



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 06:20 PM EDT

PDB ID : 1PPJ / pdb_00001ppj
Title : Bovine cytochrome bc1 complex with stigmatellin and antimycin
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2003-06-16
Resolution : 2.10 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

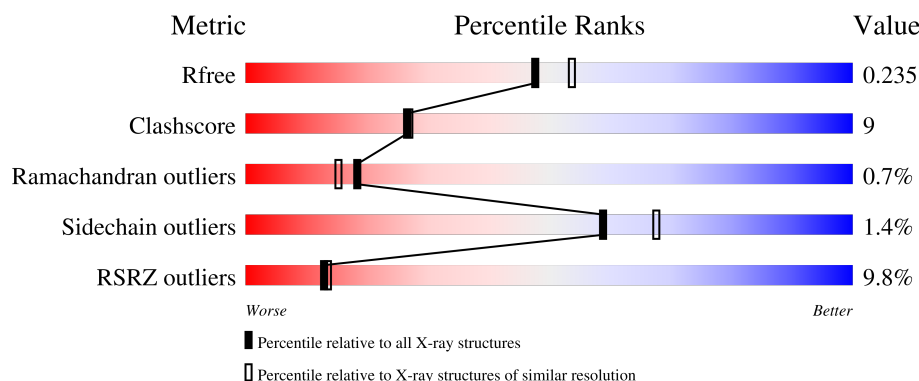
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



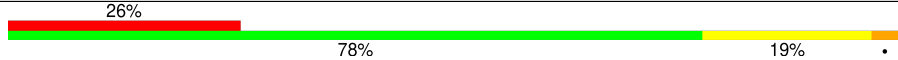
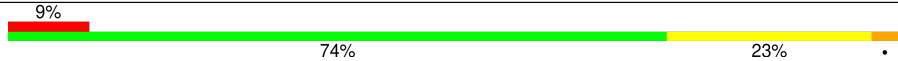
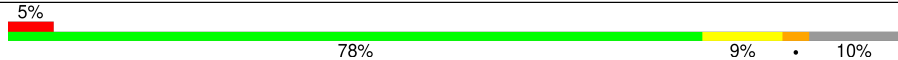
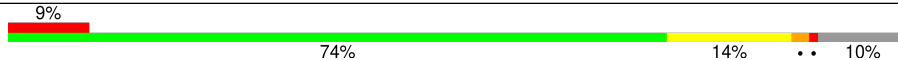
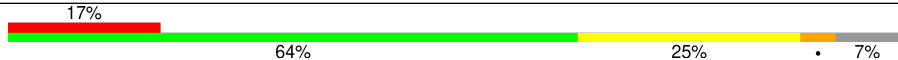
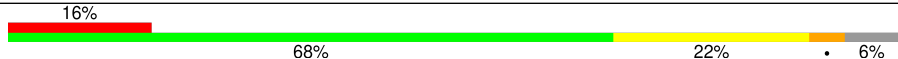
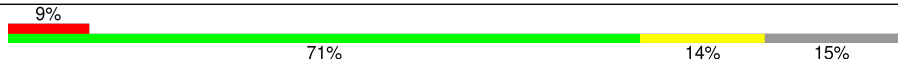
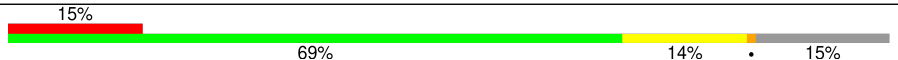
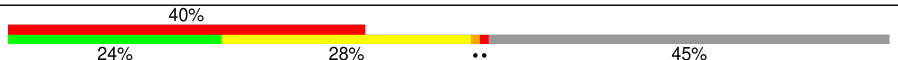
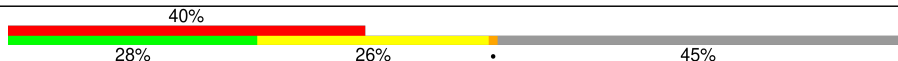
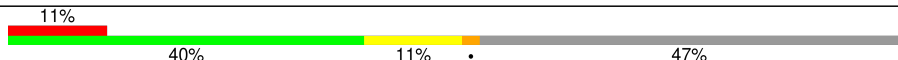
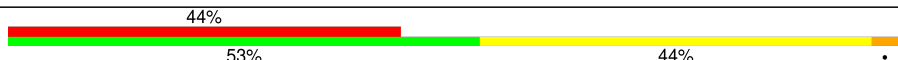
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	5% 78% 19% ..
1	N	446	9% 78% 19% ..
2	B	439	4% 78% 18% ..
2	O	439	10% 80% 16% .
3	C	379	2% 78% 16% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	379	
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	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

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
13	AZI	A	4011	-	X	-	X
13	AZI	C	2005	-	X	-	-
13	AZI	G	4009	-	X	-	-
13	AZI	O	4010	-	X	-	-
13	AZI	P	3005	-	X	-	-
18	ANY	P	3002	X	-	-	-
19	HEC	D	501	X	-	-	-
19	HEC	Q	501	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33549 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 Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	1
			3396	2117	601	658	20			
1	N	442	Total	C	N	O	S	10	0	1
			3396	2117	601	658	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3178	1997	562	612	7			
2	O	424	Total	C	N	O	S	0	0	1
			3156	1984	558	607	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2892	1940	450	485	17			
3	P	365	Total	C	N	O	S	0	0	0
			2891	1940	449	485	17			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1510	954	263	285	8			
5	R	196	Total	C	N	O	S	0	0	0
			1517	956	263	290	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

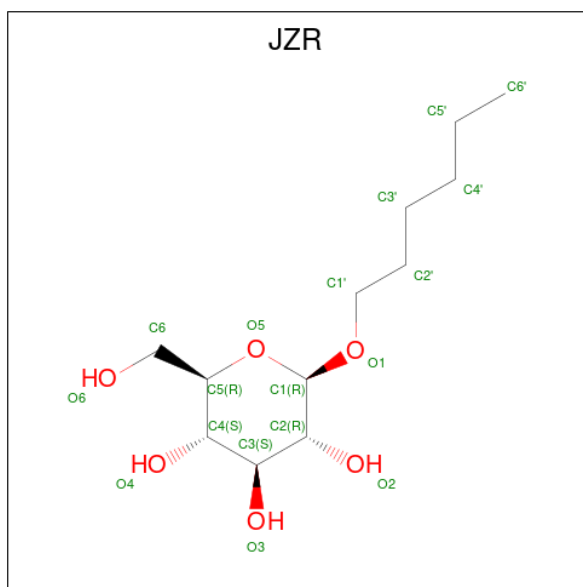
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	43	Total	C	N	O	S	0	0	0
			285	175	53	56	1			
9	V	43	Total	C	N	O	S	0	0	0
			285	175	53	56	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

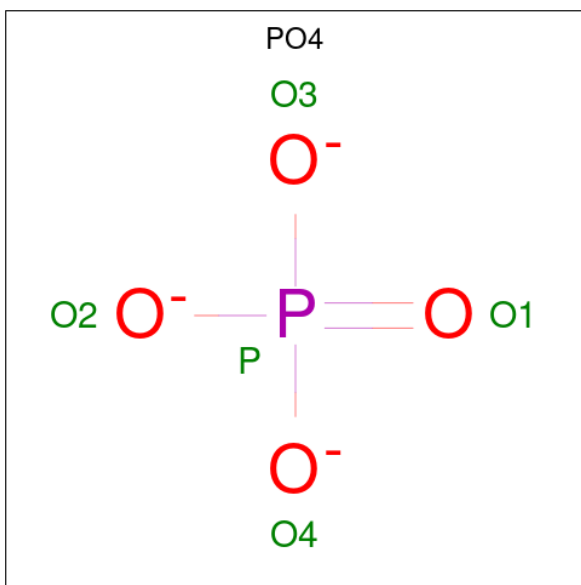
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	33	Total	C	N	O	0	0	1
			284	185	50	49			
10	W	62	Total	C	N	O	0	0	1
			506	332	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: C₁₂H₂₄O₆).



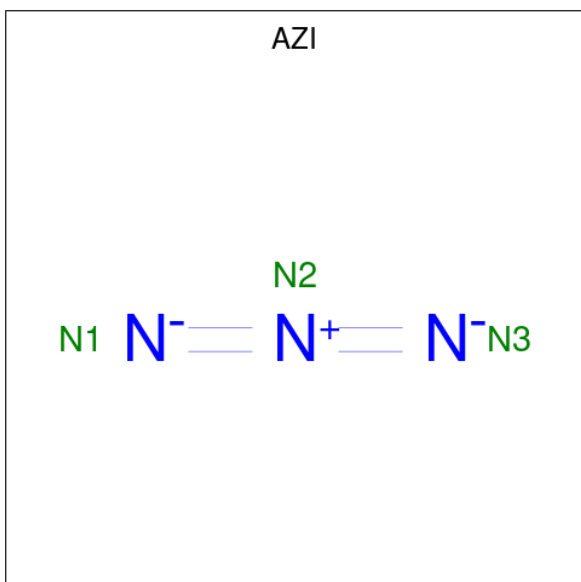
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	D	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	R	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



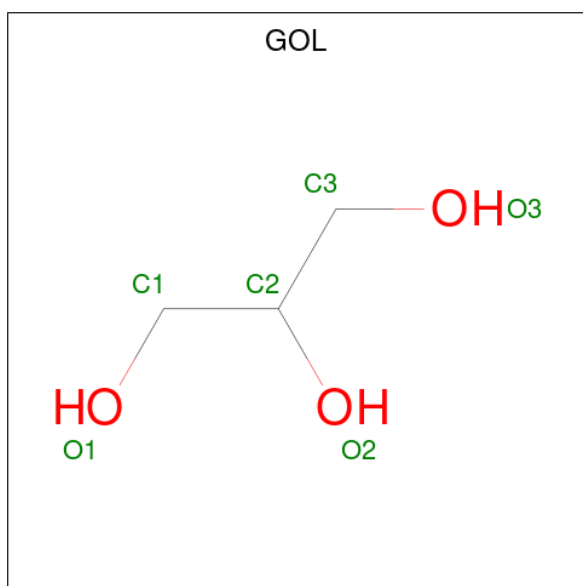
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			5	4	1		
12	C	1	Total	O	P	0	0
			5	4	1		
12	F	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		
12	S	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is AZIDE ION (CCD ID: AZI) (formula: N₃).



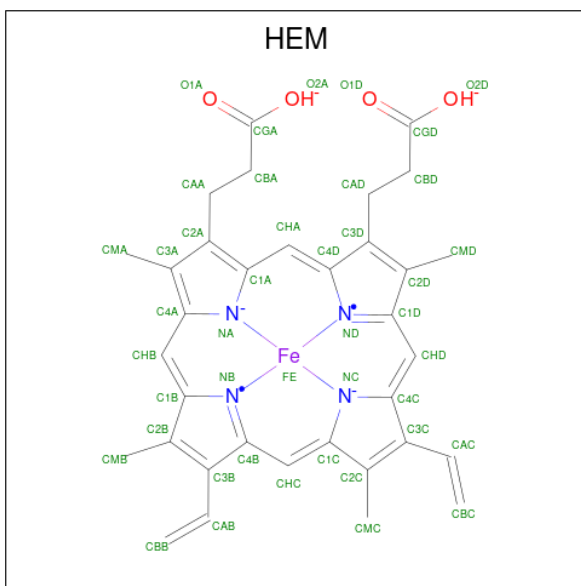
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total N 3 3	0	0
13	C	1	Total N 3 3	0	0
13	G	1	Total N 3 3	0	0
13	O	1	Total N 3 3	0	0
13	P	1	Total N 3 3	0	0

- Molecule 14 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



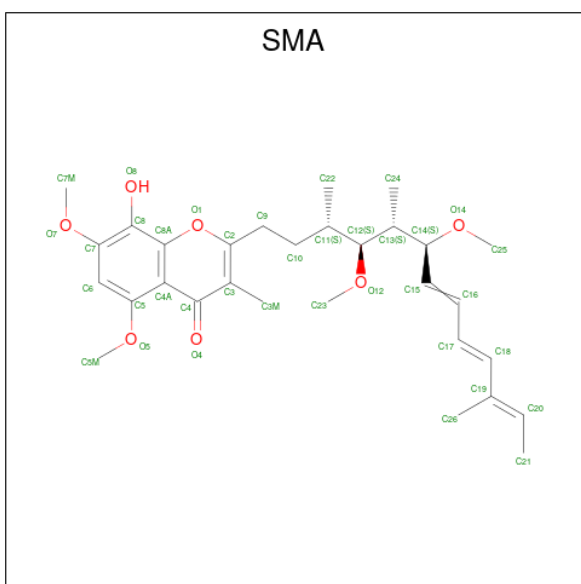
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C O 6 3 3	0	0
14	C	1	Total C O 6 3 3	0	0
14	C	1	Total C O 6 3 3	0	0
14	O	1	Total C O 6 3 3	0	0
14	P	1	Total C O 6 3 3	0	0
14	R	1	Total C O 6 3 3	0	0

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$$\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4).$$


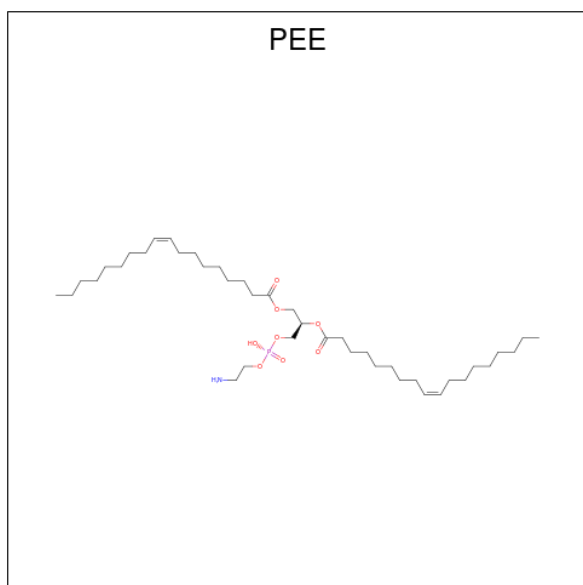
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
15	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
15	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
15	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 16 is STIGMATELLIN A (CCD ID: SMA) (formula: $\text{C}_{30}\text{H}_{42}\text{O}_7$).



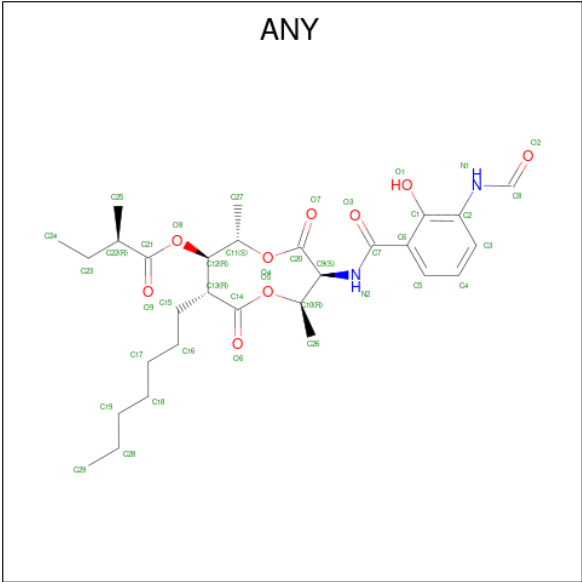
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			37	30	7		
16	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



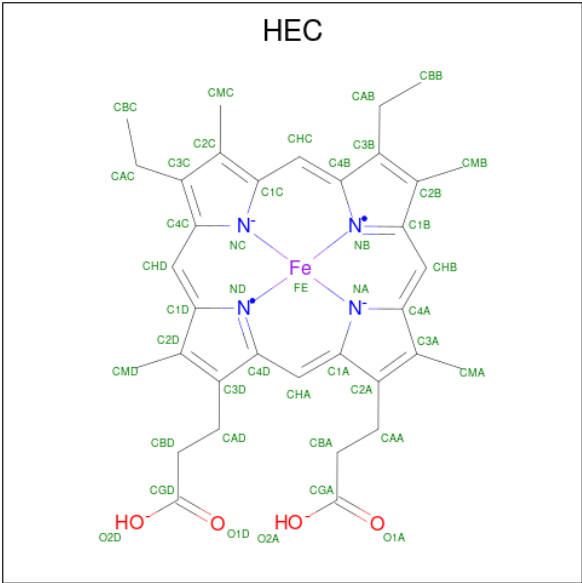
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
17	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
17	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
17	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 18 is 2-METHYL-BUTYRIC ACID 3-(3-FORMYLAMINO-2-HYDROXY-BENZ OYLAMINO)-8-HEPTYL-2,6-DIMETHYL-4,9-DIOXO-[1,5]DIOXONAN-7-YL ESTER (CCD ID: ANY) (formula: $C_{29}H_{42}N_2O_9$).



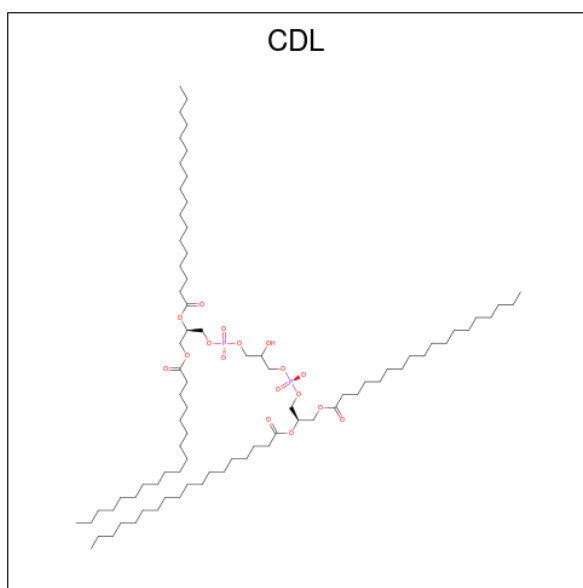
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	N	O	0	0
			37	26	2	9		
18	P	1	Total	C	N	O	0	0
			37	26	2	9		

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



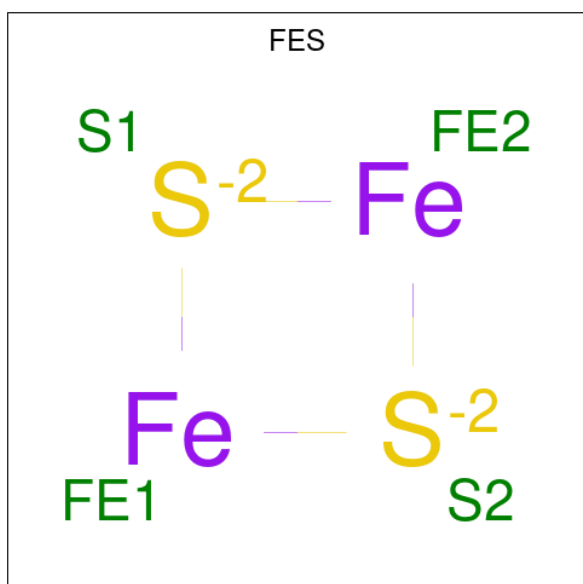
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
19	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	D	1	Total	C	O	P	0	0
			39	24	13	2		
20	G	1	Total	C	O	P	0	0
			44	25	17	2		
20	P	1	Total	C	O	P	0	0
			39	24	13	2		
20	T	1	Total	C	O	P	0	0
			49	30	17	2		

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



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

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	219	Total	O	0	0
			219	219		
22	B	167	Total	O	0	0
			167	167		
22	C	123	Total	O	0	0
			123	123		
22	D	96	Total	O	0	0
			96	96		
22	E	50	Total	O	0	0
			50	50		
22	F	63	Total	O	0	0
			63	63		
22	G	17	Total	O	0	0
			17	17		
22	H	17	Total	O	0	0
			17	17		
22	I	16	Total	O	0	0
			16	16		
22	J	4	Total	O	0	0
			4	4		
22	N	98	Total	O	0	0
			98	98		
22	O	127	Total	O	0	0
			127	127		
22	P	115	Total	O	0	0
			115	115		
22	Q	89	Total	O	0	0
			89	89		
22	R	63	Total	O	0	0
			63	63		
22	S	63	Total	O	0	0
			63	63		
22	T	20	Total	O	0	0
			20	20		
22	U	6	Total	O	0	0
			6	6		

Continued on next page...

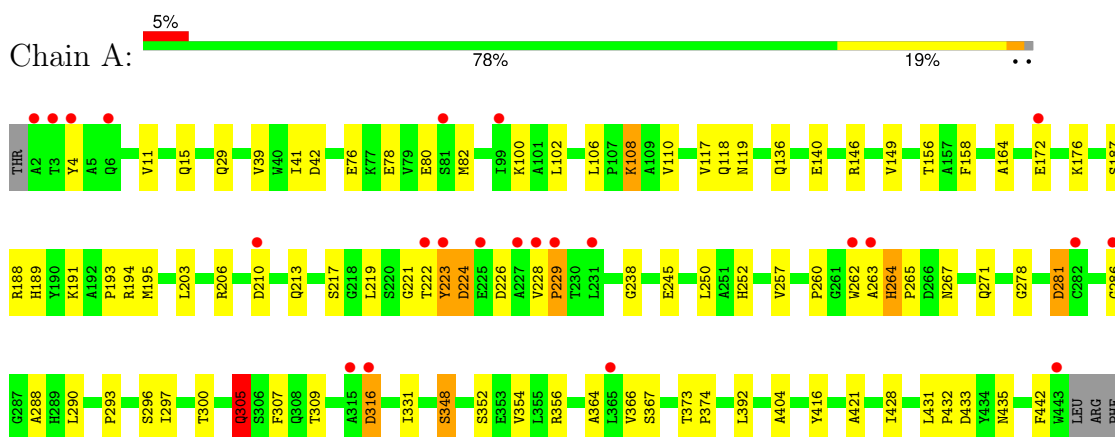
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	V	8	Total	O	0	0
			8	8		
22	W	9	Total	O	0	0
			9	9		

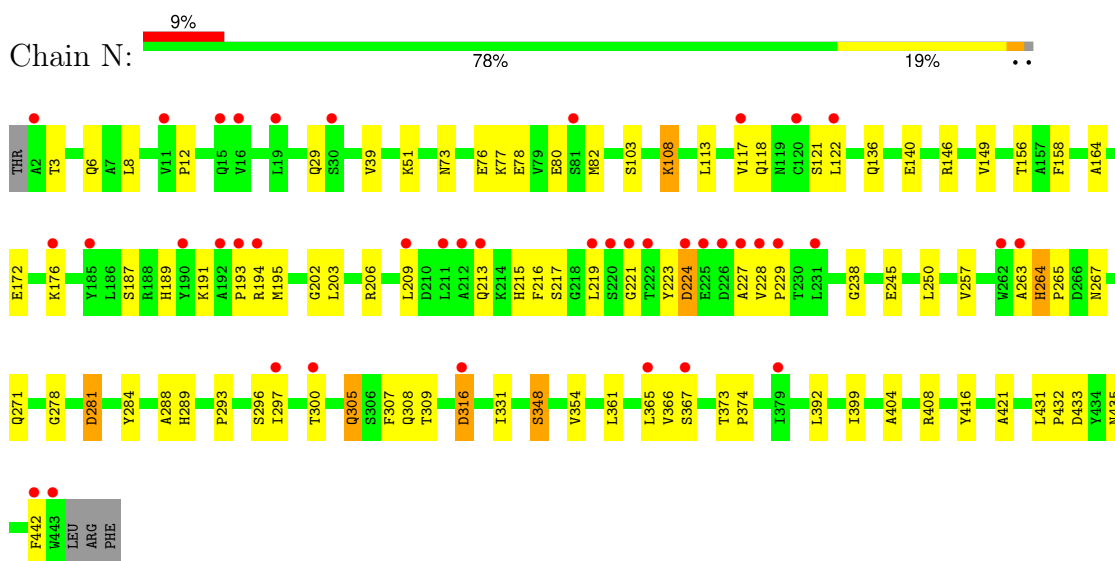
3 Residue-property plots [i](#)

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.

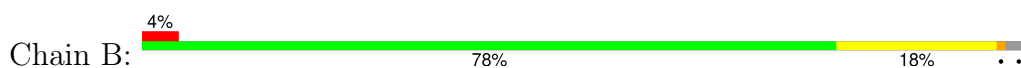
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

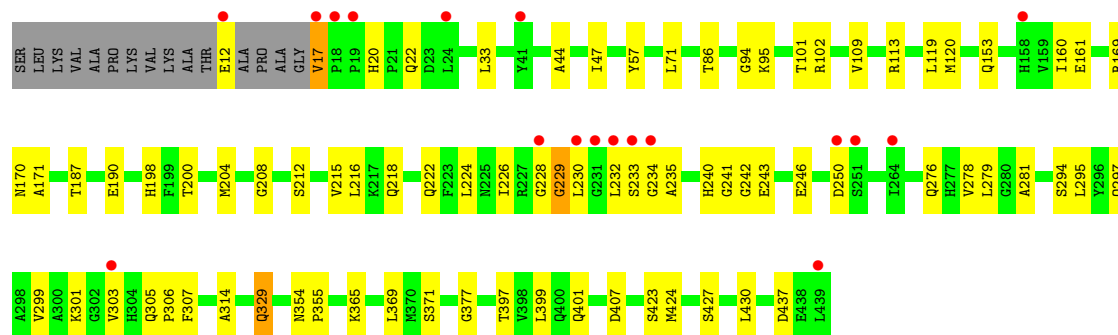


- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

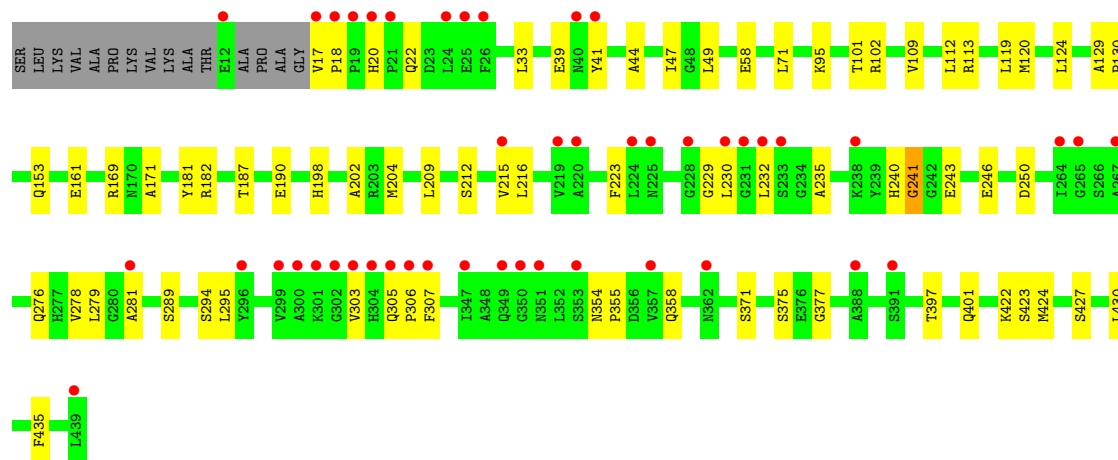
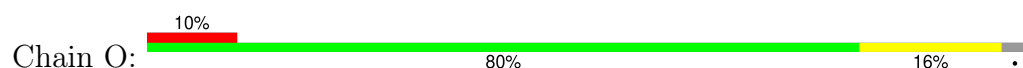


- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

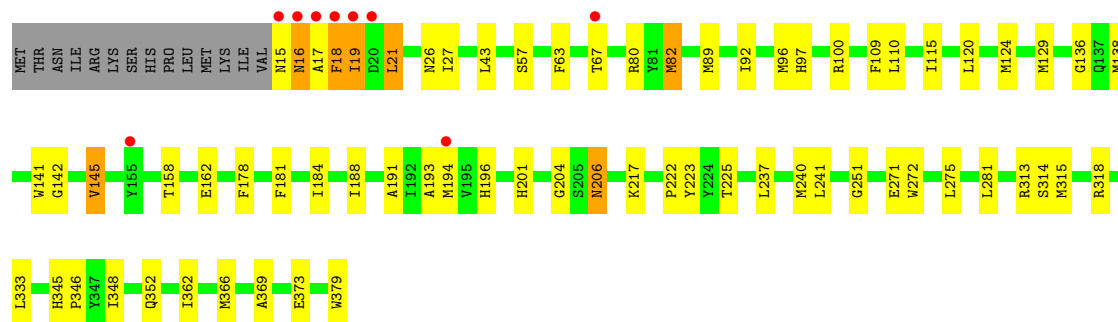
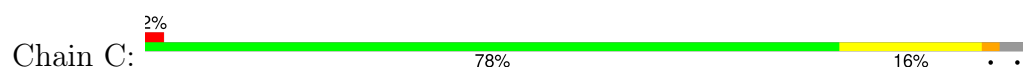




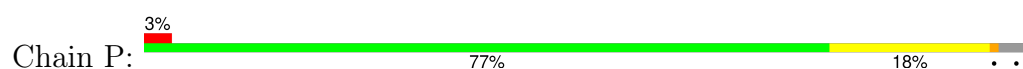
• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

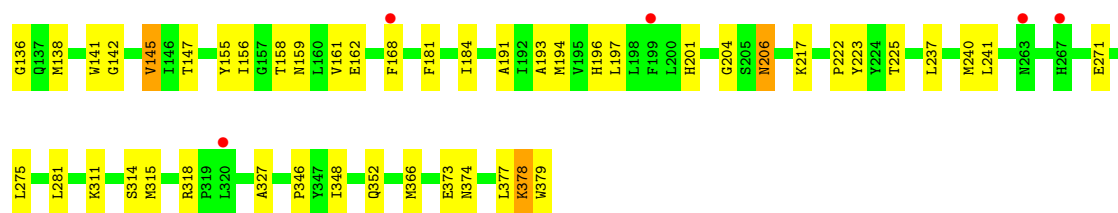


• Molecule 3: Cytochrome b

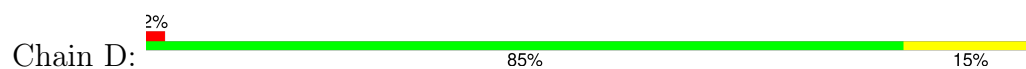


• Molecule 3: Cytochrome b

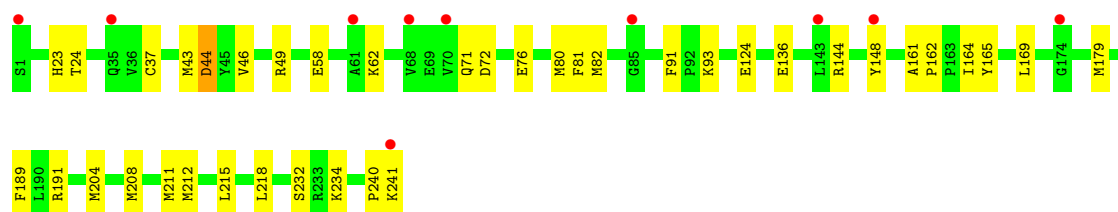
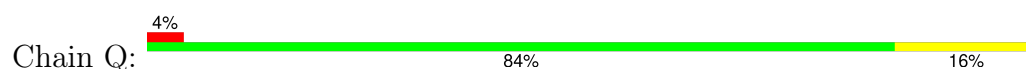




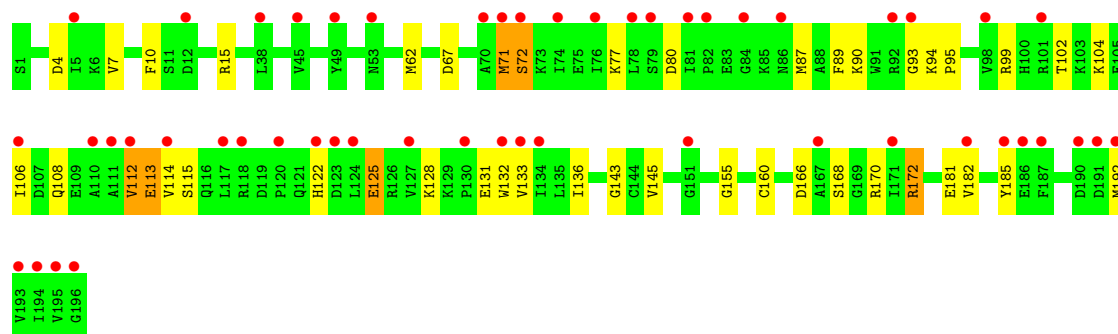
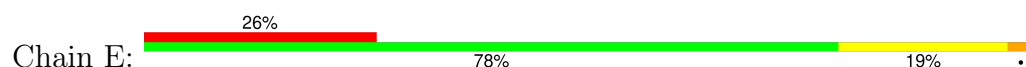
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



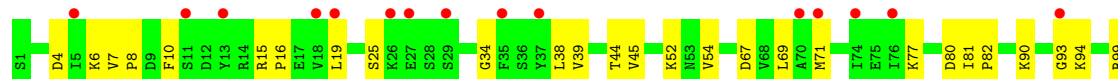
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

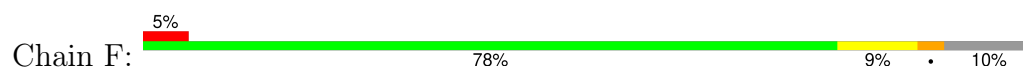


- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial





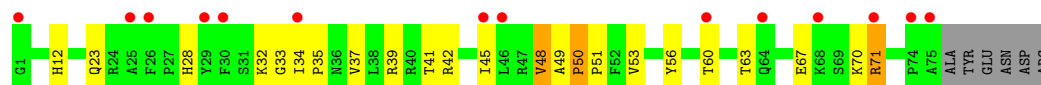
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



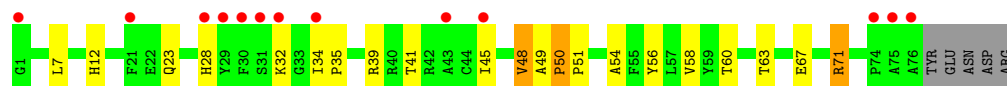
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



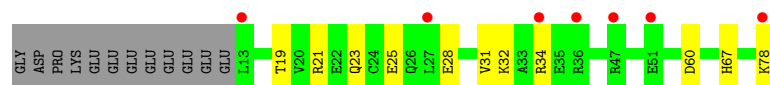
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



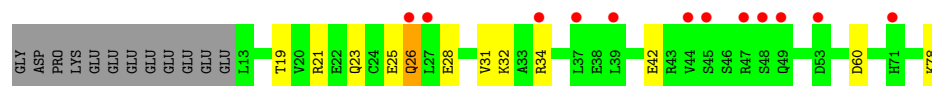
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



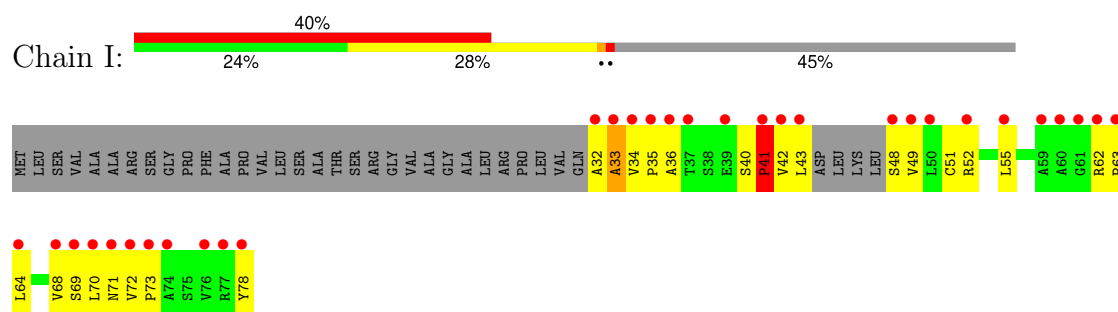
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



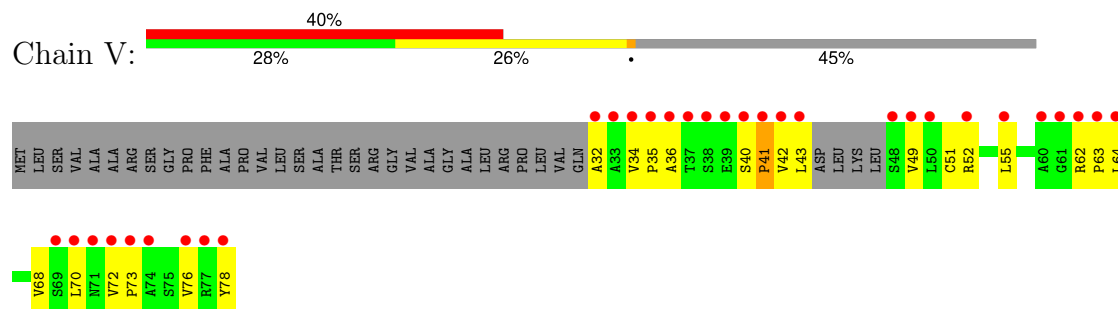
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



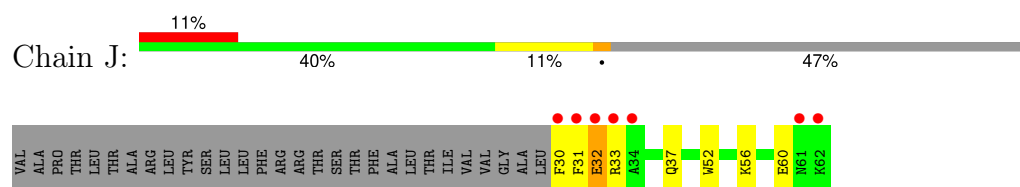
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



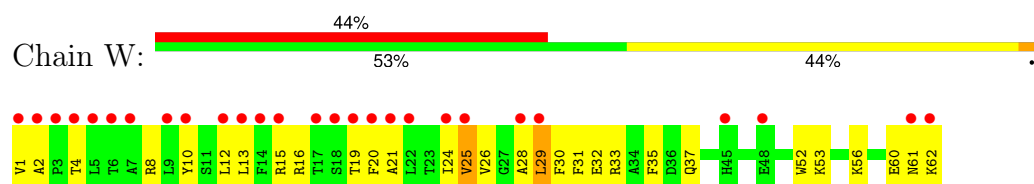
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein



- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.53Å 168.75Å 231.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.53 – 2.10 93.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (93.53-2.10) 97.8 (93.53-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.260 0.220 , 0.235	Depositor DCC
R_{free} test set	14181 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33549	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SMA, PO4, AZI, PEE, ANY, FES, JZR, CDL, HEM, 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	0.41	0/3465	0.97	17/4704 (0.4%)
1	N	0.37	0/3465	0.95	13/4704 (0.3%)
2	B	0.41	0/3236	0.93	10/4388 (0.2%)
2	O	0.39	0/3213	0.94	11/4354 (0.3%)
3	C	0.42	0/2986	1.00	23/4089 (0.6%)
3	P	0.42	0/2985	1.01	20/4087 (0.5%)
4	D	0.39	0/1978	0.96	7/2684 (0.3%)
4	Q	0.39	0/1978	0.93	7/2684 (0.3%)
5	E	0.37	0/1544	0.99	6/2087 (0.3%)
5	R	0.38	0/1551	1.01	11/2097 (0.5%)
6	F	0.40	0/878	0.96	5/1175 (0.4%)
6	S	0.37	0/878	0.91	4/1175 (0.3%)
7	G	0.37	0/642	0.97	6/869 (0.7%)
7	T	0.35	0/647	0.96	5/876 (0.6%)
8	H	0.35	0/544	0.93	1/729 (0.1%)
8	U	0.35	0/544	0.92	1/729 (0.1%)
9	I	0.49	0/286	1.35	4/387 (1.0%)
9	V	0.48	0/286	1.30	4/387 (1.0%)
10	J	0.34	0/292	0.74	0/386
10	W	0.35	0/518	0.83	0/696
All	All	0.40	0/31916	0.97	155/43287 (0.4%)

There are no bond length outliers.

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	143	GLY	N-CA-C	8.72	127.35	115.32
5	E	143	GLY	N-CA-C	8.51	127.06	115.32
3	P	26	ASN	N-CA-C	8.38	122.81	112.59
3	C	26	ASN	N-CA-C	8.16	122.55	112.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	153	GLN	N-CA-C	-7.67	103.90	113.18

There are no chirality outliers.

There are no planarity outliers.

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	3396	0	3292	68	0
1	N	3396	0	3292	60	0
2	B	3178	0	3153	74	0
2	O	3156	0	3123	51	0
3	C	2892	0	2938	41	0
3	P	2891	0	2937	49	0
4	D	1919	0	1868	33	0
4	Q	1919	0	1868	37	0
5	E	1510	0	1495	33	0
5	R	1517	0	1499	35	0
6	F	861	0	854	12	0
6	S	861	0	854	19	0
7	G	621	0	626	15	0
7	T	626	0	631	15	0
8	H	539	0	524	11	0
8	U	539	0	524	10	0
9	I	285	0	280	50	0
9	V	285	0	280	24	0
10	J	284	0	264	5	0
10	W	506	0	512	35	0
11	A	18	0	24	0	0
11	C	36	0	48	2	0
11	D	18	0	24	3	0
11	F	36	0	48	3	0
11	P	18	0	24	0	0
11	R	18	0	24	1	0
11	S	18	0	24	3	0
12	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	5	0	0	0	0
12	F	5	0	0	0	0
12	P	5	0	0	0	0
12	S	5	0	0	0	0
13	A	3	0	0	0	0
13	C	3	0	0	0	0
13	G	3	0	0	0	0
13	O	3	0	0	0	0
13	P	3	0	0	0	0
14	B	6	0	8	0	0
14	C	12	0	16	1	0
14	O	6	0	8	0	0
14	P	6	0	8	0	0
14	R	6	0	8	2	0
15	C	86	0	60	3	0
15	P	86	0	60	2	0
16	C	37	0	42	2	0
16	P	37	0	42	2	0
17	C	49	0	72	0	0
17	D	26	0	26	3	0
17	P	49	0	72	1	0
17	Q	51	0	82	4	0
18	C	37	0	28	1	0
18	P	37	0	29	2	0
19	D	43	0	30	2	0
19	Q	43	0	30	0	0
20	D	39	0	39	1	0
20	G	44	0	32	0	0
20	P	39	0	39	2	0
20	T	49	0	42	2	0
21	E	4	0	0	0	0
21	R	4	0	0	0	0
22	A	219	0	0	7	0
22	B	167	0	0	5	0
22	C	123	0	0	1	0
22	D	96	0	0	1	0
22	E	50	0	0	0	0
22	F	63	0	0	0	0
22	G	17	0	0	0	0
22	H	17	0	0	0	0
22	I	16	0	0	2	0
22	J	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	N	98	0	0	1	0
22	O	127	0	0	2	0
22	P	115	0	0	5	0
22	Q	89	0	0	0	0
22	R	63	0	0	5	0
22	S	63	0	0	1	0
22	T	20	0	0	0	0
22	U	6	0	0	0	0
22	V	8	0	0	1	0
22	W	9	0	0	0	0
All	All	33549	0	31803	595	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 9.

The worst 5 of 595 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.41	1.03
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.23	1.01
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.21	1.01
2:B:95:LYS:HE2	9:I:32:ALA:HB3	1.47	0.94
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.48	0.94

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	440/446 (99%)	425 (97%)	11 (2%)	4 (1%)	14	10
1	N	440/446 (99%)	425 (97%)	11 (2%)	4 (1%)	14	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	418/439 (95%)	405 (97%)	10 (2%)	3 (1%)	18	15
2	O	419/439 (95%)	404 (96%)	13 (3%)	2 (0%)	24	22
3	C	363/379 (96%)	352 (97%)	9 (2%)	2 (1%)	21	18
3	P	363/379 (96%)	352 (97%)	10 (3%)	1 (0%)	36	36
4	D	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
4	Q	239/241 (99%)	232 (97%)	7 (3%)	0	100	100
5	E	194/196 (99%)	181 (93%)	10 (5%)	3 (2%)	8	4
5	R	194/196 (99%)	183 (94%)	8 (4%)	3 (2%)	8	4
6	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
6	S	97/110 (88%)	94 (97%)	1 (1%)	2 (2%)	5	2
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	69 (93%)	5 (7%)	0	100	100
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	64 (100%)	0	0	100	100
9	I	39/78 (50%)	37 (95%)	1 (3%)	1 (3%)	4	1
9	V	39/78 (50%)	36 (92%)	2 (5%)	1 (3%)	4	1
10	J	30/62 (48%)	28 (93%)	2 (7%)	0	100	100
10	W	59/62 (95%)	54 (92%)	4 (7%)	1 (2%)	7	3
All	All	3945/4220 (94%)	3803 (96%)	115 (3%)	27 (1%)	18	15

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP
3	C	19	ILE
5	E	71	MET
5	E	72	SER
9	I	41	PRO

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	363/370 (98%)	355 (98%)	8 (2%)	45	53
1	N	363/370 (98%)	357 (98%)	6 (2%)	53	62
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	328/343 (96%)	327 (100%)	1 (0%)	86	91
3	C	312/327 (95%)	308 (99%)	4 (1%)	61	69
3	P	311/327 (95%)	307 (99%)	4 (1%)	61	69
4	D	206/206 (100%)	205 (100%)	1 (0%)	81	88
4	Q	206/206 (100%)	204 (99%)	2 (1%)	68	76
5	E	165/168 (98%)	163 (99%)	2 (1%)	63	72
5	R	167/168 (99%)	164 (98%)	3 (2%)	51	60
6	F	90/98 (92%)	88 (98%)	2 (2%)	45	53
6	S	90/98 (92%)	87 (97%)	3 (3%)	33	37
7	G	66/71 (93%)	65 (98%)	1 (2%)	57	65
7	T	66/71 (93%)	65 (98%)	1 (2%)	57	65
8	H	63/74 (85%)	63 (100%)	0	100	100
8	U	63/74 (85%)	61 (97%)	2 (3%)	34	38
9	I	27/60 (45%)	26 (96%)	1 (4%)	30	33
9	V	27/60 (45%)	26 (96%)	1 (4%)	30	33
10	J	27/52 (52%)	25 (93%)	2 (7%)	13	10
10	W	51/52 (98%)	50 (98%)	1 (2%)	48	56
All	All	3323/3538 (94%)	3278 (99%)	45 (1%)	59	67

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	16	ASN
5	R	113	GLU
3	P	21	LEU
4	Q	76	GLU
6	S	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	159	GLN
2	O	218	GLN
9	V	71	ASN
1	N	165	GLN
1	N	267	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](#)

45 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	$\# Z > 2$
15	HEM	C	501	3	50,50,50	1.44	4 (8%)	67,82,82	1.03	3 (4%)
20	CDL	G	2004	-	43,43,99	1.12	3 (6%)	49,55,111	1.24	6 (12%)
13	AZI	O	4010	-	2,2,2	3.49	2 (100%)	0,1,1	-	-
20	CDL	P	3003	-	38,38,99	1.04	1 (2%)	42,47,111	1.04	4 (9%)
11	JZR	P	3010	-	18,18,18	1.82	5 (27%)	23,23,23	0.70	0
11	JZR	S	2011	-	18,18,18	1.79	3 (16%)	23,23,23	0.73	0
19	HEC	D	501	4	50,50,50	0.95	1 (2%)	68,82,82	1.19	3 (4%)
18	ANY	C	2002	-	38,38,41	1.88	11 (28%)	32,52,55	1.73	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	GOL	P	3008	-	5,5,5	1.28	0	5,5,5	0.56	0
16	SMA	P	3001	-	38,38,38	1.62	8 (21%)	47,52,52	0.88	2 (4%)
13	AZI	A	4011	-	2,2,2	4.67	2 (100%)	0,1,1	-	-
20	CDL	D	2003	-	38,38,99	1.07	1 (2%)	42,47,111	1.04	3 (7%)
15	HEM	P	502	3	50,50,50	1.53	4 (8%)	67,82,82	1.02	2 (2%)
12	PO4	A	2013	-	4,4,4	1.42	1 (25%)	6,6,6	0.90	0
21	FES	E	501	5	0,4,4	-	-	-	-	-
11	JZR	F	4001	-	18,18,18	1.84	5 (27%)	23,23,23	0.71	0
20	CDL	T	3004	-	48,48,99	1.15	3 (6%)	54,60,111	1.19	3 (5%)
14	GOL	R	4005	-	5,5,5	1.30	0	5,5,5	0.56	0
11	JZR	C	2010	-	18,18,18	1.81	4 (22%)	23,23,23	0.70	0
16	SMA	C	2001	-	38,38,38	1.64	9 (23%)	47,52,52	0.89	2 (4%)
14	GOL	B	2009	-	5,5,5	1.21	0	5,5,5	0.56	0
14	GOL	C	4006	-	5,5,5	1.32	0	5,5,5	0.61	0
11	JZR	F	3011	-	18,18,18	1.80	5 (27%)	23,23,23	0.67	0
17	PEE	D	2006	-	25,25,50	1.50	6 (24%)	28,30,55	0.77	1 (3%)
14	GOL	O	3009	-	5,5,5	1.15	0	5,5,5	0.50	0
11	JZR	R	4007	-	18,18,18	1.85	4 (22%)	23,23,23	0.71	0
13	AZI	C	2005	-	2,2,2	4.06	2 (100%)	0,1,1	-	-
11	JZR	A	4004	-	18,18,18	1.58	3 (16%)	23,23,23	0.62	0
12	PO4	P	3013	-	4,4,4	1.41	1 (25%)	6,6,6	0.87	0
11	JZR	C	4002	-	18,18,18	1.87	4 (22%)	23,23,23	0.76	1 (4%)
13	AZI	P	3005	-	2,2,2	3.88	2 (100%)	0,1,1	-	-
12	PO4	C	4008	-	4,4,4	1.46	1 (25%)	6,6,6	0.89	0
17	PEE	C	2007	-	48,48,50	1.29	5 (10%)	51,53,55	0.75	2 (3%)
14	GOL	C	2008	-	5,5,5	1.45	0	5,5,5	0.75	0
12	PO4	S	3012	-	4,4,4	1.40	1 (25%)	6,6,6	0.89	0
15	HEM	C	502	3	50,50,50	1.46	5 (10%)	67,82,82	1.04	2 (2%)
15	HEM	P	501	3	50,50,50	1.49	5 (10%)	67,82,82	0.99	2 (2%)
11	JZR	D	4003	-	18,18,18	1.84	4 (22%)	23,23,23	0.72	0
12	PO4	F	2012	-	4,4,4	1.34	1 (25%)	6,6,6	0.89	0
21	FES	R	501	5	0,4,4	-	-	-	-	-
19	HEC	Q	501	4	50,50,50	0.93	1 (2%)	68,82,82	1.28	5 (7%)
18	ANY	P	3002	-	38,38,41	1.88	12 (31%)	32,52,55	1.59	6 (18%)
17	PEE	Q	3006	-	50,50,50	1.33	5 (10%)	53,55,55	0.75	2 (3%)
13	AZI	G	4009	-	2,2,2	3.80	2 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PEE	P	3007	-	48,48,50	1.30	5 (10%)	51,53,55	0.75	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	HEM	C	501	3	-	5/14/54/54	-
20	CDL	G	2004	-	-	34/52/52/110	-
20	CDL	P	3003	-	-	23/43/43/110	-
11	JZR	P	3010	-	-	5/9/29/29	0/1/1/1
11	JZR	S	2011	-	-	5/9/29/29	0/1/1/1
19	HEC	D	501	4	1/1/3/7	8/14/54/54	-
18	ANY	C	2002	-	-	2/37/52/56	0/1/2/2
14	GOL	P	3008	-	-	2/4/4/4	-
16	SMA	P	3001	-	-	0/34/34/34	0/2/2/2
20	CDL	D	2003	-	-	19/43/43/110	-
15	HEM	P	502	3	-	4/14/54/54	-
21	FES	E	501	5	-	-	0/1/1/1
11	JZR	F	4001	-	-	2/9/29/29	0/1/1/1
20	CDL	T	3004	-	-	27/57/57/110	-
14	GOL	R	4005	-	-	2/4/4/4	-
11	JZR	C	2010	-	-	4/9/29/29	0/1/1/1
16	SMA	C	2001	-	-	2/34/34/34	0/2/2/2
14	GOL	B	2009	-	-	2/4/4/4	-
14	GOL	C	4006	-	-	3/4/4/4	-
11	JZR	F	3011	-	-	3/9/29/29	0/1/1/1
17	PEE	D	2006	-	-	18/29/29/54	-
14	GOL	O	3009	-	-	4/4/4/4	-
11	JZR	R	4007	-	-	2/9/29/29	0/1/1/1
11	JZR	A	4004	-	-	0/9/29/29	0/1/1/1
11	JZR	C	4002	-	-	3/9/29/29	0/1/1/1
17	PEE	C	2007	-	-	19/52/52/54	-
14	GOL	C	2008	-	-	4/4/4/4	-
15	HEM	C	502	3	-	4/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEM	P	501	3	-	5/14/54/54	-
11	JZR	D	4003	-	-	4/9/29/29	0/1/1/1
21	FES	R	501	5	-	-	0/1/1/1
19	HEC	Q	501	4	1/1/3/7	7/14/54/54	-
18	ANY	P	3002	-	1/1/10/13	3/37/52/56	0/1/2/2
17	PEE	Q	3006	-	-	24/54/54/54	-
17	PEE	P	3007	-	-	19/52/52/54	-

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	502	HEM	CBB-CAB	5.48	1.56	1.30
15	P	501	HEM	CBB-CAB	5.42	1.56	1.30
15	C	501	HEM	CBC-CAC	5.33	1.56	1.30
15	P	501	HEM	CBC-CAC	5.00	1.54	1.30
15	C	502	HEM	CBC-CAC	5.00	1.54	1.30

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	2002	ANY	C25-C22-C23	5.41	133.03	111.60
19	Q	501	HEC	CAC-C3C-C4C	-4.79	118.33	124.91
20	T	3004	CDL	CB4-OB6-CB5	-4.54	109.82	117.85
19	Q	501	HEC	CAC-C3C-C2C	4.31	133.70	126.89
20	G	2004	CDL	CB4-OB6-CB5	-4.01	110.77	117.85

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	P	3002	ANY	C22
19	D	501	HEC	NA
19	Q	501	HEC	NA

5 of 268 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	2008	GOL	C1-C2-C3-O3
14	O	3009	GOL	O1-C1-C2-C3
14	O	3009	GOL	C1-C2-C3-O3
14	P	3008	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

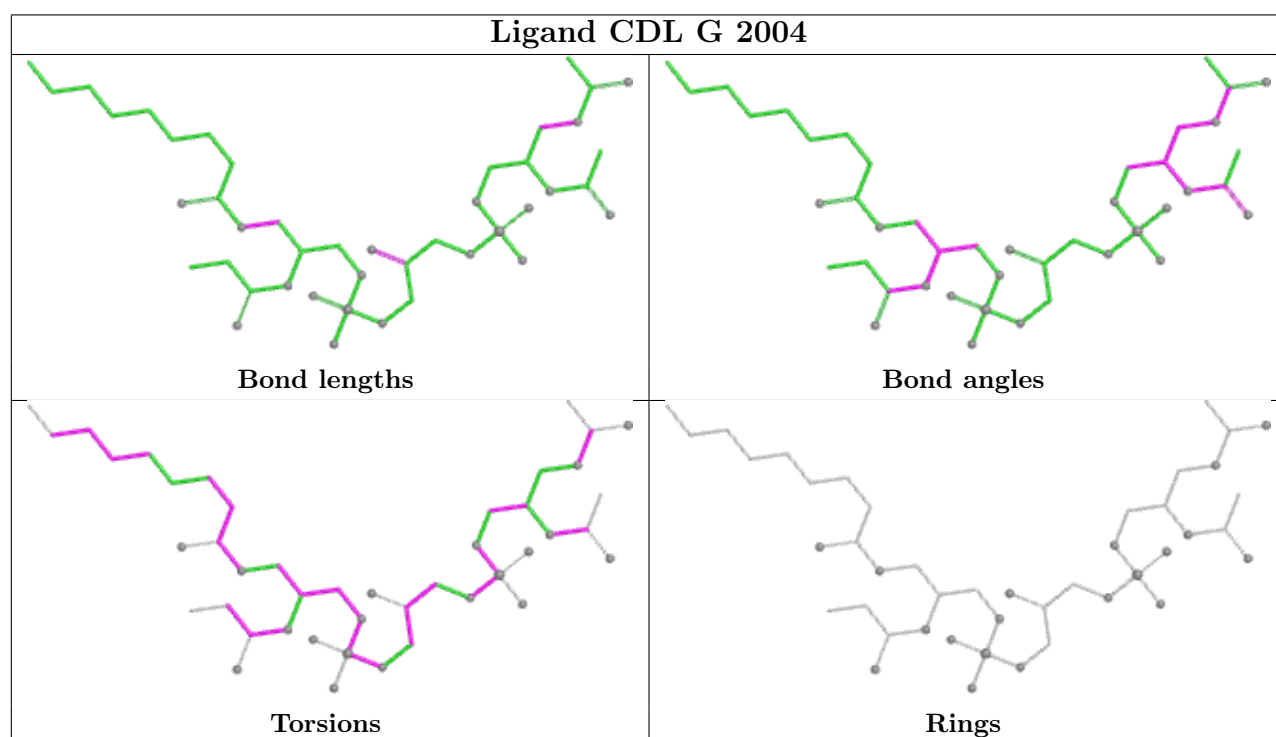
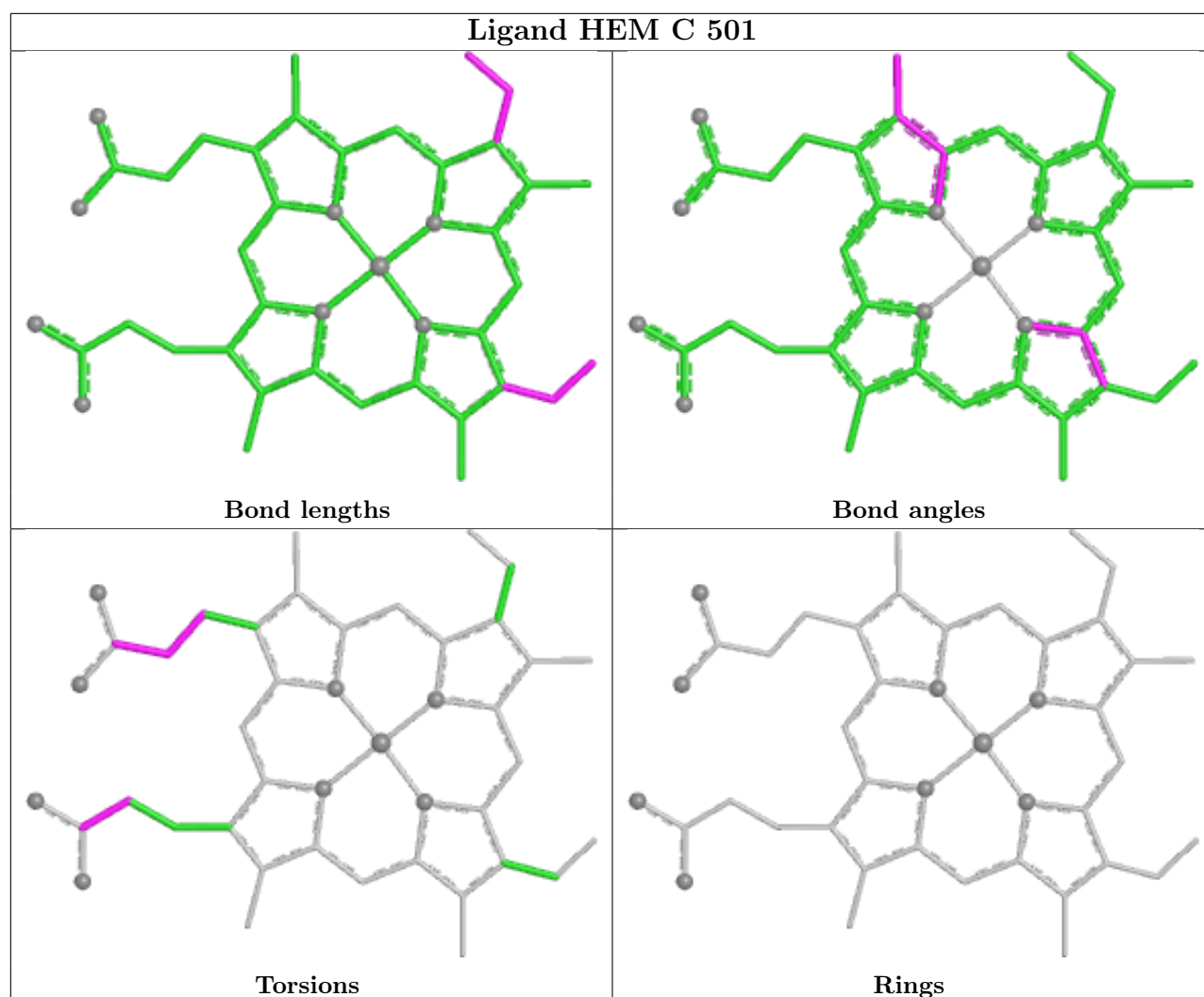
Mol	Chain	Res	Type	Atoms
14	R	4005	GOL	O1-C1-C2-C3

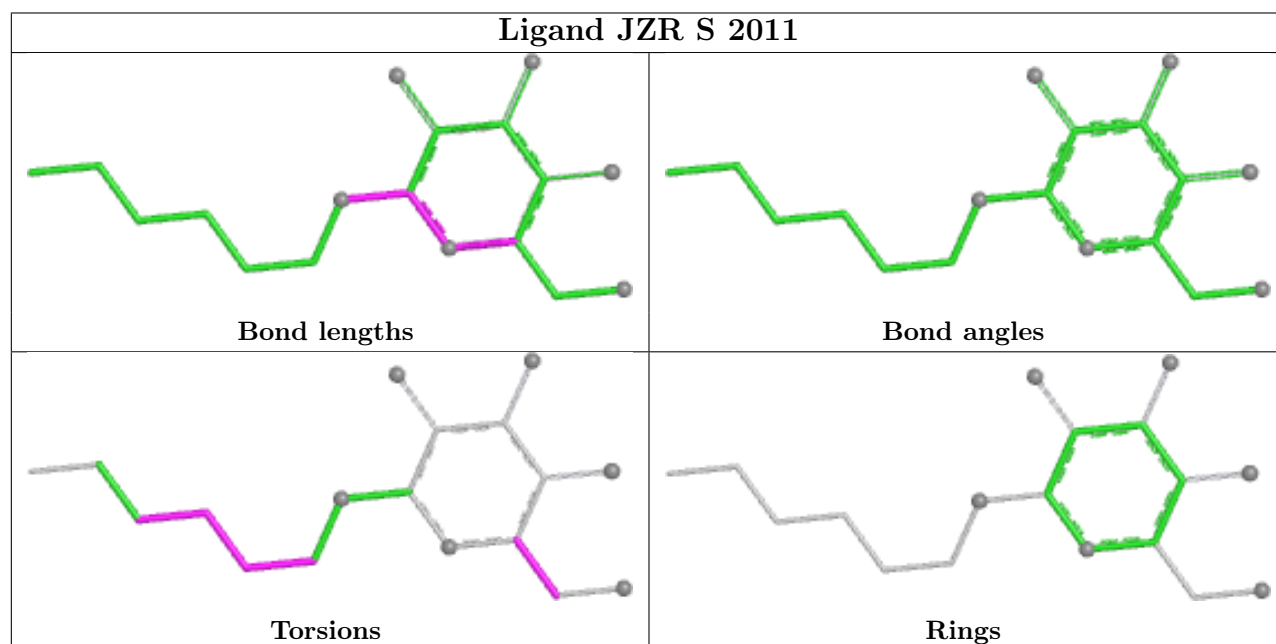
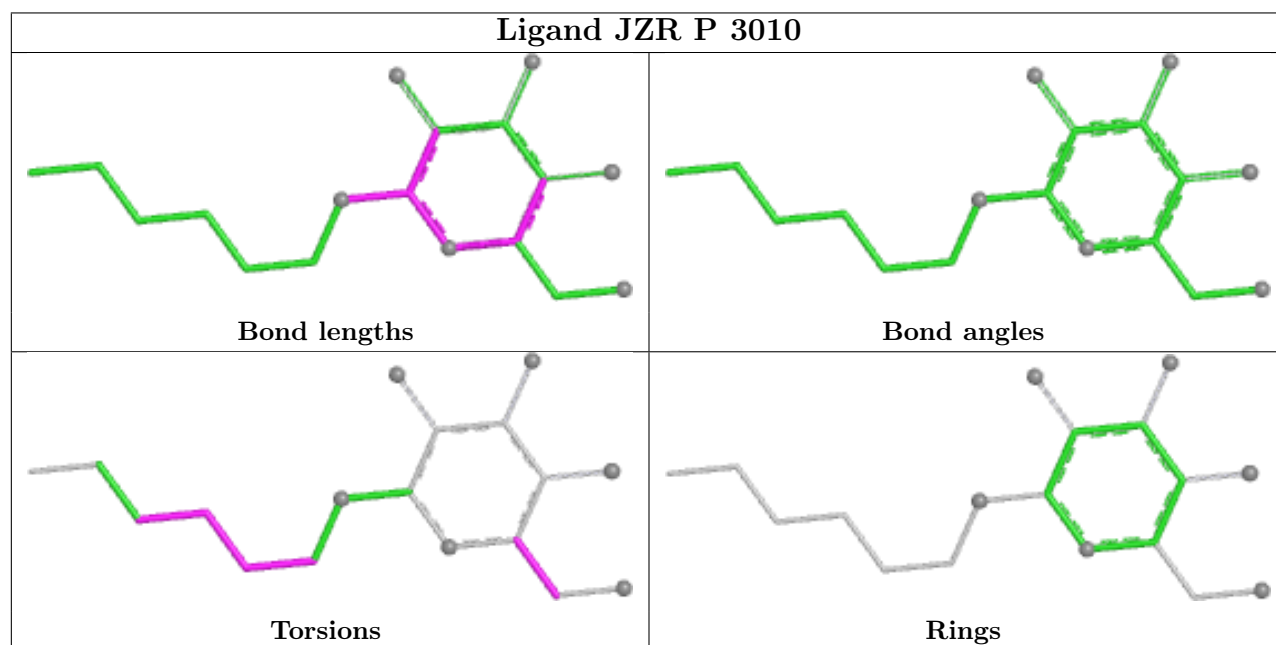
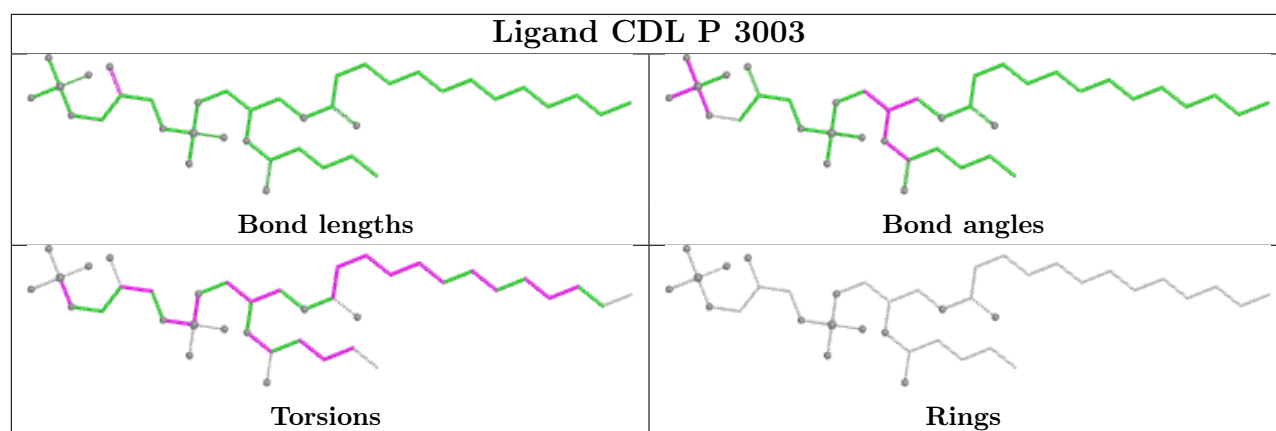
There are no ring outliers.

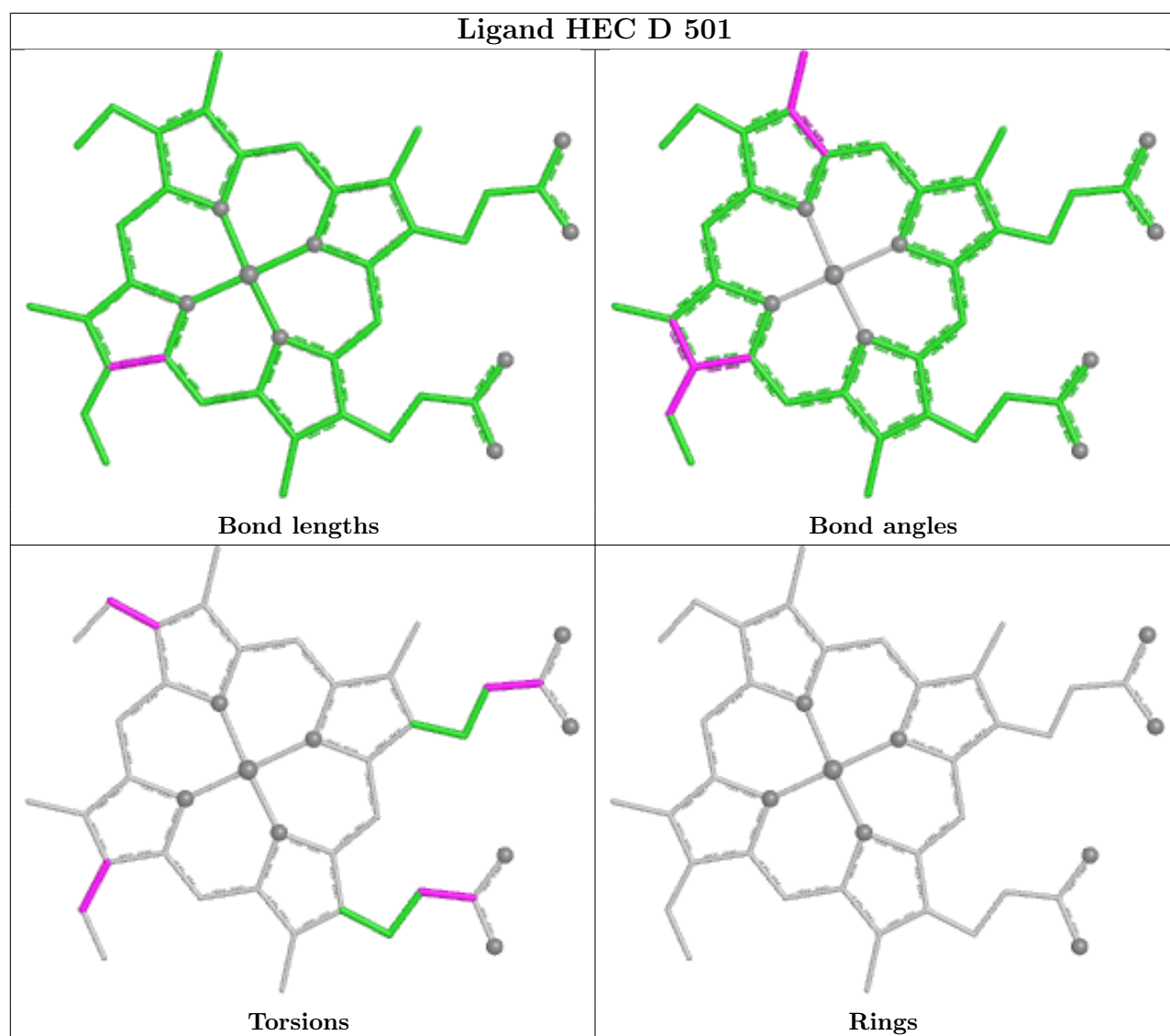
23 monomers are involved in 41 short contacts:

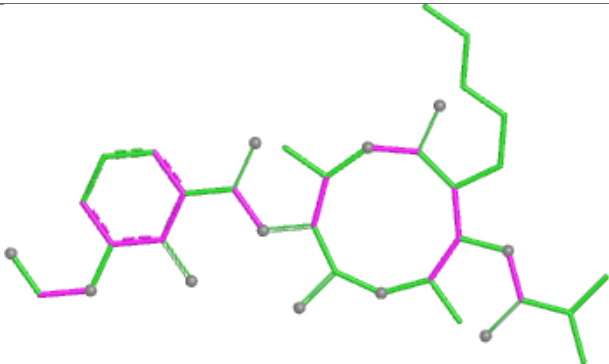
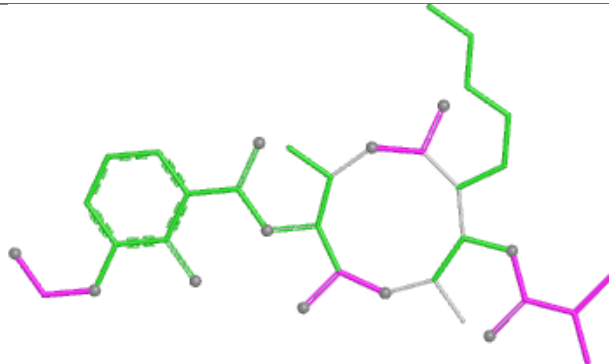
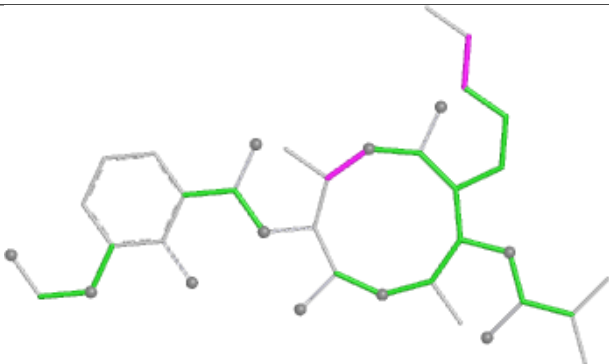
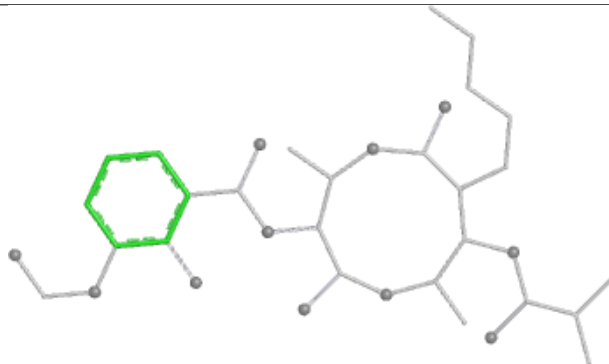
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	501	HEM	1	0
20	P	3003	CDL	2	0
11	S	2011	JZR	3	0
19	D	501	HEC	2	0
18	C	2002	ANY	1	0
16	P	3001	SMA	2	0
20	D	2003	CDL	1	0
15	P	502	HEM	1	0
11	F	4001	JZR	1	0
20	T	3004	CDL	2	0
14	R	4005	GOL	2	0
16	C	2001	SMA	2	0
11	F	3011	JZR	2	0
17	D	2006	PEE	3	0
11	R	4007	JZR	1	0
11	C	4002	JZR	2	0
14	C	2008	GOL	1	0
15	C	502	HEM	2	0
15	P	501	HEM	1	0
11	D	4003	JZR	3	0
18	P	3002	ANY	2	0
17	Q	3006	PEE	4	0
17	P	3007	PEE	1	0

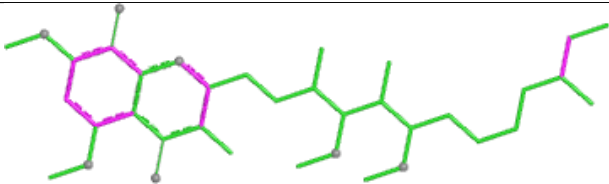
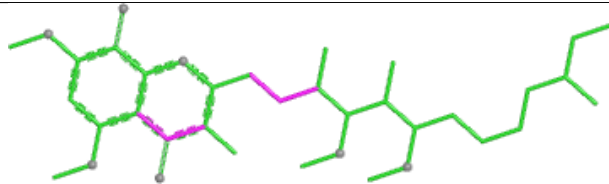
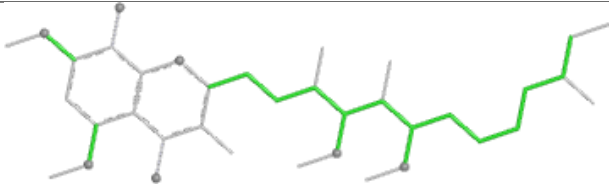
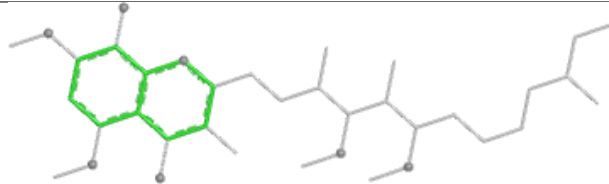
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

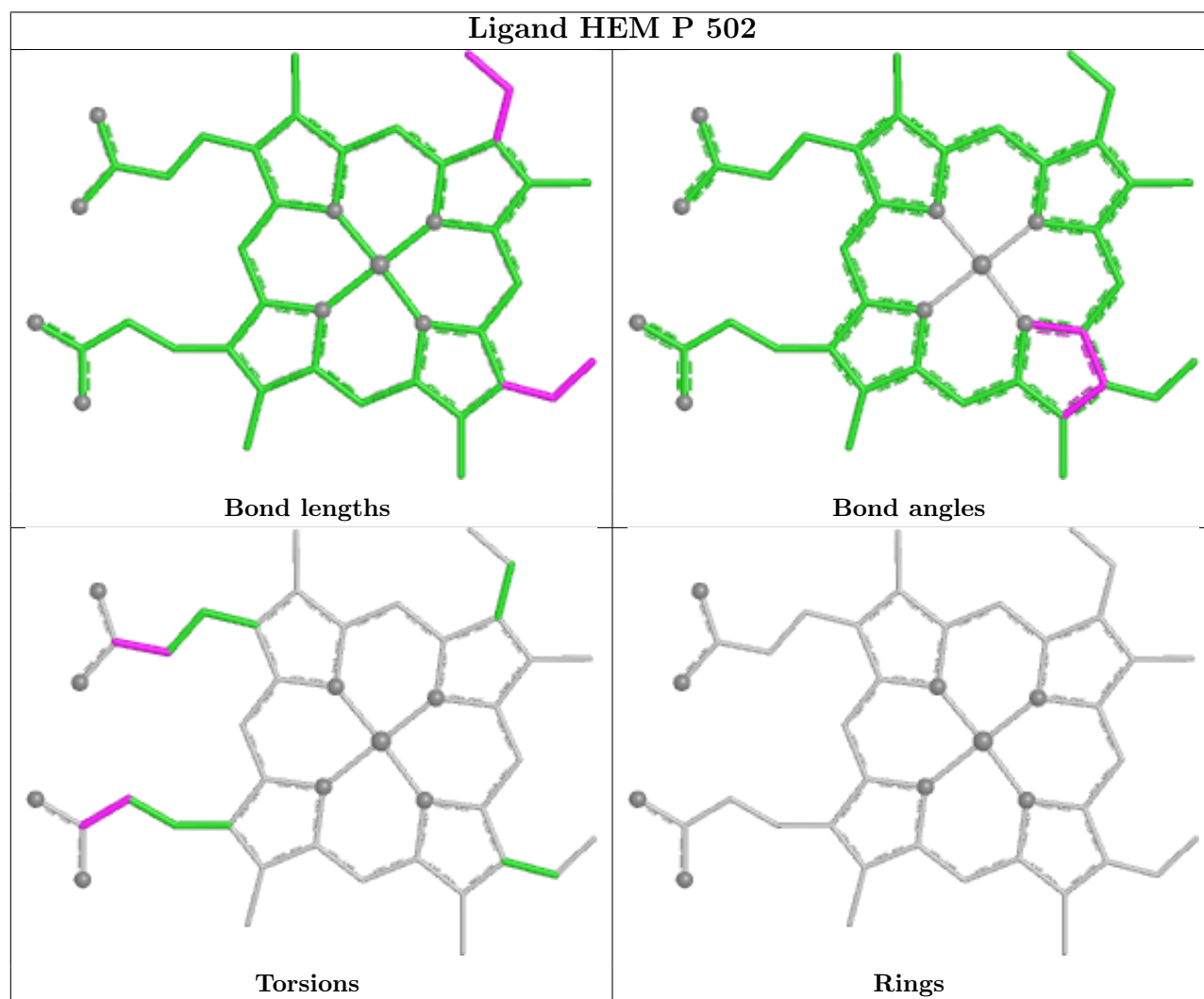
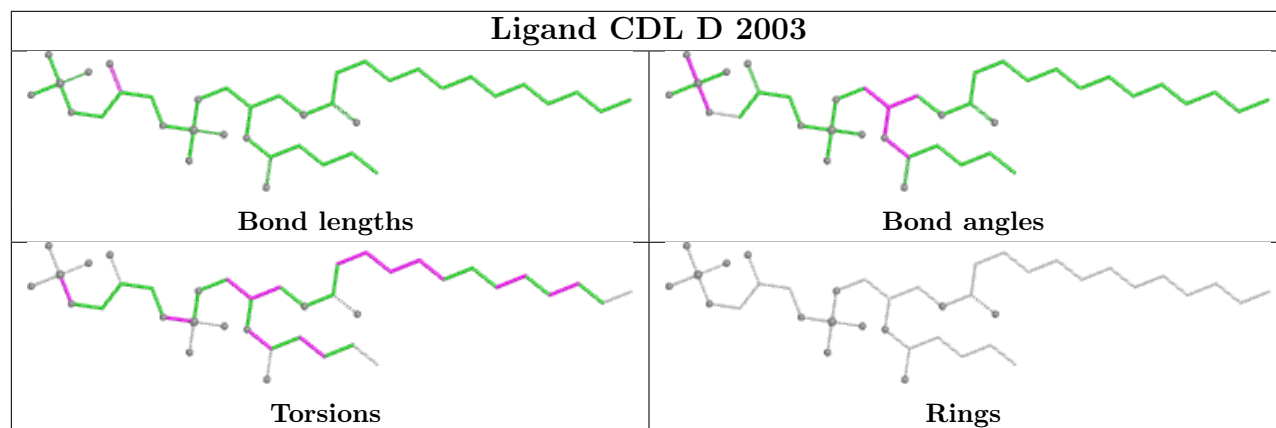


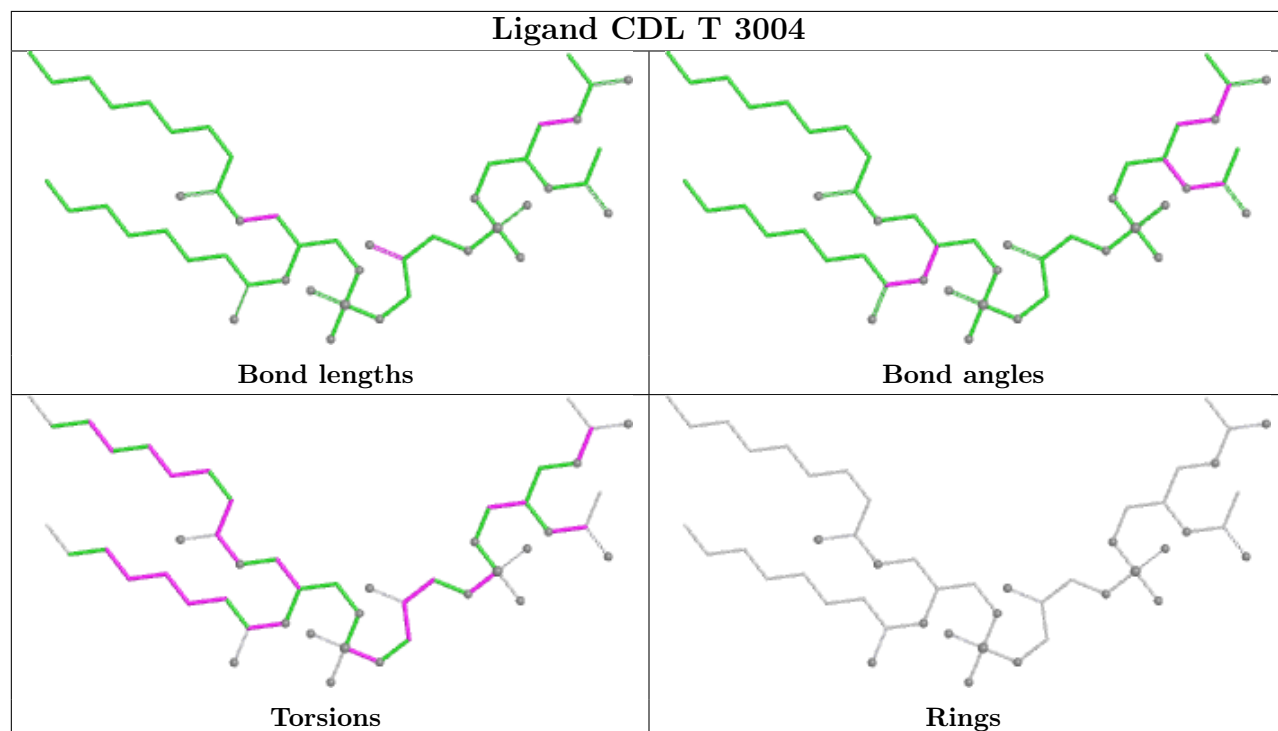
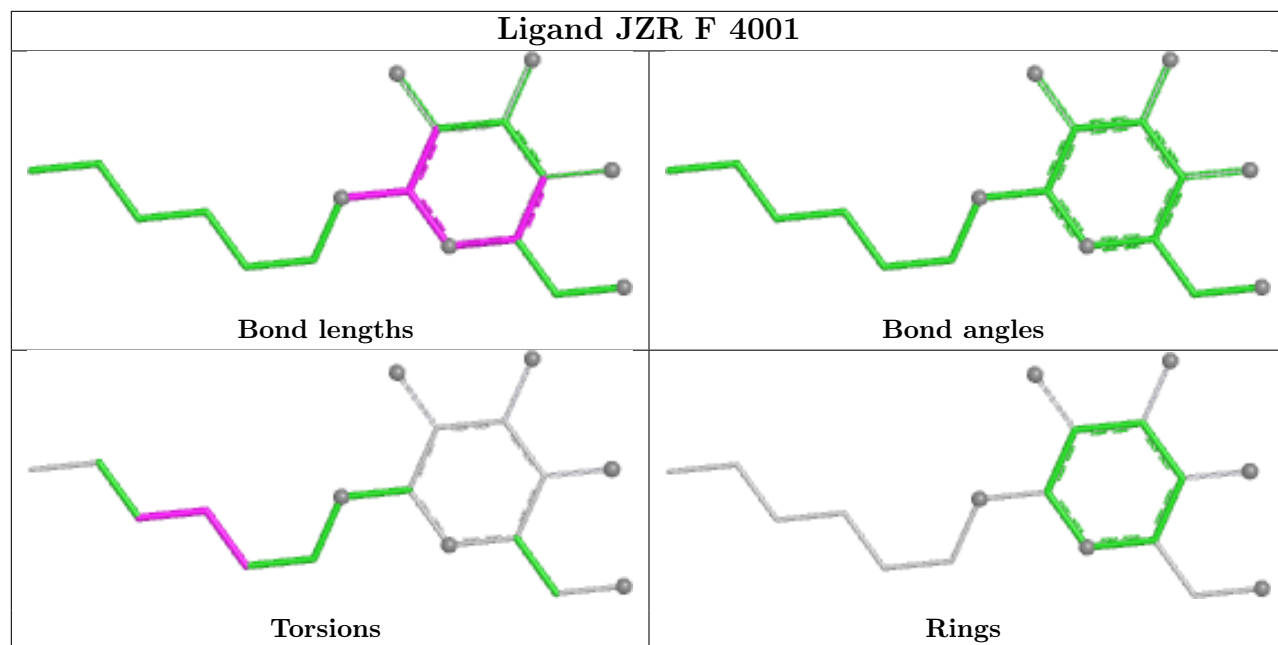


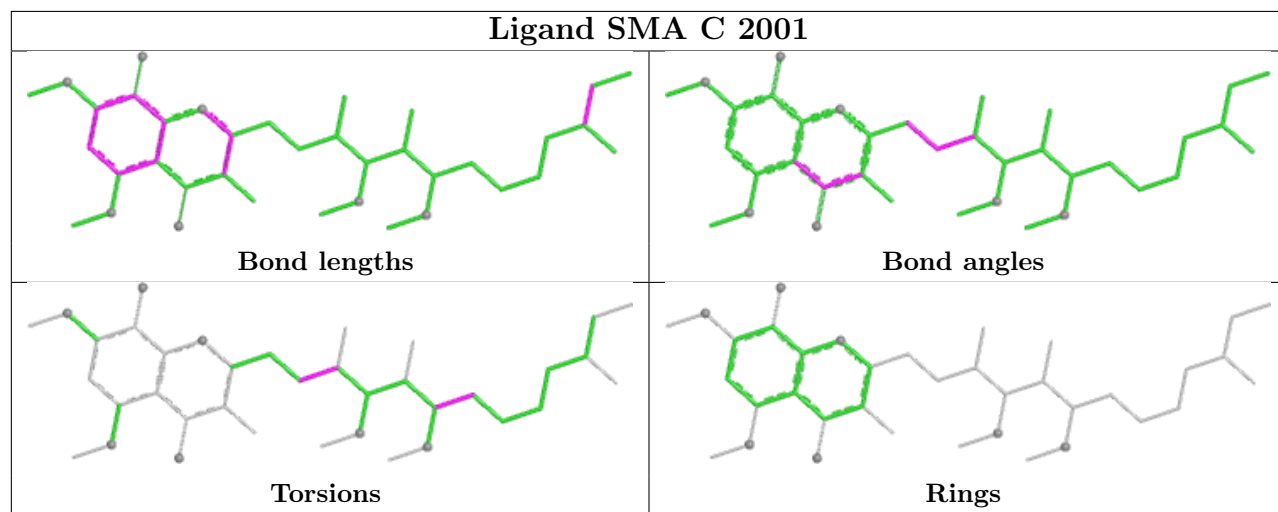
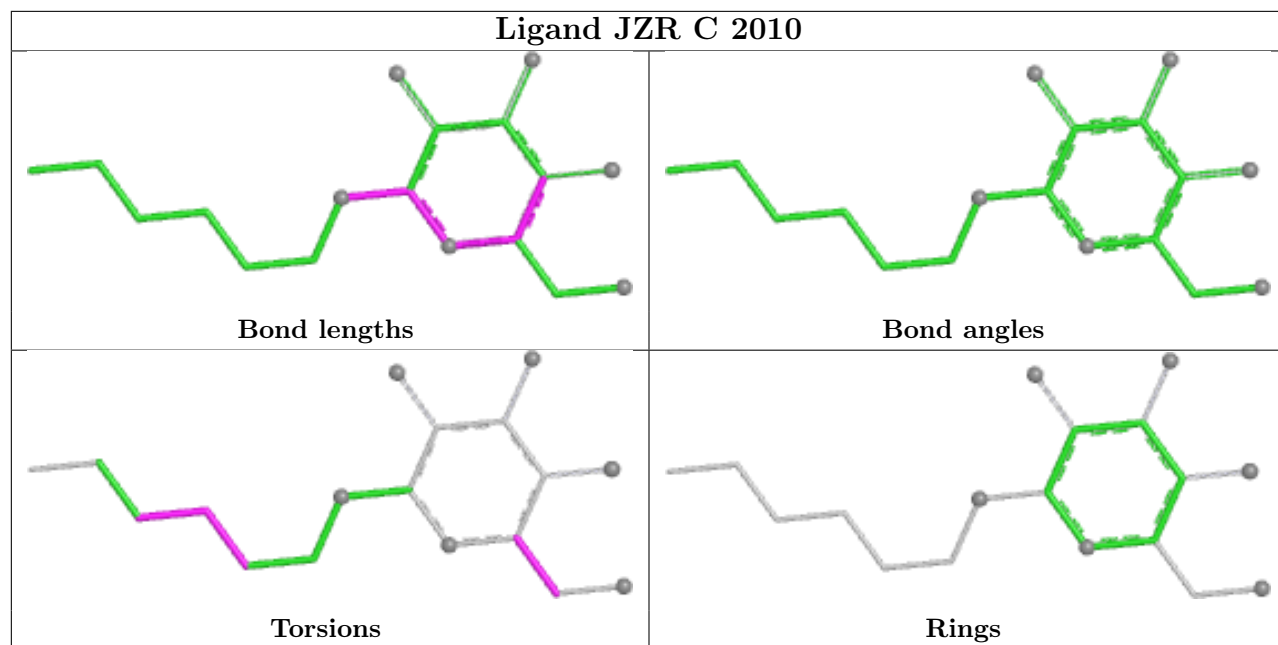


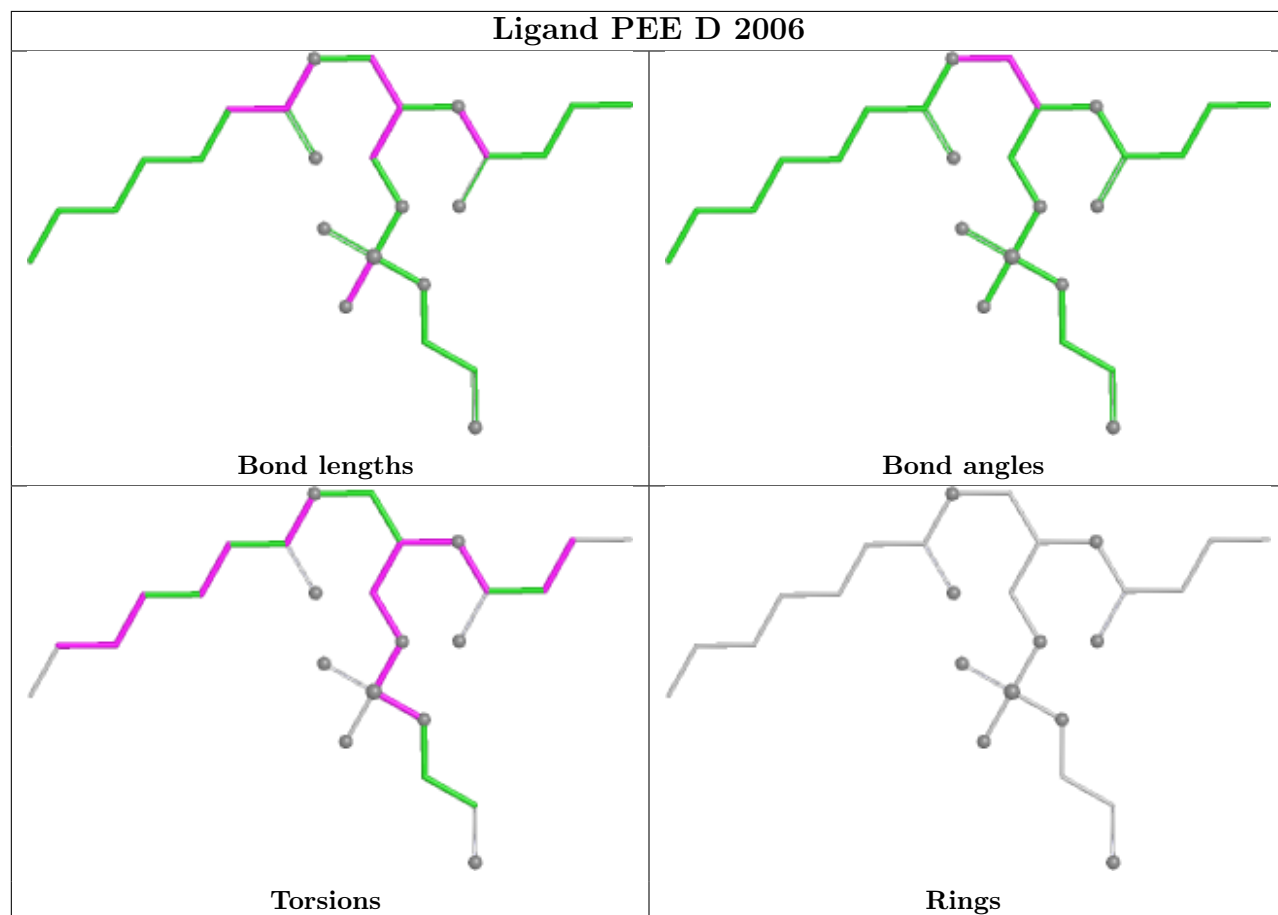
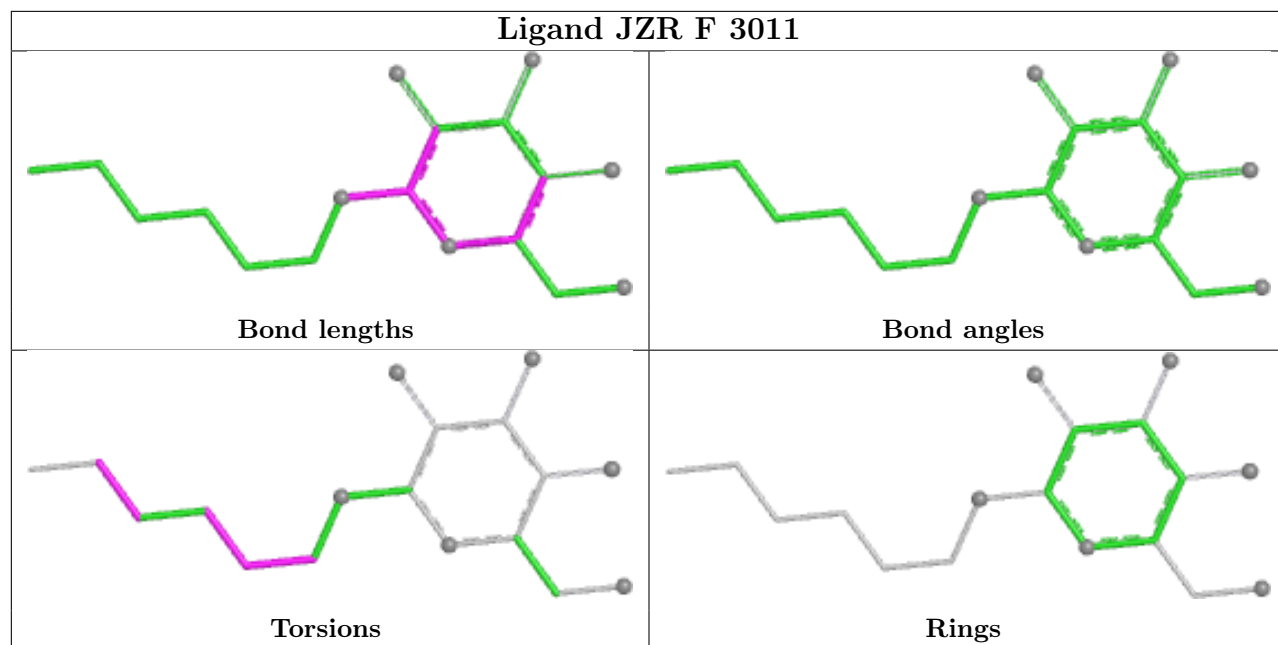
Ligand ANY C 2002	
	
Bond lengths	Bond angles
	
Torsions	Rings

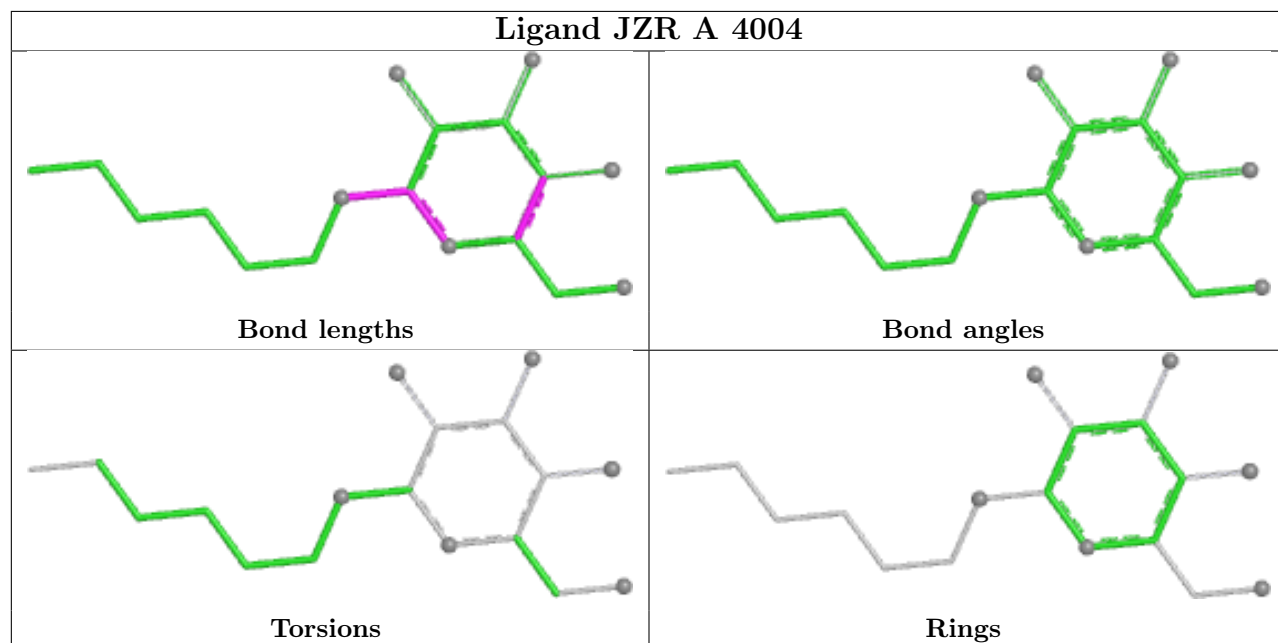
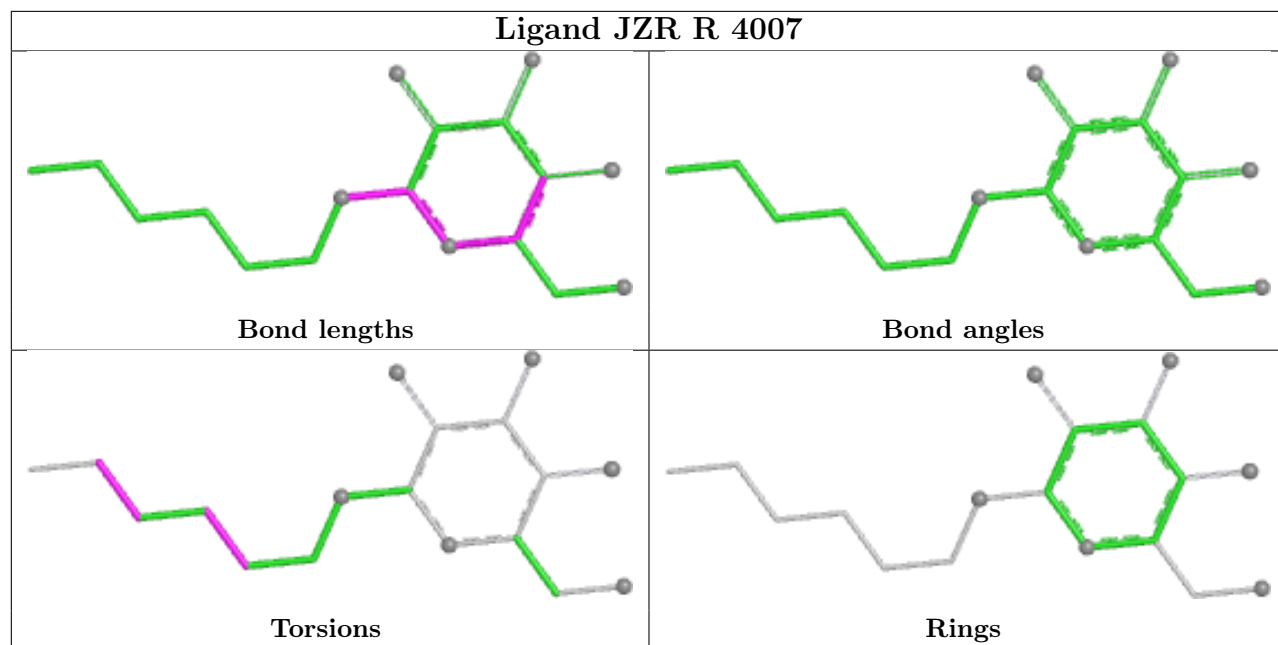
Ligand SMA P 3001	
	
Bond lengths	Bond angles
	
Torsions	Rings

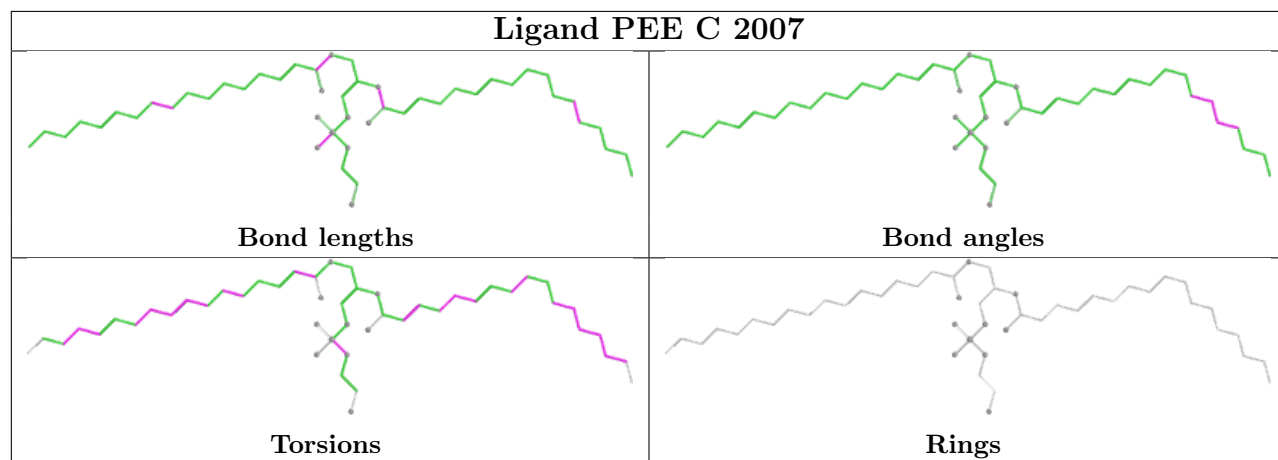
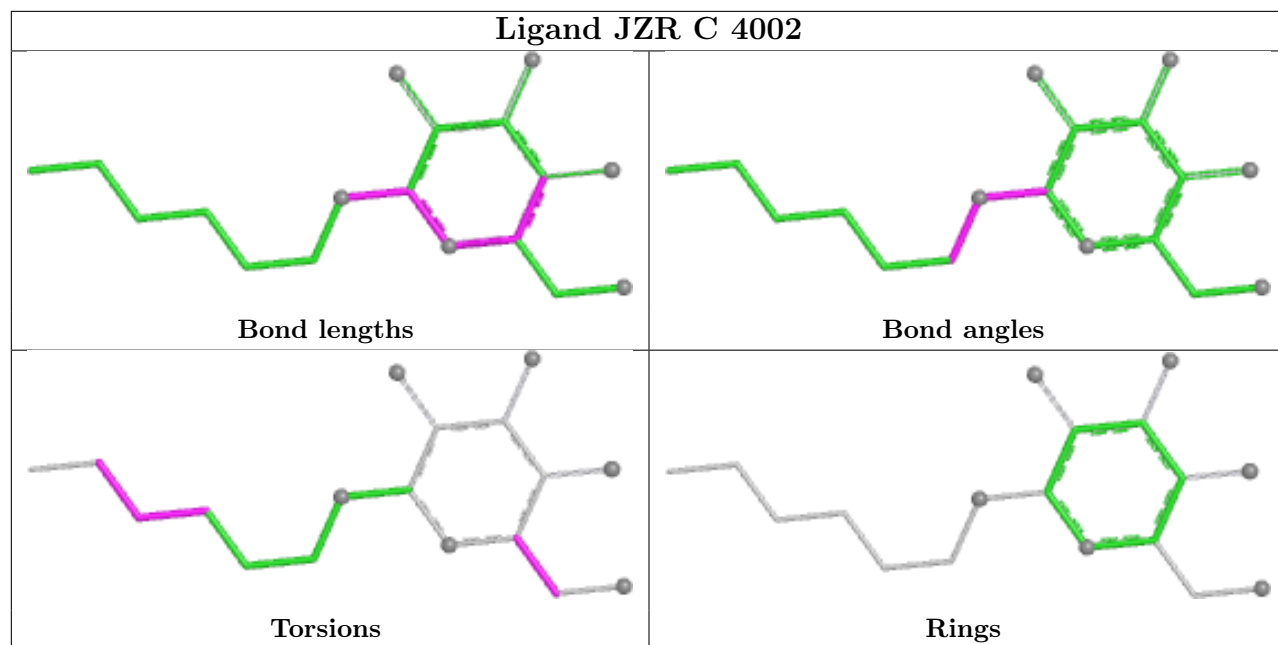


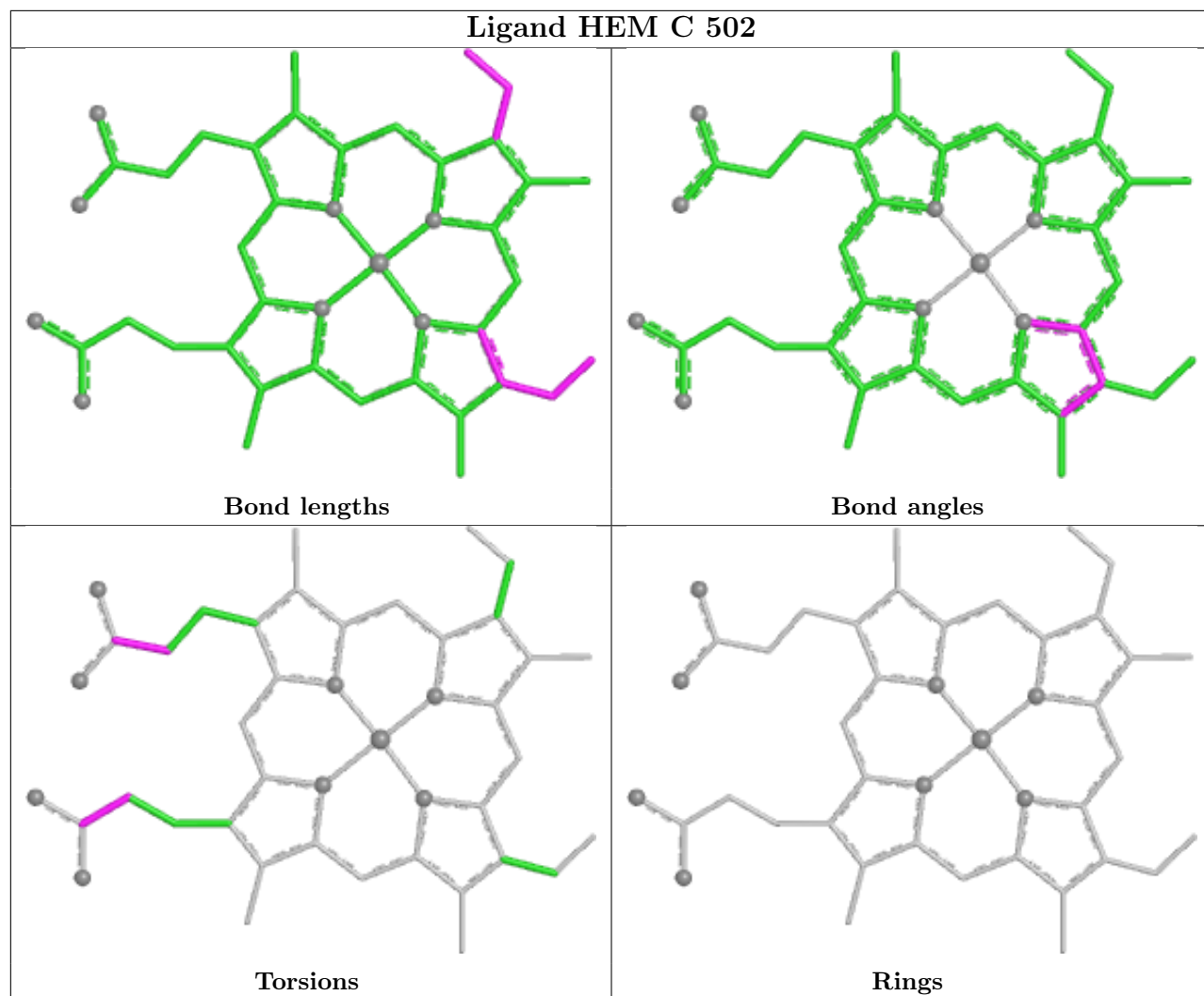


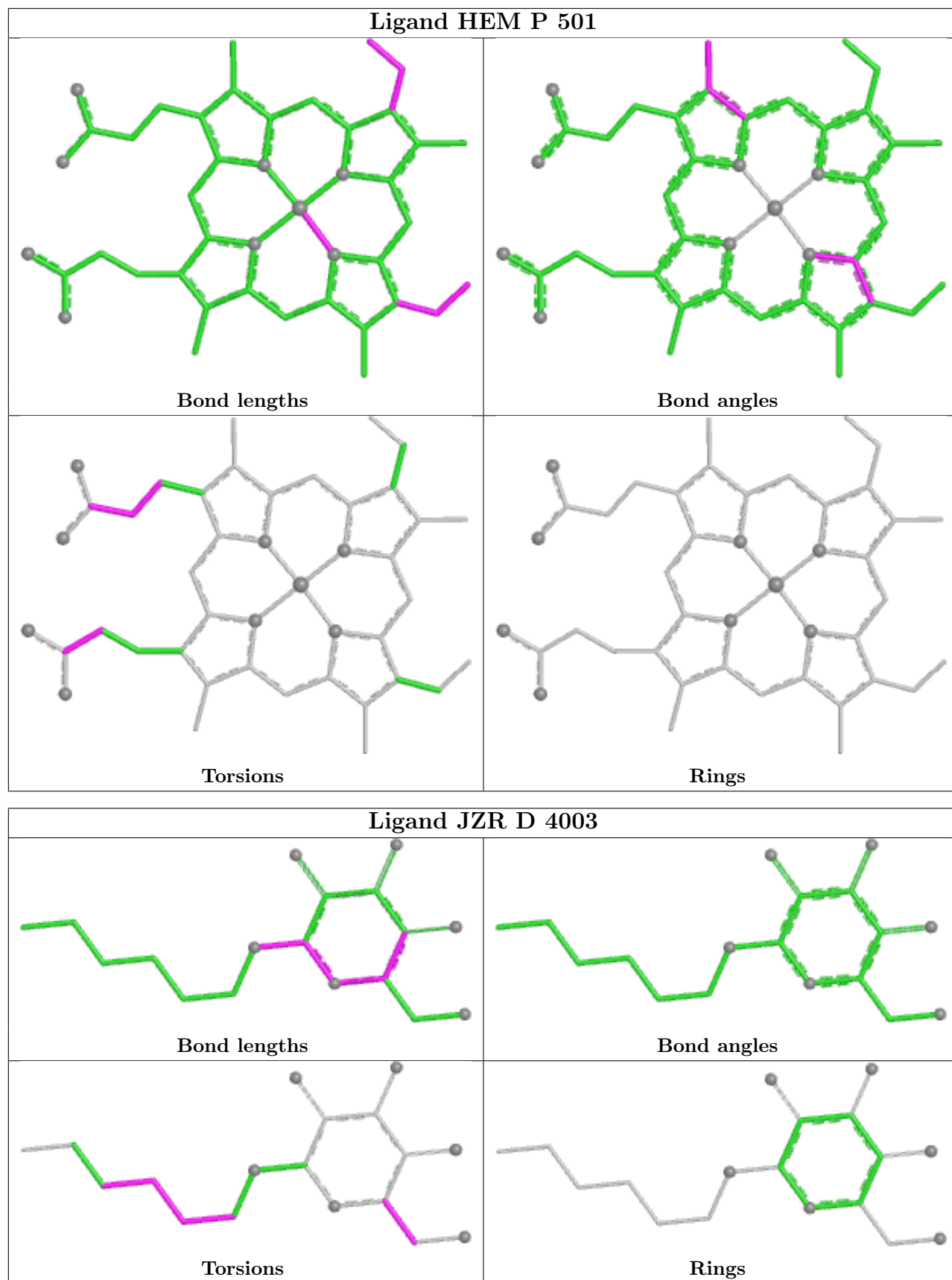


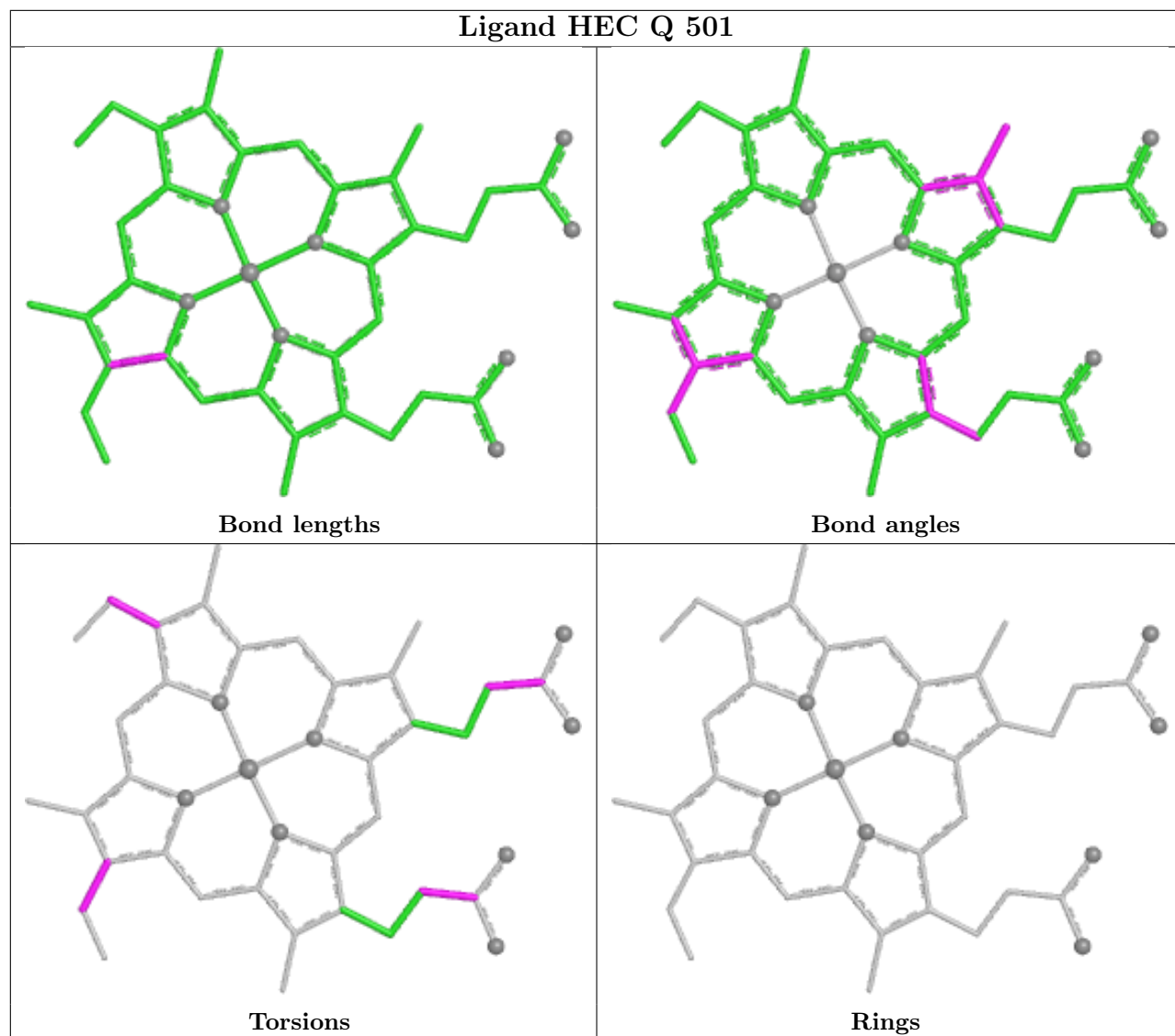




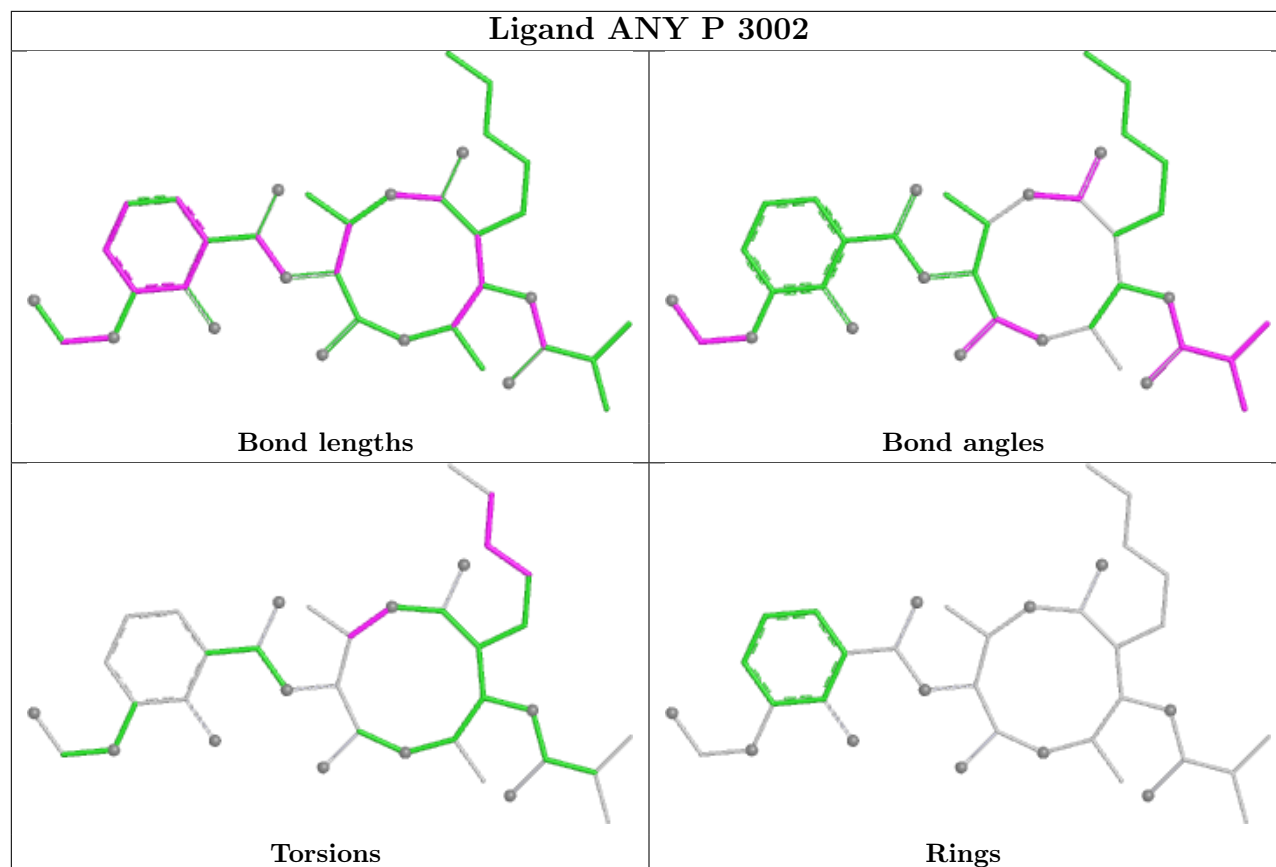




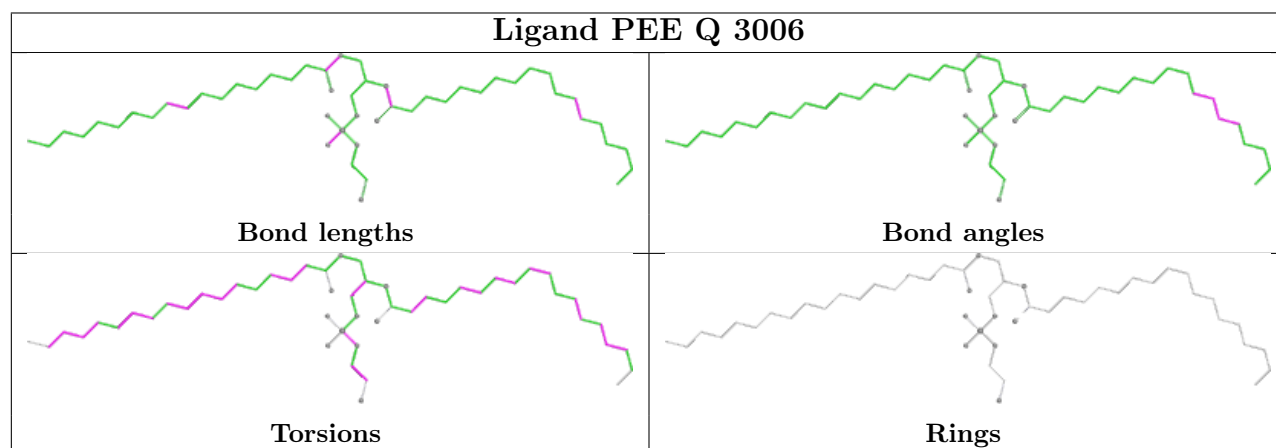




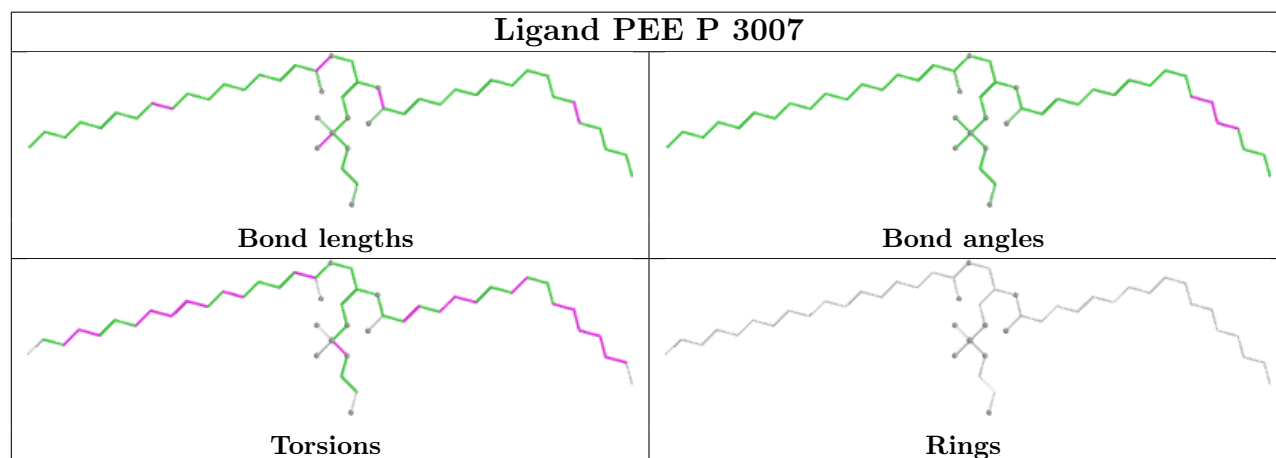
Ligand ANY P 3002



Ligand PEE Q 3006



Ligand PEE P 3007



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/446 (99%)	0.42	23 (5%) 33 35	25, 39, 60, 115	0
1	N	441/446 (98%)	0.91	41 (9%) 14 15	30, 52, 76, 139	1 (0%)
2	B	424/439 (96%)	0.52	18 (4%) 40 42	29, 42, 66, 94	0
2	O	424/439 (96%)	0.83	46 (10%) 11 11	30, 47, 70, 124	0
3	C	365/379 (96%)	0.30	9 (2%) 58 61	23, 36, 53, 108	0
3	P	365/379 (96%)	0.38	11 (3%) 52 55	29, 39, 53, 106	0
4	D	241/241 (100%)	0.52	5 (2%) 63 66	31, 44, 64, 82	0
4	Q	241/241 (100%)	0.73	10 (4%) 41 43	35, 48, 67, 89	0
5	E	196/196 (100%)	1.46	51 (26%) 1 1	35, 62, 106, 111	0
5	R	196/196 (100%)	0.91	18 (9%) 14 15	34, 51, 77, 95	0
6	F	99/110 (90%)	0.47	6 (6%) 27 29	27, 40, 69, 78	0
6	S	99/110 (90%)	0.77	10 (10%) 12 13	33, 42, 80, 102	0
7	G	75/81 (92%)	1.20	14 (18%) 3 3	29, 53, 76, 89	0
7	T	76/81 (93%)	1.32	13 (17%) 4 4	37, 63, 93, 95	0
8	H	66/78 (84%)	0.98	7 (10%) 11 12	43, 59, 77, 81	0
8	U	66/78 (84%)	1.30	12 (18%) 3 3	50, 66, 89, 104	0
9	I	43/78 (55%)	2.87	31 (72%) 0 0	34, 65, 84, 89	0
9	V	43/78 (55%)	2.79	31 (72%) 0 0	38, 72, 86, 90	0
10	J	33/62 (53%)	1.24	7 (21%) 2 2	37, 54, 115, 130	0
10	W	62/62 (100%)	1.76	27 (43%) 0 1	44, 74, 129, 144	0
All	All	3997/4220 (94%)	0.76	390 (9%) 13 13	23, 45, 81, 144	1 (0%)

The worst 5 of 390 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	1	GLY	8.5
1	N	222	THR	8.0
6	S	13	LEU	7.2
2	B	231	GLY	7.0
9	I	78	TYR	6.9

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	JZR	F	4001	18/18	0.19	0.28	146,154,157,158	0
14	GOL	C	4006	6/6	0.54	0.16	96,98,99,100	0
11	JZR	S	2011	18/18	0.62	0.28	61,89,94,98	0
13	AZI	C	2005	3/3	0.64	0.32	54,54,56,58	0
11	JZR	F	3011	18/18	0.64	0.29	108,113,116,116	0
13	AZI	A	4011	3/3	0.66	0.44	61,61,66,69	0
12	PO4	A	2013	5/5	0.68	0.13	119,120,121,122	0
14	GOL	R	4005	6/6	0.68	0.17	81,83,84,85	0
13	AZI	P	3005	3/3	0.69	0.26	51,51,54,56	0
14	GOL	B	2009	6/6	0.69	0.25	84,85,86,86	0
11	JZR	R	4007	18/18	0.70	0.19	85,95,98,99	0
12	PO4	C	4008	5/5	0.71	0.19	153,153,153,153	0
11	JZR	C	2010	18/18	0.72	0.23	94,103,108,108	0
11	JZR	D	4003	18/18	0.73	0.31	160,169,171,171	0
12	PO4	S	3012	5/5	0.73	0.15	97,97,99,100	0
14	GOL	O	3009	6/6	0.77	0.19	82,84,85,85	0
13	AZI	O	4010	3/3	0.78	0.14	102,102,104,104	0
14	GOL	P	3008	6/6	0.78	0.27	67,69,71,71	0
11	JZR	P	3010	18/18	0.78	0.24	103,107,112,112	0

Continued on next page...

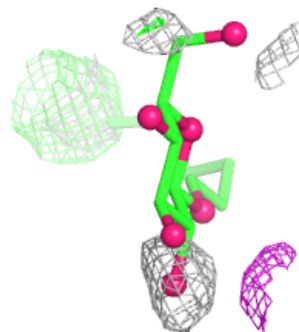
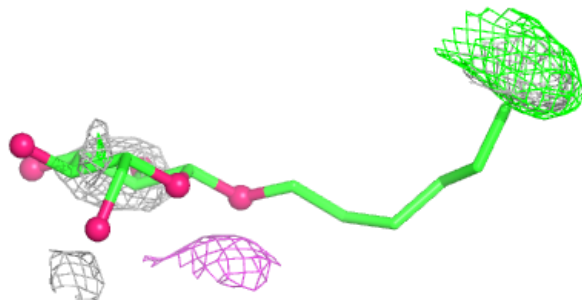
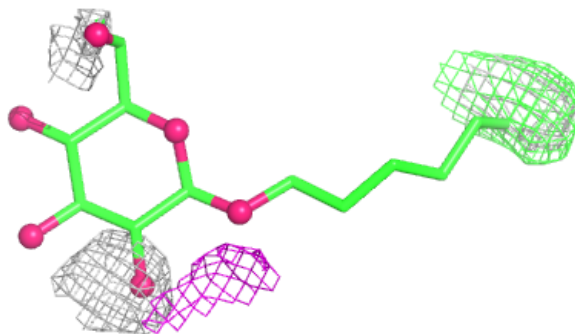
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	PEE	D	2006	26/51	0.78	0.27	85,98,108,109	0
12	PO4	P	3013	5/5	0.80	0.11	104,105,106,106	0
20	CDL	D	2003	39/100	0.80	0.18	53,78,93,94	0
11	JZR	C	4002	18/18	0.81	0.24	114,122,125,125	0
20	CDL	G	2004	44/100	0.83	0.20	73,87,99,102	0
20	CDL	P	3003	39/100	0.83	0.18	61,89,111,111	0
20	CDL	T	3004	49/100	0.83	0.21	74,89,107,107	0
12	PO4	F	2012	5/5	0.84	0.11	81,82,83,84	0
17	PEE	Q	3006	51/51	0.86	0.20	65,75,98,100	0
14	GOL	C	2008	6/6	0.88	0.23	61,65,68,75	0
13	AZI	G	4009	3/3	0.90	0.25	66,66,67,68	0
17	PEE	P	3007	49/51	0.91	0.17	41,57,81,81	0
17	PEE	C	2007	49/51	0.92	0.15	35,55,81,83	0
11	JZR	A	4004	18/18	0.93	0.09	28,34,40,42	0
18	ANY	C	2002	37/40	0.94	0.10	31,39,65,70	0
18	ANY	P	3002	37/40	0.94	0.11	33,39,67,71	0
16	SMA	C	2001	37/37	0.95	0.08	31,39,44,48	0
16	SMA	P	3001	37/37	0.95	0.09	27,40,44,46	0
19	HEC	Q	501	43/43	0.96	0.09	38,45,48,51	0
19	HEC	D	501	43/43	0.97	0.08	35,41,44,45	0
15	HEM	C	501	43/43	0.97	0.08	20,31,38,47	0
15	HEM	P	502	43/43	0.97	0.08	27,31,36,40	0
21	FES	E	501	4/4	0.97	0.06	41,41,43,43	0
15	HEM	C	502	43/43	0.98	0.07	22,28,34,37	0
15	HEM	P	501	43/43	0.98	0.07	30,34,42,46	0
21	FES	R	501	4/4	0.98	0.04	35,35,37,37	0

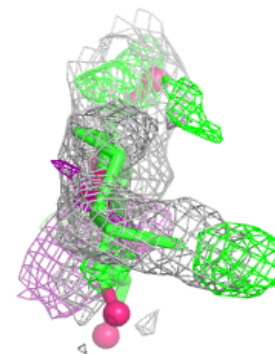
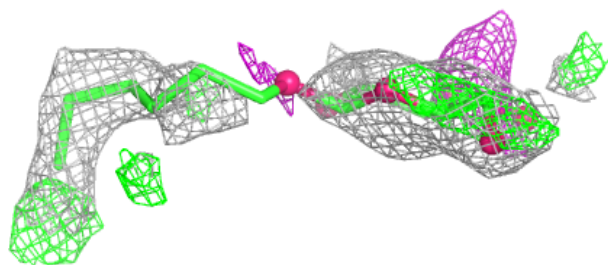
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JZR F 4001:

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

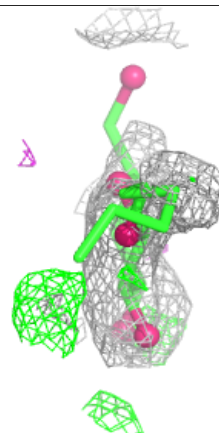
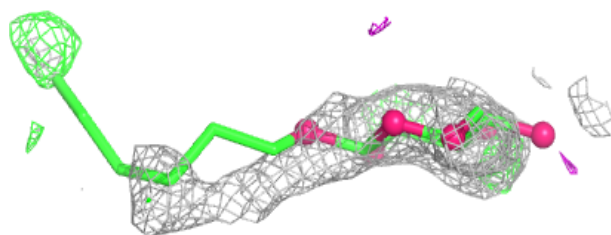
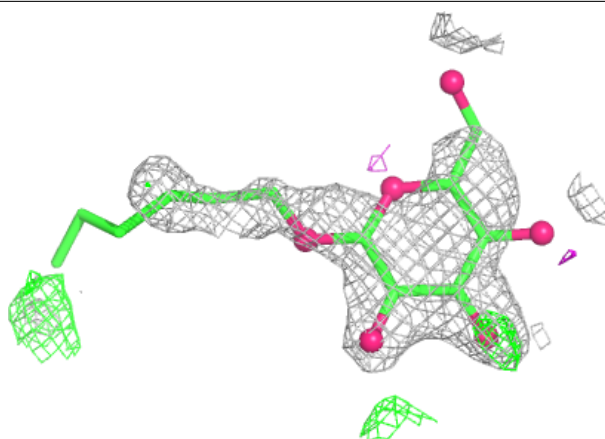
**Electron density around JZR S 2011:**

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



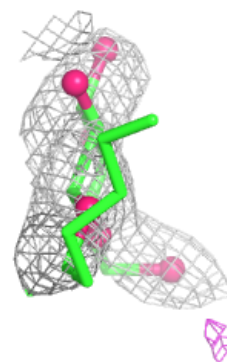
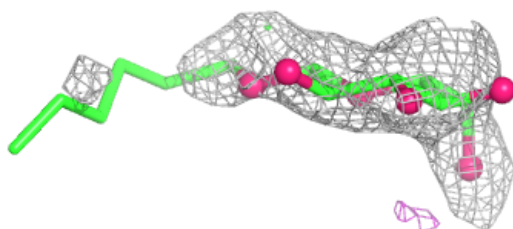
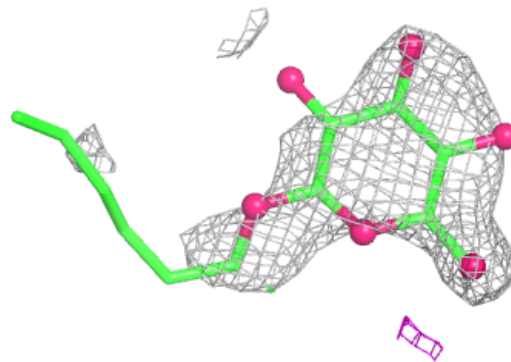
Electron density around JZR F 3011:

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

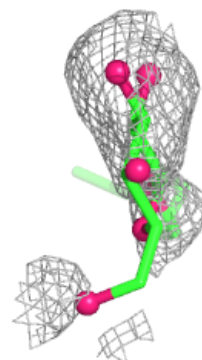
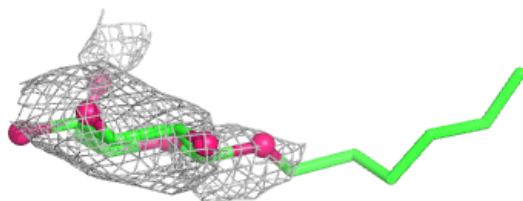


Electron density around JZR R 4007:

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

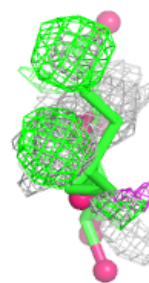
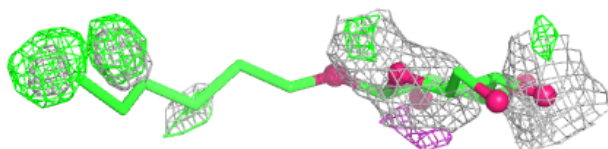
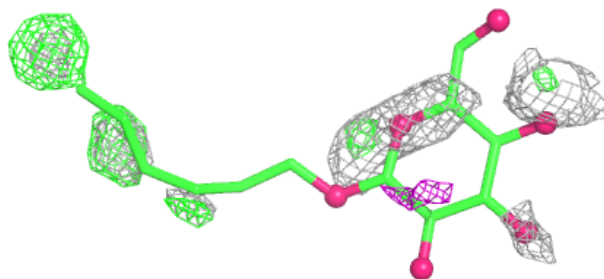
**Electron density around JZR C 2010:**

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

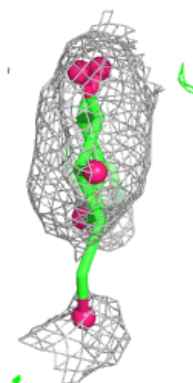
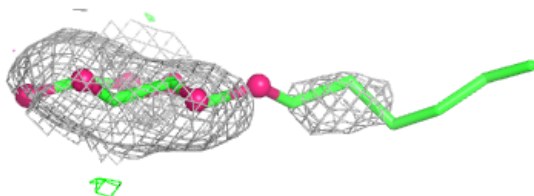
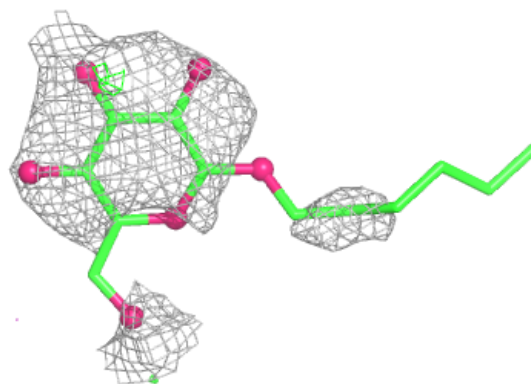


Electron density around JZR D 4003:

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

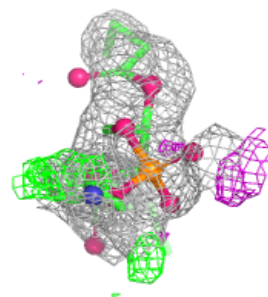
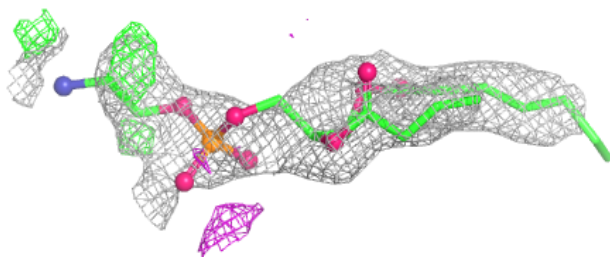
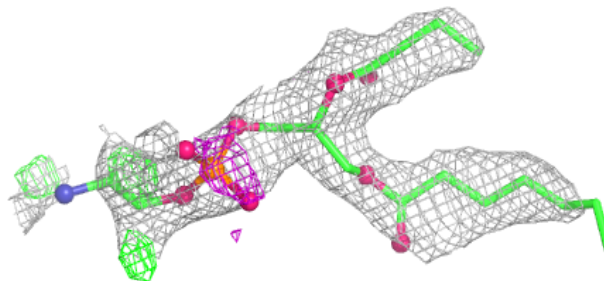
**Electron density around JZR P 3010:**

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

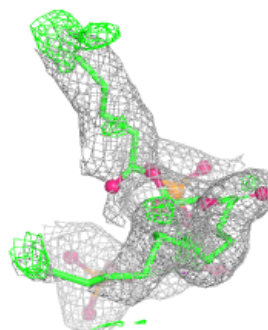
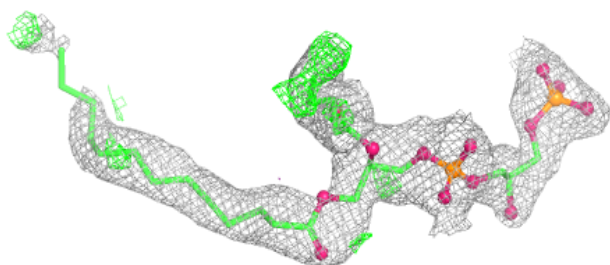
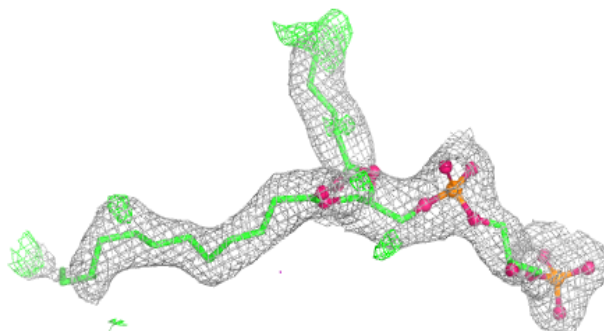


Electron density around PEE D 2006:

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

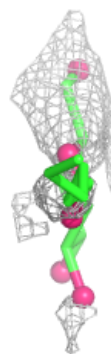
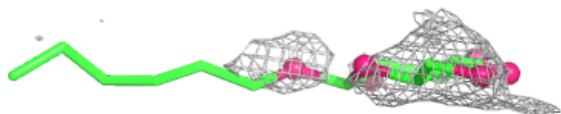
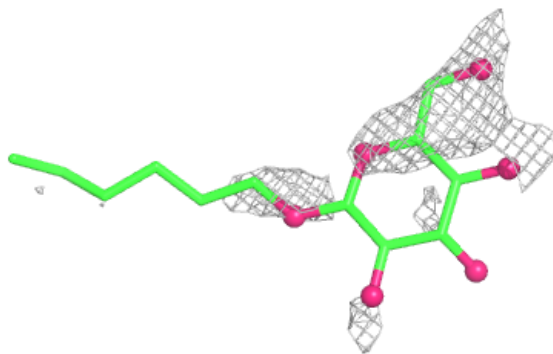
**Electron density around CDL D 2003:**

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

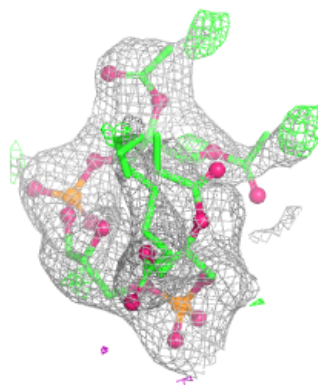
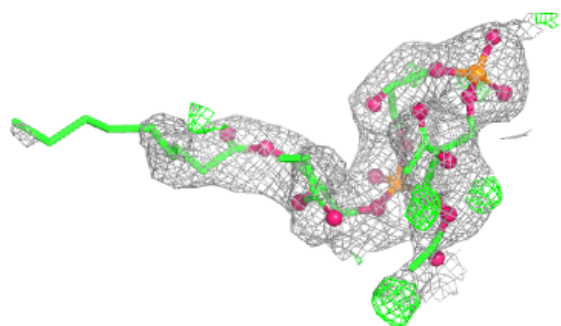
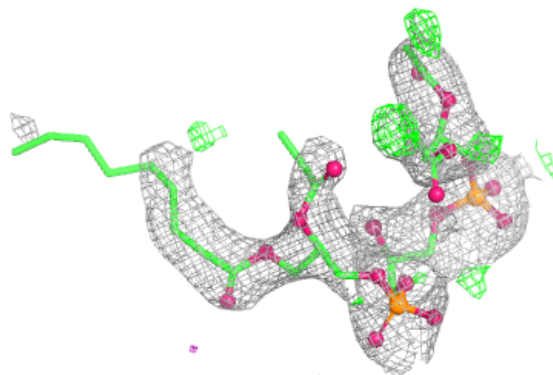


Electron density around JZR C 4002:

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

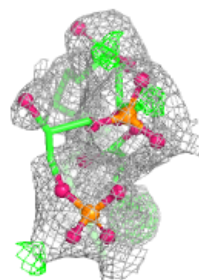
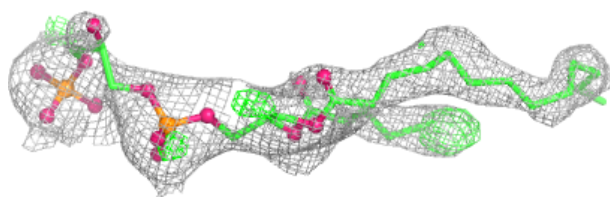
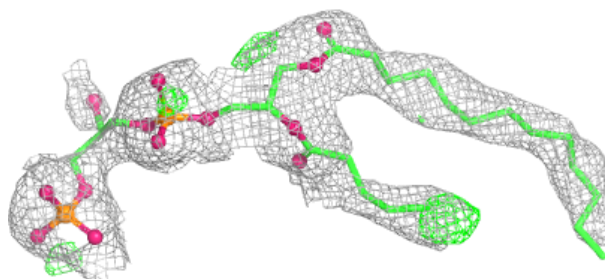
**Electron density around CDL G 2004:**

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

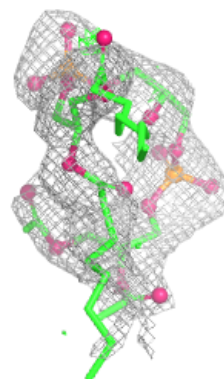
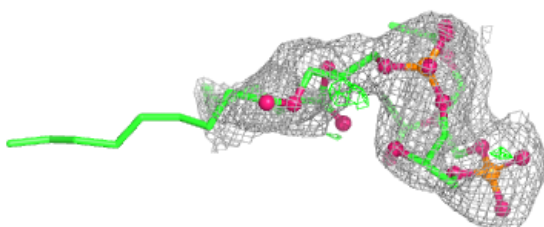
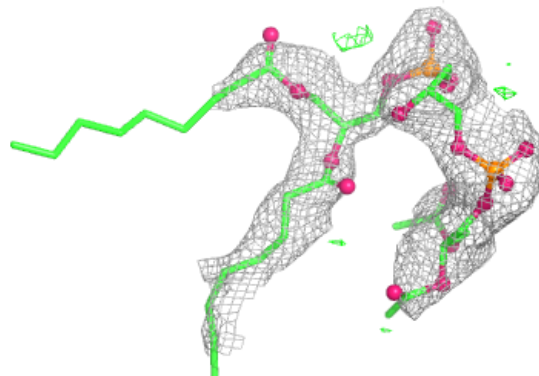


Electron density around CDL P 3003:

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

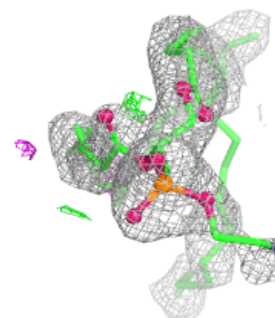
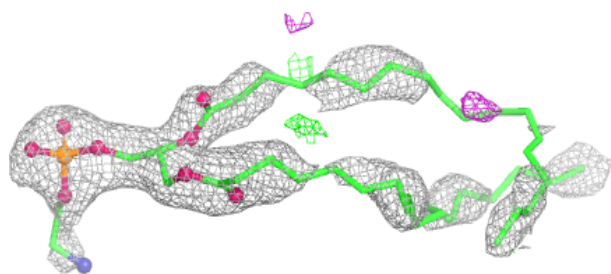
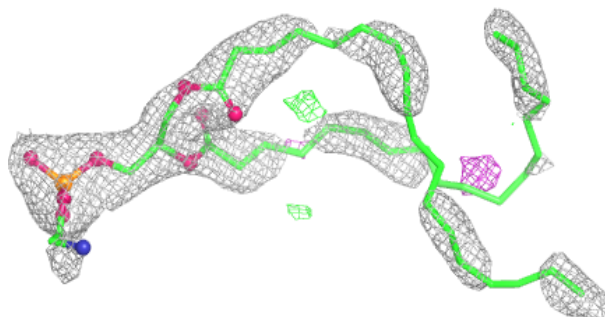
**Electron density around CDL T 3004:**

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

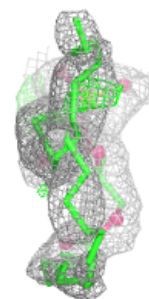
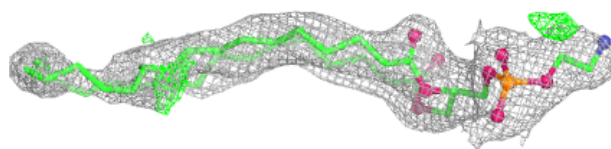
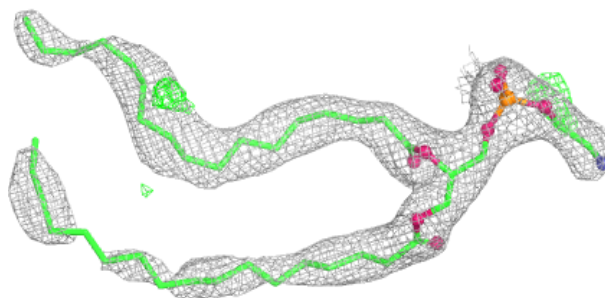


Electron density around PEE Q 3006:

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

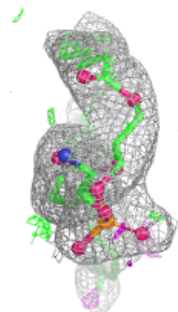
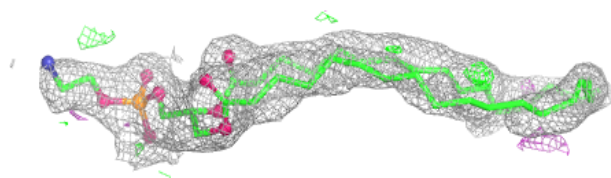
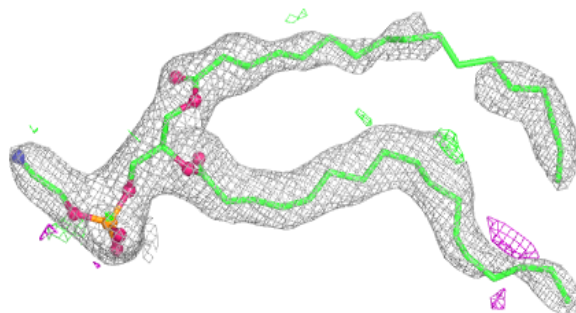
**Electron density around PEE P 3007:**

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

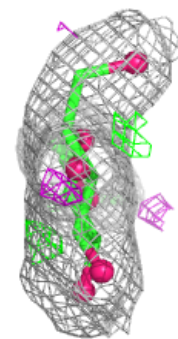
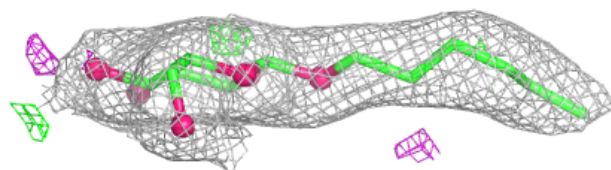
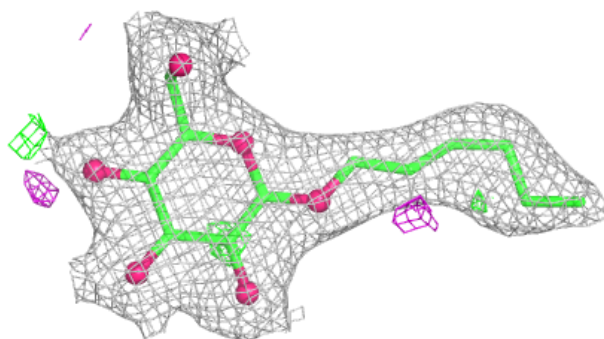


Electron density around PEE C 2007:

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

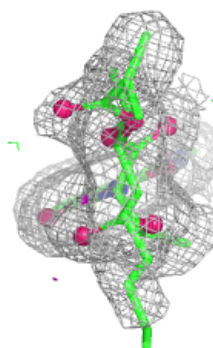
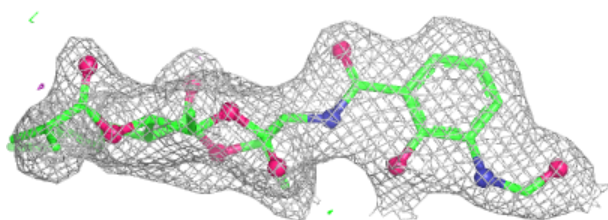
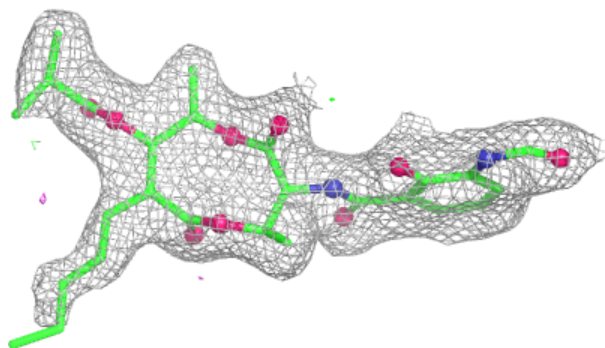
**Electron density around JZR A 4004:**

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

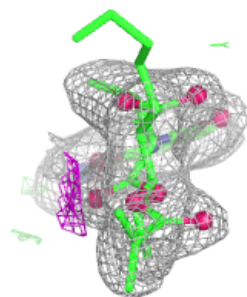
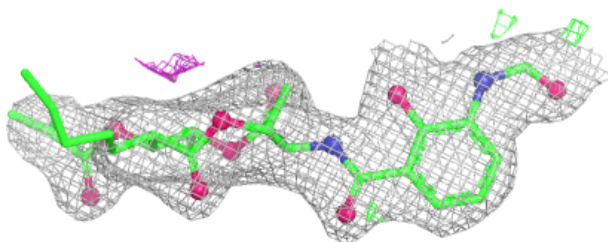
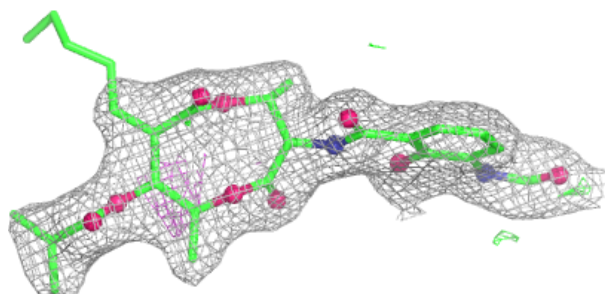


Electron density around ANY C 2002:

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

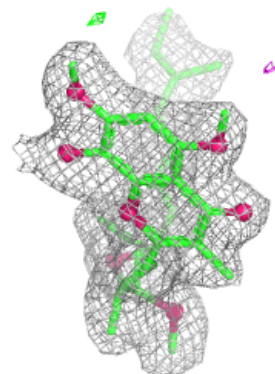
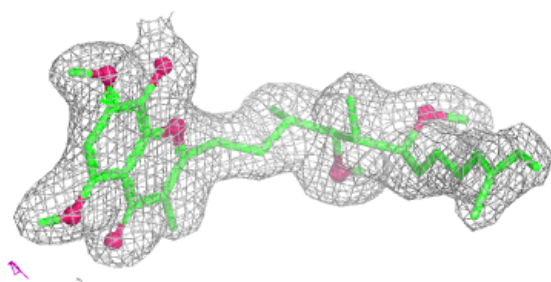
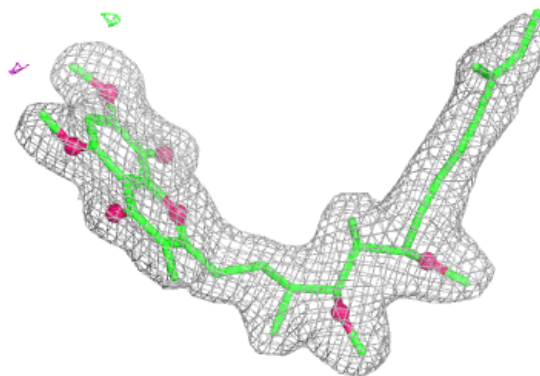
**Electron density around ANY P 3002:**

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

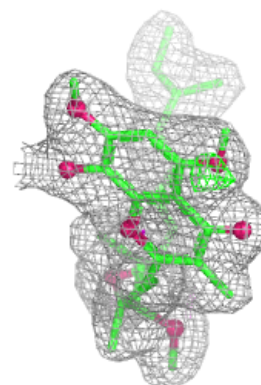
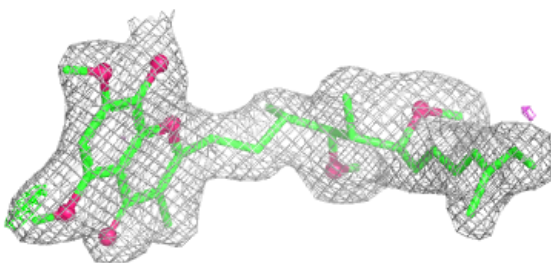
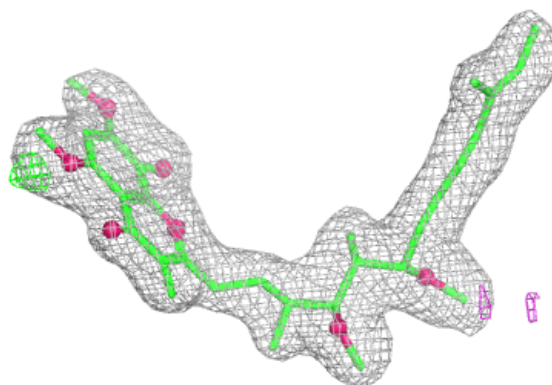


Electron density around SMA C 2001:

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

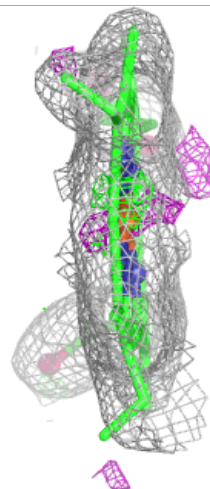
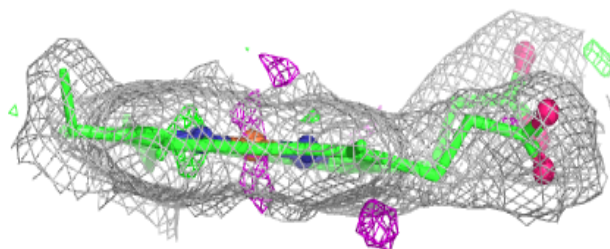
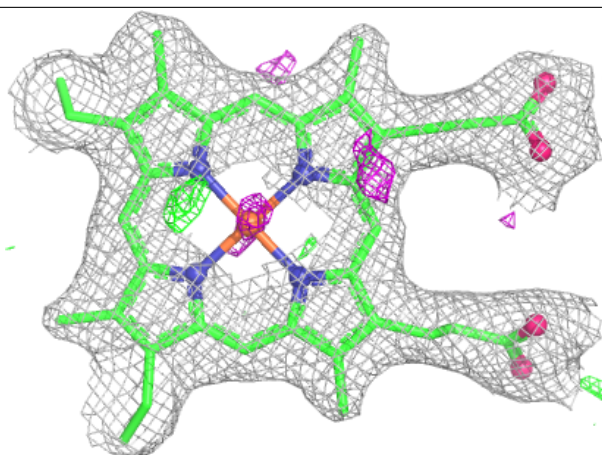
**Electron density around SMA P 3001:**

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



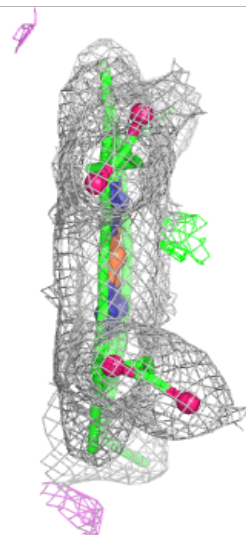
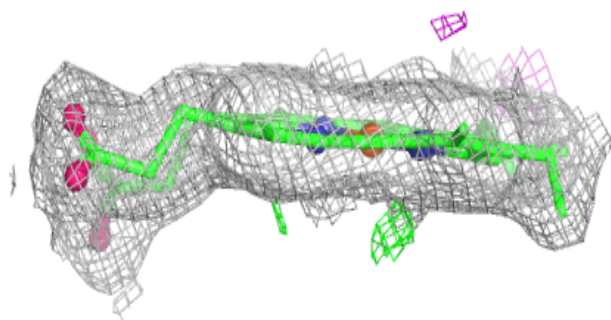
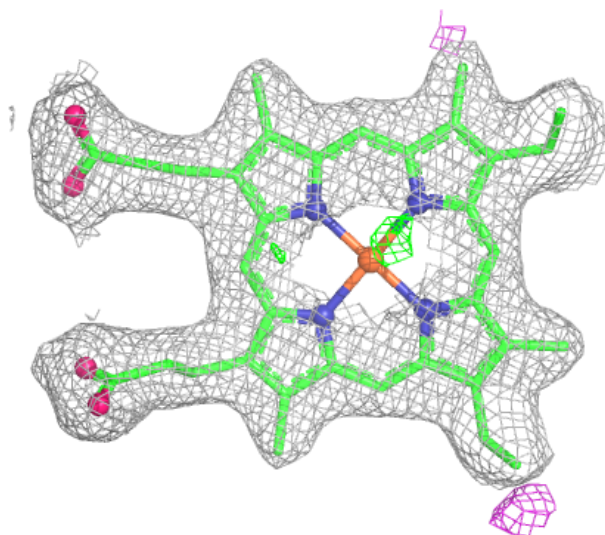
Electron density around HEC Q 501:

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



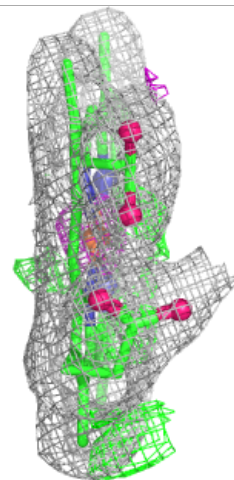
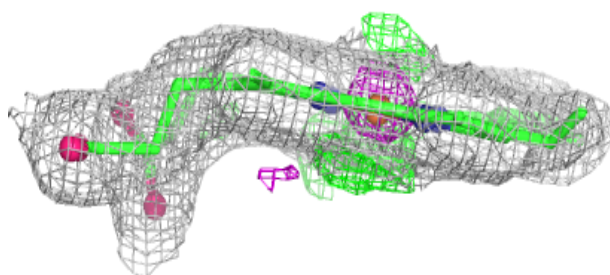
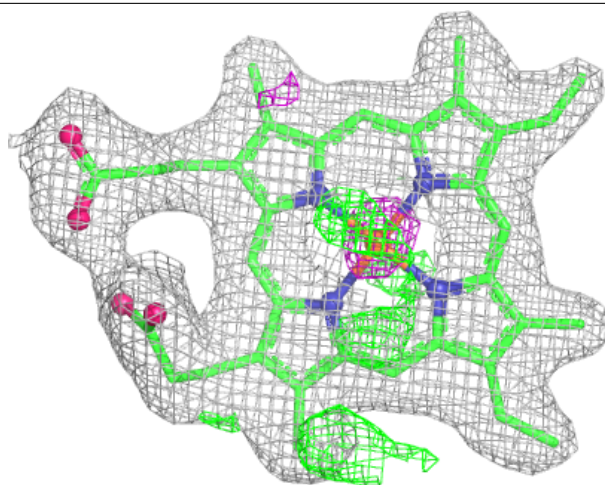
Electron density around HEC D 501:

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



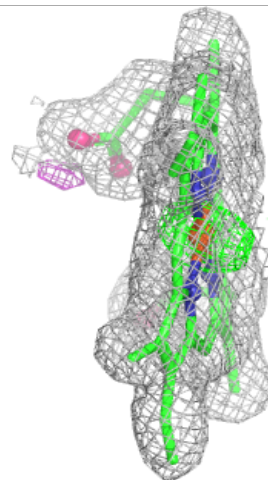
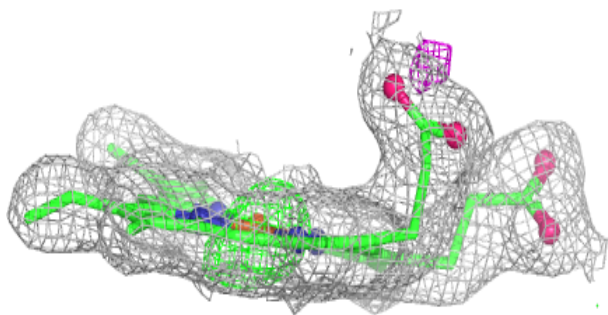
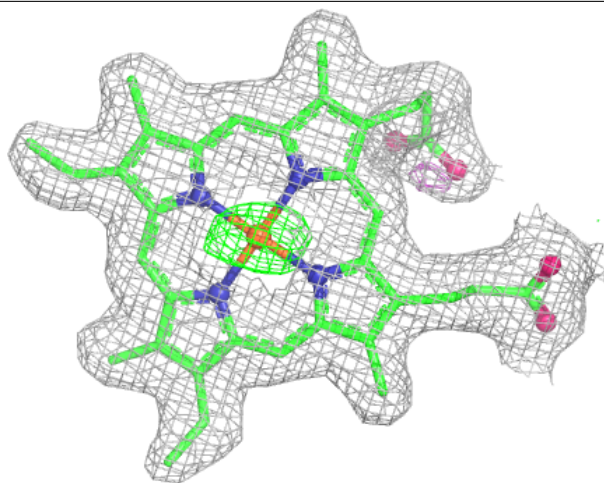
Electron density around HEM C 501:

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



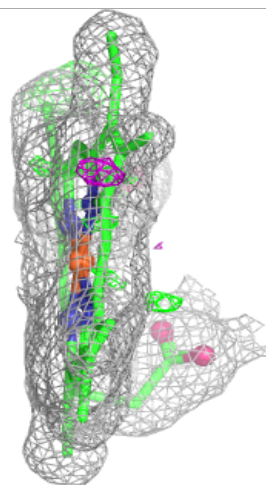
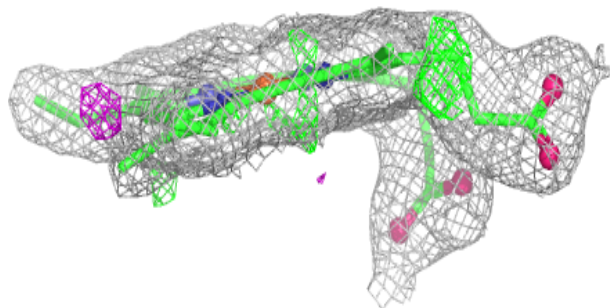
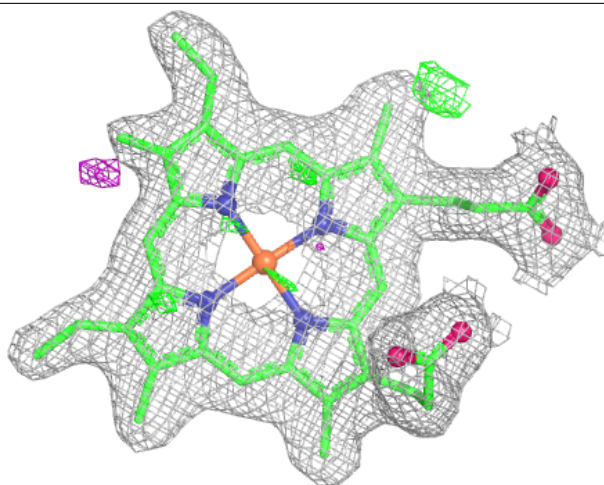
Electron density around HEM P 502:

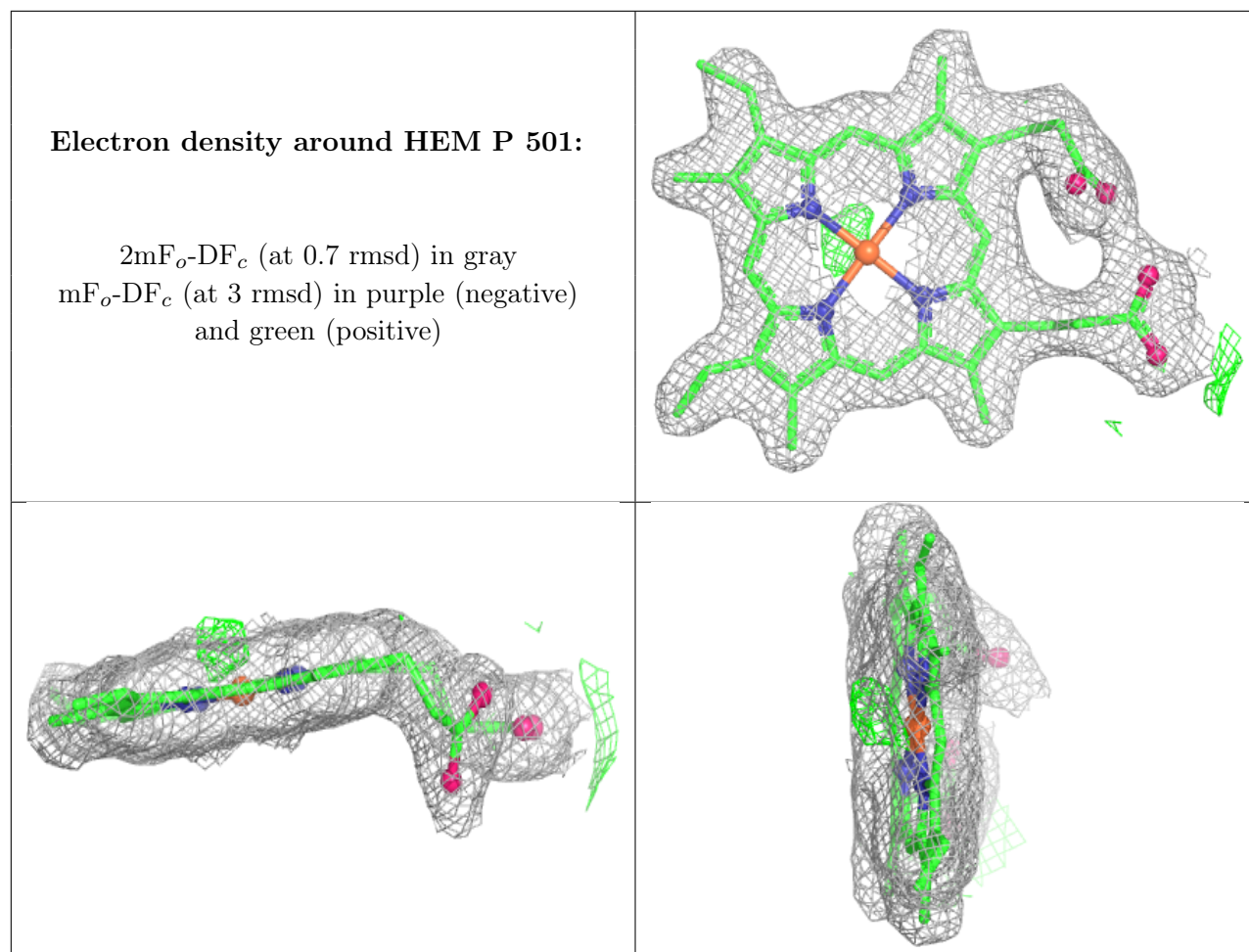
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.