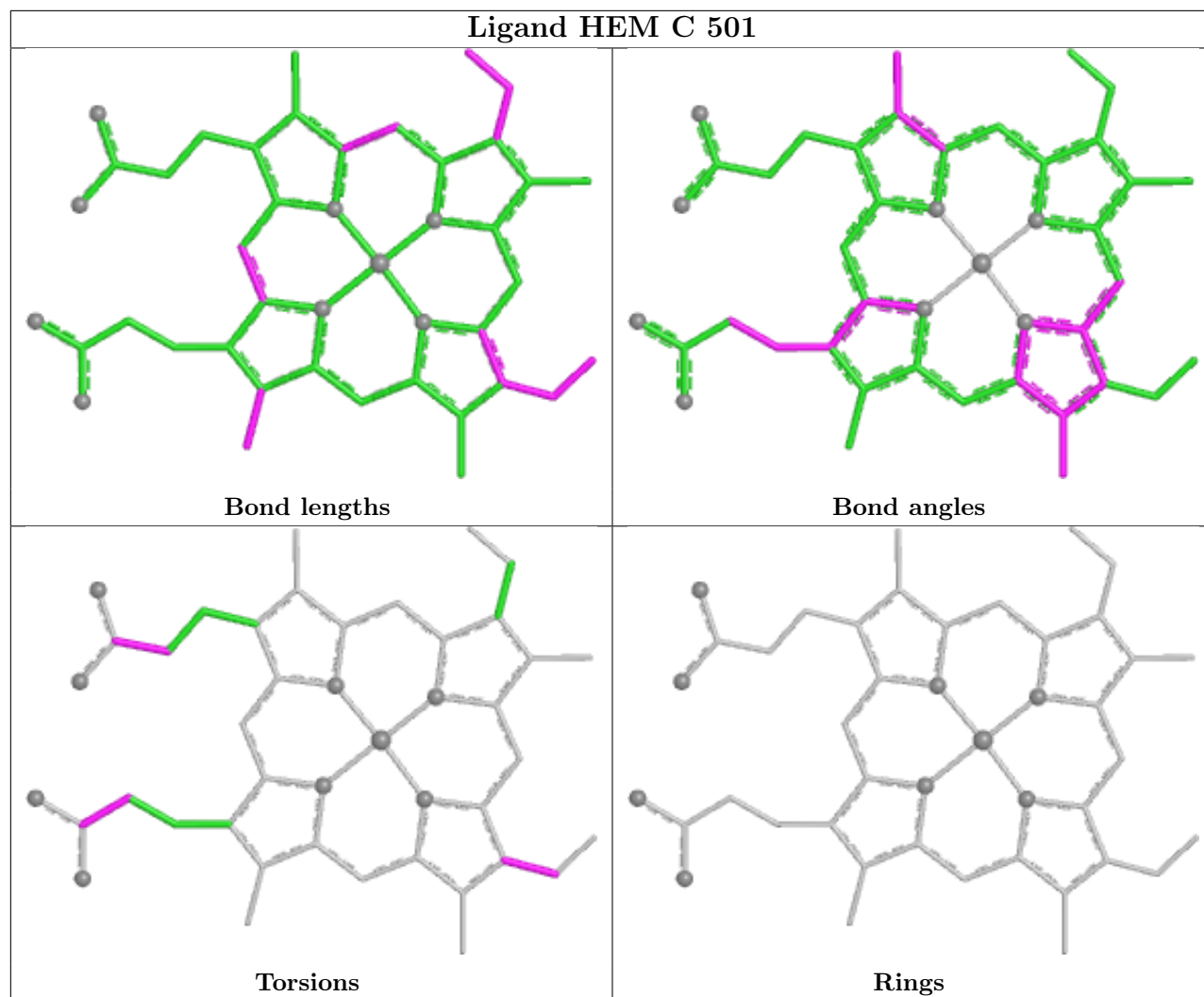


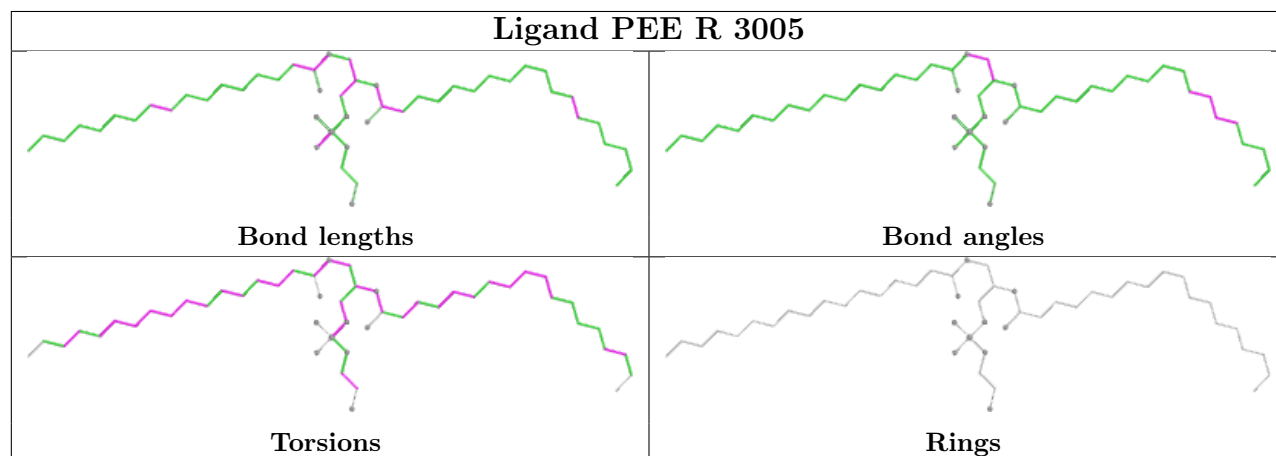
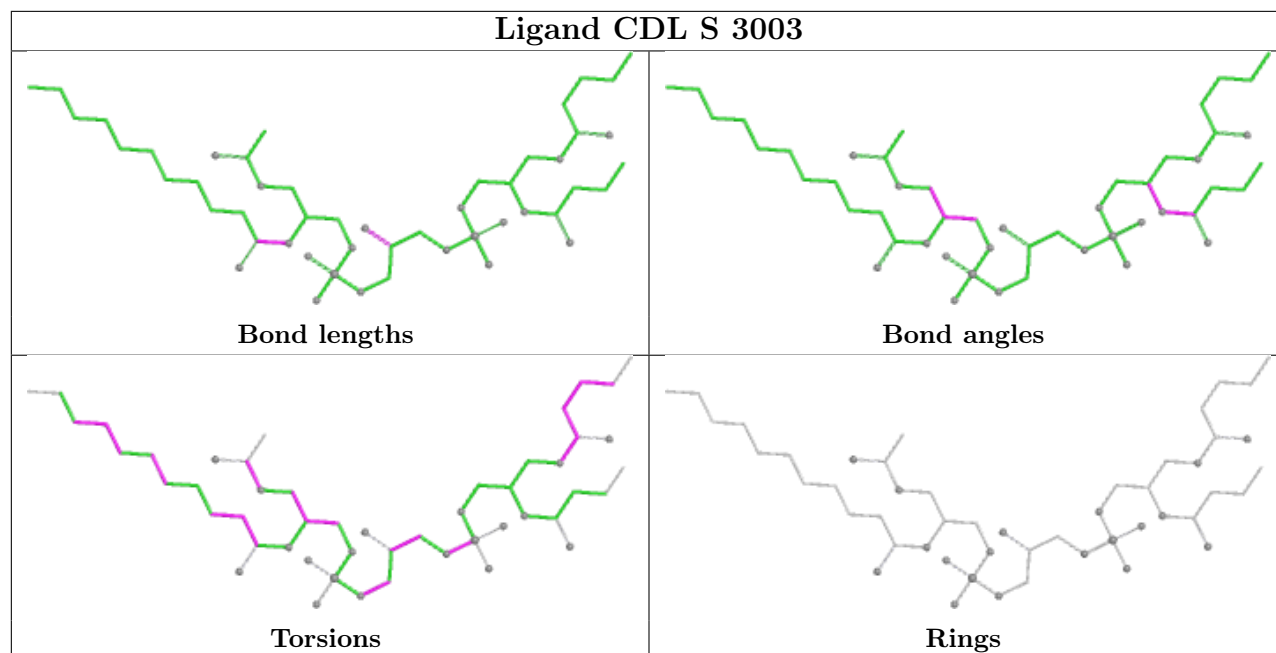
Torsions

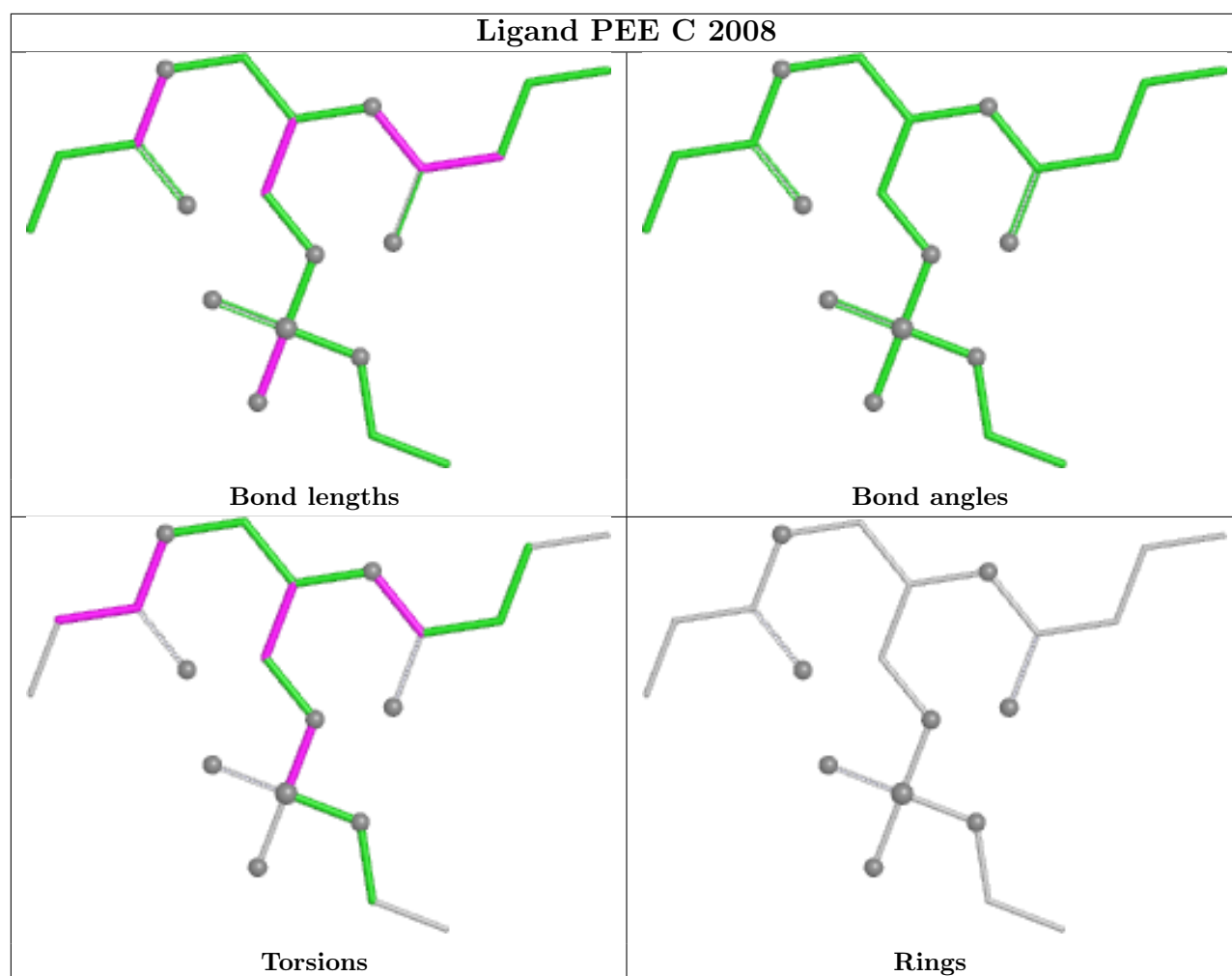


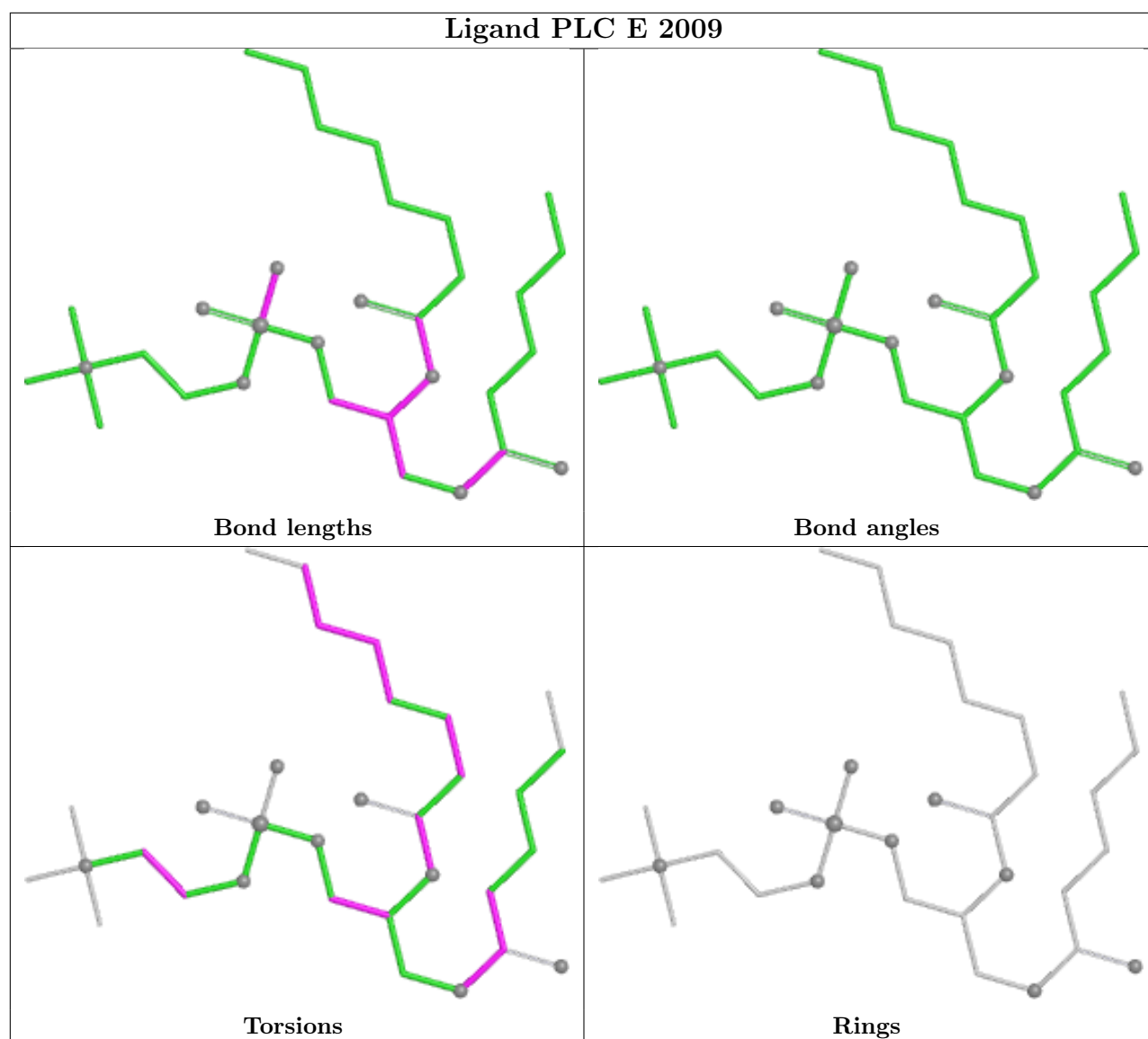
Rings

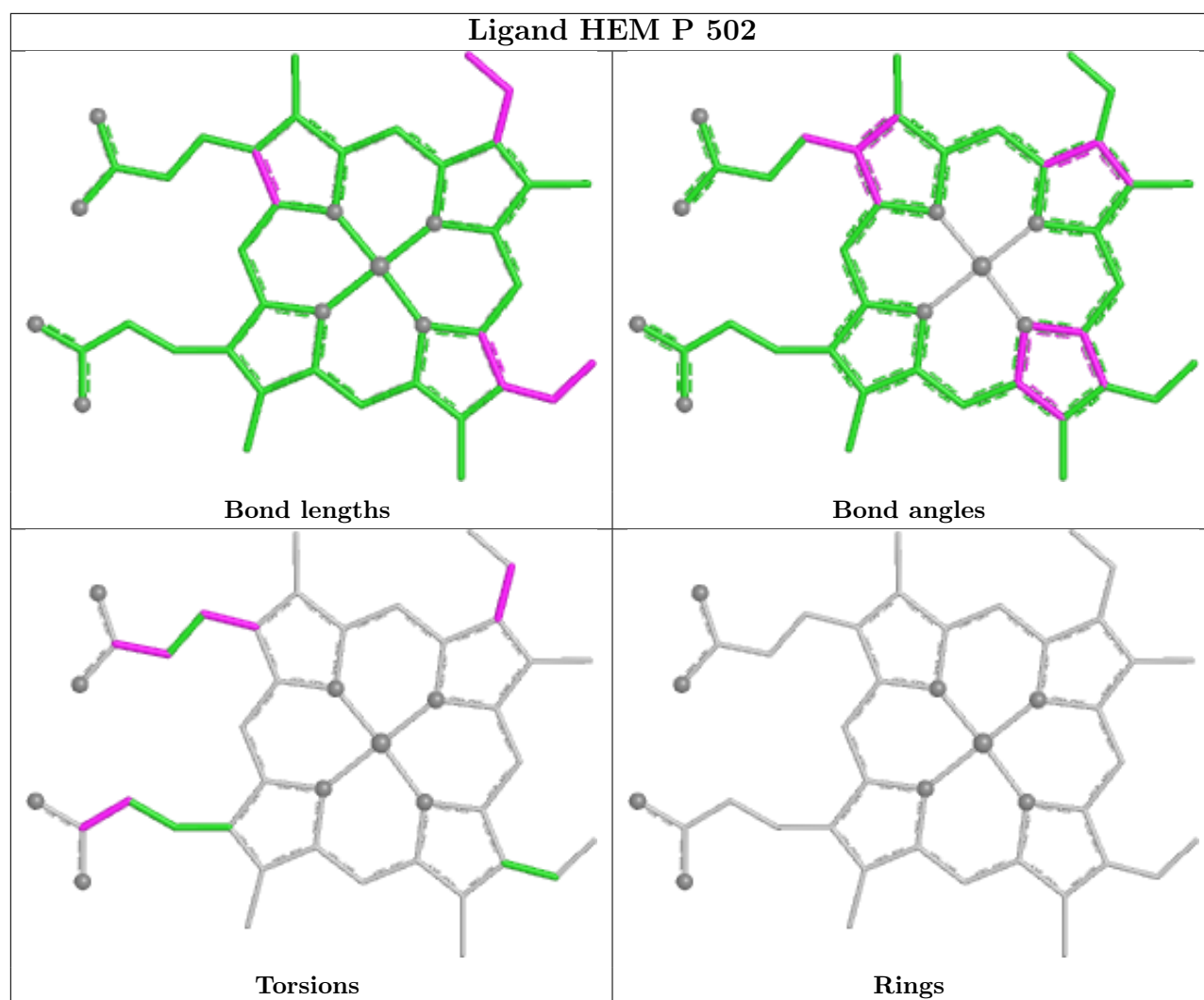


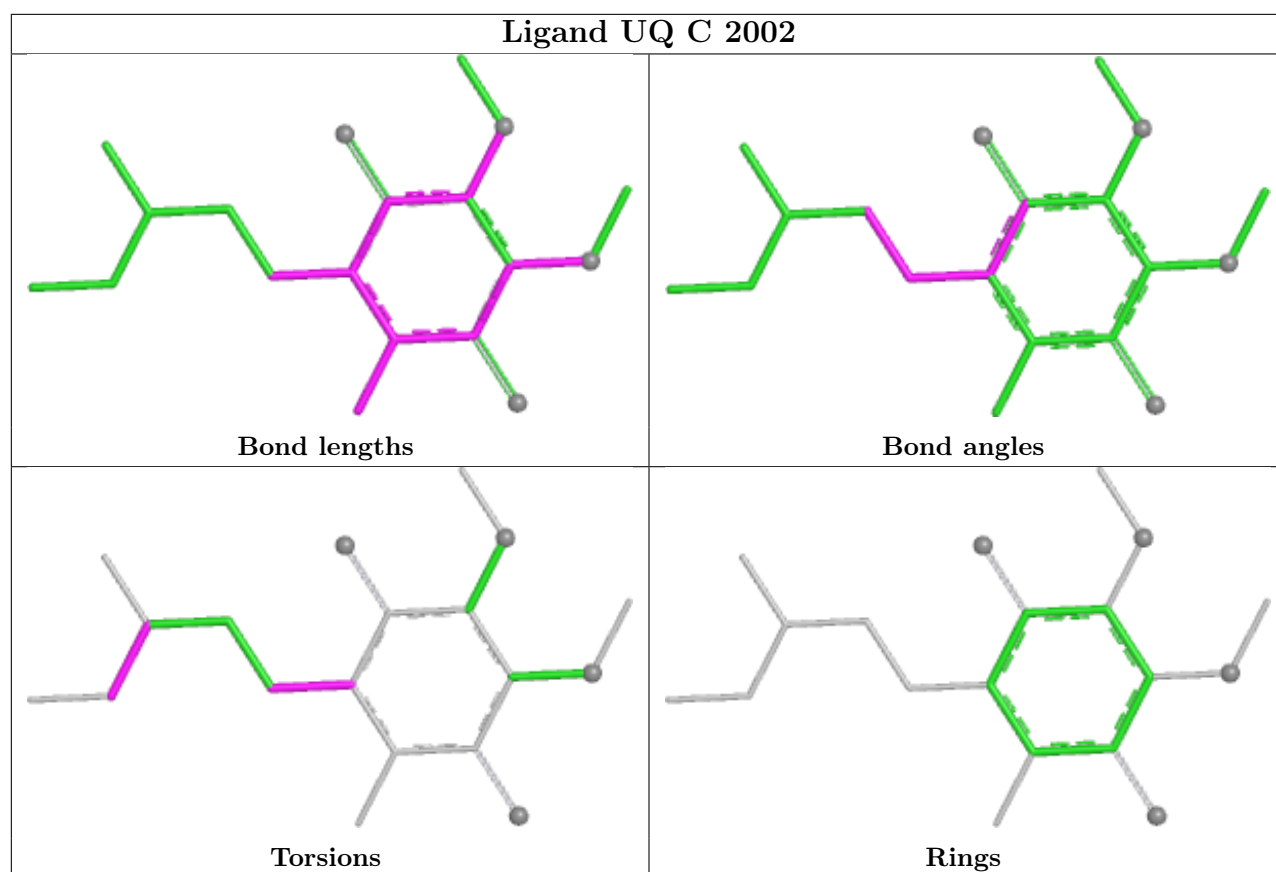




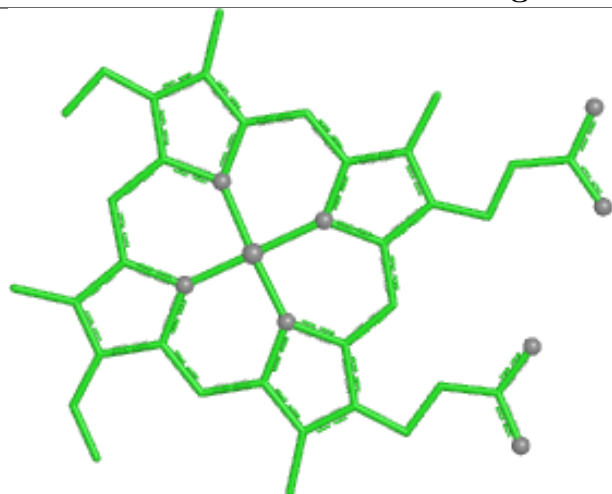




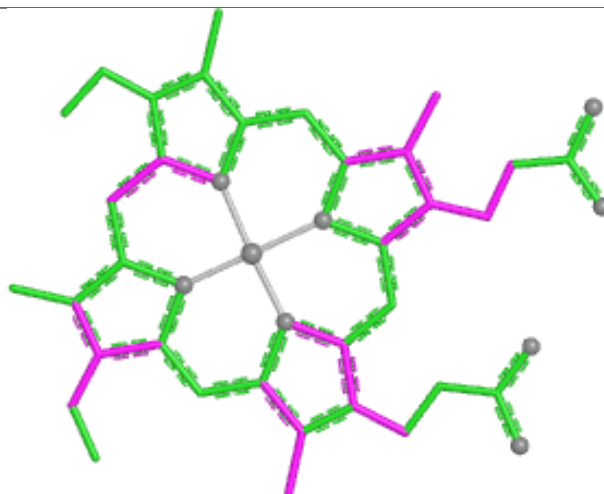




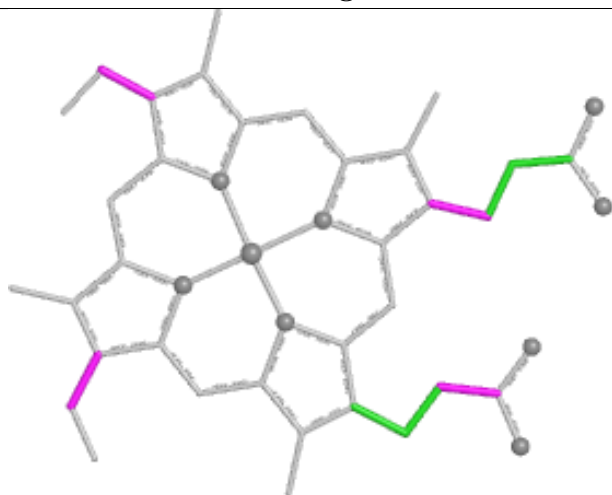
Ligand HEC D 501



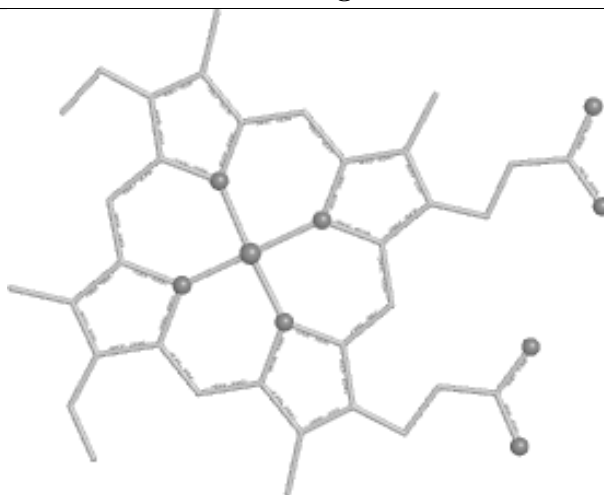
Bond lengths



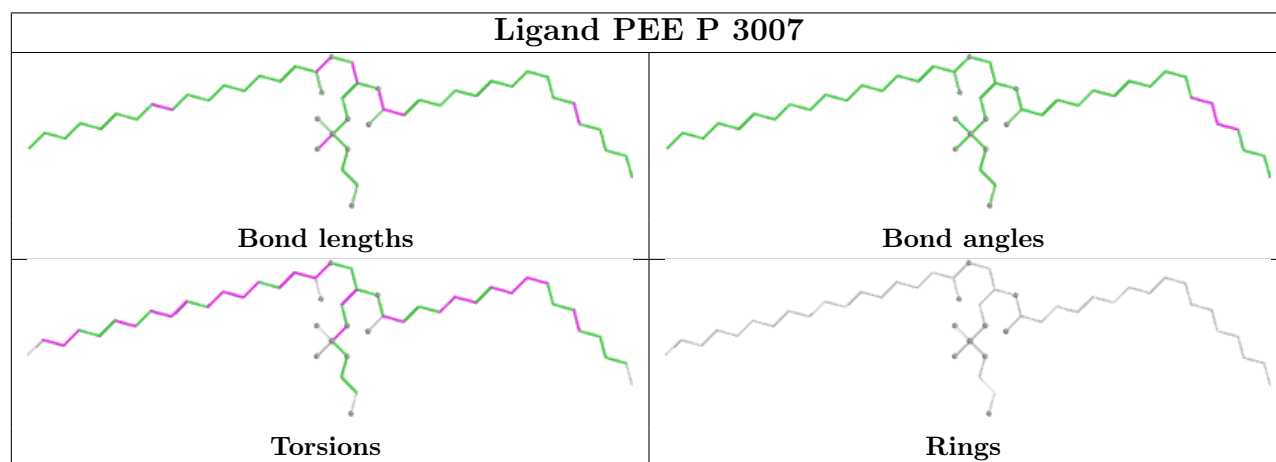
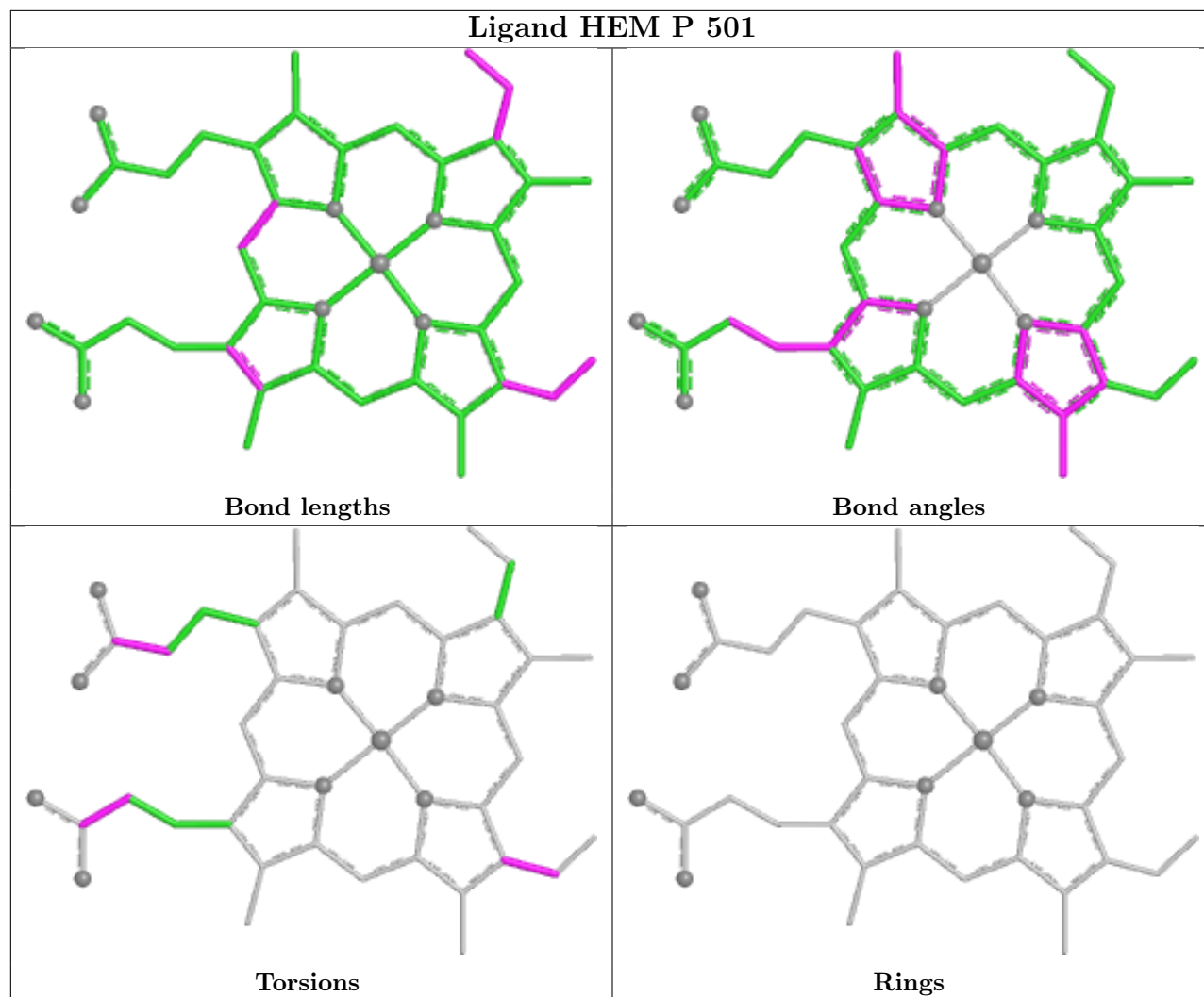
Bond angles

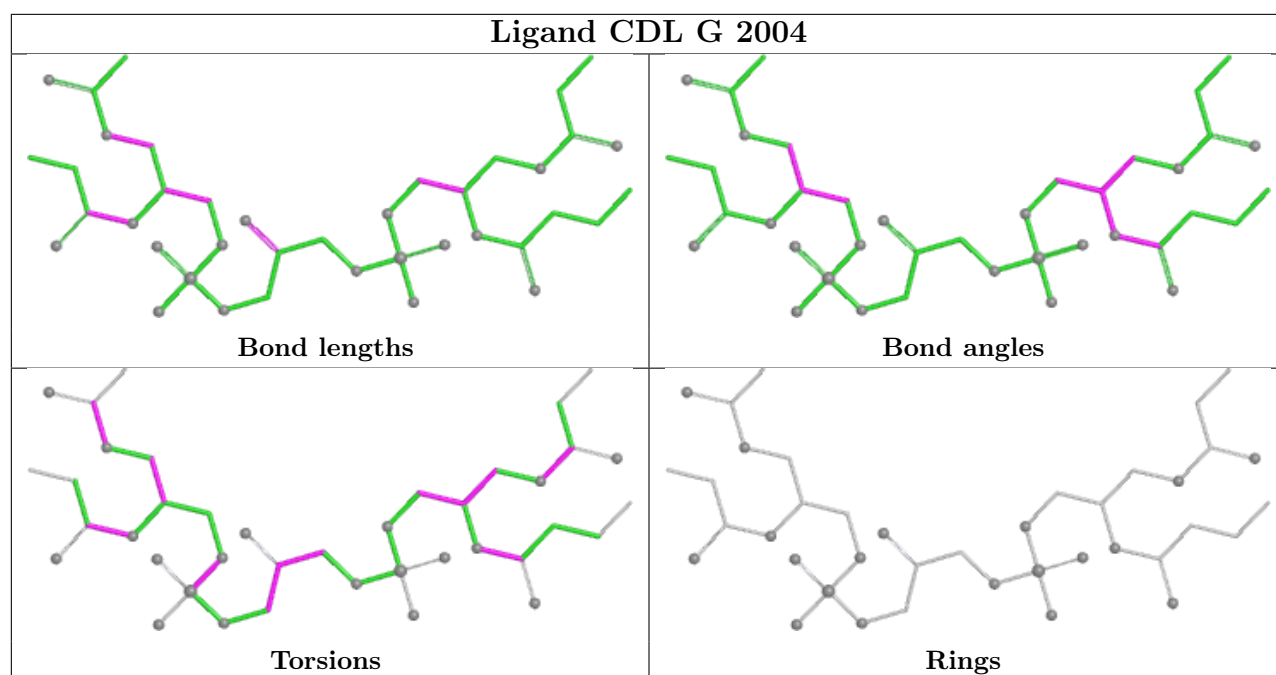


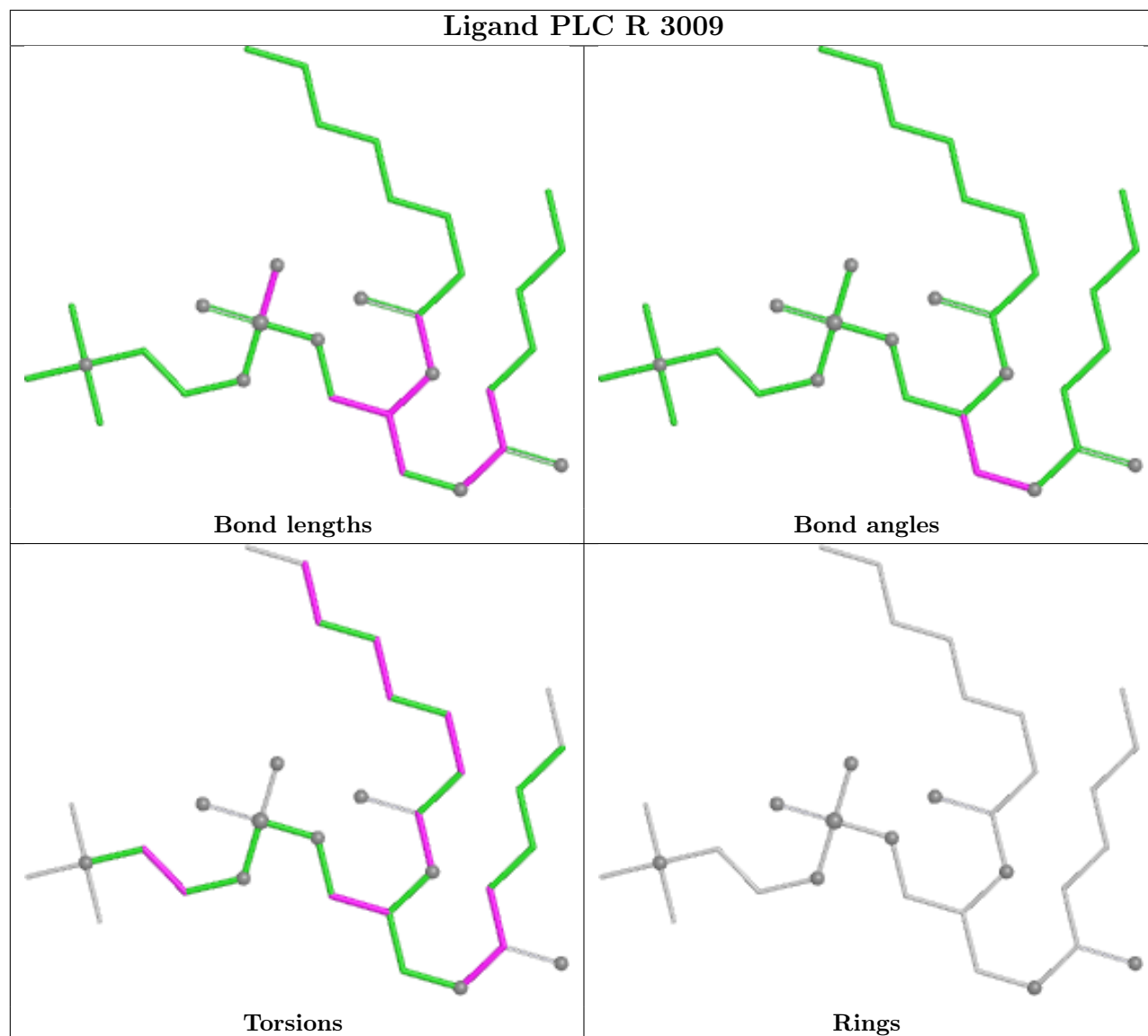
Torsions

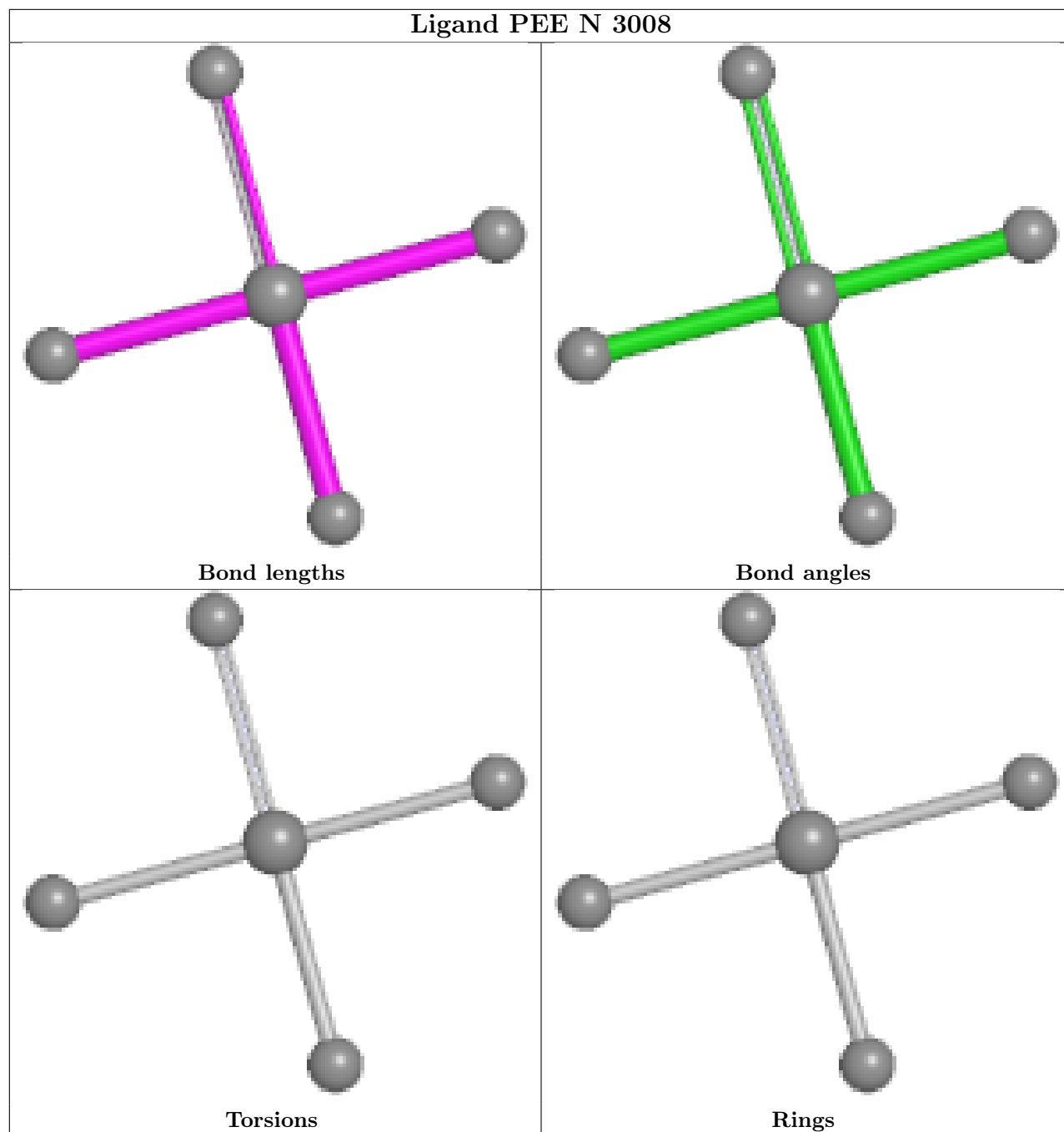


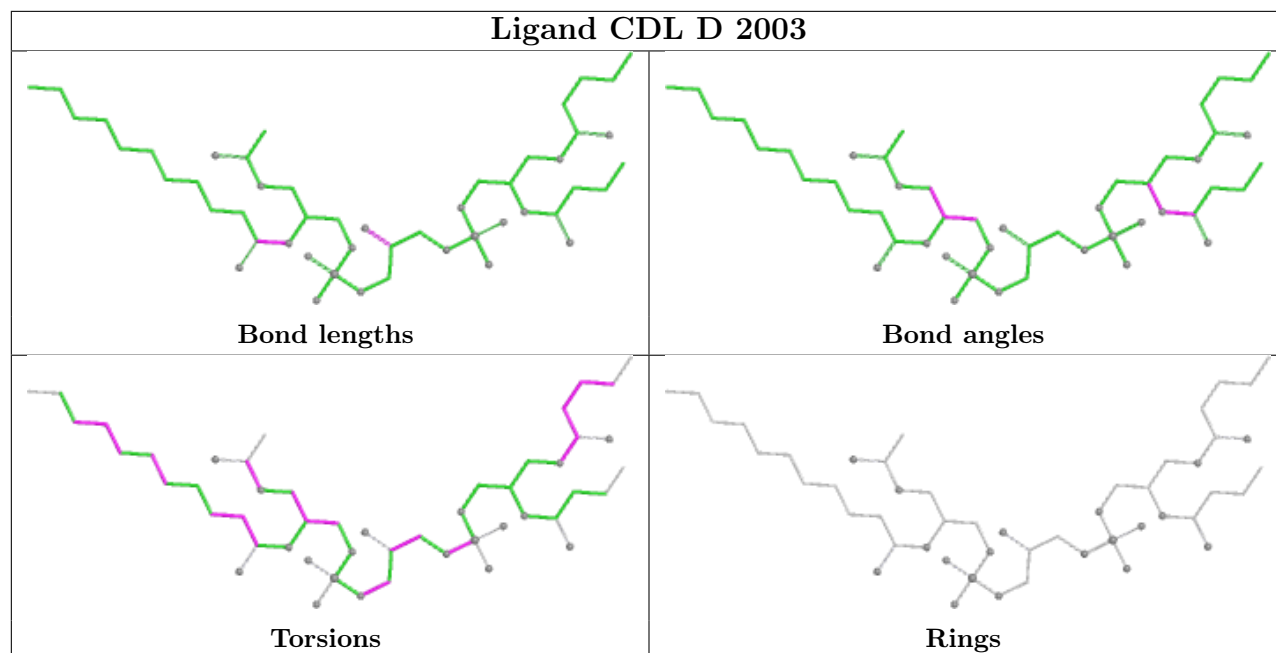
Rings











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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.01	2 (0%) 87 72	44, 77, 105, 114	0
1	N	442/446 (99%)	0.23	9 (2%) 65 41	54, 80, 102, 110	0
2	B	421/441 (95%)	0.43	14 (3%) 49 28	66, 93, 122, 140	0
2	O	422/441 (95%)	0.21	9 (2%) 63 40	52, 85, 111, 124	0
3	C	380/380 (100%)	-0.44	4 (1%) 78 57	33, 49, 84, 140	0
3	P	379/380 (99%)	0.06	11 (2%) 53 31	44, 75, 99, 119	0
4	D	241/241 (100%)	-0.44	0 100 100	42, 55, 86, 114	0
4	Q	241/241 (100%)	0.36	8 (3%) 49 28	59, 86, 112, 127	0
5	E	196/196 (100%)	0.62	16 (8%) 17 9	48, 113, 165, 172	0
5	R	196/196 (100%)	0.38	3 (1%) 72 49	54, 85, 134, 151	0
6	F	101/110 (91%)	-0.50	0 100 100	37, 53, 67, 99	0
6	S	101/110 (91%)	0.11	0 100 100	64, 84, 112, 141	0
7	G	81/81 (100%)	0.09	2 (2%) 58 35	48, 62, 94, 113	0
7	T	79/81 (97%)	0.70	7 (8%) 15 8	69, 95, 147, 164	0
8	H	70/77 (90%)	0.05	1 (1%) 73 51	48, 73, 90, 133	0
8	U	67/77 (87%)	1.03	8 (11%) 9 5	102, 125, 148, 154	0
9	I	31/47 (65%)	2.41	18 (58%) 0 0	94, 127, 172, 178	0
9	V	31/47 (65%)	2.61	21 (67%) 0 0	93, 125, 184, 184	0
10	J	61/61 (100%)	-0.12	1 (1%) 70 47	57, 71, 109, 151	0
10	W	59/61 (96%)	0.14	0 100 100	69, 85, 101, 117	0
All	All	4042/4160 (97%)	0.16	134 (3%) 49 28	33, 79, 125, 184	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	49	LEU	6.5
1	A	444	ILE	5.9
9	V	61	ARG	5.8
9	I	63	ASP	5.5
9	V	50	LEU	5.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	PEE	N	3008	5/51	0.72	0.13	135,135,136,136	0
15	PEE	C	2008	21/51	0.77	0.23	139,142,144,144	0
18	CDL	P	3004	40/100	0.81	0.22	106,114,120,121	0
18	CDL	S	3003	50/100	0.81	0.30	126,140,153,153	0
20	PLC	E	2009	32/42	0.81	0.24	67,83,97,98	0
11	UNL	E	3103	1/-	0.83	0.14	45,45,45,45	0
18	CDL	D	2003	50/100	0.84	0.25	79,112,130,131	0
18	CDL	G	2004	40/100	0.85	0.17	81,90,97,98	0
11	UNL	A	3016	1/-	0.86	0.23	55,55,55,55	0
20	PLC	R	3009	32/42	0.86	0.26	91,99,116,116	0
14	UQ	P	3002	19/63	0.89	0.28	116,121,122,122	0
15	PEE	E	2005	50/51	0.90	0.19	76,90,95,95	0
14	UQ	C	2002	19/63	0.90	0.26	85,88,90,91	0
15	PEE	R	3005	50/51	0.90	0.20	95,108,116,119	0
15	PEE	P	3007	49/51	0.91	0.20	73,98,107,108	0
11	UNL	C	3015	1/-	0.91	0.12	47,47,47,47	0
15	PEE	C	2007	49/51	0.92	0.17	52,68,87,89	0
11	UNL	P	2015	1/-	0.92	0.10	33,33,33,33	0
11	UNL	P	3104	1/-	0.93	0.08	59,59,59,59	0

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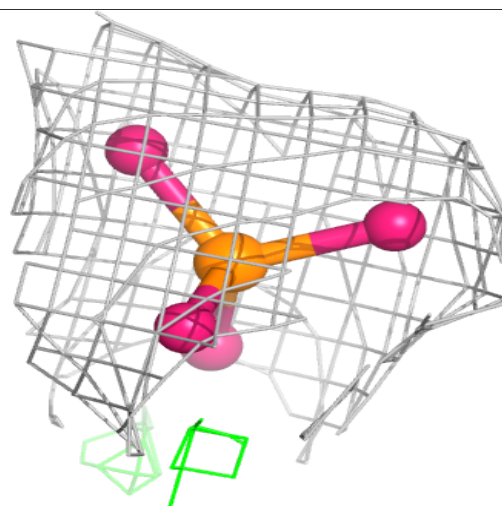
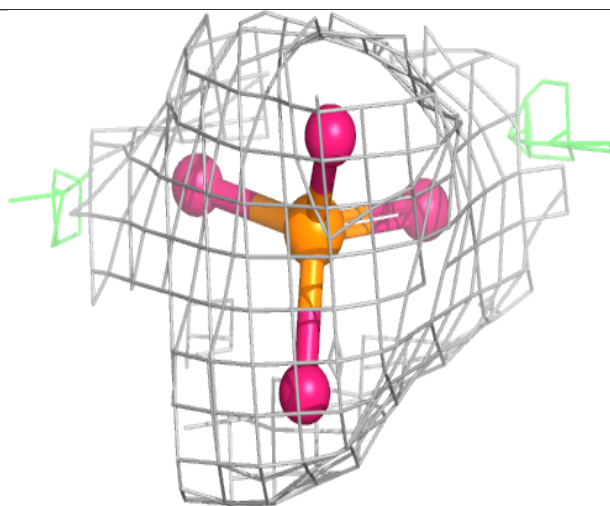
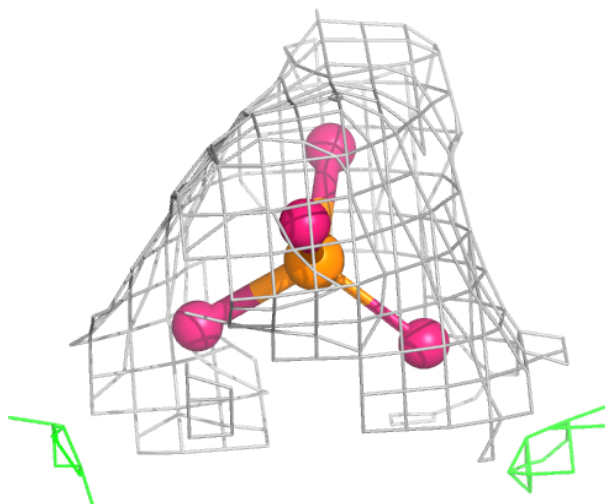
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	GOL	C	2011	6/6	0.94	0.18	79,81,82,83	0
16	GOL	P	3011	6/6	0.94	0.18	69,71,72,72	0
11	UNL	E	2105	1/-	0.95	0.07	62,62,62,62	0
11	UNL	R	2103	1/-	0.95	0.12	45,45,45,45	0
11	UNL	C	2104	1/-	0.96	0.11	71,71,71,71	0
13	SMA	P	3001	37/37	0.96	0.12	67,73,75,78	0
11	UNL	C	2010	1/-	0.97	0.22	53,53,53,53	0
11	UNL	P	3010	1/-	0.97	0.22	67,67,67,67	0
12	HEM	P	501	43/43	0.97	0.10	56,61,69,75	0
17	HEC	Q	501	43/43	0.97	0.10	67,71,76,78	0
13	SMA	C	2001	37/37	0.97	0.09	41,44,46,52	0
19	FES	E	501	4/4	0.98	0.05	92,93,95,95	0
17	HEC	D	501	43/43	0.98	0.07	44,46,50,53	0
12	HEM	C	501	43/43	0.98	0.08	44,48,50,53	0
12	HEM	P	502	43/43	0.99	0.06	59,63,71,77	0
12	HEM	C	502	43/43	0.99	0.06	34,40,50,54	0
19	FES	R	501	4/4	1.00	0.02	52,54,56,57	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.

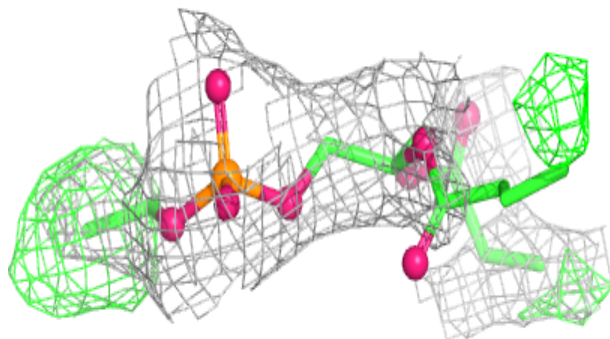
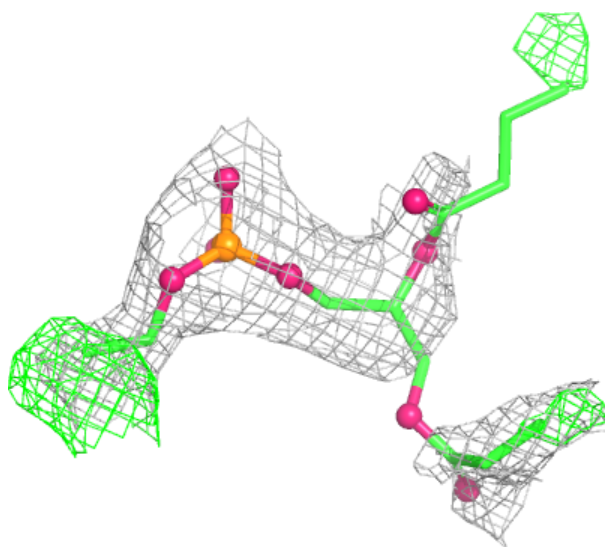
Electron density around PEE N 3008:

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



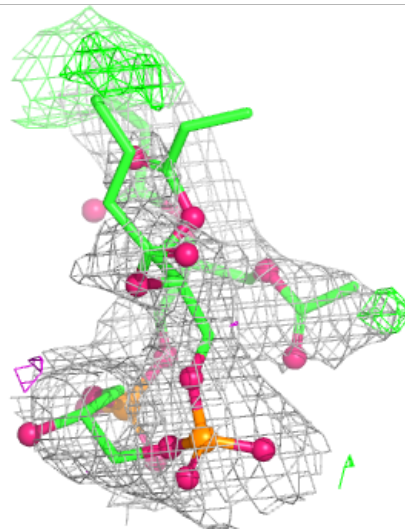
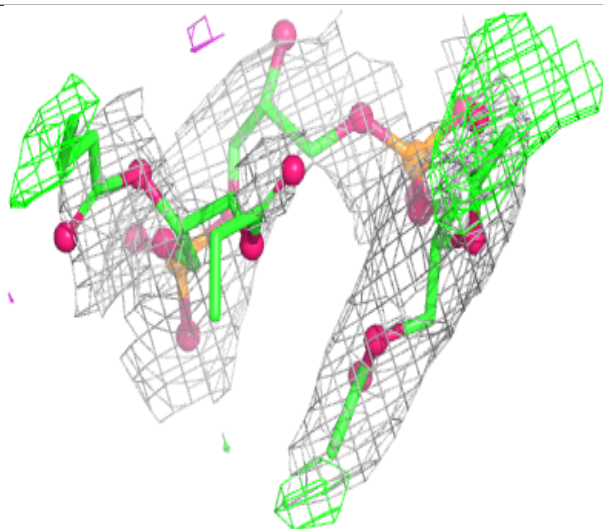
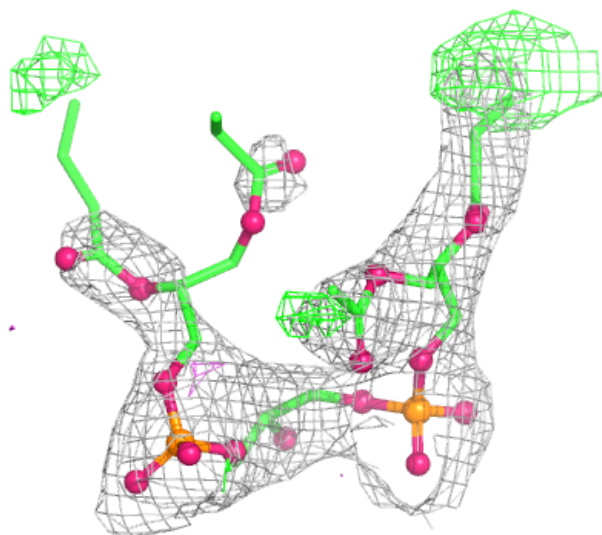
Electron density around PEE C 2008:

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



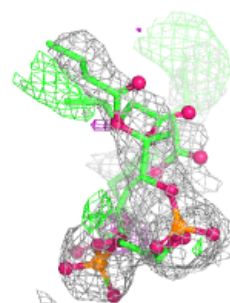
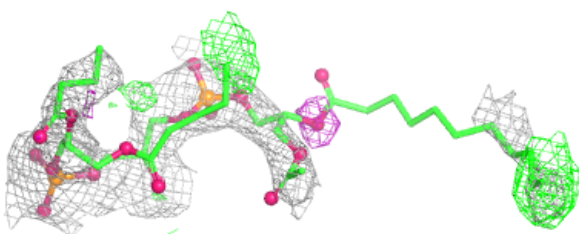
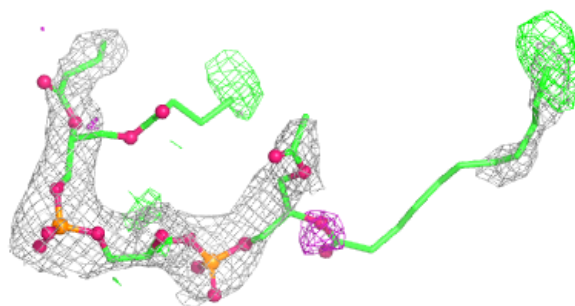
Electron density around CDL P 3004:

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

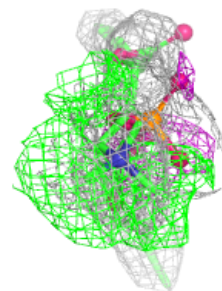
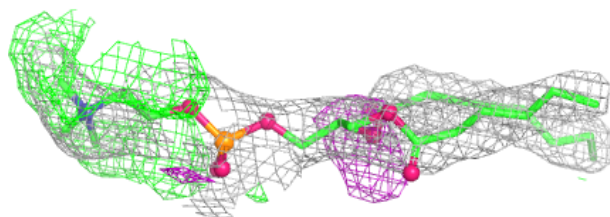
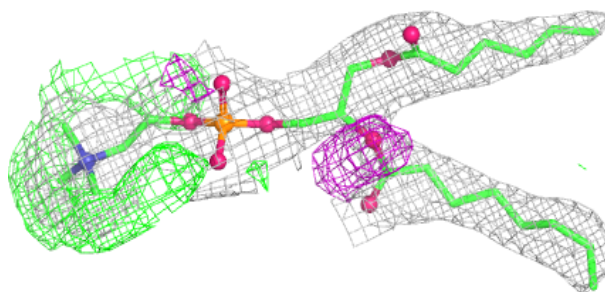


Electron density around CDL S 3003:

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

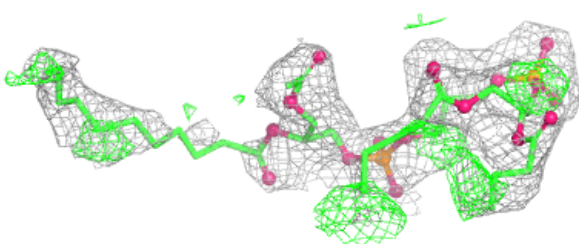
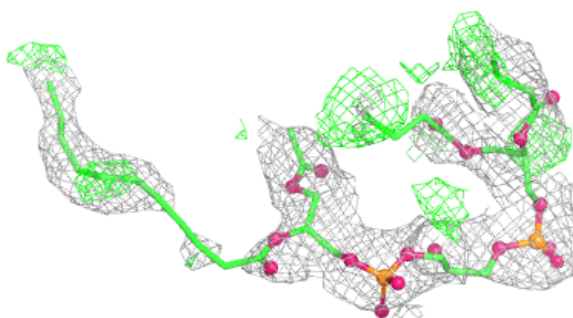
**Electron density around PLC E 2009:**

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



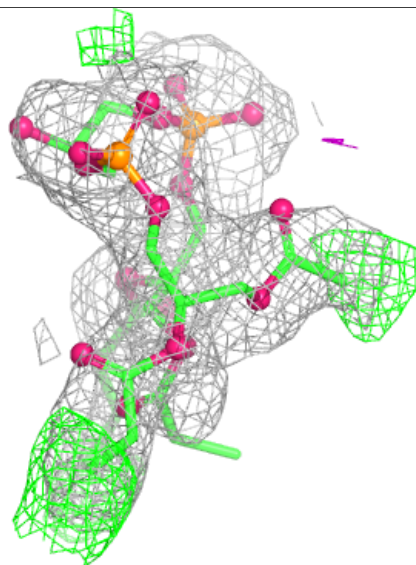
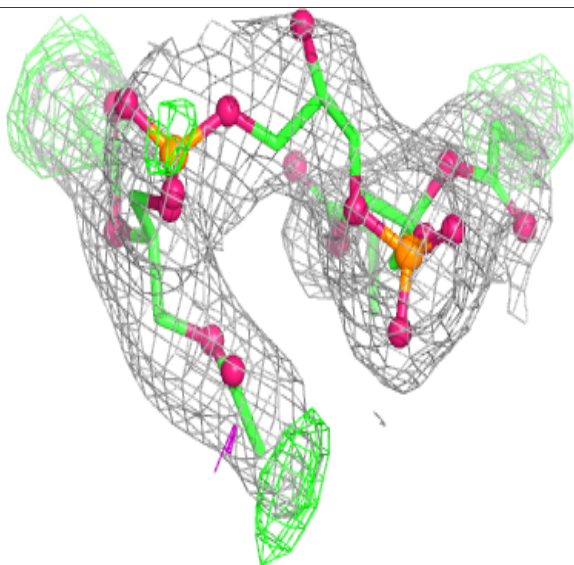
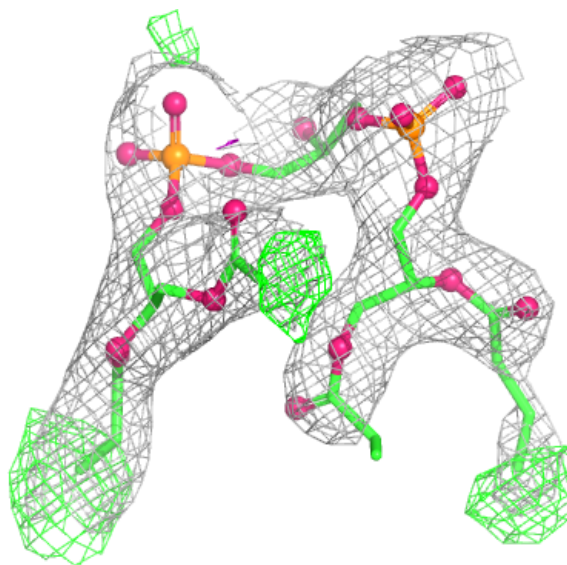
Electron density around CDL D 2003:

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



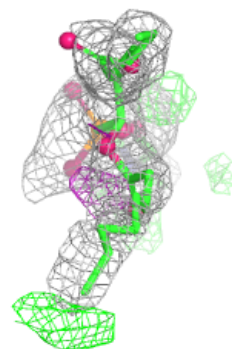
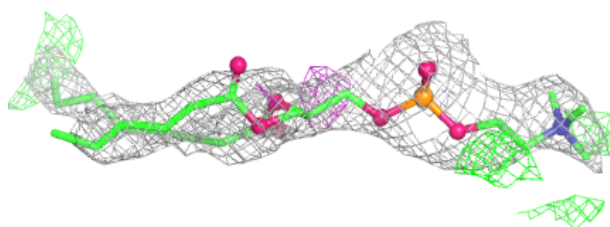
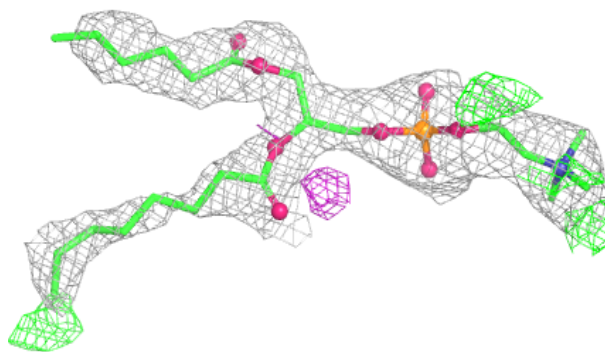
Electron density around CDL G 2004:

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

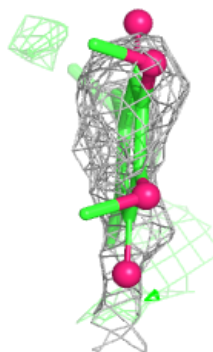
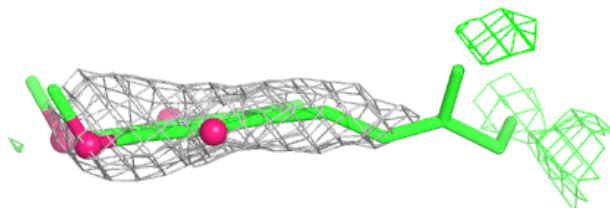
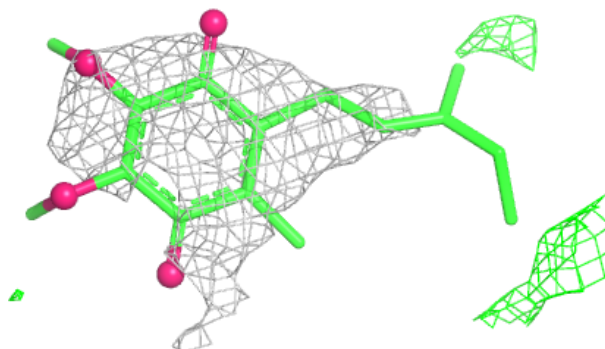


Electron density around PLC R 3009:

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

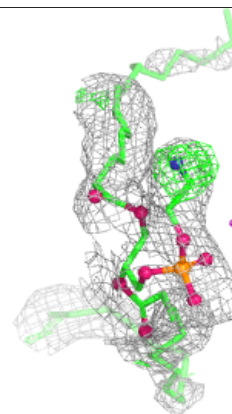
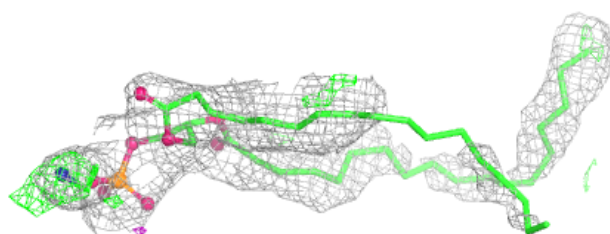
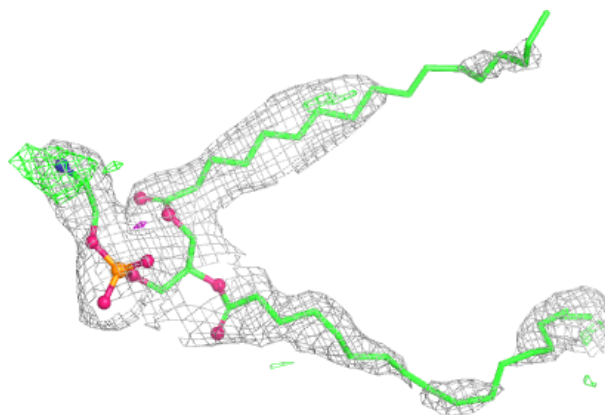
**Electron density around UQ P 3002:**

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

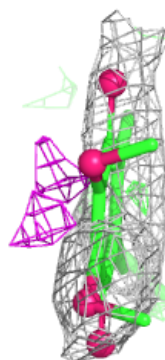
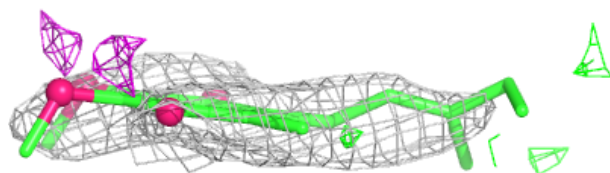
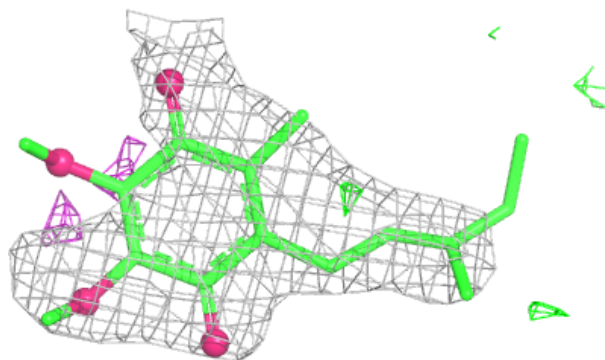


Electron density around PEE E 2005:

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

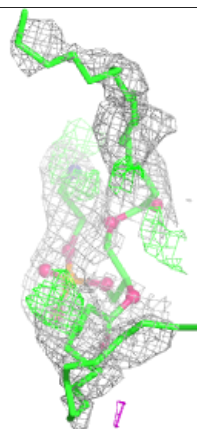
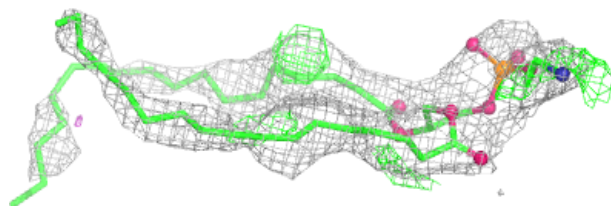
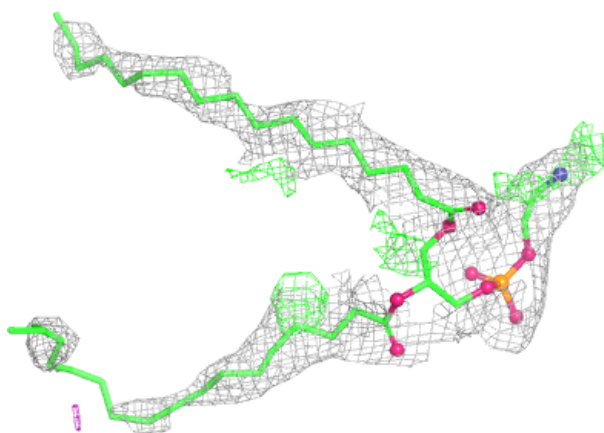
**Electron density around UQ C 2002:**

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

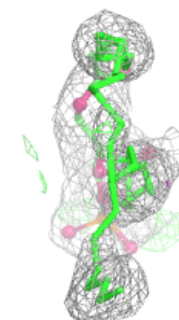
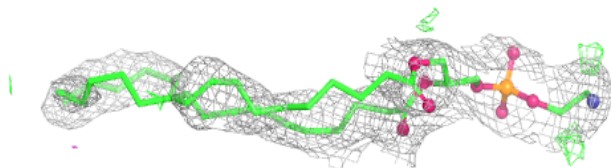
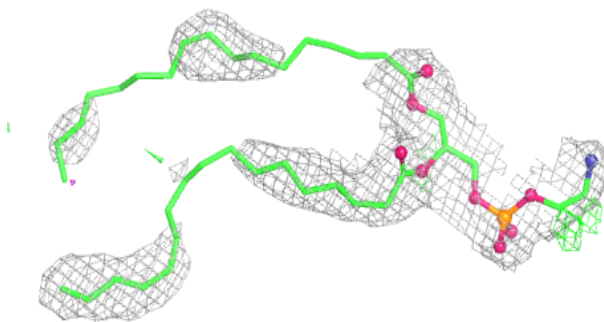


Electron density around PEE R 3005:

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

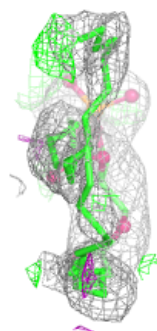
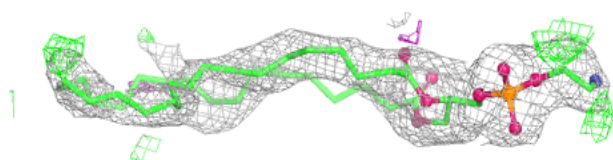
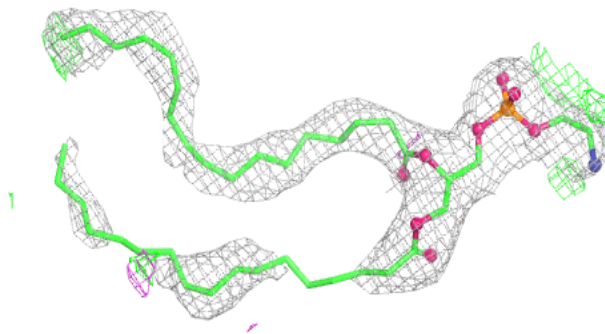
**Electron density around PEE P 3007:**

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

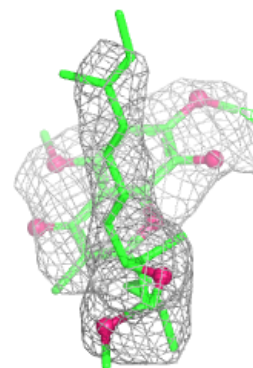
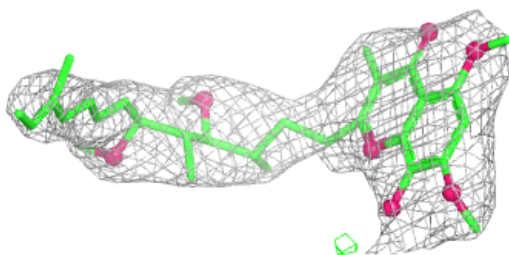
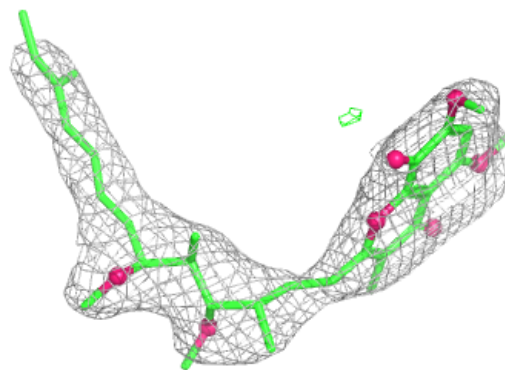


Electron density around PEE C 2007:

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

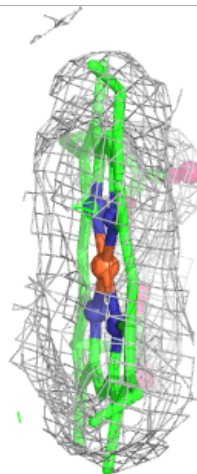
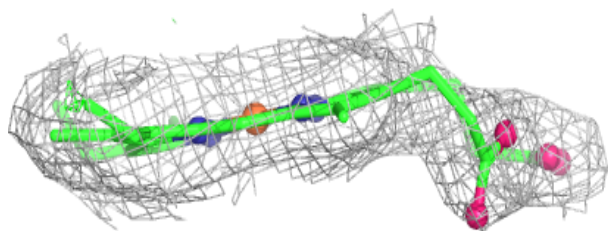
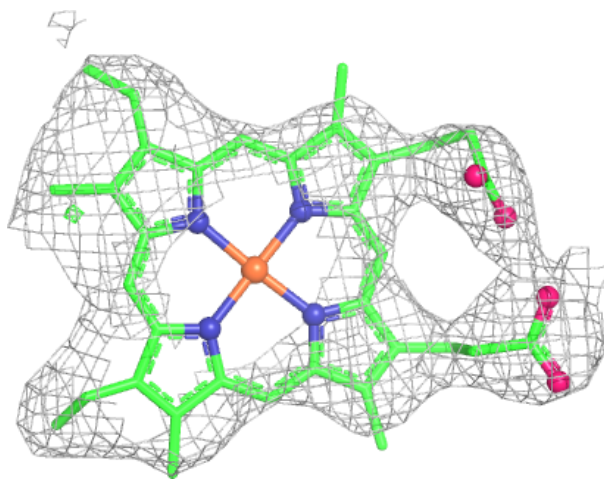
**Electron density around SMA P 3001:**

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



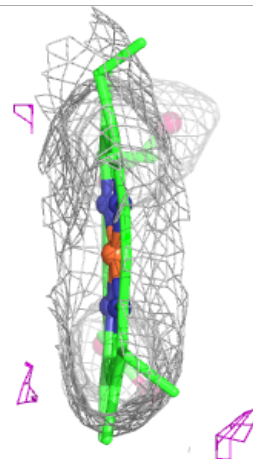
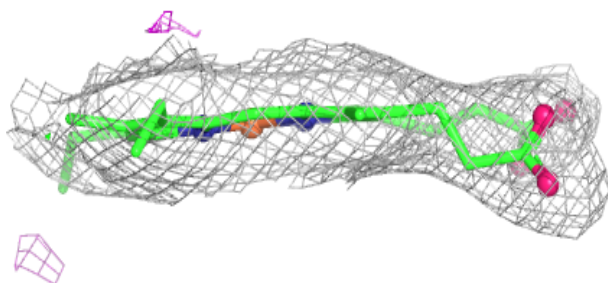
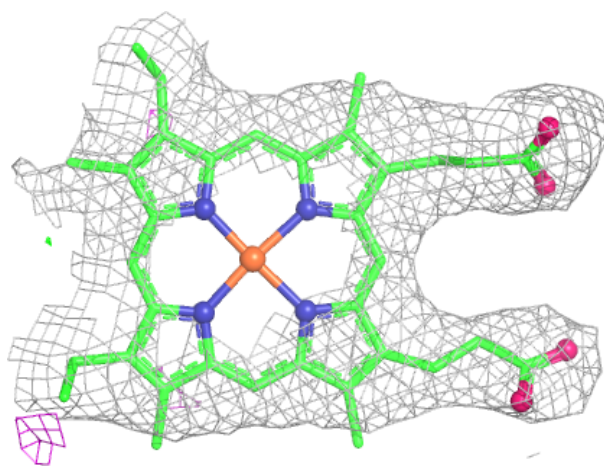
Electron density around HEM P 501:

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



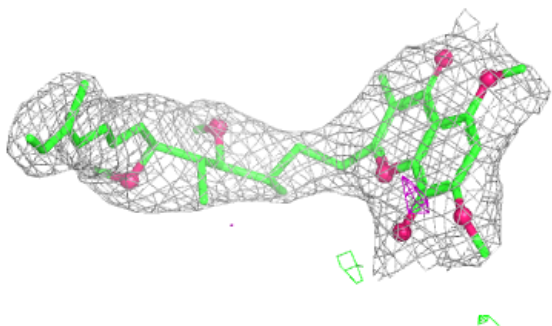
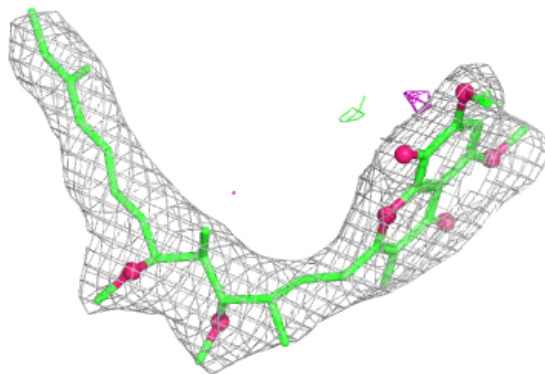
Electron density around HEC Q 501:

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



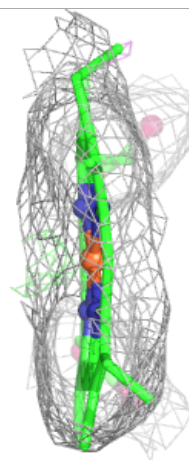
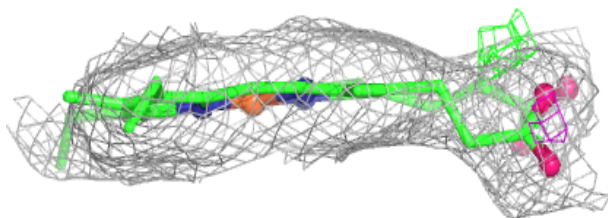
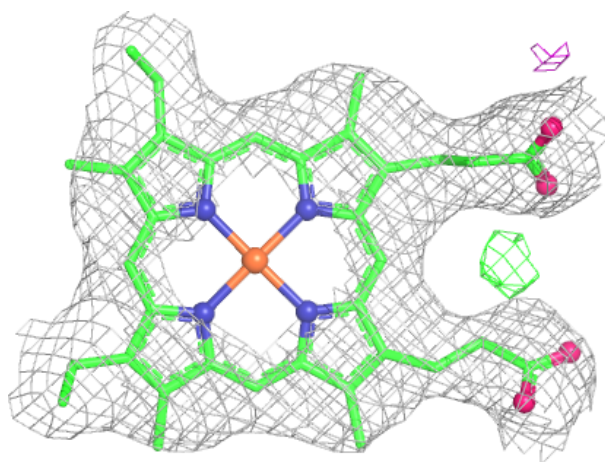
Electron density around SMA C 2001:

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



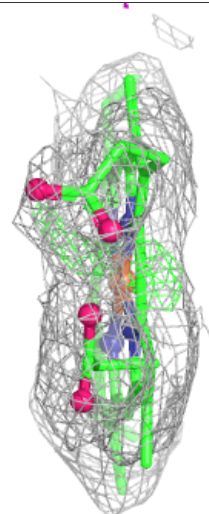
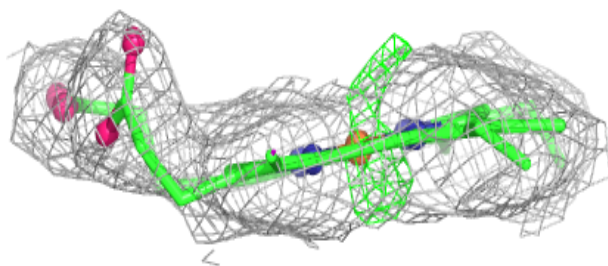
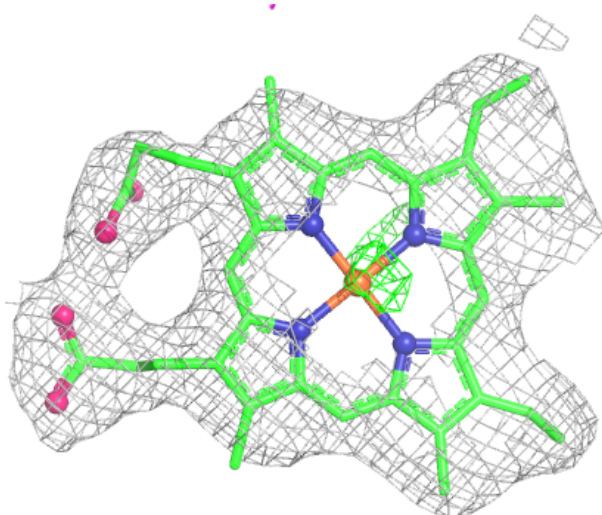
Electron density around HEC D 501:

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



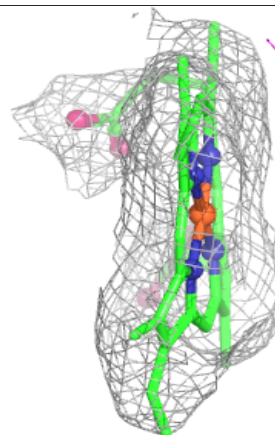
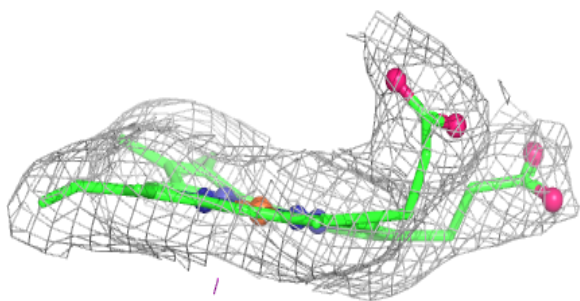
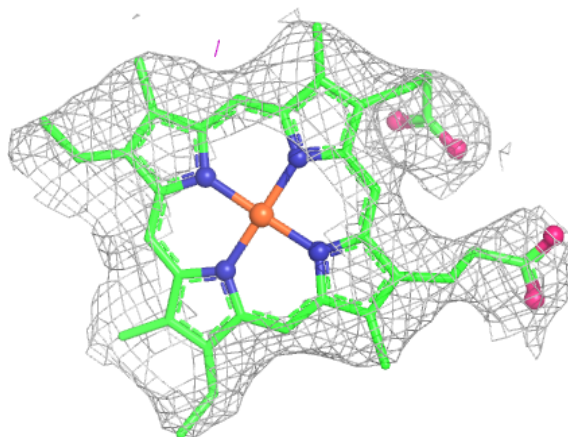
Electron density around HEM C 501:

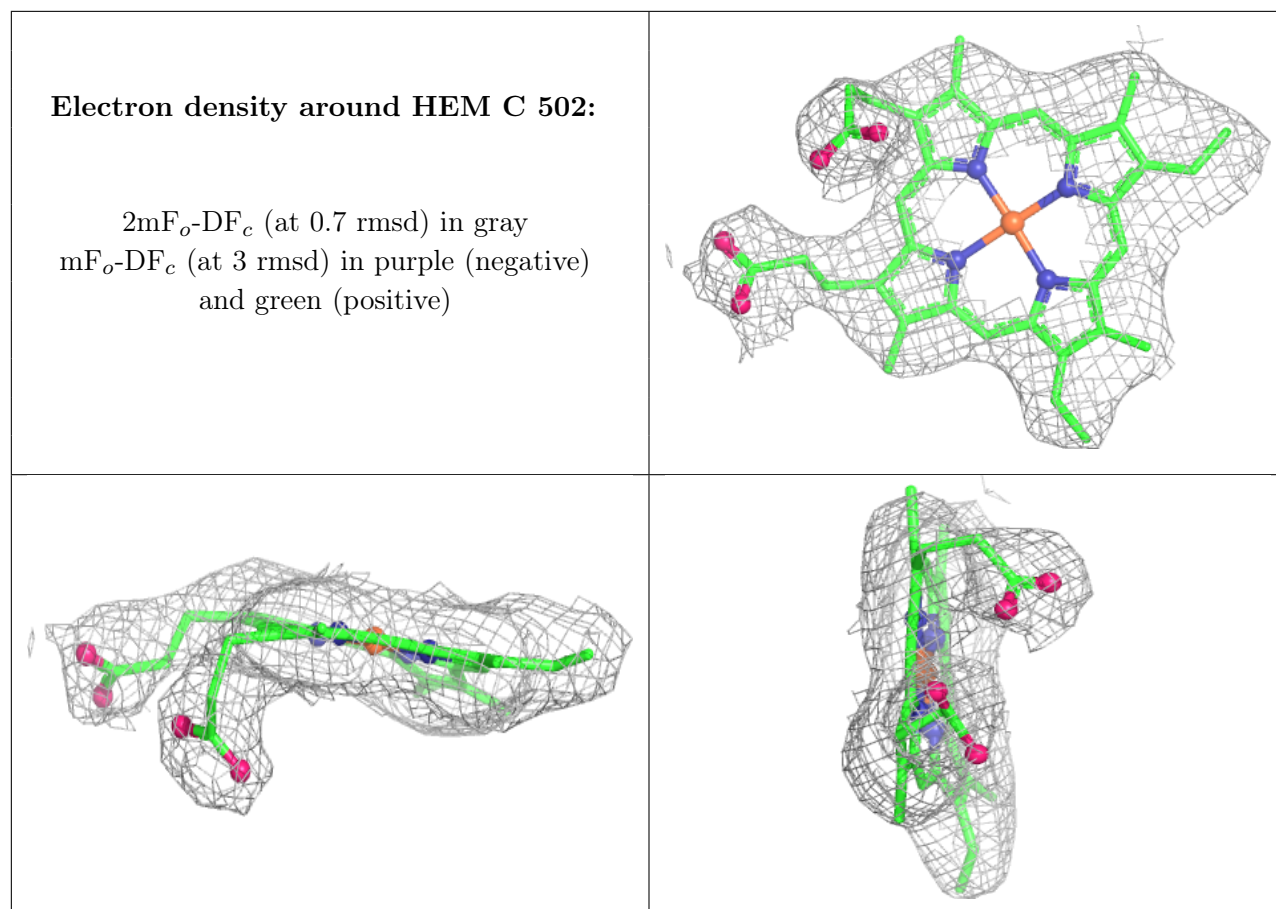
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.