



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 9FKS / pdb_00009fks
EMDB ID : EMD-50526
Title : Respiratory supercomplex CIII2-CIV2 from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-06-04
Resolution : 4.31 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

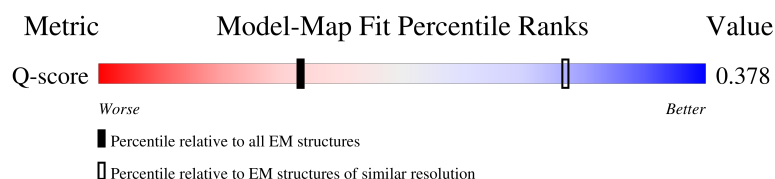
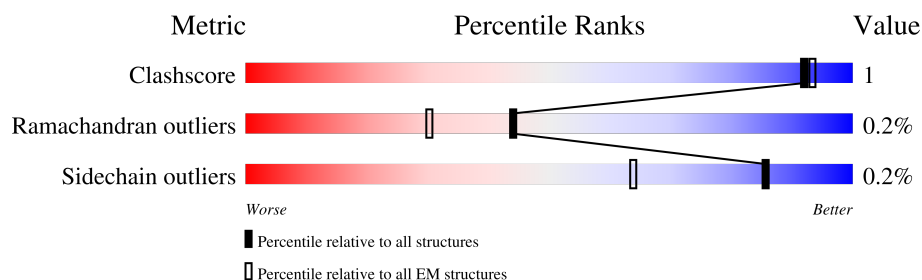
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.31 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3904 (3.81 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	440	<div> <div>21%</div> <div>93%</div> <div>5%</div> </div>
1	d	440	<div> <div>22%</div> <div>95%</div> <div>.</div> </div>
2	b	450	<div> <div>12%</div> <div>52%</div> <div>47%</div> </div>
2	e	450	<div> <div>12%</div> <div>52%</div> <div>47%</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	195	<div> <div>56%</div> <div>88%</div> <div>5%</div> <div>8%</div> </div>
3	f	195	<div> <div>56%</div> <div>91%</div> <div>7%</div> </div>
4	g	558	<div> <div>39%</div> <div>93%</div> </div>
4	k	558	<div> <div>40%</div> <div>92%</div> <div>5%</div> </div>
5	h	298	<div> <div>48%</div> <div>83%</div> <div>15%</div> </div>
5	l	298	<div> <div>47%</div> <div>84%</div> <div>15%</div> </div>
6	i	274	<div> <div>35%</div> <div>98%</div> </div>
6	m	274	<div> <div>35%</div> <div>95%</div> </div>
7	j	66	<div> <div>47%</div> <div>65%</div> <div>35%</div> </div>
7	n	66	<div> <div>44%</div> <div>62%</div> <div>35%</div> </div>
8	o	176	<div> <div>7%</div> <div>24%</div> <div>75%</div> </div>
8	p	176	<div> <div>10%</div> <div>24%</div> <div>74%</div> </div>

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 34791 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	433	Total	C	N	O	S	0	0
			3504	2373	552	561	18		
1	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
2	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	180	Total	C	N	O	S	0	0
			1353	838	245	263	7		
3	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		
4	k	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		
5	l	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 6 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		
6	m	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

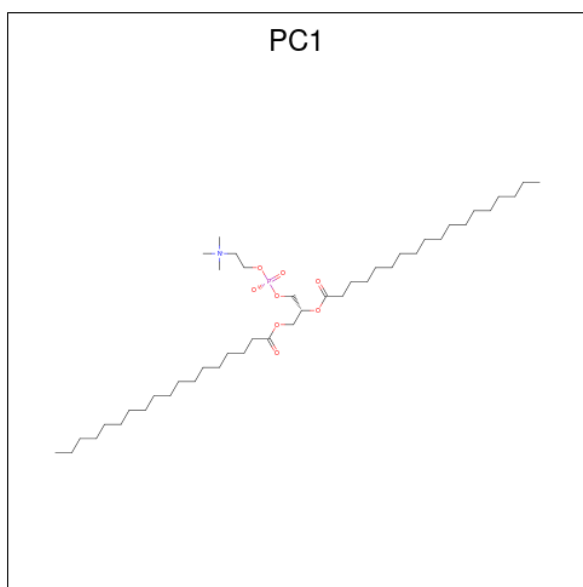
- Molecule 7 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		
7	n	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

- Molecule 8 is a protein called Cytochrome c, class I.

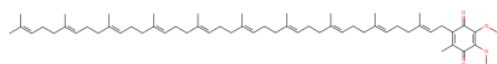
Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	44	Total	C	N	O	S	0	0
			324	215	49	58	2		
8	p	45	Total	C	N	O	S	0	0
			330	218	50	60	2		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).

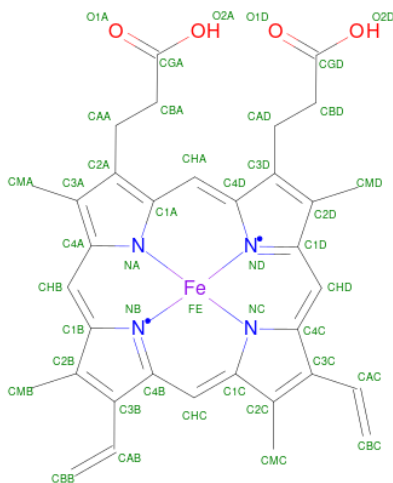


Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	d	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	j	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	n	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	o	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 10 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

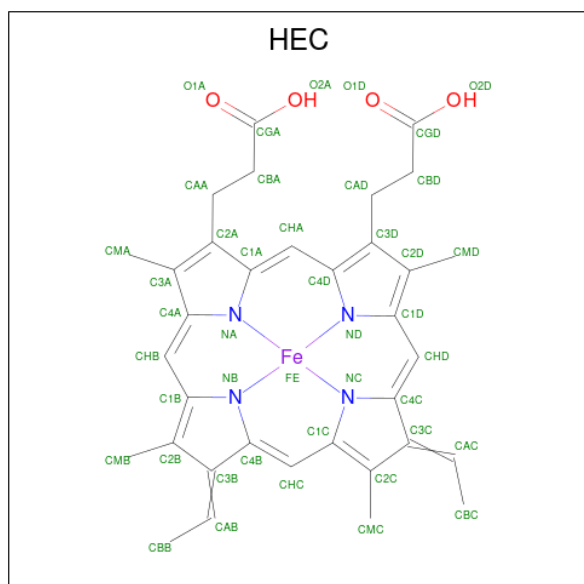


Mol	Chain	Residues	Atoms					AltConf
11	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	d	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	d	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
12	b	1	Total Ca 1 1	0
12	e	1	Total Ca 1 1	0
12	g	1	Total Ca 1 1	0
12	k	1	Total Ca 1 1	0

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



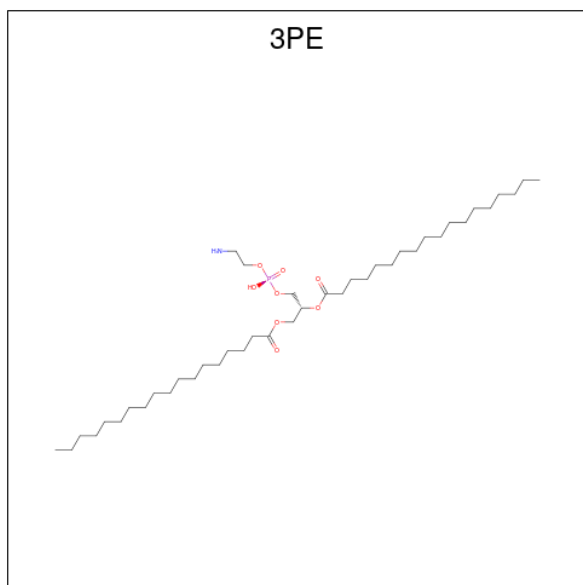
Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 43	C 34	Fe 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



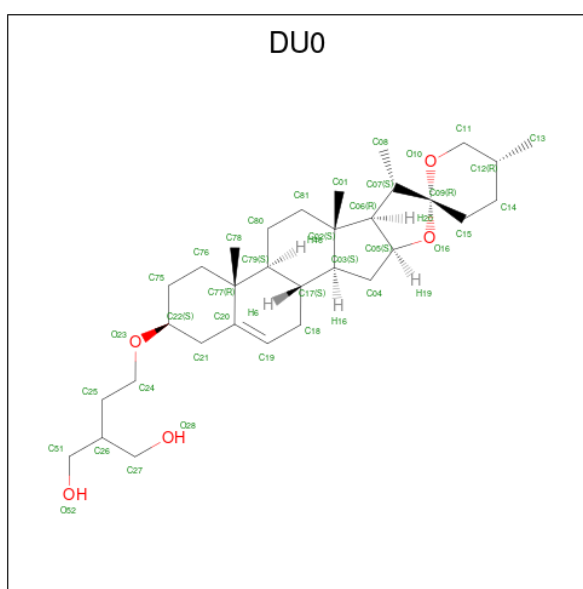
Mol	Chain	Residues	Atoms					AltConf
14	c	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	e	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	e	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	g	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	k	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
14	n	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 15 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



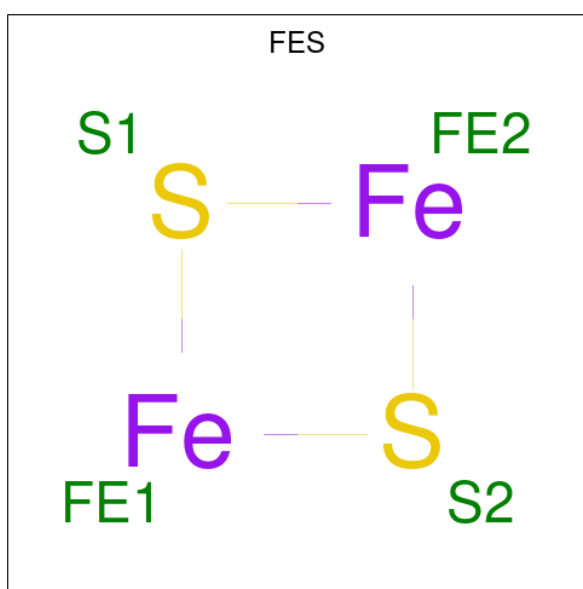
Mol	Chain	Residues	Atoms			AltConf
15	c	1	Total	C	O	0
			37	32	5	
15	c	1	Total	C	O	0
			37	32	5	
15	d	1	Total	C	O	0
			37	32	5	
15	d	1	Total	C	O	0
			37	32	5	
15	f	1	Total	C	O	0
			37	32	5	
15	f	1	Total	C	O	0
			37	32	5	
15	i	1	Total	C	O	0
			37	32	5	

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Mol	Chain	Residues	Atoms			AltConf
15	i	1	Total	C	O	0
			37	32	5	
15	k	1	Total	C	O	0
			37	32	5	
15	m	1	Total	C	O	0
			37	32	5	
15	m	1	Total	C	O	0
			37	32	5	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



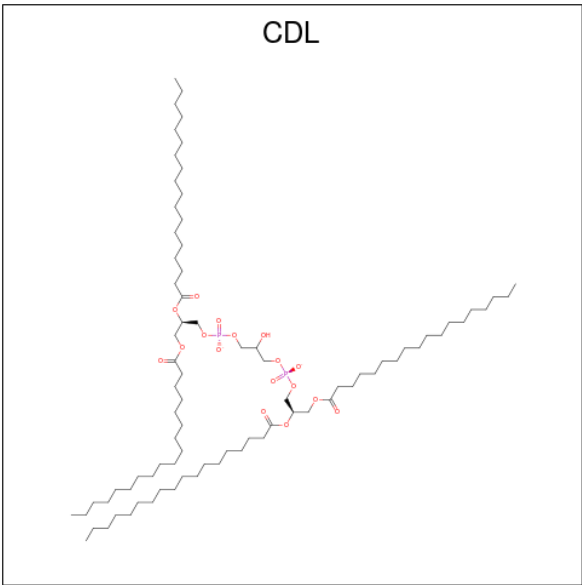
Mol	Chain	Residues	Atoms			AltConf
16	c	1	Total	Fe	S	0
			4	2	2	
16	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $\text{C}_{39}\text{H}_{77}\text{O}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



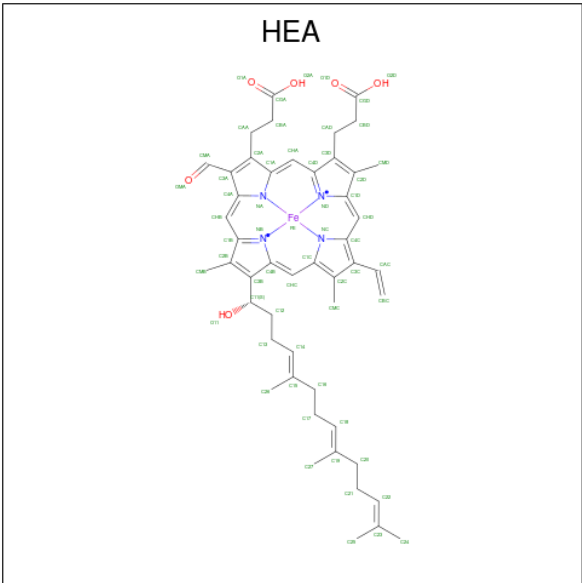
Mol	Chain	Residues	Atoms				AltConf
17	c	1	Total	C	O	P	0
			48	39	8	1	
17	d	1	Total	C	O	P	0
			48	39	8	1	
17	f	1	Total	C	O	P	0
			48	39	8	1	
17	g	1	Total	C	O	P	0
			48	39	8	1	
17	i	1	Total	C	O	P	0
			48	39	8	1	
17	k	1	Total	C	O	P	0
			48	39	8	1	
17	m	1	Total	C	O	P	0
			48	39	8	1	
17	m	1	Total	C	O	P	0
			48	39	8	1	
17	m	1	Total	C	O	P	0
			48	39	8	1	
17	p	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
18	d	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 19 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	g	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
19	g	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
19	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
19	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

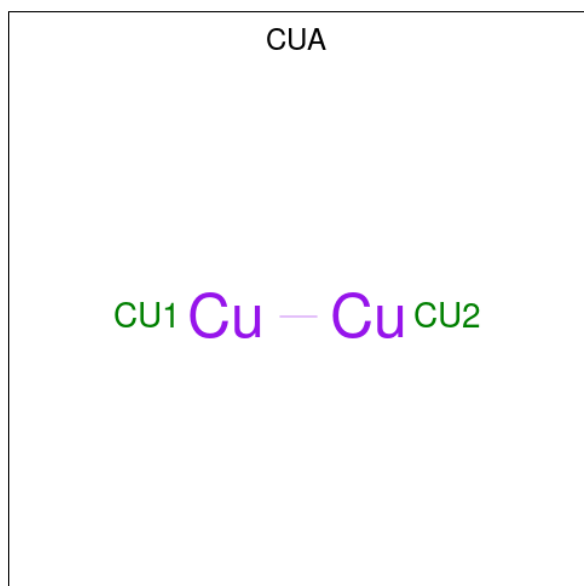
- Molecule 20 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
20	g	1	Total	Cu	0
			1	1	
20	k	1	Total	Cu	0
			1	1	

- Molecule 21 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
21	g	1	Total	Mn	0
			1	1	
21	k	1	Total	Mn	0
			1	1	

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
22	h	1	Total	Cu	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
22	l	1	Total	Cu	0
			2	2	

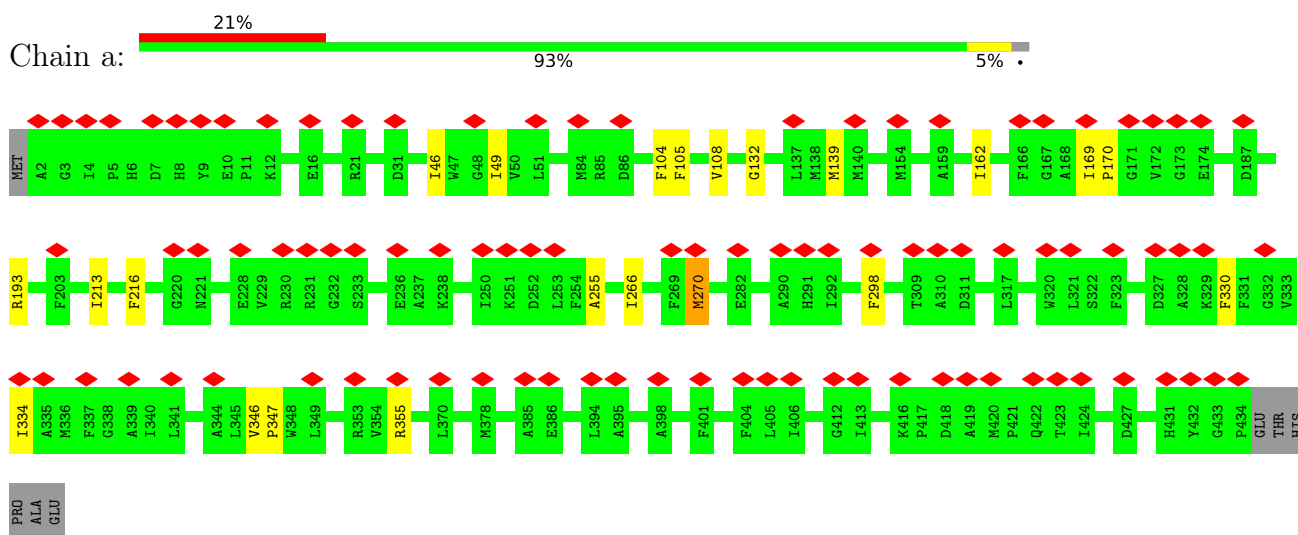
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	i	1	Total	Zn	0
			1	1	
23	m	1	Total	Zn	0
			1	1	

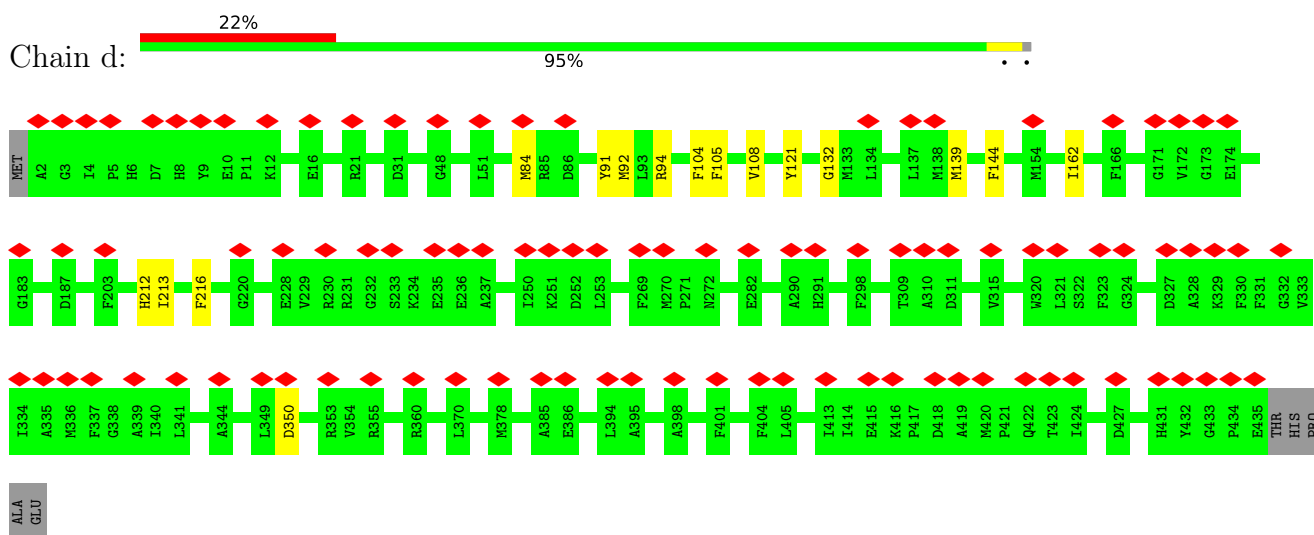
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Cytochrome b

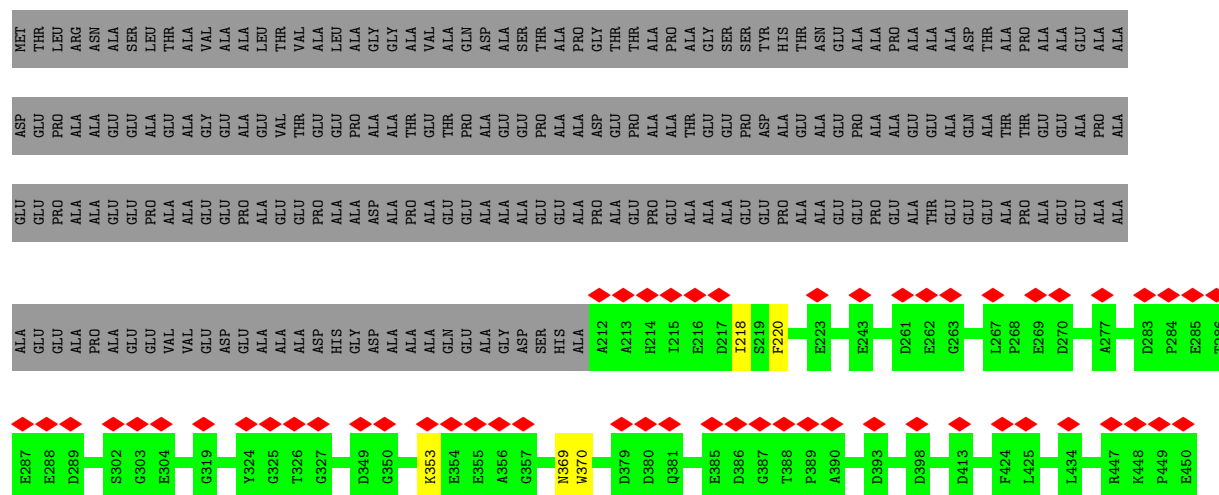


- Molecule 1: Cytochrome b



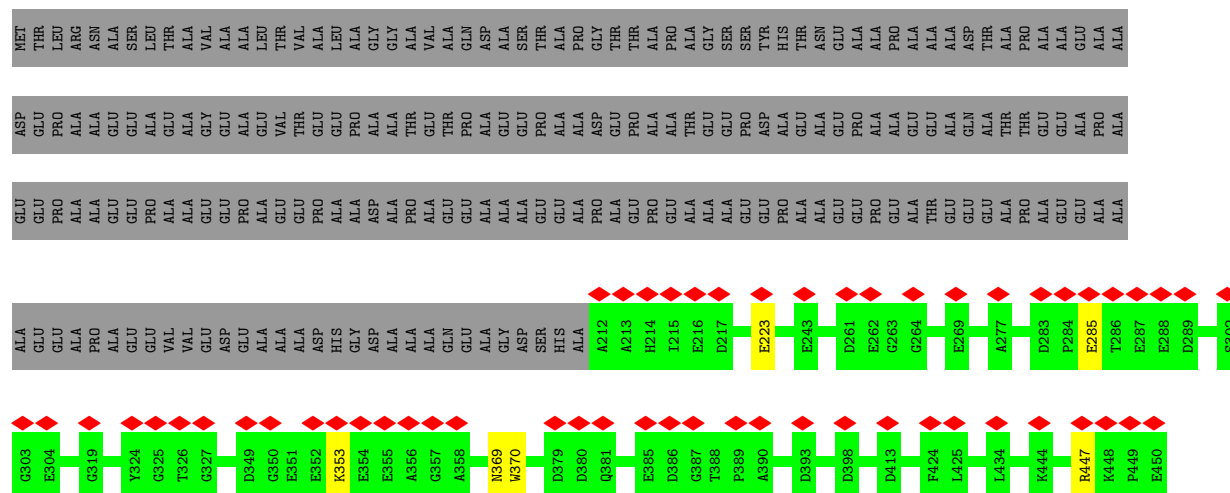
- Molecule 2: Cytochrome c1





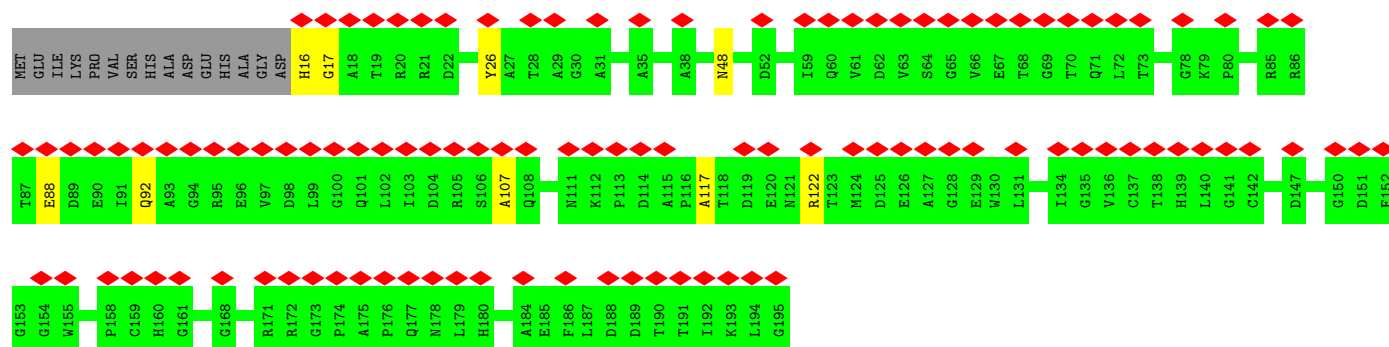
• Molecule 2: Cytochrome c1

Chain e: 12% 52% 47%

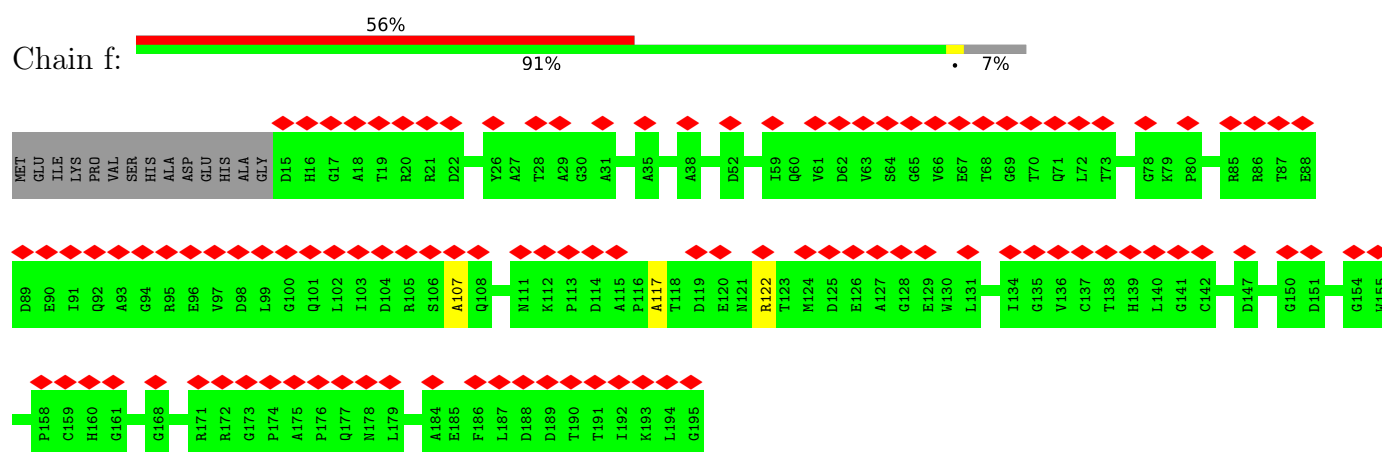


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

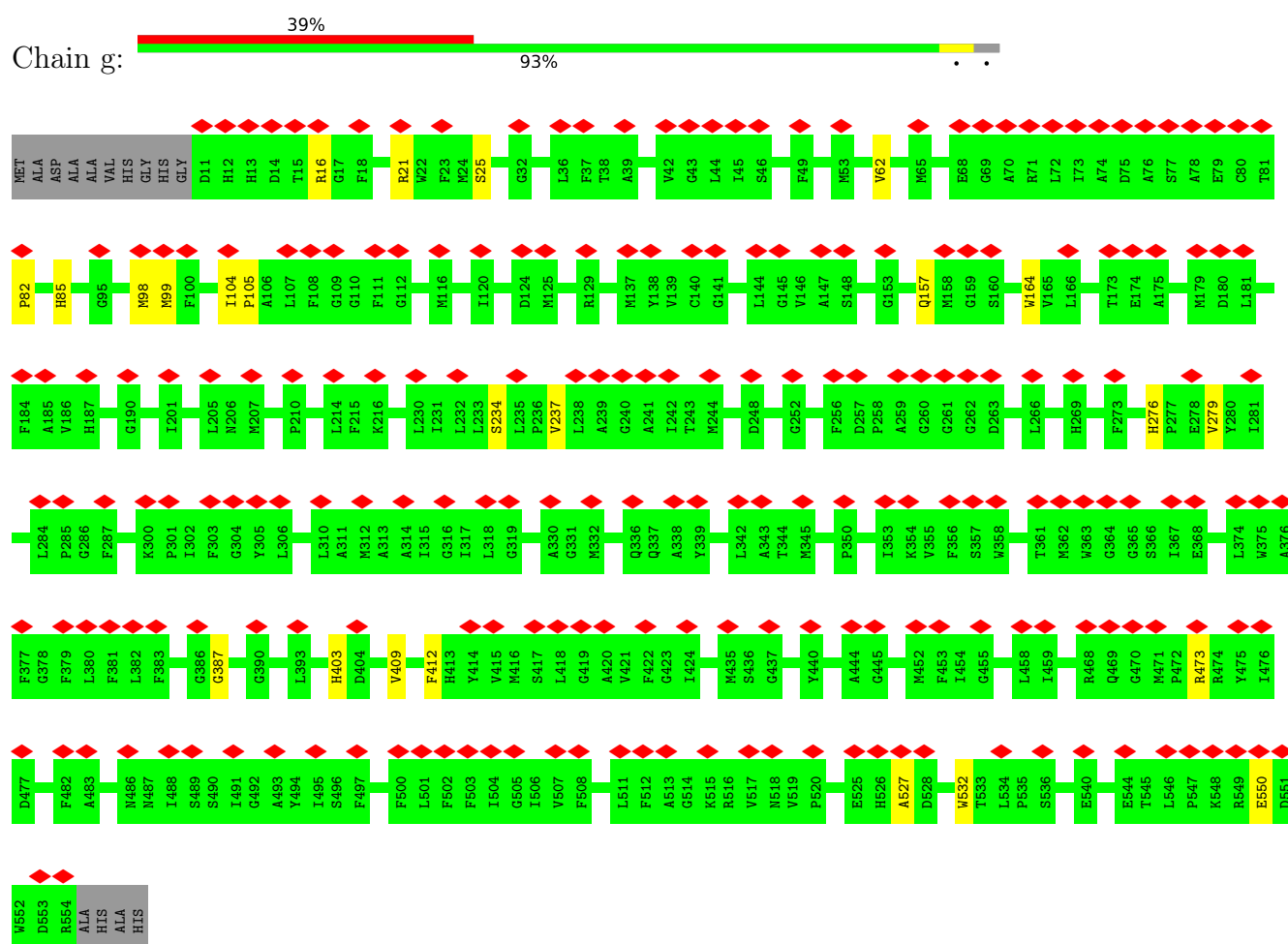
Chain c: 56% 88% 5% 8%



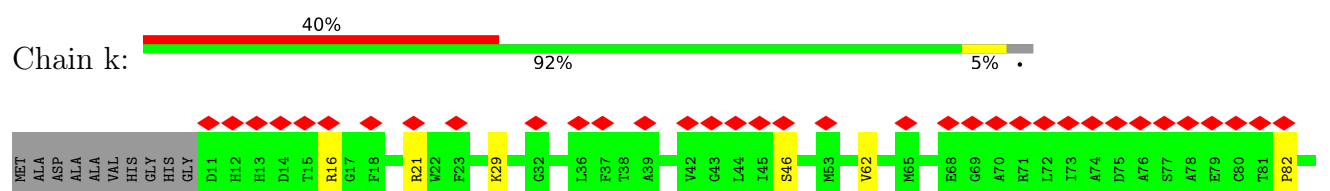
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

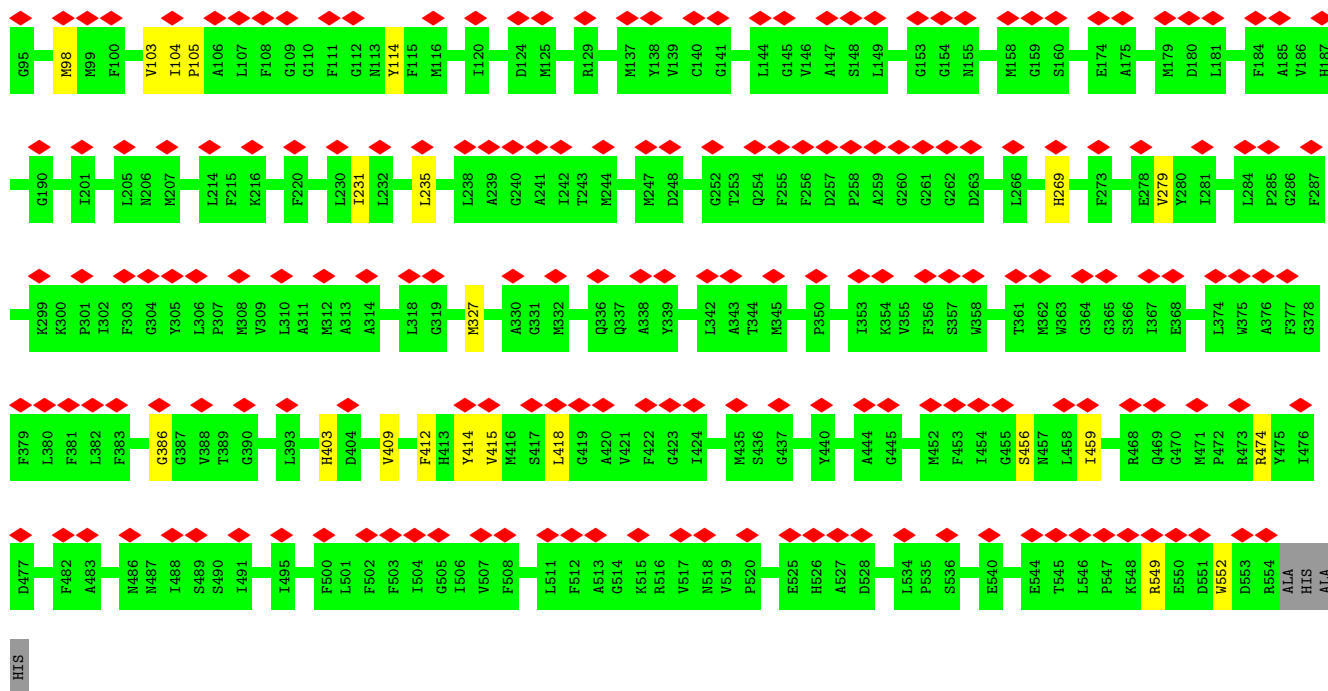


• Molecule 4: Cytochrome c oxidase subunit 1

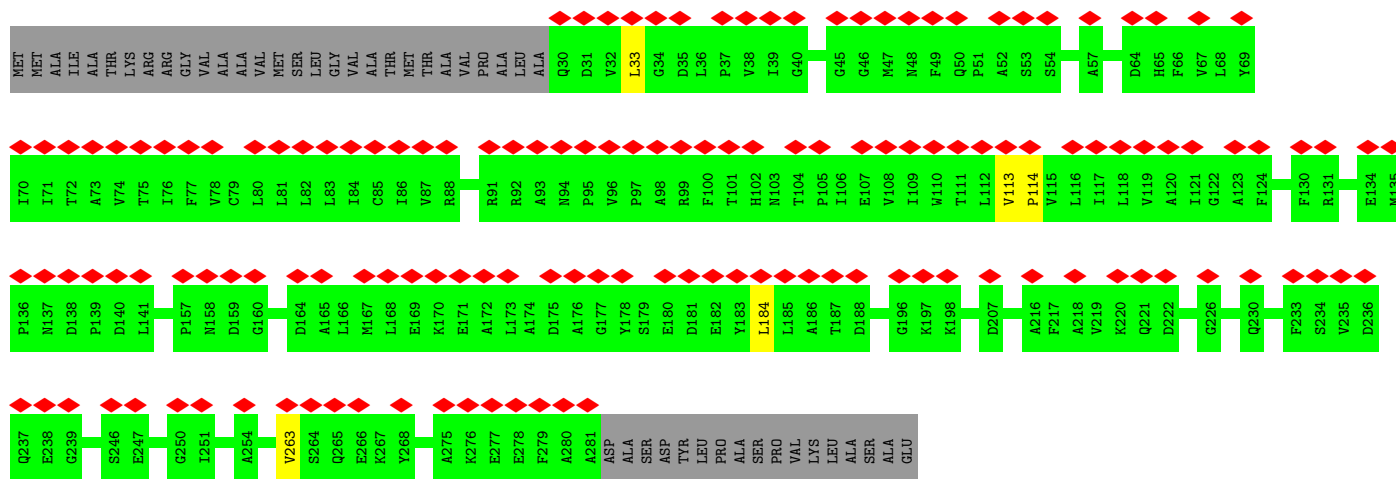
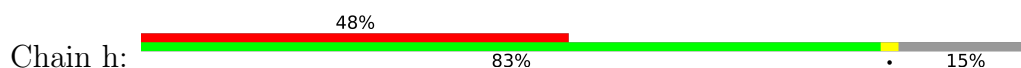


• Molecule 4: Cytochrome c oxidase subunit 1

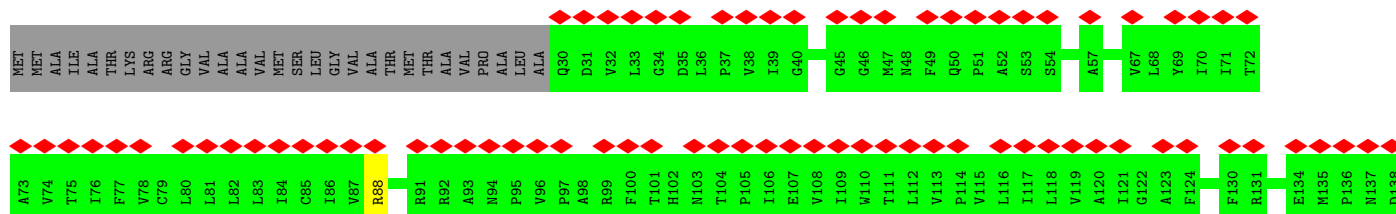
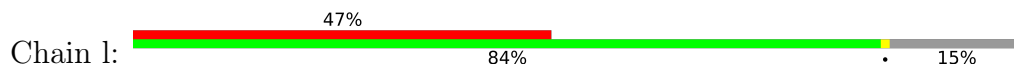


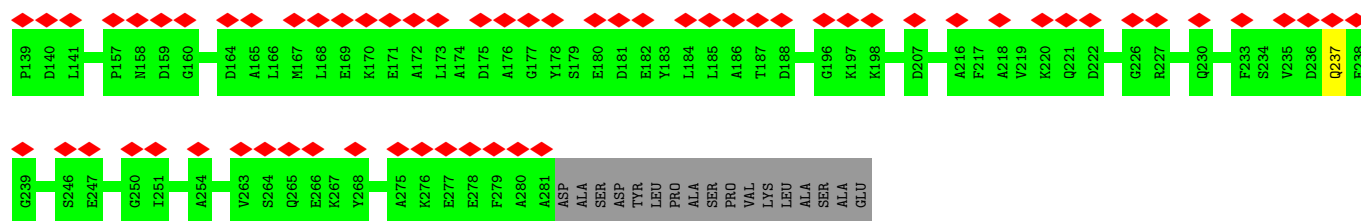


• Molecule 5: Cytochrome c oxidase subunit 2



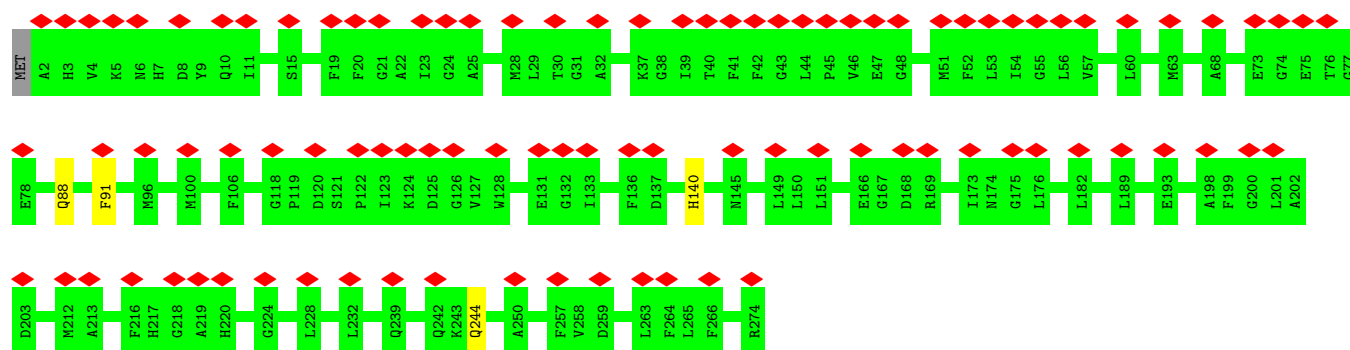
• Molecule 5: Cytochrome c oxidase subunit 2





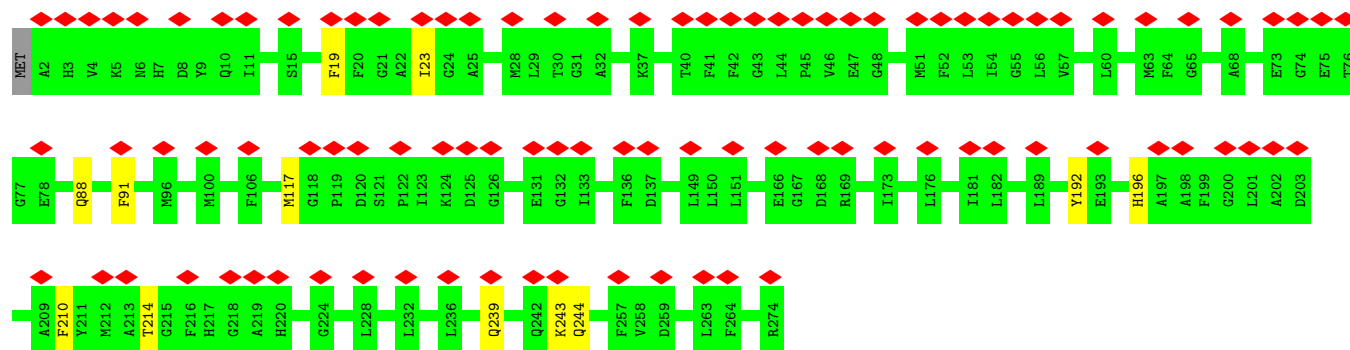
• Molecule 6: cytochrome-c oxidase

Chain i: 35% 98%



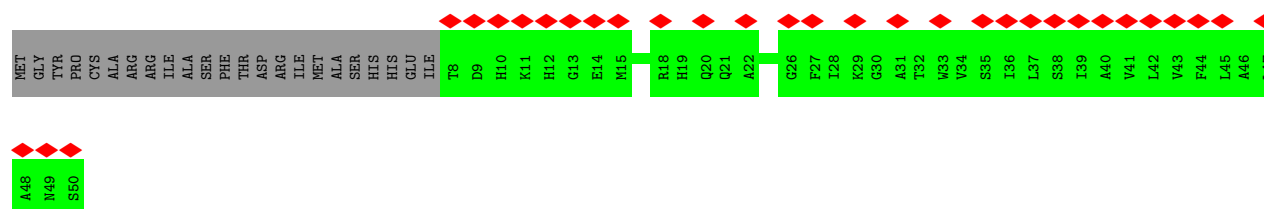
• Molecule 6: cytochrome-c oxidase

Chain m: 35% 95%

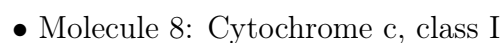


• Molecule 7: Aa3 type cytochrome c oxidase subunit IV

Chain j: 47% 65% 35%



• Molecule 7: Aa3 type cytochrome c oxidase subunit IV



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	10322	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.028	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (\AA)	393.0, 393.0, 393.0	wwPDB
Map dimensions	375, 375, 375	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, HEC, DU0, ZN, 3PE, HEM, FES, PC1, CUA, MN, HEA, CDL, CA, U10, CU

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	0.31	0/3641	0.51	0/4993
1	d	0.31	0/3650	0.49	0/5005
2	b	0.26	0/1906	0.48	0/2592
2	e	0.26	0/1906	0.50	0/2592
3	c	0.21	0/1382	0.48	0/1880
3	f	0.21	0/1390	0.50	0/1891
4	g	0.24	0/4483	0.51	0/6118
4	k	0.25	0/4483	0.51	0/6118
5	h	0.19	0/2033	0.50	0/2787
5	l	0.19	0/2033	0.49	0/2787
6	i	0.24	0/2270	0.46	0/3107
6	m	0.25	0/2270	0.47	0/3107
7	j	0.20	0/339	0.40	0/457
7	n	0.20	0/339	0.47	0/457
8	o	0.23	0/330	0.46	0/448
8	p	0.25	0/336	0.48	0/456
All	All	0.25	0/32791	0.49	0/44795

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
1	a	0	1
4	g	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	355	ARG	Sidechain
4	g	473	ARG	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	3504	0	3483	15	0
1	d	3513	0	3489	12	0
2	b	1855	0	1773	2	0
2	e	1855	0	1773	3	0
3	c	1353	0	1297	5	0
3	f	1361	0	1301	1	0
4	g	4322	0	4225	16	0
4	k	4322	0	4225	18	0
5	h	1976	0	1960	2	0
5	l	1976	0	1960	0	0
6	i	2183	0	2144	2	0
6	m	2183	0	2144	8	0
7	j	332	0	331	0	0
7	n	332	0	331	1	0
8	o	324	0	330	1	0
8	p	330	0	335	2	0
9	a	108	0	176	1	0
9	b	54	0	88	0	0
9	d	54	0	88	0	0
9	i	108	0	176	1	0
9	j	54	0	88	0	0
9	m	162	0	264	2	0
9	n	54	0	88	0	0
9	o	54	0	88	0	0
10	a	126	0	180	7	0
10	d	126	0	180	8	0
11	a	86	0	60	1	0
11	d	86	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	b	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	k	1	0	0	0	0
13	b	43	0	30	2	0
13	e	43	0	30	3	0
14	c	51	0	82	0	0
14	e	102	0	164	1	0
14	g	51	0	82	0	0
14	i	153	0	246	0	0
14	k	51	0	82	0	0
14	m	204	0	328	1	0
14	n	51	0	82	0	0
15	c	74	0	0	1	0
15	d	74	0	0	0	0
15	f	74	0	0	0	0
15	i	74	0	0	0	0
15	k	37	0	0	0	0
15	m	74	0	0	0	0
16	c	4	0	0	0	0
16	f	4	0	0	0	0
17	c	48	0	75	0	0
17	d	48	0	75	0	0
17	f	48	0	75	0	0
17	g	48	0	75	0	0
17	i	48	0	75	0	0
17	k	48	0	75	0	0
17	m	144	0	225	0	0
17	p	48	0	75	0	0
18	d	100	0	156	0	0
19	g	120	0	108	7	0
19	k	120	0	108	7	0
20	g	1	0	0	0	0
20	k	1	0	0	0	0
21	g	1	0	0	0	0
21	k	1	0	0	0	0
22	h	2	0	0	0	0
22	l	2	0	0	0	0
23	i	1	0	0	0	0
23	m	1	0	0	1	0
All	All	34791	0	34885	104	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 1.

The worst 5 of 104 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)
4:g:98:MET:HB3	19:g:603:HEA:CBC	2.15	0.77
1:d:162:ILE:HG13	10:d:508:U10:H3M3	1.76	0.68
14:m:308:3PE:O14	23:m:309:ZN:ZN	1.42	0.68
10:a:506:U10:H452	10:d:508:U10:H253	1.77	0.66
10:a:502:U10:H253	10:d:506:U10:H43	1.77	0.65

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 PDB entries followed by that with respect to all EM entries.

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	431/440 (98%)	422 (98%)	9 (2%)	0	100	100
1	d	432/440 (98%)	417 (96%)	15 (4%)	0	100	100
2	b	237/450 (53%)	231 (98%)	5 (2%)	1 (0%)	30	66
2	e	237/450 (53%)	233 (98%)	3 (1%)	1 (0%)	30	66
3	c	178/195 (91%)	171 (96%)	6 (3%)	1 (1%)	21	58
3	f	179/195 (92%)	173 (97%)	5 (3%)	1 (1%)	21	58
4	g	542/558 (97%)	521 (96%)	21 (4%)	0	100	100
4	k	542/558 (97%)	525 (97%)	17 (3%)	0	100	100
5	h	250/298 (84%)	241 (96%)	8 (3%)	1 (0%)	30	66
5	l	250/298 (84%)	239 (96%)	11 (4%)	0	100	100
6	i	271/274 (99%)	265 (98%)	5 (2%)	1 (0%)	30	66
6	m	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
7	j	41/66 (62%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	n	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
8	o	40/176 (23%)	39 (98%)	1 (2%)	0	100	100
8	p	41/176 (23%)	41 (100%)	0	0	100	100
All	All	3983/4914 (81%)	3860 (97%)	117 (3%)	6 (0%)	44	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	369	ASN
3	f	117	ALA
3	c	117	ALA
6	i	140	HIS
2	e	369	ASN

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 PDB entries followed by that with respect to all EM entries.

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	360/366 (98%)	359 (100%)	1 (0%)	86	84
1	d	361/366 (99%)	361 (100%)	0	100	100
2	b	192/319 (60%)	192 (100%)	0	100	100
2	e	192/319 (60%)	191 (100%)	1 (0%)	81	81
3	c	139/151 (92%)	139 (100%)	0	100	100
3	f	140/151 (93%)	140 (100%)	0	100	100
4	g	447/454 (98%)	447 (100%)	0	100	100
4	k	447/454 (98%)	446 (100%)	1 (0%)	87	85
5	h	211/243 (87%)	211 (100%)	0	100	100
5	l	211/243 (87%)	209 (99%)	2 (1%)	70	76
6	i	220/221 (100%)	220 (100%)	0	100	100
6	m	220/221 (100%)	220 (100%)	0	100	100
7	j	34/53 (64%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	n	34/53 (64%)	34 (100%)	0	100	100
8	o	33/126 (26%)	33 (100%)	0	100	100
8	p	34/126 (27%)	34 (100%)	0	100	100
All	All	3275/3866 (85%)	3270 (100%)	5 (0%)	85	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	270	MET
2	e	447	ARG
4	k	279	VAL
5	l	88	ARG
5	l	237	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
5	l	202	GLN
5	l	230	GLN
6	m	165	HIS
4	g	155	ASN
4	g	83	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 75 ligands modelled in this entry, 10 are monoatomic - leaving 65 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	DU0	i	301	-	42,42,42	0.67	0	64,66,66	0.91	1 (1%)
15	DU0	k	605	-	42,42,42	0.64	0	64,66,66	0.82	2 (3%)
9	PC1	a	501	-	53,53,53	0.96	3 (5%)	59,61,61	0.85	2 (3%)
14	3PE	g	607	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	4 (7%)
17	3PH	m	301	-	47,47,47	1.37	5 (10%)	50,52,52	1.05	5 (10%)
14	3PE	m	313	-	50,50,50	0.95	4 (8%)	53,55,55	1.04	2 (3%)
11	HEM	a	504	1	50,50,50	1.27	5 (10%)	67,82,82	0.88	0
18	CDL	d	501	-	99,99,99	0.91	8 (8%)	105,111,111	0.92	5 (4%)
14	3PE	i	308	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	3 (5%)
17	3PH	i	304	-	47,47,47	1.39	5 (10%)	50,52,52	1.02	5 (10%)
17	3PH	g	601	-	47,47,47	1.39	5 (10%)	50,52,52	1.04	3 (6%)
15	DU0	c	202	-	42,42,42	0.69	0	64,66,66	0.88	2 (3%)
9	PC1	j	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.91	3 (5%)
13	HEC	b	503	2	46,50,50	1.90	6 (13%)	58,82,82	1.62	8 (13%)
15	DU0	i	302	-	42,42,42	0.63	0	64,66,66	0.80	1 (1%)
17	3PH	f	204	-	47,47,47	1.37	5 (10%)	50,52,52	1.06	4 (8%)
15	DU0	d	502	-	42,42,42	0.61	0	64,66,66	0.96	4 (6%)
11	HEM	d	505	1	50,50,50	1.27	6 (12%)	67,82,82	1.03	3 (4%)
19	HEA	g	605	4	67,67,67	1.35	6 (8%)	81,103,103	2.33	27 (33%)
9	PC1	d	503	-	53,53,53	0.93	3 (5%)	59,61,61	0.91	2 (3%)
14	3PE	e	501	-	50,50,50	0.96	4 (8%)	53,55,55	0.98	2 (3%)
15	DU0	m	312	-	42,42,42	0.61	0	64,66,66	0.92	2 (3%)
14	3PE	i	309	-	50,50,50	0.97	4 (8%)	53,55,55	1.06	4 (7%)
17	3PH	k	602	-	47,47,47	1.38	5 (10%)	50,52,52	1.03	6 (12%)
14	3PE	m	306	-	50,50,50	0.97	4 (8%)	53,55,55	1.00	3 (5%)
16	FES	f	202	3	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	3PH	c	205	-	47,47,47	1.38	5 (10%)	50,52,52	1.14	5 (10%)
9	PC1	m	303	-	53,53,53	0.97	3 (5%)	59,61,61	0.85	3 (5%)
14	3PE	m	305	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	3 (5%)
9	PC1	a	503	-	53,53,53	0.95	3 (5%)	59,61,61	0.82	1 (1%)
11	HEM	d	504	1	50,50,50	1.25	4 (8%)	67,82,82	0.93	1 (1%)
9	PC1	b	501	-	53,53,53	0.95	3 (5%)	59,61,61	0.87	1 (1%)
10	U10	a	502	-	63,63,63	0.71	0	78,79,79	0.94	4 (5%)
10	U10	a	506	-	63,63,63	0.68	0	78,79,79	0.72	1 (1%)
14	3PE	e	504	-	50,50,50	0.95	4 (8%)	53,55,55	0.99	4 (7%)
15	DU0	c	203	-	42,42,42	0.66	0	64,66,66	1.10	4 (6%)
15	DU0	f	203	-	42,42,42	0.67	0	64,66,66	0.81	0
9	PC1	m	307	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	3 (5%)
9	PC1	i	303	-	53,53,53	0.97	3 (5%)	59,61,61	0.89	4 (6%)
14	3PE	i	305	-	50,50,50	0.97	4 (8%)	53,55,55	1.17	3 (5%)
9	PC1	o	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.86	1 (1%)
15	DU0	d	509	-	42,42,42	0.65	0	64,66,66	0.90	1 (1%)
14	3PE	k	608	-	50,50,50	0.96	4 (8%)	53,55,55	0.98	4 (7%)
15	DU0	f	201	-	42,42,42	0.68	0	64,66,66	0.97	3 (4%)
17	3PH	m	302	-	47,47,47	1.37	5 (10%)	50,52,52	1.00	4 (8%)
17	3PH	m	304	-	47,47,47	1.38	5 (10%)	50,52,52	1.10	6 (12%)
17	3PH	p	1000	-	47,47,47	1.38	5 (10%)	50,52,52	1.02	4 (8%)
19	HEA	k	606	4	67,67,67	1.37	7 (10%)	81,103,103	2.35	29 (35%)
22	CUA	h	301	5	0,1,1	-	-	-	-	-
9	PC1	m	310	-	53,53,53	0.95	3 (5%)	59,61,61	0.95	3 (5%)
22	CUA	l	301	5	0,1,1	-	-	-	-	-
19	HEA	k	601	4	67,67,67	1.35	6 (8%)	81,103,103	2.28	28 (34%)
9	PC1	n	102	-	53,53,53	0.97	3 (5%)	59,61,61	0.86	3 (5%)
14	3PE	n	101	-	50,50,50	0.98	4 (8%)	53,55,55	0.92	2 (3%)
9	PC1	i	307	-	53,53,53	0.96	3 (5%)	59,61,61	0.85	3 (5%)
10	U10	d	506	-	63,63,63	0.66	0	78,79,79	1.01	3 (3%)
16	FES	c	204	3	0,4,4	-	-	-	-	-
15	DU0	m	311	-	42,42,42	0.68	0	64,66,66	0.88	2 (3%)
17	3PH	d	507	-	47,47,47	1.38	5 (10%)	50,52,52	1.00	4 (8%)
14	3PE	m	308	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	2 (3%)
19	HEA	g	603	4	67,67,67	1.38	7 (10%)	81,103,103	2.33	26 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HEM	a	505	1	50,50,50	1.27	6 (12%)	67,82,82	0.94	3 (4%)
10	U10	d	508	-	63,63,63	0.66	0	78,79,79	1.12	4 (5%)
14	3PE	c	201	-	50,50,50	0.96	4 (8%)	53,55,55	1.18	4 (7%)
13	HEC	e	503	2	46,50,50	1.90	6 (13%)	58,82,82	1.53	6 (10%)

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	DU0	i	301	-	-	2/10/98/98	0/6/6/6
15	DU0	k	605	-	-	0/10/98/98	0/6/6/6
9	PC1	a	501	-	-	11/57/57/57	-
14	3PE	g	607	-	-	11/54/54/54	-
17	3PH	m	301	-	-	2/49/49/49	-
14	3PE	m	313	-	-	12/54/54/54	-
11	HEM	a	504	1	-	5/14/54/54	-
18	CDL	d	501	-	-	24/110/110/110	-
14	3PE	i	308	-	-	7/54/54/54	-
17	3PH	i	304	-	-	10/49/49/49	-
17	3PH	g	601	-	-	5/49/49/49	-
15	DU0	c	202	-	-	2/10/98/98	0/6/6/6
9	PC1	j	1001	-	-	16/57/57/57	-
13	HEC	b	503	2	-	8/14/54/54	-
15	DU0	i	302	-	-	2/10/98/98	0/6/6/6
17	3PH	f	204	-	-	15/49/49/49	-
15	DU0	d	502	-	-	1/10/98/98	0/6/6/6
11	HEM	d	505	1	-	8/14/54/54	-
19	HEA	g	605	4	-	2/36/76/76	-
9	PC1	d	503	-	-	15/57/57/57	-
14	3PE	e	501	-	-	12/54/54/54	-
15	DU0	m	312	-	-	0/10/98/98	0/6/6/6
14	3PE	i	309	-	-	10/54/54/54	-
17	3PH	k	602	-	-	7/49/49/49	-
14	3PE	m	306	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	3PH	c	205	-	-	4/49/49/49	-
16	FES	f	202	3	-	-	0/1/1/1
9	PC1	m	303	-	-	12/57/57/57	-
14	3PE	m	305	-	-	5/54/54/54	-
9	PC1	a	503	-	-	13/57/57/57	-
11	HEM	d	504	1	-	8/14/54/54	-
9	PC1	b	501	-	-	13/57/57/57	-
10	U10	a	502	-	-	8/63/87/87	0/1/1/1
10	U10	a	506	-	-	13/63/87/87	0/1/1/1
14	3PE	e	504	-	-	11/54/54/54	-
15	DU0	c	203	-	-	3/10/98/98	0/6/6/6
15	DU0	f	203	-	-	1/10/98/98	0/6/6/6
9	PC1	m	307	-	-	18/57/57/57	-
9	PC1	i	303	-	-	7/57/57/57	-
14	3PE	i	305	-	-	14/54/54/54	-
9	PC1	o	1001	-	-	12/57/57/57	-
15	DU0	d	509	-	-	1/10/98/98	0/6/6/6
14	3PE	k	608	-	-	11/54/54/54	-
15	DU0	f	201	-	-	0/10/98/98	0/6/6/6
17	3PH	m	302	-	-	14/49/49/49	-
17	3PH	m	304	-	-	8/49/49/49	-
17	3PH	p	1000	-	-	5/49/49/49	-
19	HEA	k	606	4	-	6/36/76/76	-
9	PC1	m	310	-	-	7/57/57/57	-
19	HEA	k	601	4	-	4/36/76/76	-
9	PC1	n	102	-	-	16/57/57/57	-
14	3PE	n	101	-	-	11/54/54/54	-
9	PC1	i	307	-	-	9/57/57/57	-
10	U10	d	506	-	-	9/63/87/87	0/1/1/1
19	HEA	g	603	4	-	3/36/76/76	-
15	DU0	m	311	-	-	3/10/98/98	0/6/6/6
17	3PH	d	507	-	-	14/49/49/49	-
14	3PE	m	308	-	-	12/54/54/54	-
16	FES	c	204	3	-	-	0/1/1/1
11	HEM	a	505	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	U10	d	508	-	-	11/63/87/87	0/1/1/1
14	3PE	c	201	-	-	16/54/54/54	-
13	HEC	e	503	2	-	8/14/54/54	-

The worst 5 of 205 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	p	1000	3PH	P-O11	7.47	1.83	1.60
17	g	601	3PH	P-O11	7.47	1.83	1.60
17	k	602	3PH	P-O11	7.43	1.83	1.60
17	i	304	3PH	P-O11	7.43	1.83	1.60
17	m	304	3PH	P-O11	7.36	1.83	1.60

The worst 5 of 285 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	k	606	HEA	C3A-C2A-C1A	-7.01	100.41	107.05
19	g	605	HEA	C3A-C2A-C1A	-6.80	100.61	107.05
19	g	603	HEA	C3A-C2A-C1A	-6.77	100.64	107.05
19	k	601	HEA	C3A-C2A-C1A	-6.68	100.72	107.05
13	b	503	HEC	CBB-CAB-C3B	-6.09	115.27	127.43

There are no chirality outliers.

5 of 513 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	a	501	PC1	C1-O11-P-O12
9	a	501	PC1	O13-C11-C12-N
9	a	503	PC1	C11-O13-P-O11
9	b	501	PC1	C1-O11-P-O13
9	b	501	PC1	O13-C11-C12-N

There are no ring outliers.

18 monomers are involved in 42 short contacts:

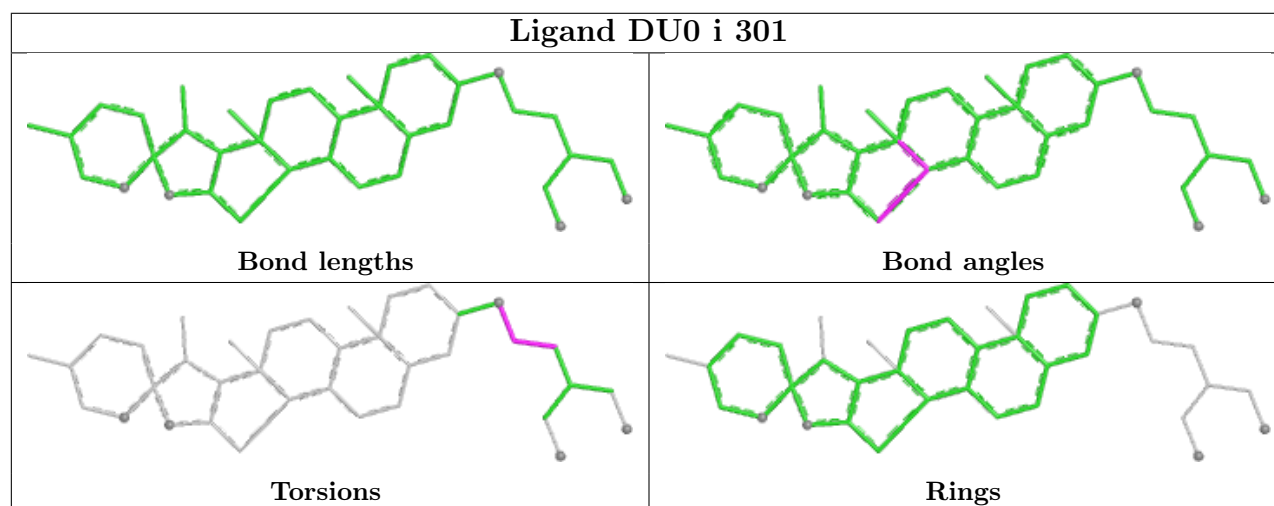
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	a	504	HEM	1	0
13	b	503	HEC	2	0
19	g	605	HEA	3	0
9	m	303	PC1	2	0

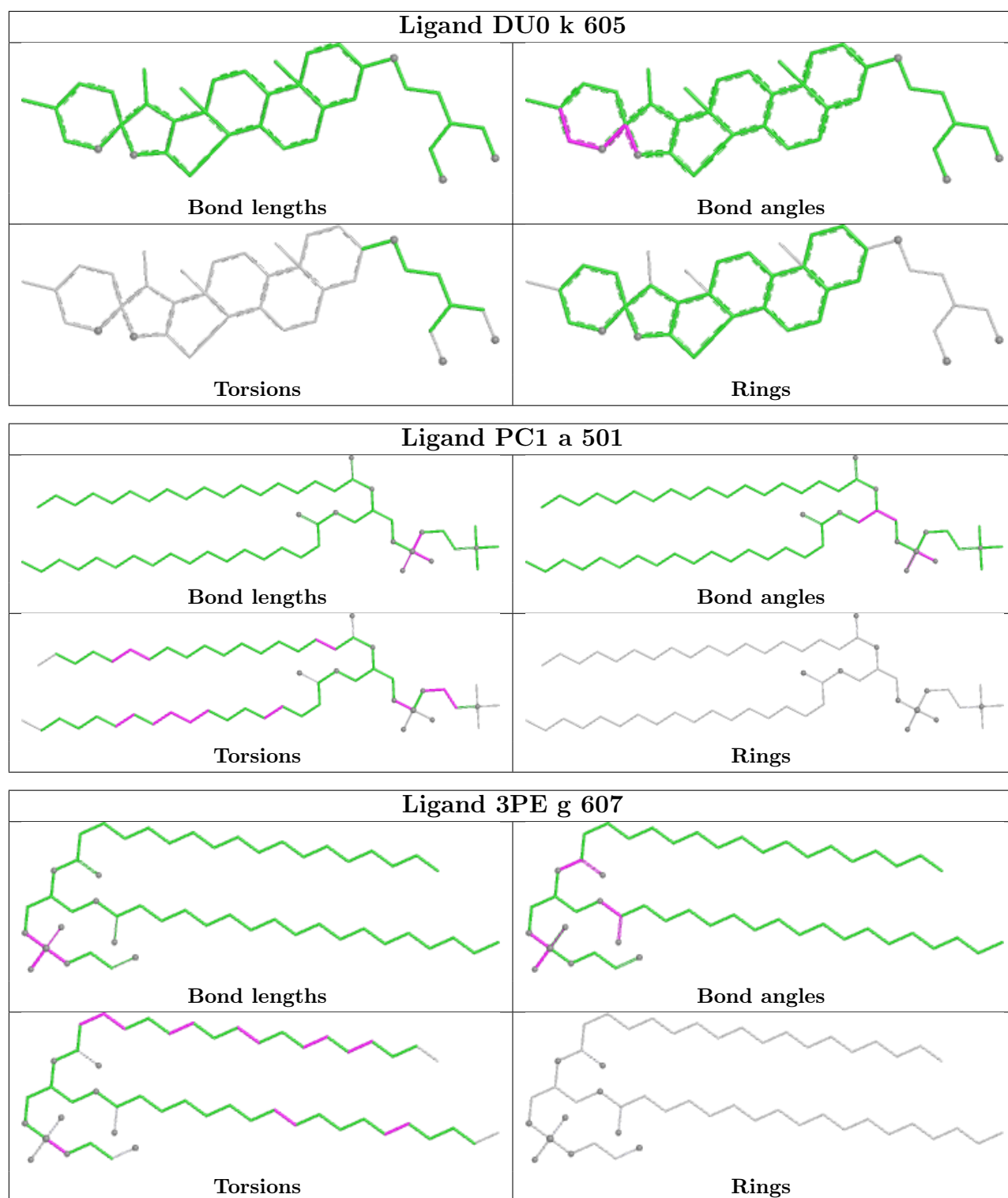
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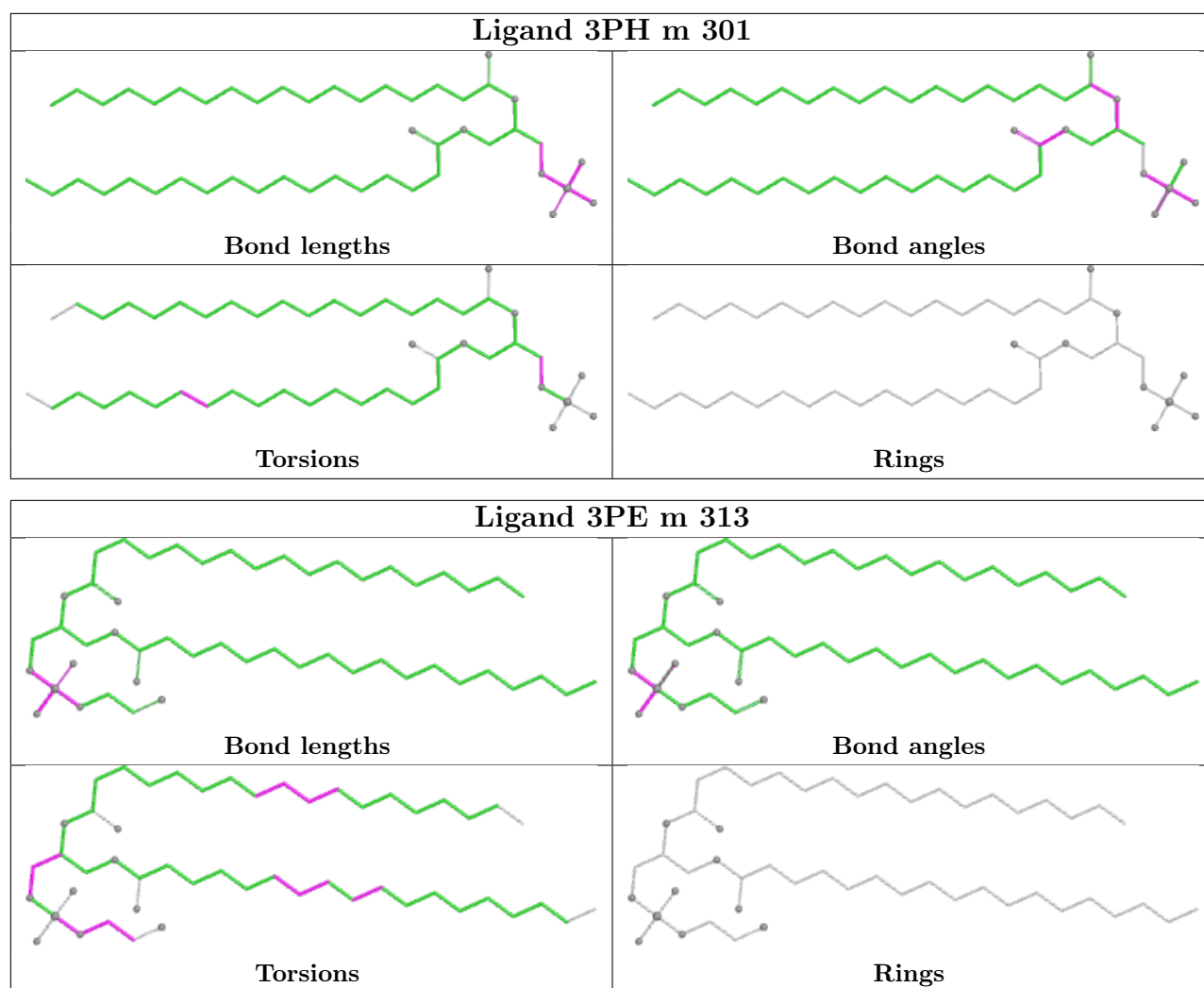
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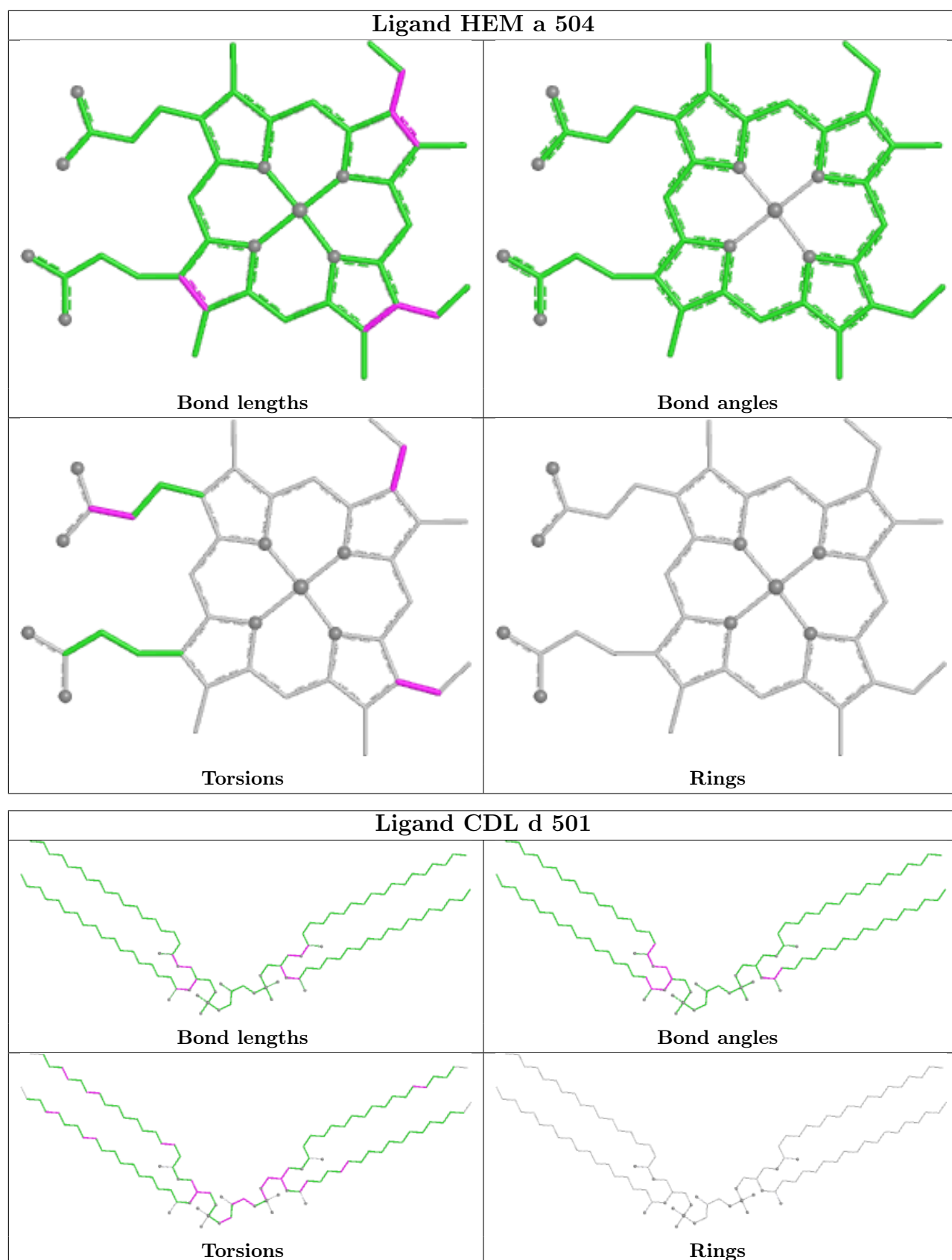
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	503	PC1	1	0
11	d	504	HEM	2	0
10	a	502	U10	4	0
10	a	506	U10	3	0
14	e	504	3PE	1	0
15	c	203	DU0	1	0
19	k	606	HEA	5	0
19	k	601	HEA	2	0
9	i	307	PC1	1	0
10	d	506	U10	2	0
14	m	308	3PE	1	0
19	g	603	HEA	4	0
10	d	508	U10	6	0
13	e	503	HEC	3	0

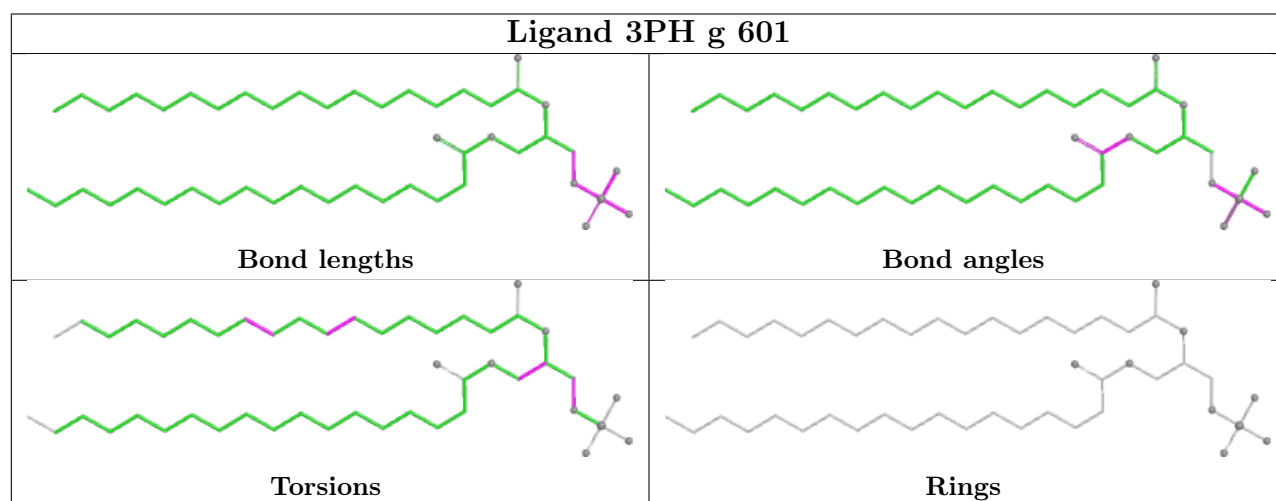
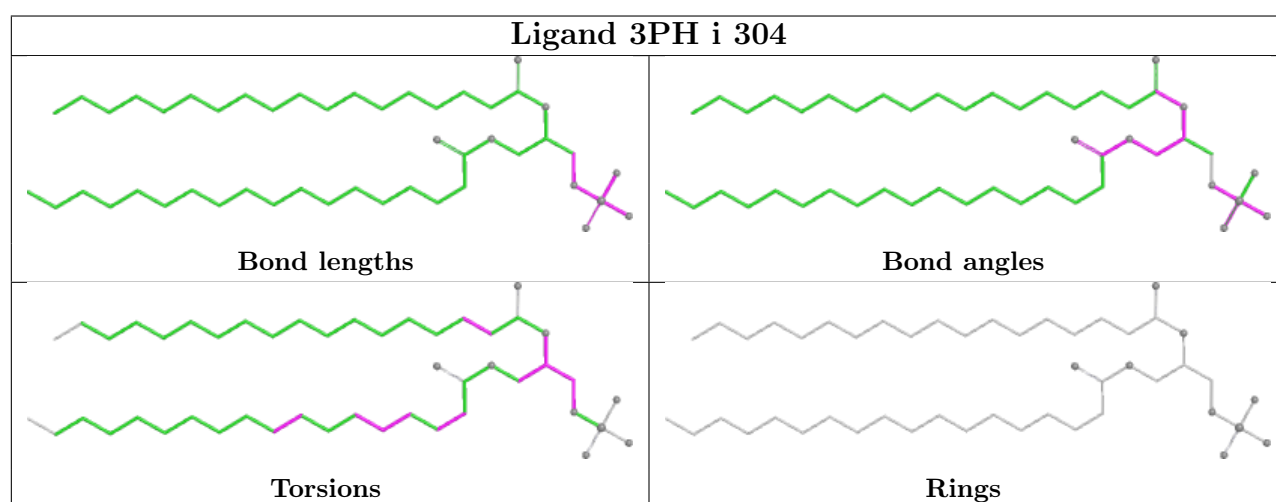
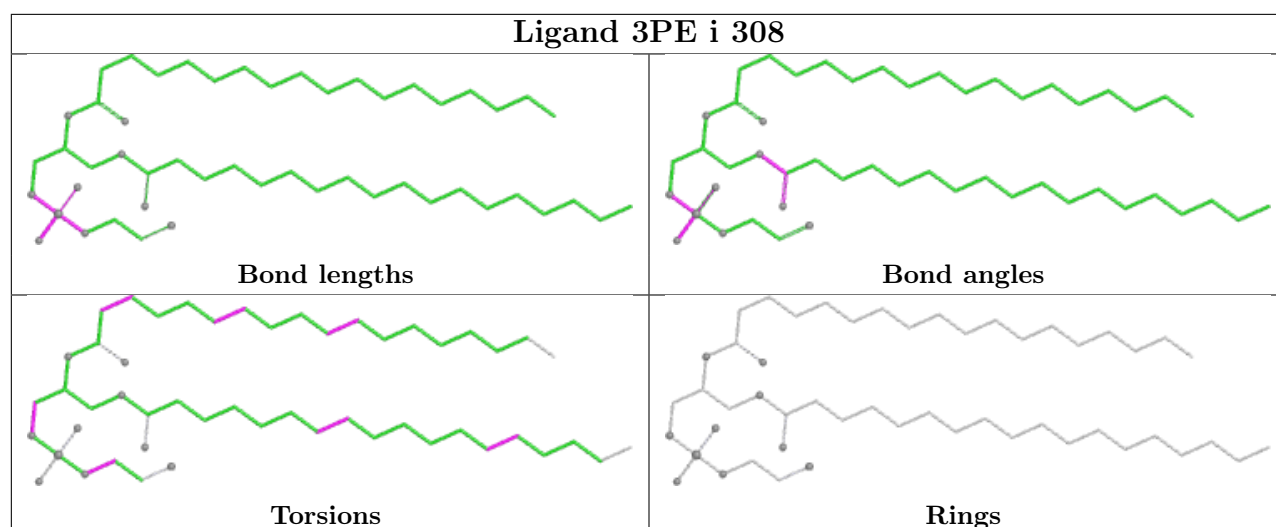
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

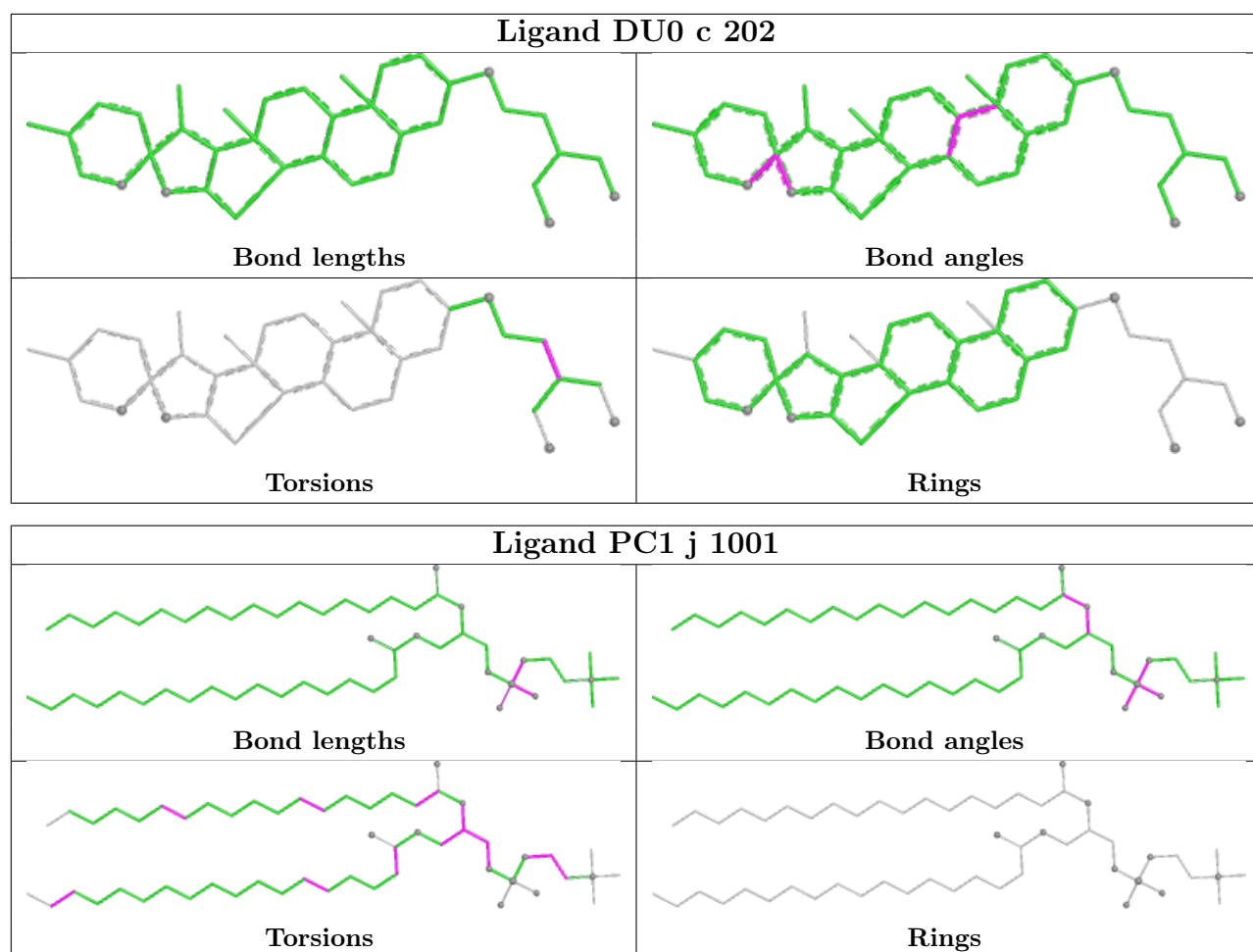




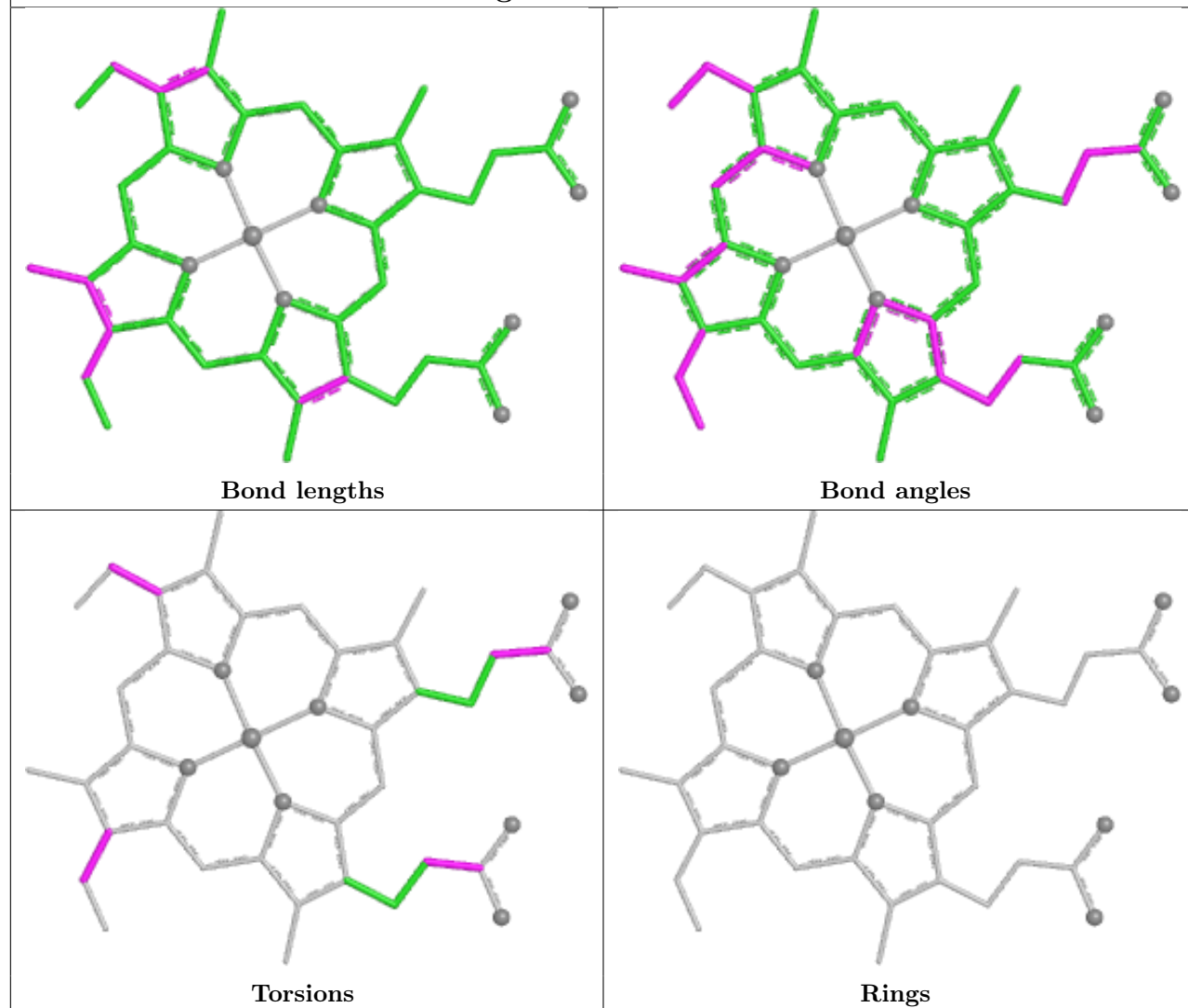




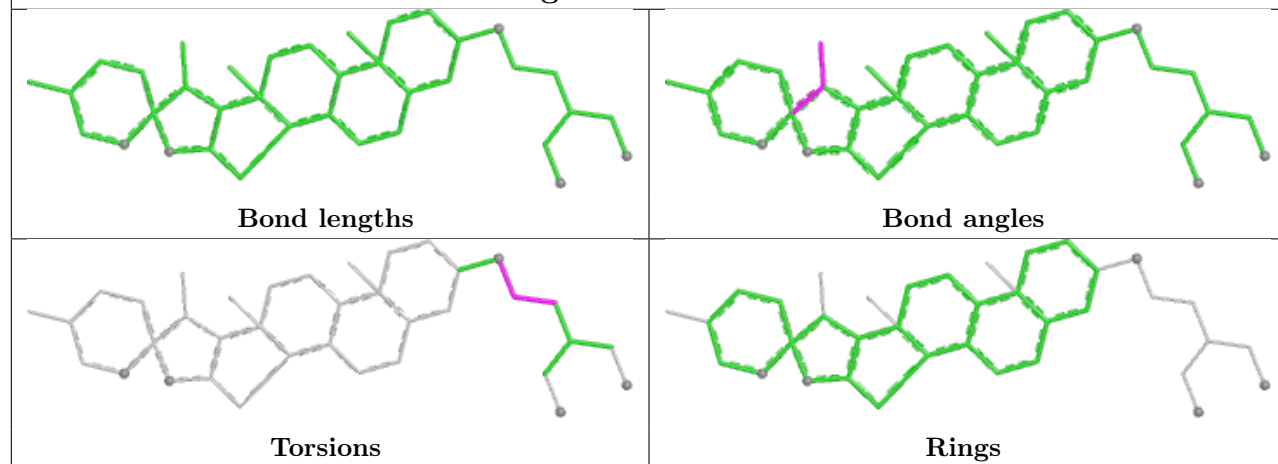


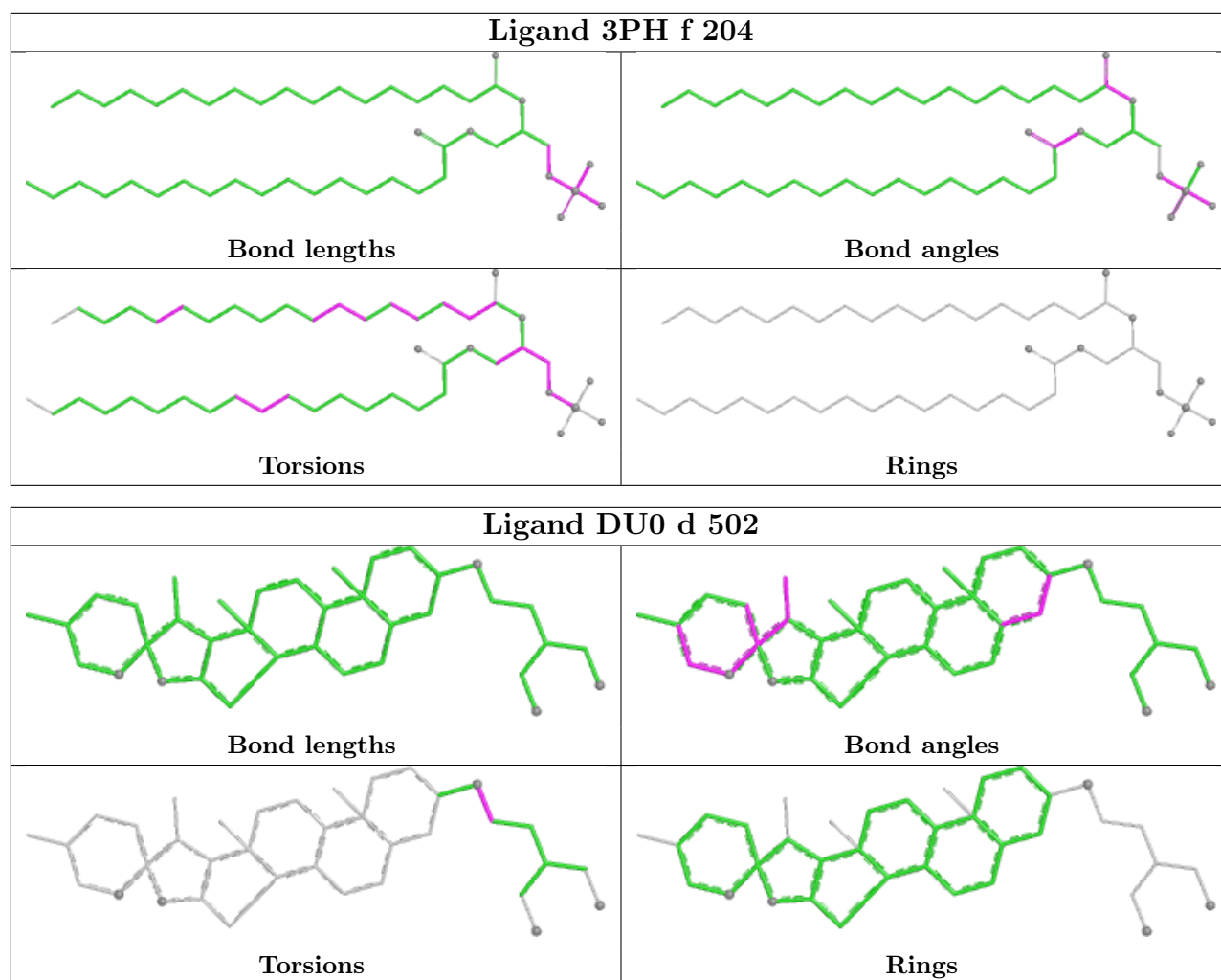


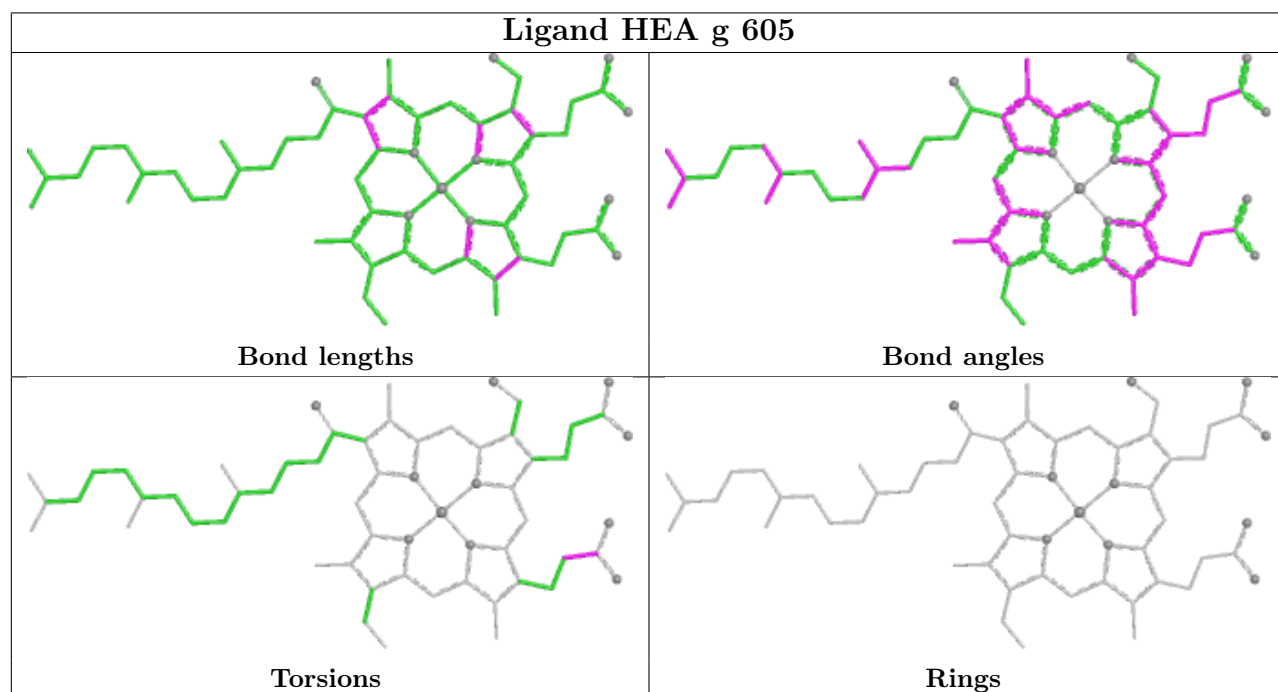
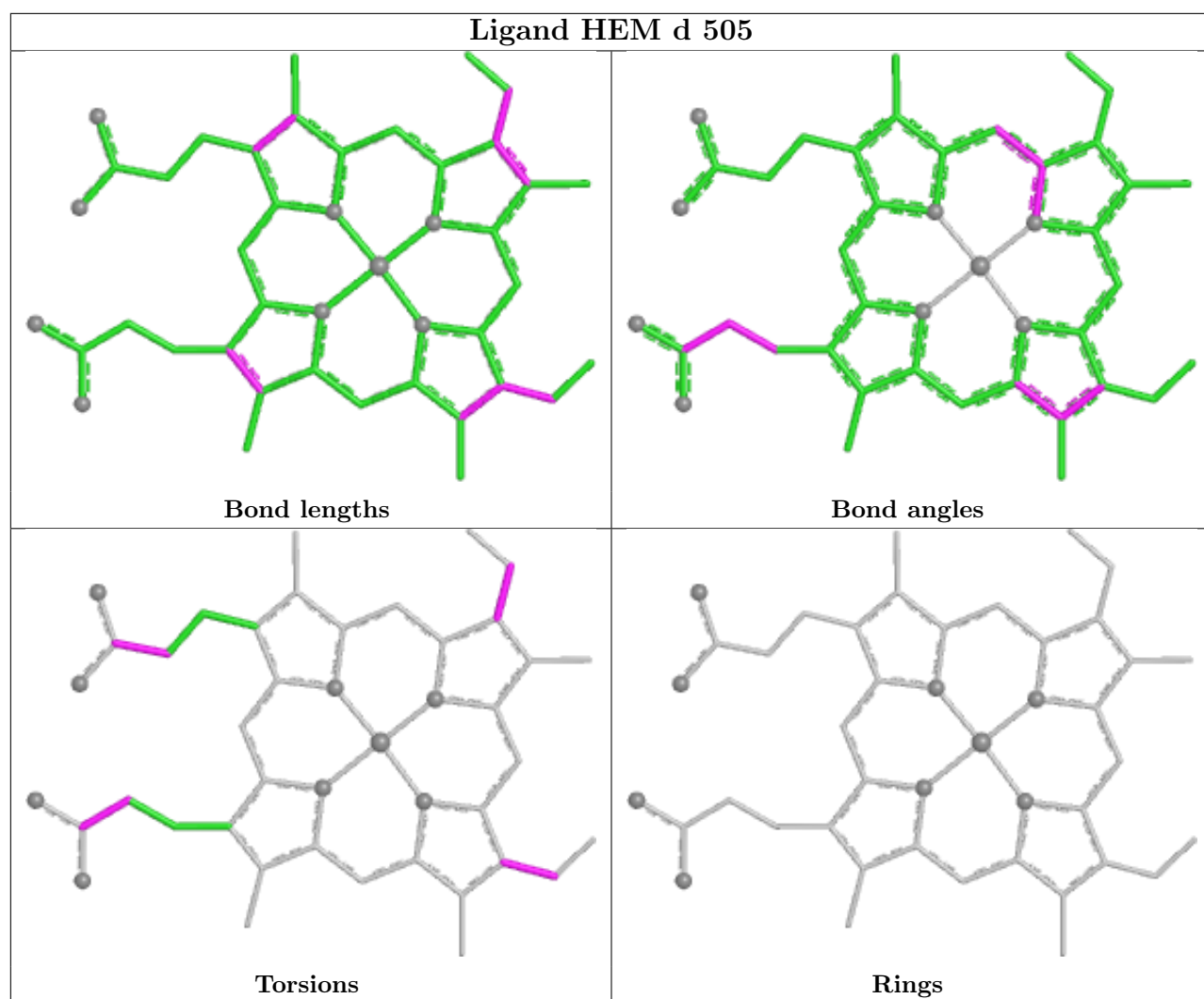
Ligand HEC b 503

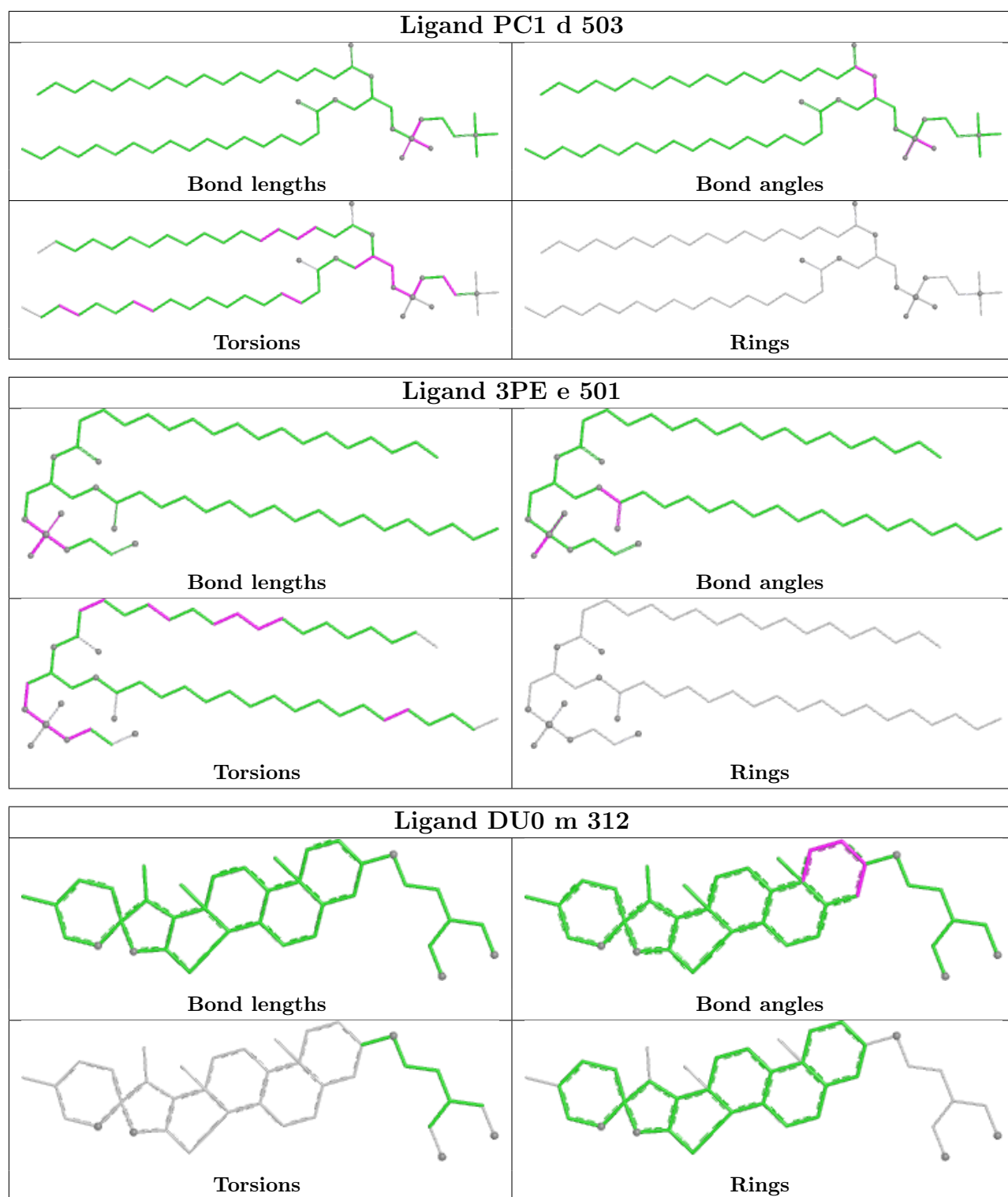


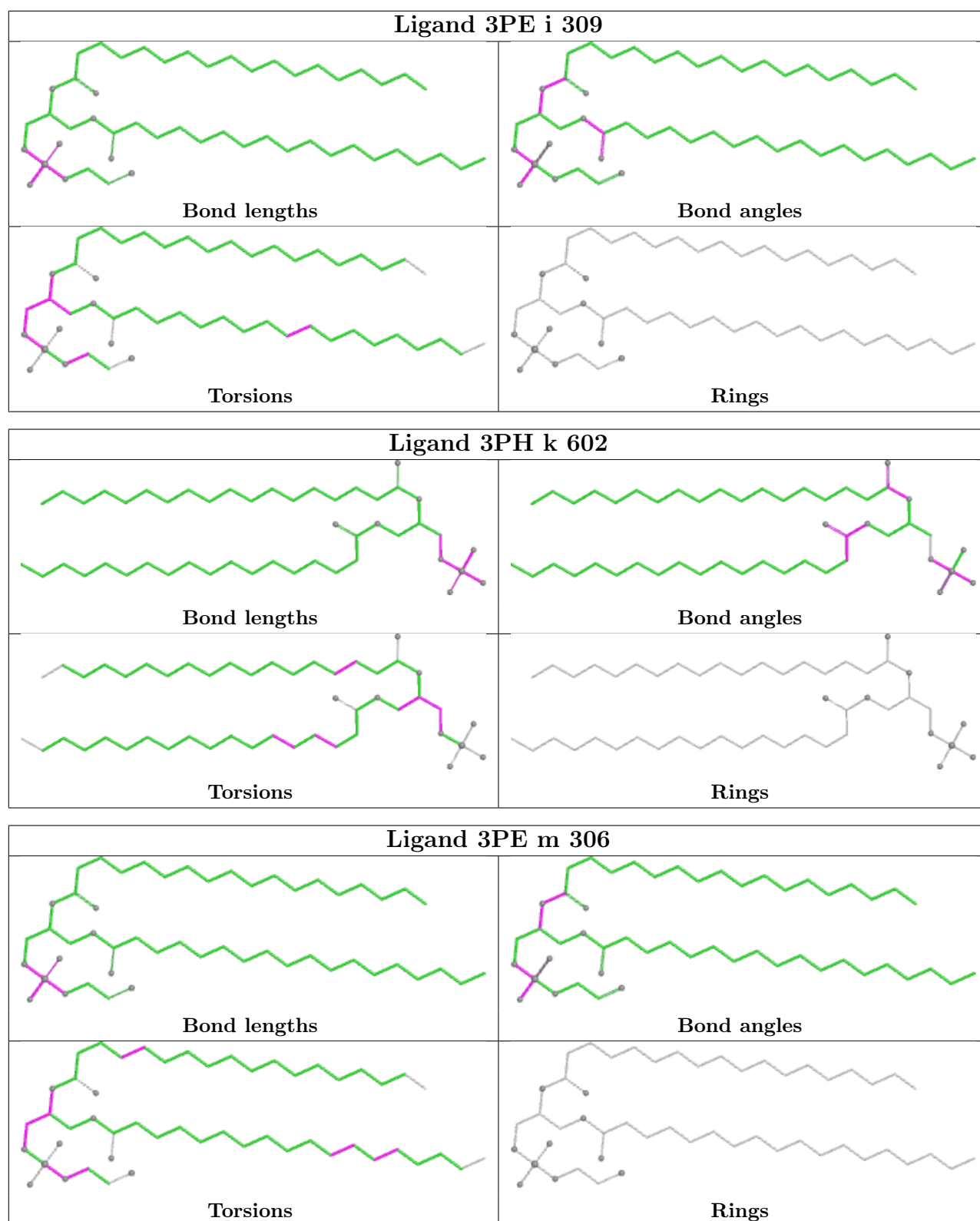
Ligand DU0 i 302

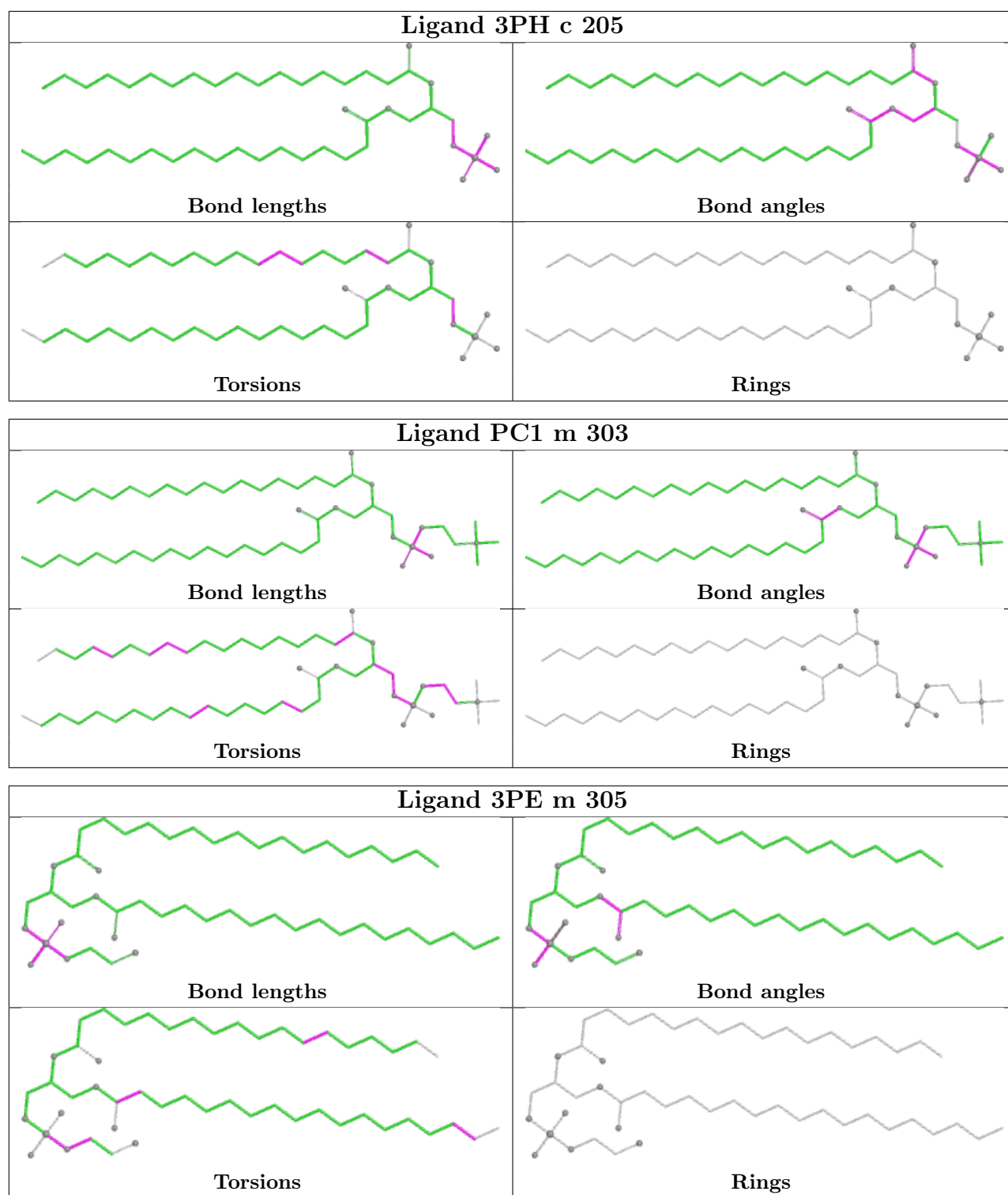


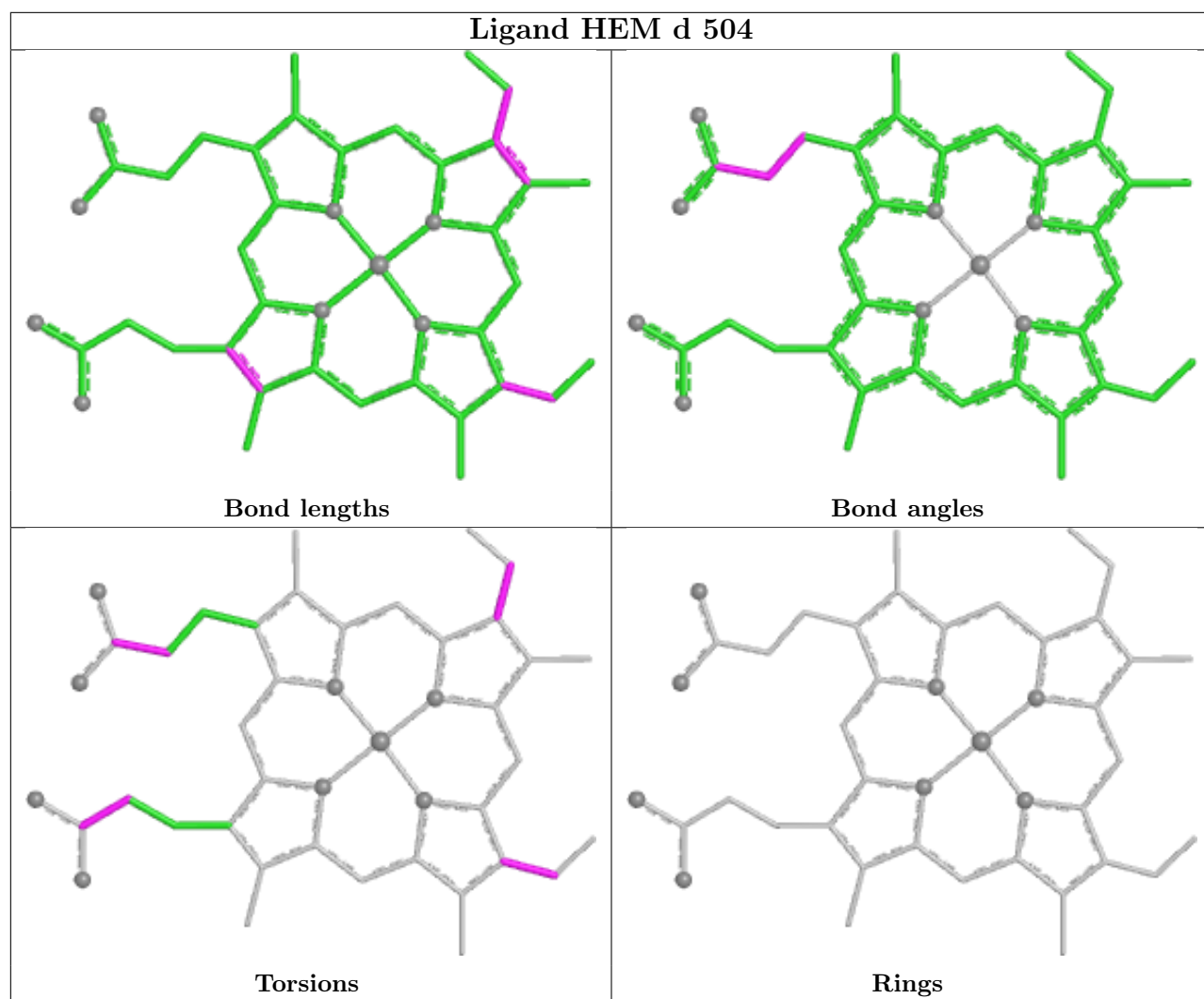
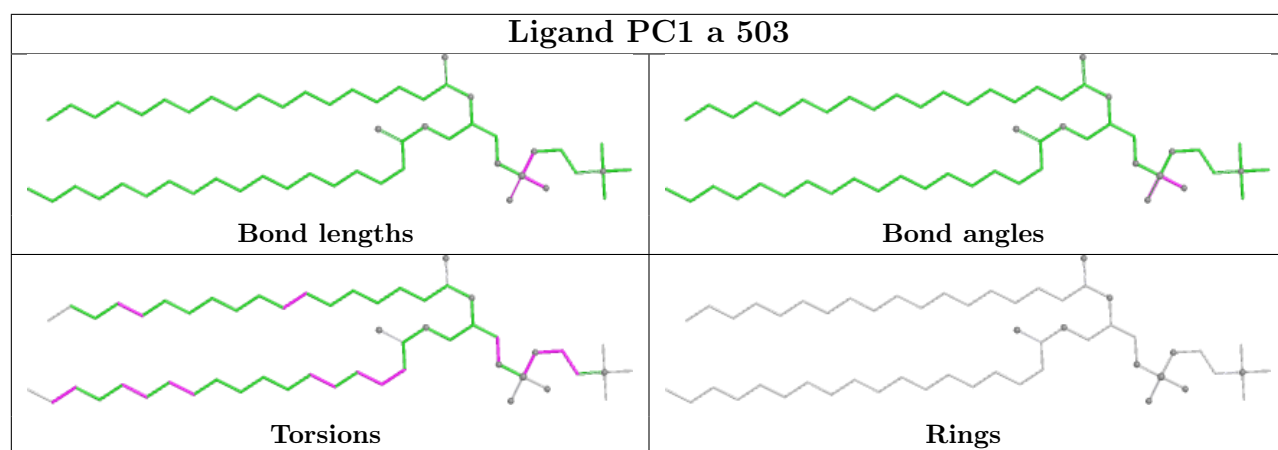


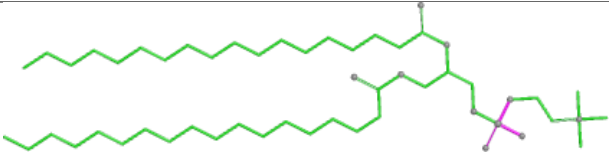
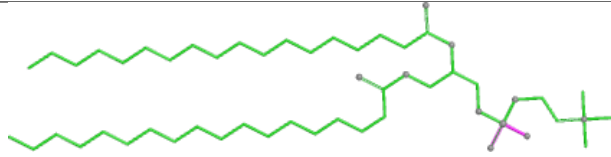
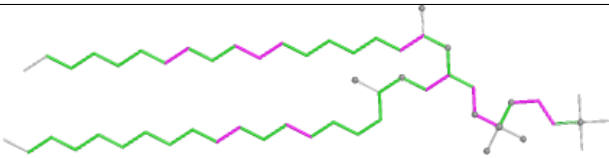
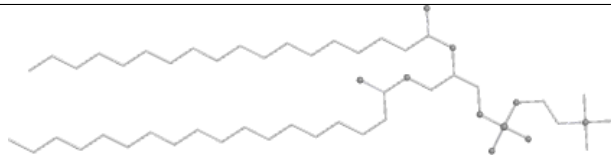
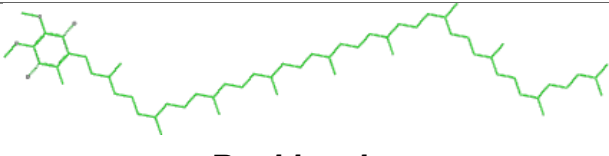
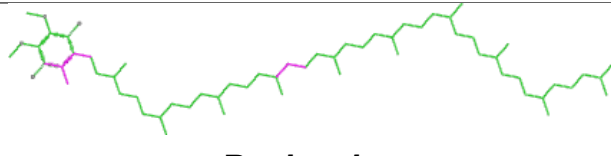
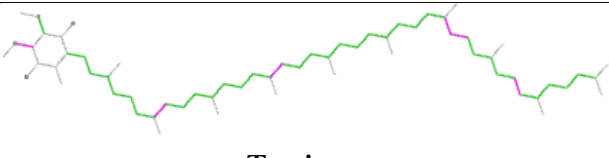
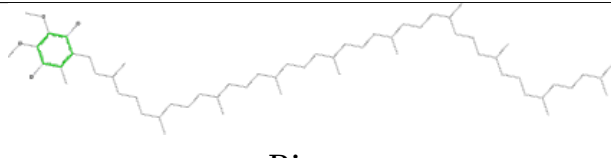
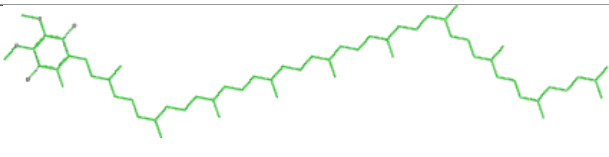
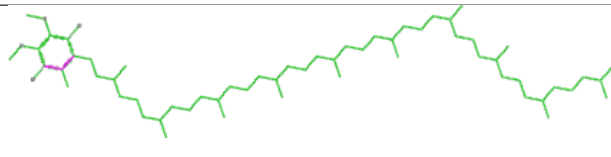
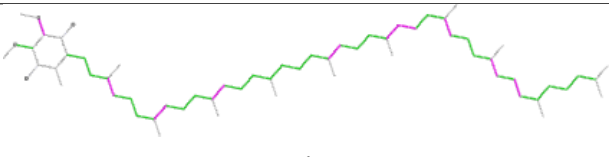
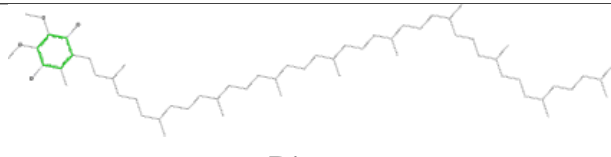


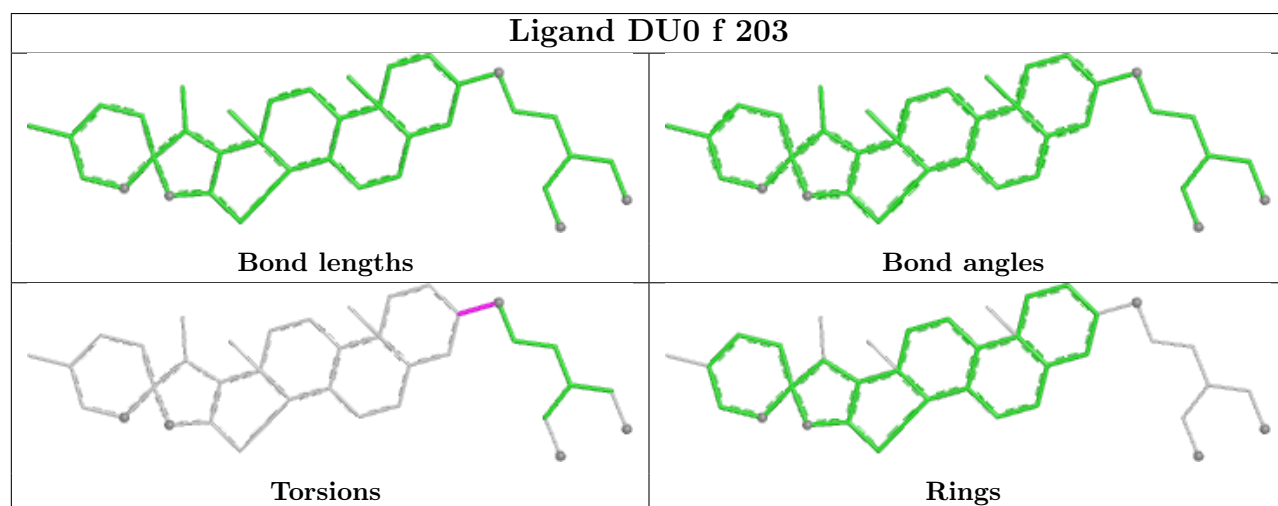
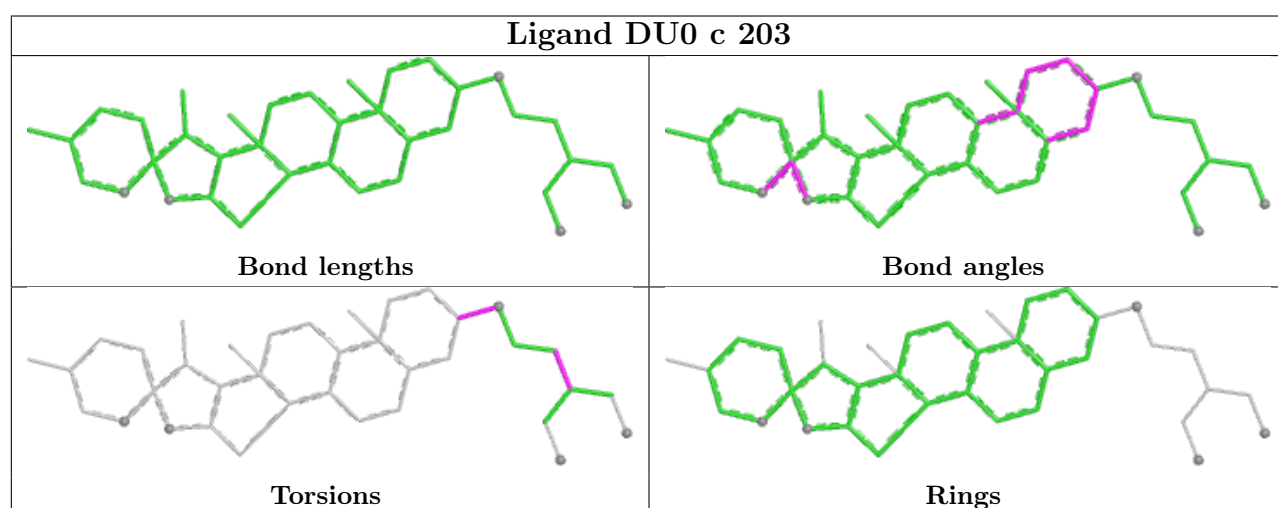
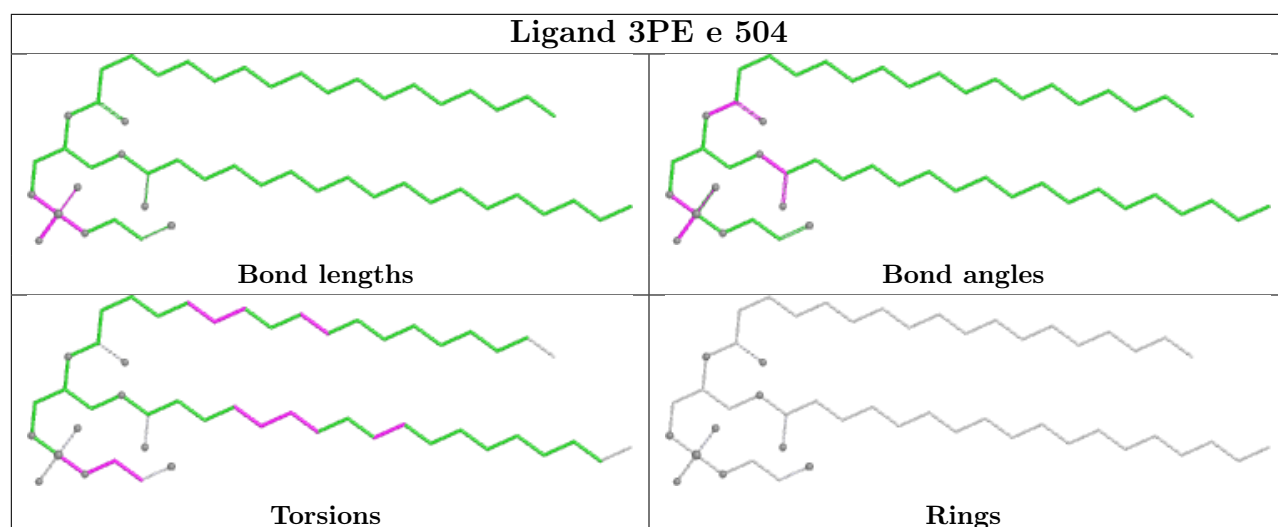


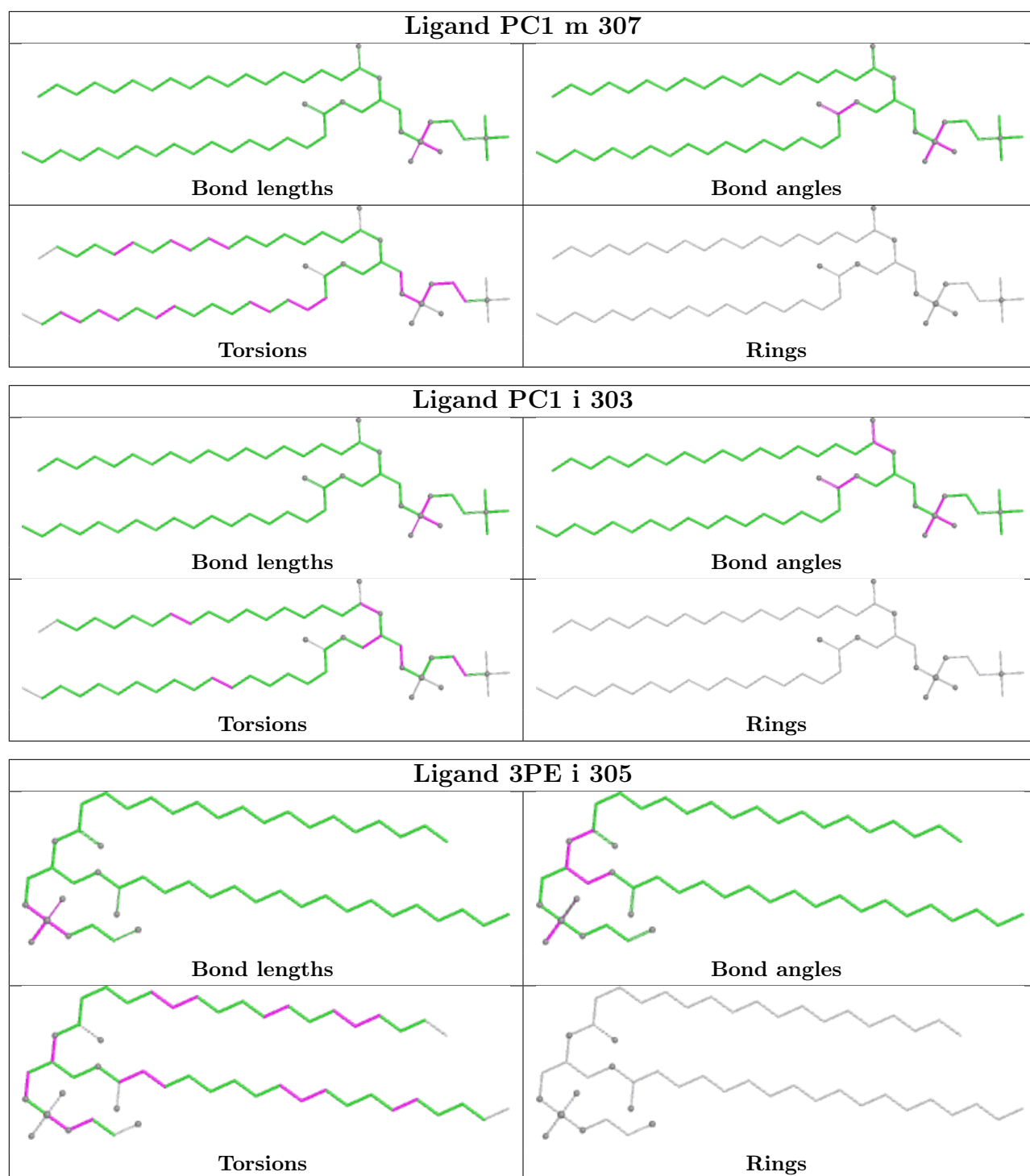


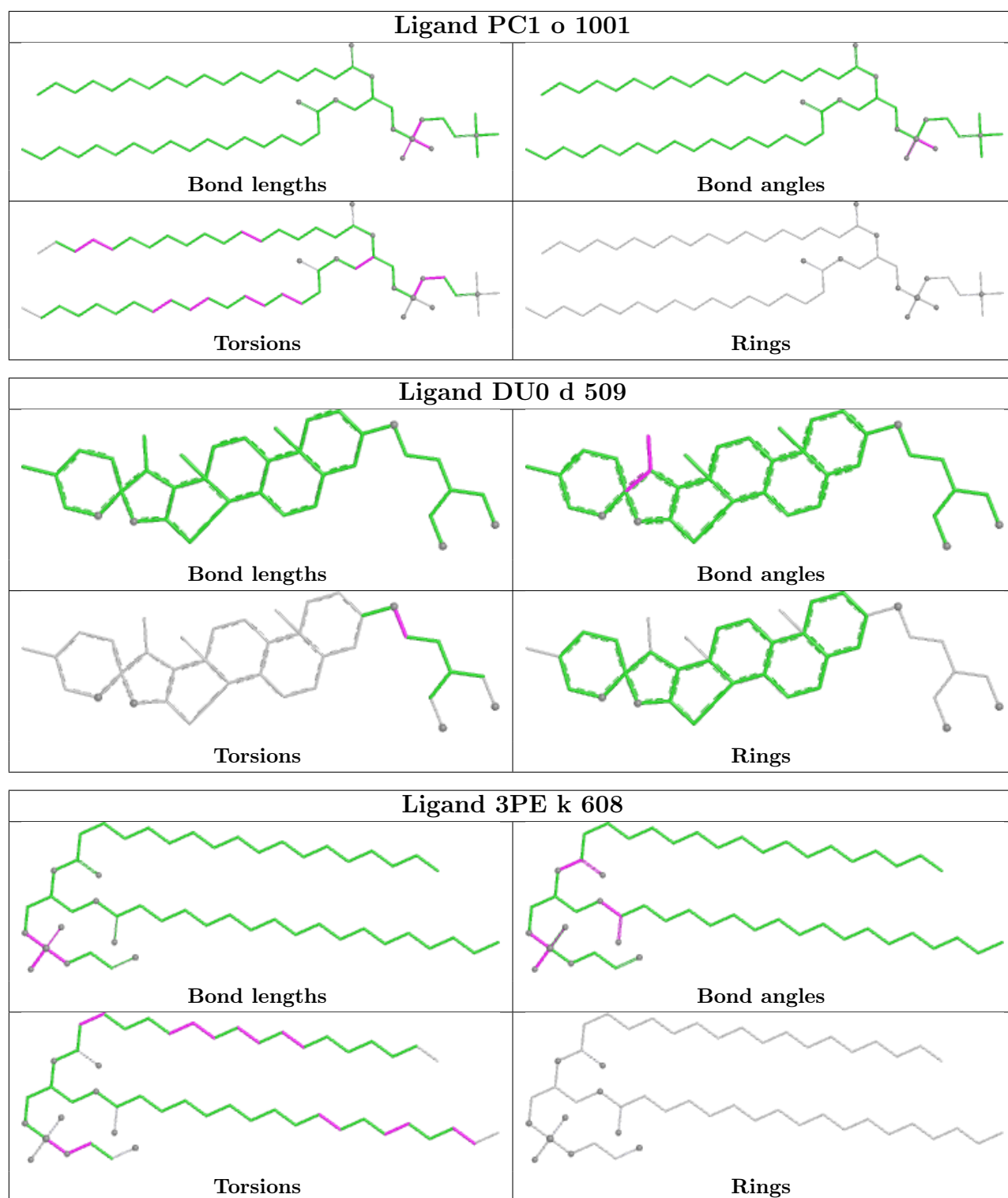


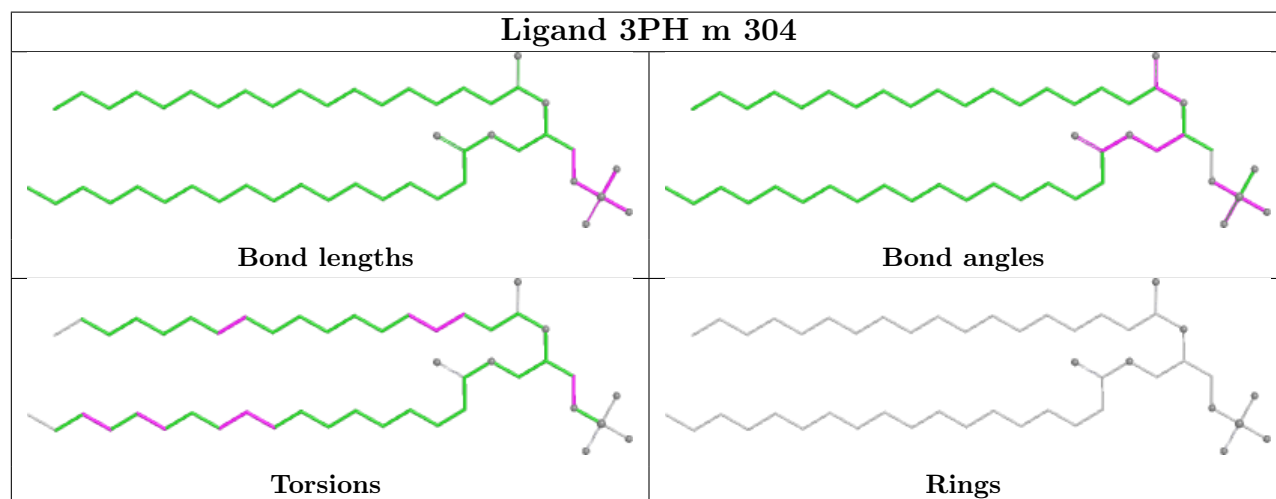
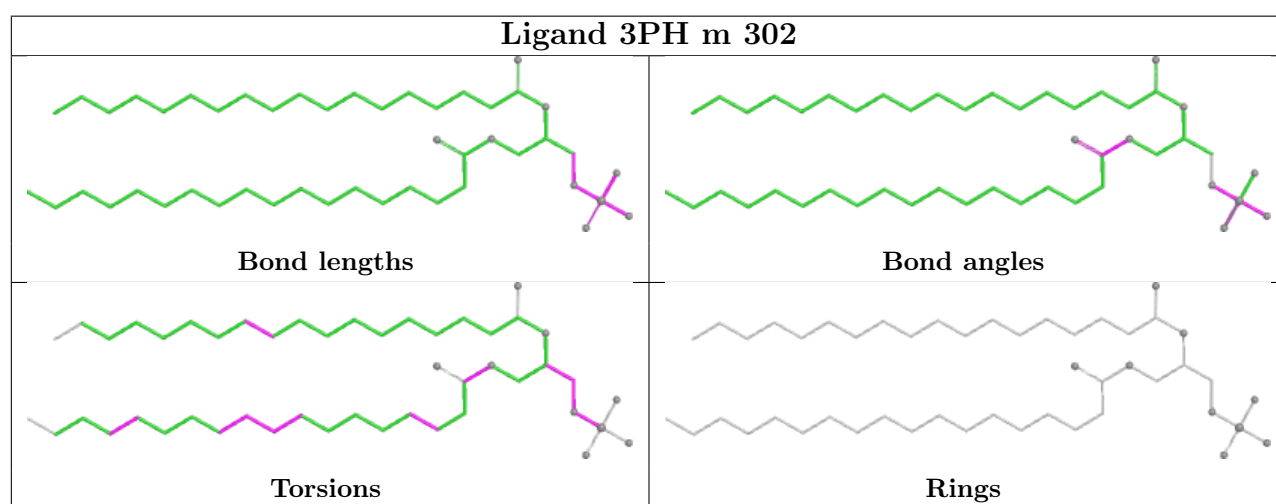
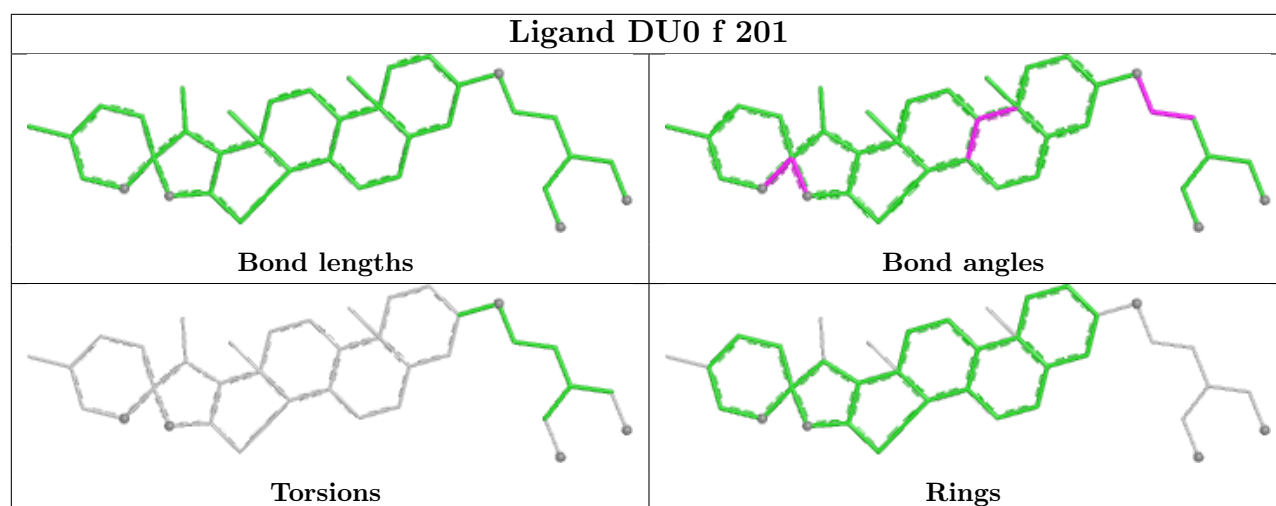


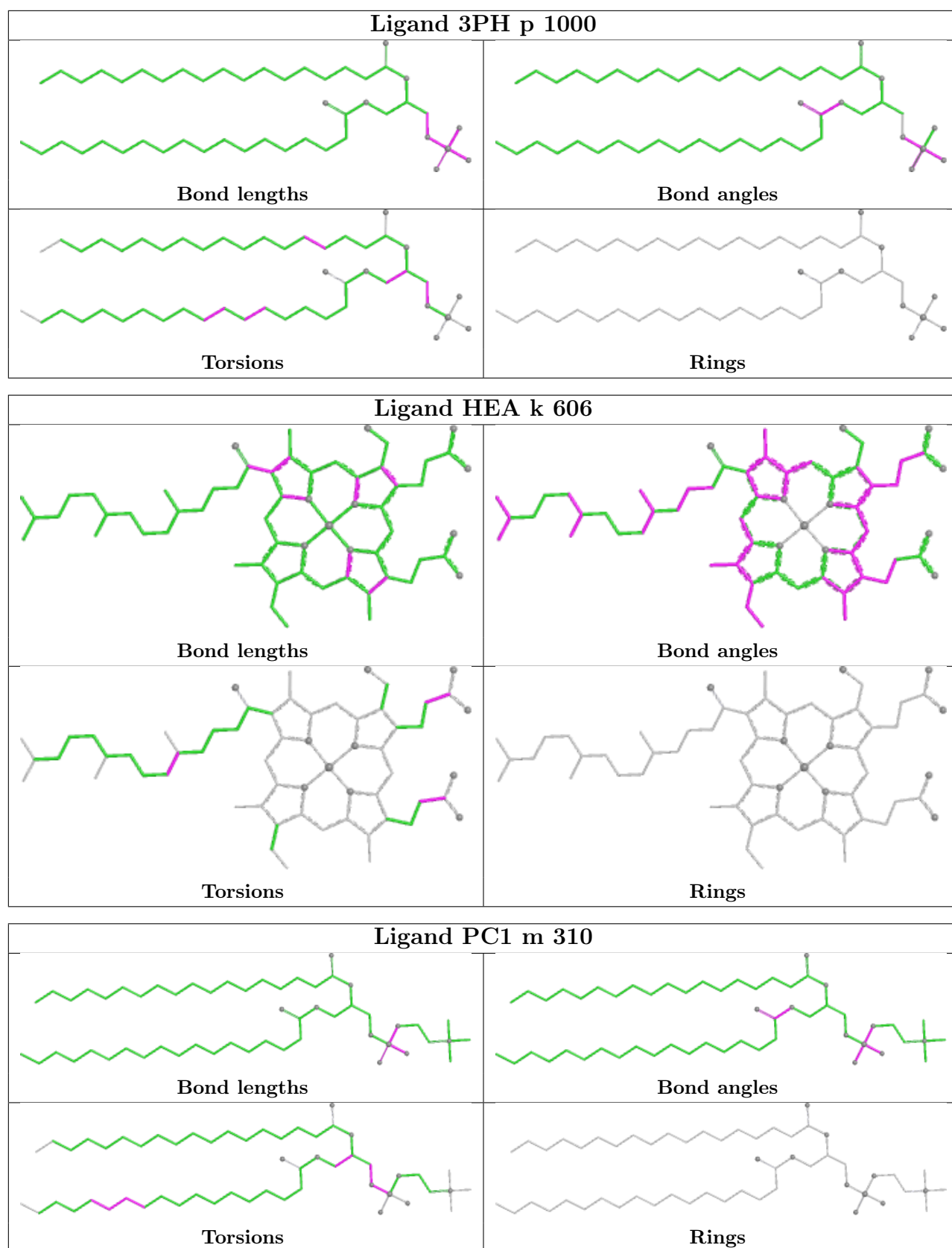
Ligand PC1 b 501	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 a 502	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 a 506	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

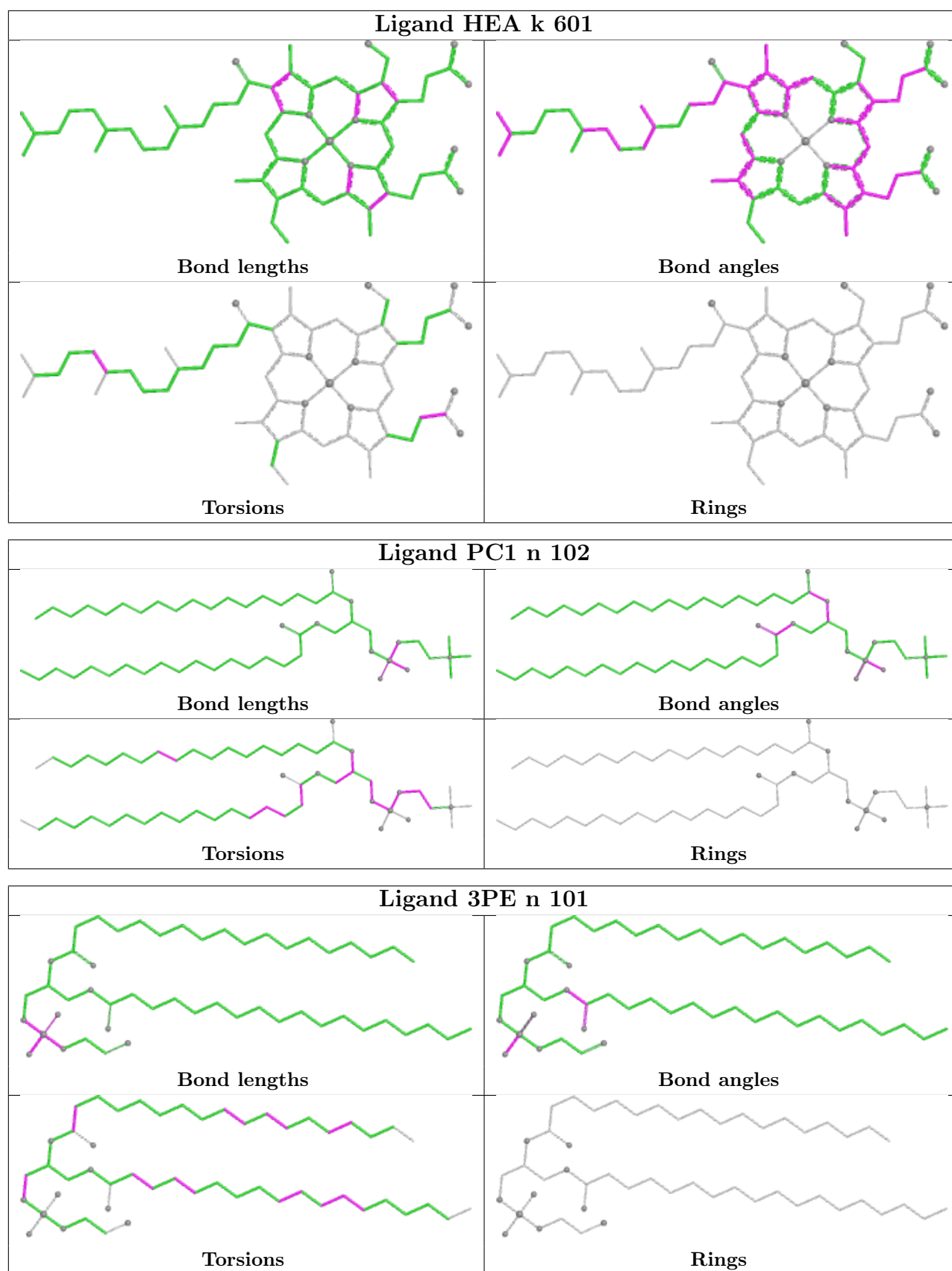


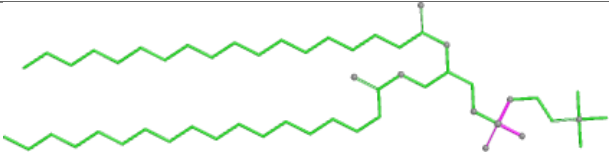
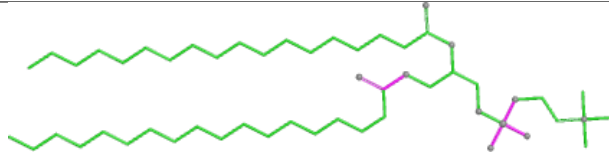
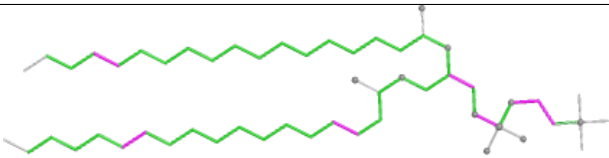
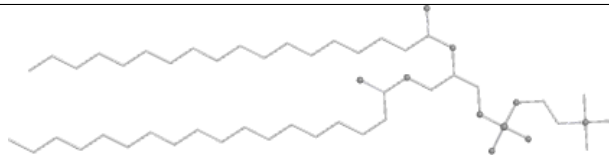
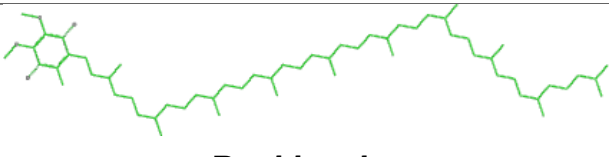
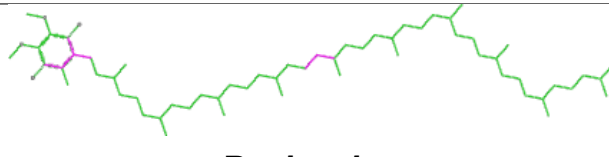
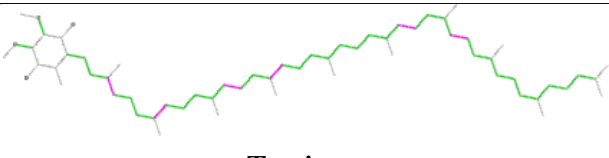
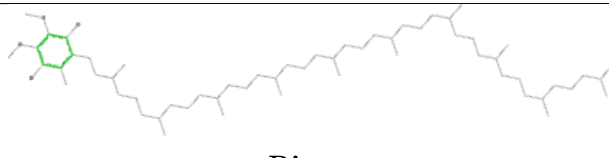
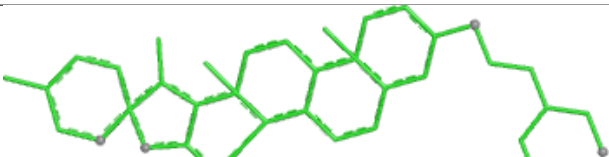
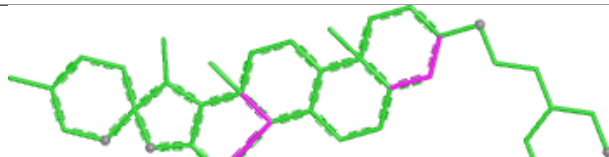
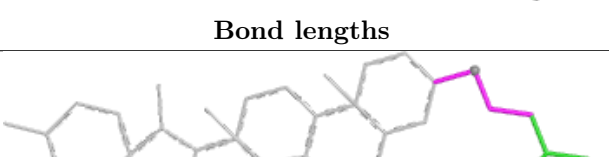
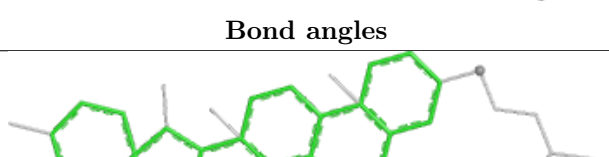


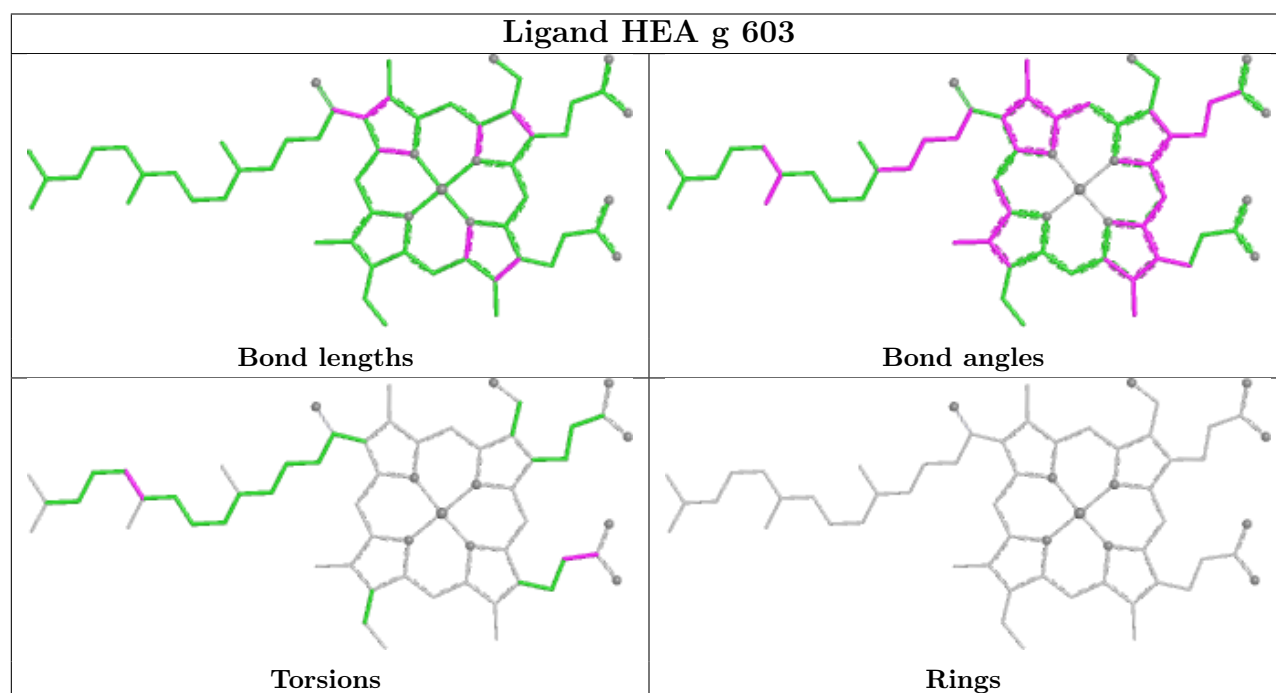
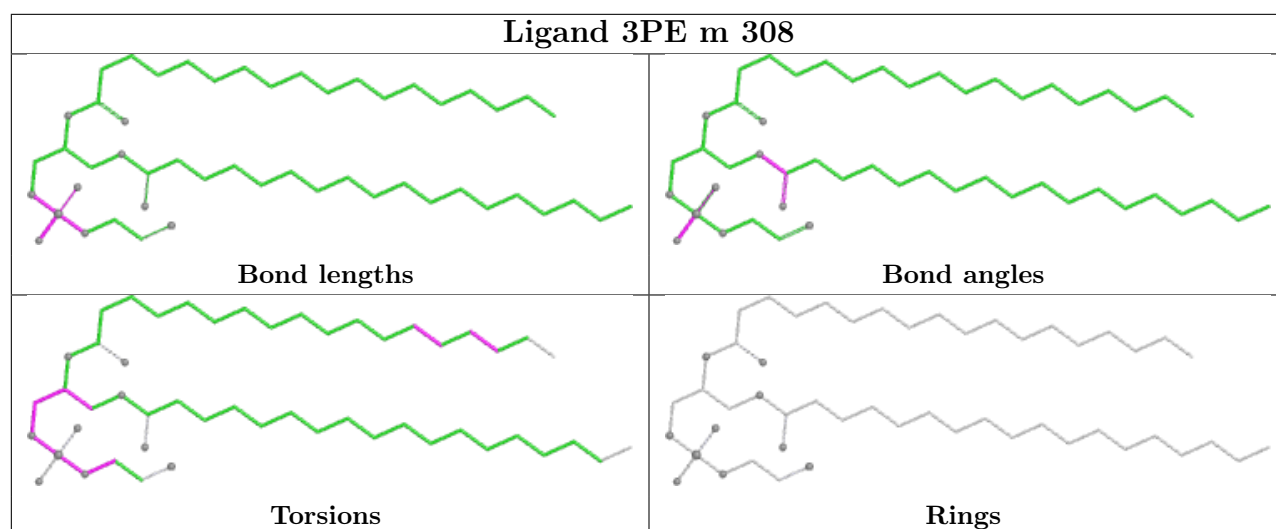
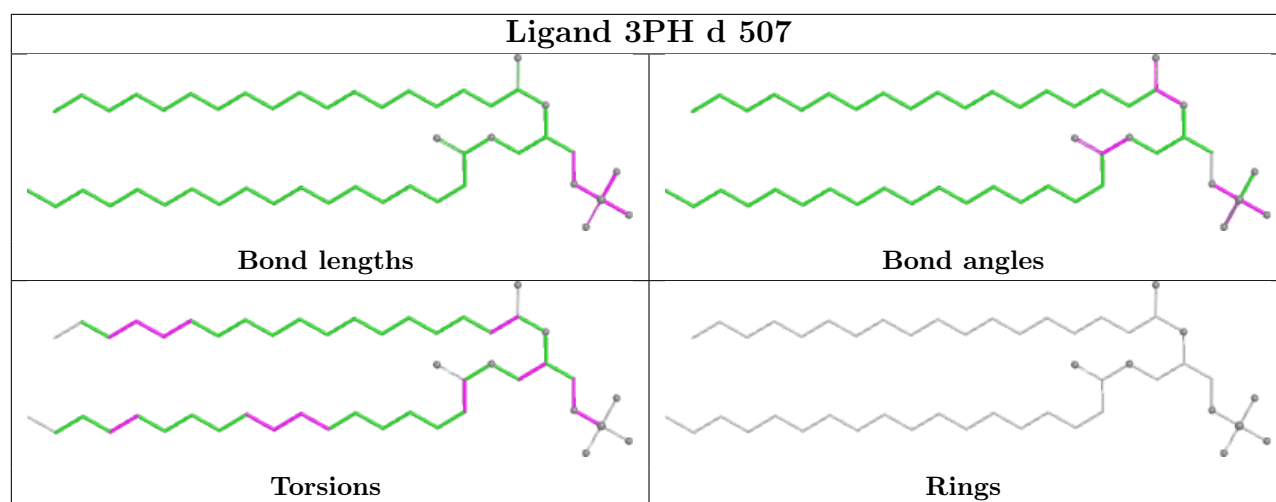


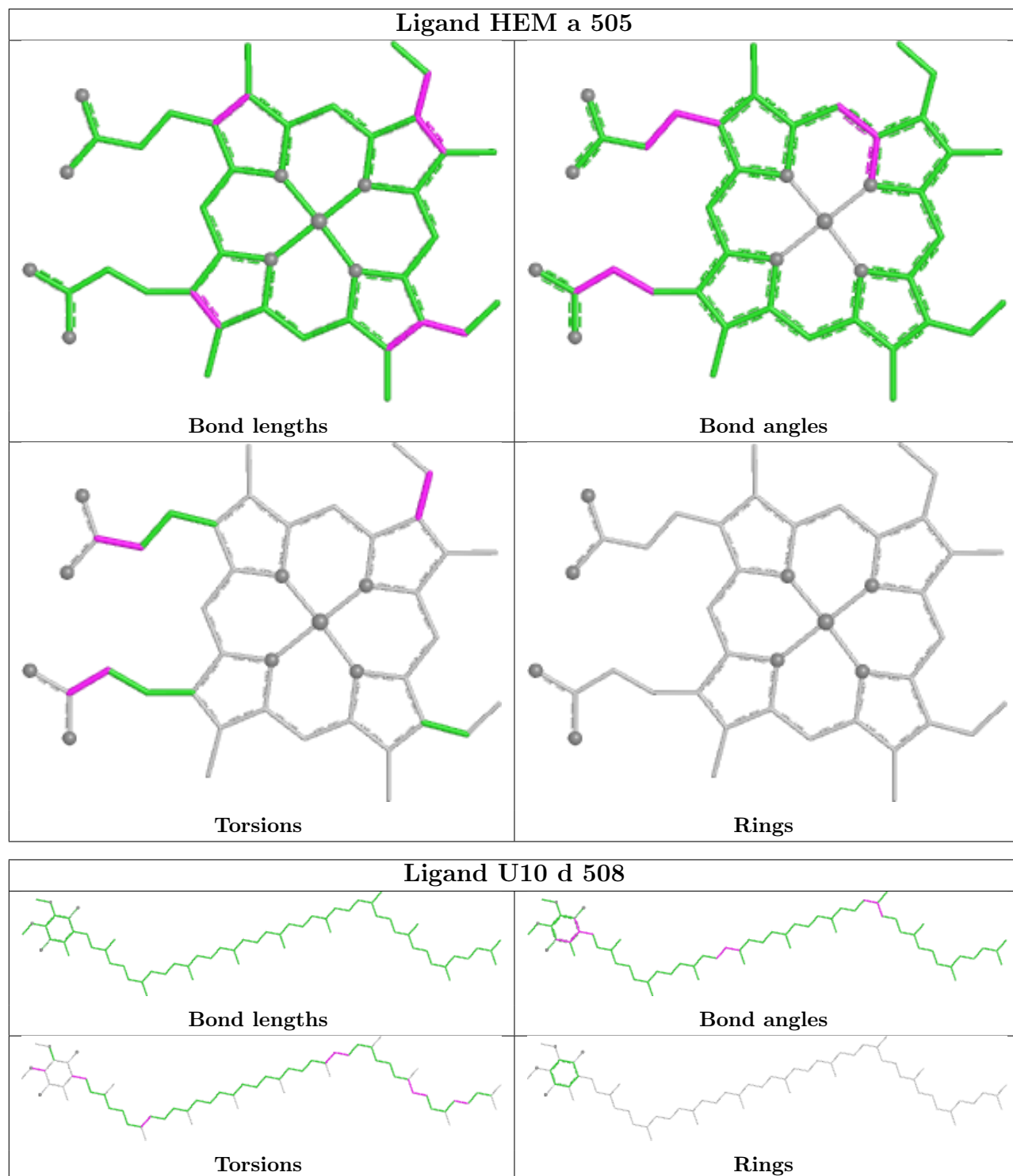


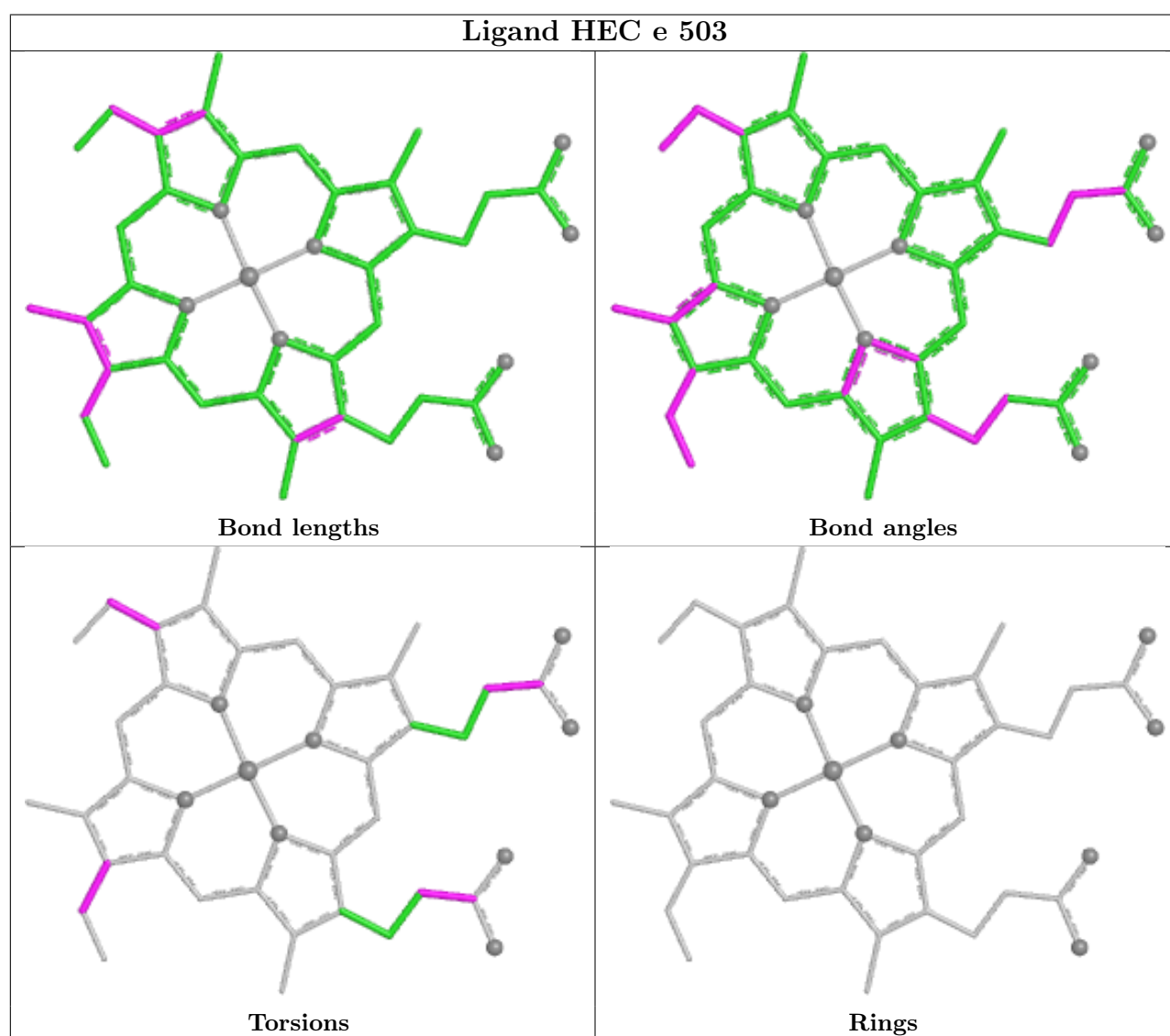
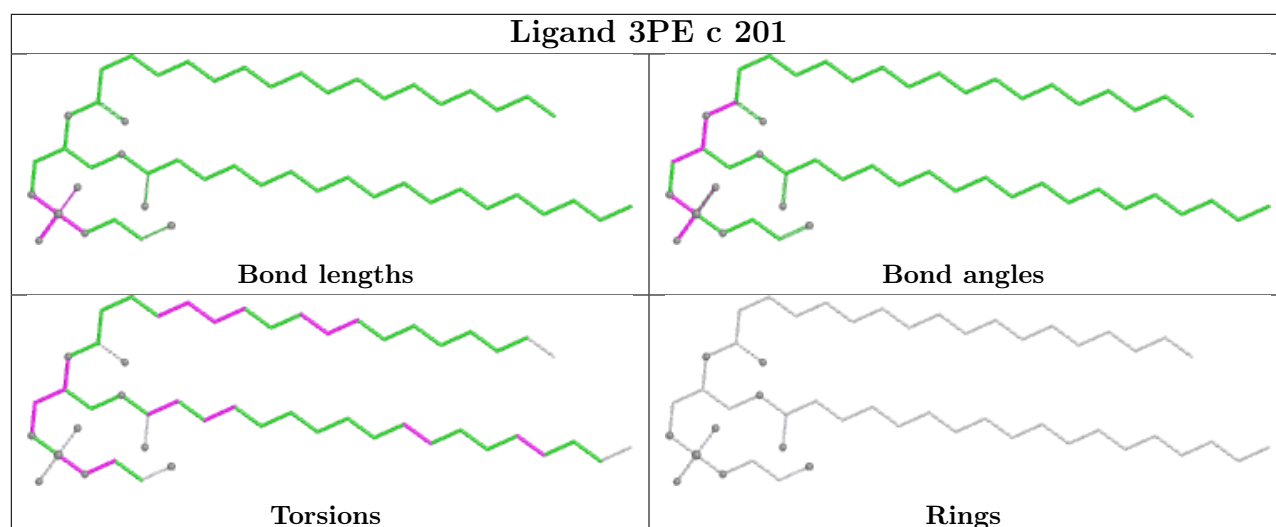




Ligand PC1 i 307	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 d 506	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DU0 m 311	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

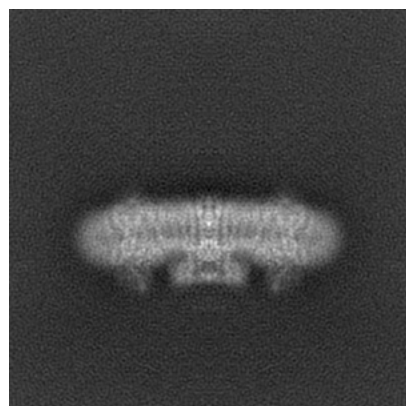
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50526. These allow visual inspection of the internal detail of the map and identification of artifacts.

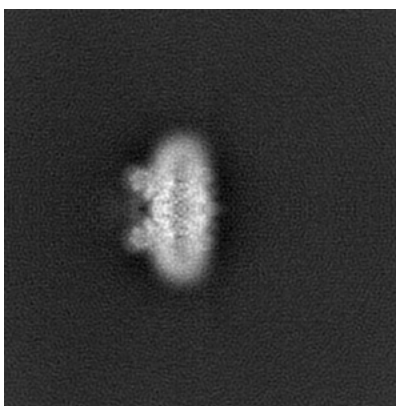
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

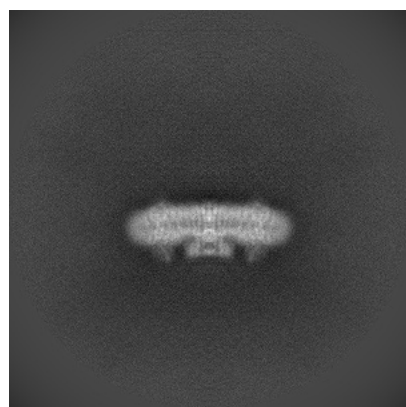


Y

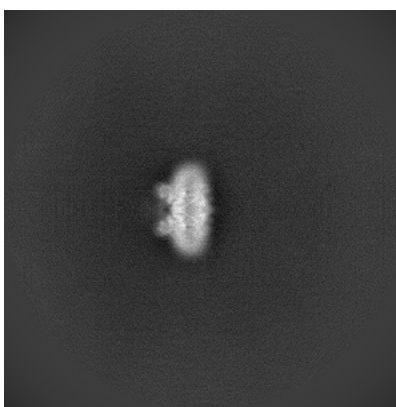


Z

6.1.2 Raw map



X



Y

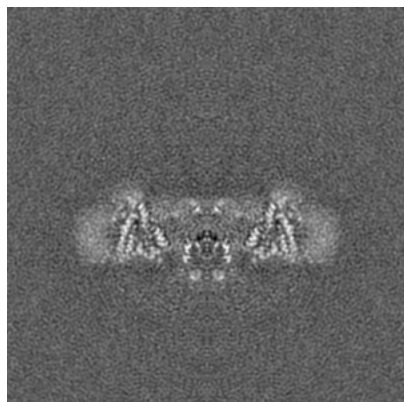


Z

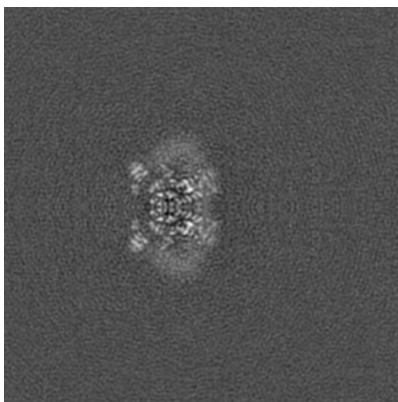
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

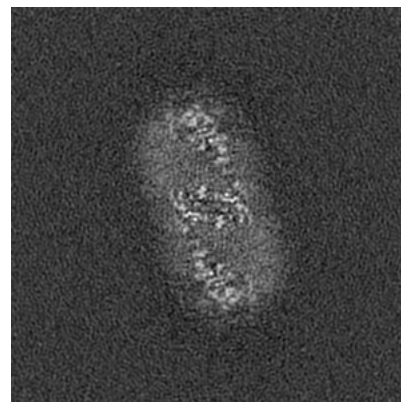
6.2.1 Primary map



X Index: 187

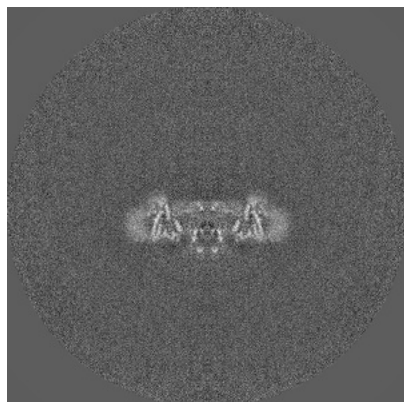


Y Index: 187

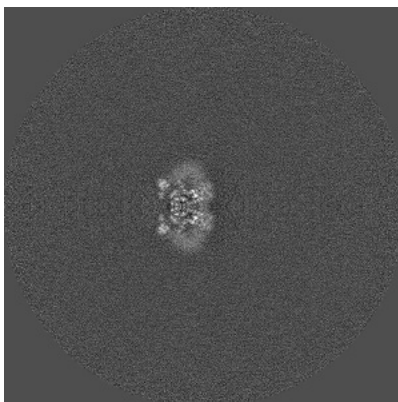


Z Index: 187

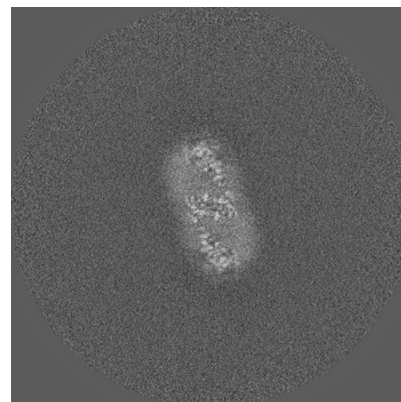
6.2.2 Raw map



X Index: 300



Y Index: 300

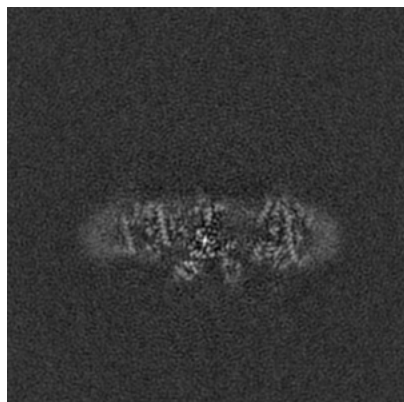


Z Index: 300

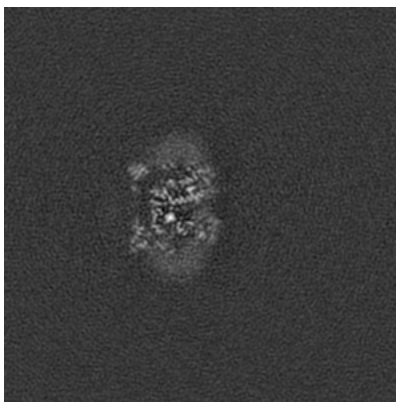
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

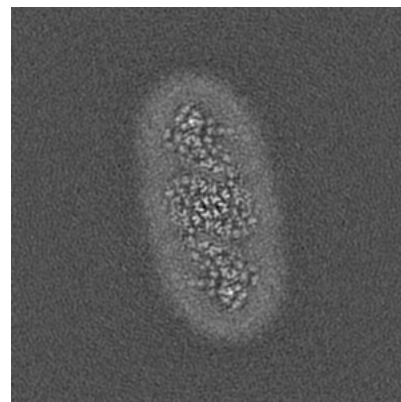
6.3.1 Primary map



X Index: 177

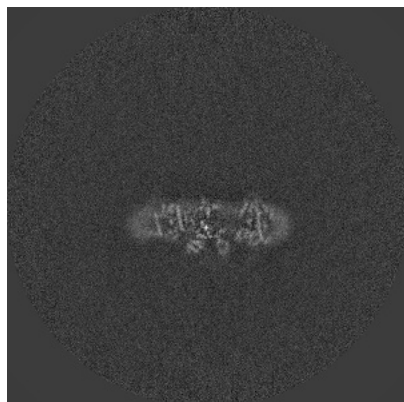


Y Index: 185

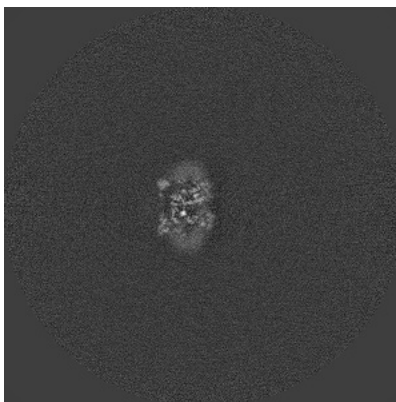


Z Index: 152

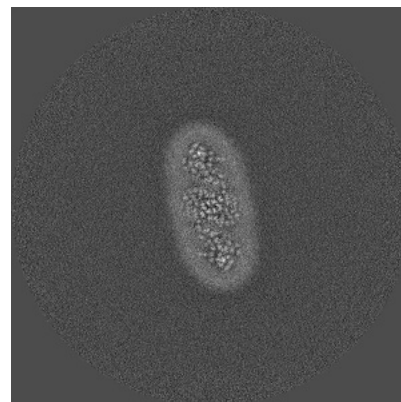
6.3.2 Raw map



X Index: 290



Y Index: 298

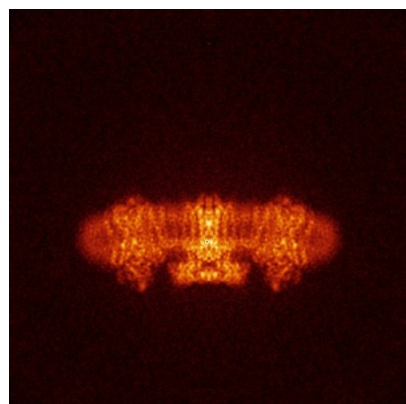


Z Index: 265

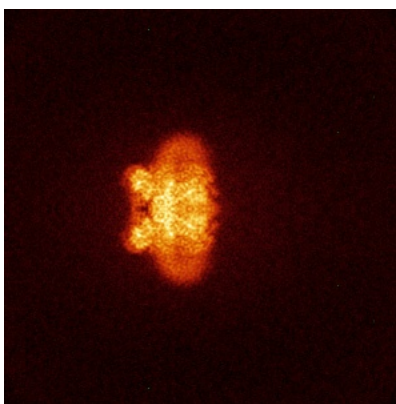
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X

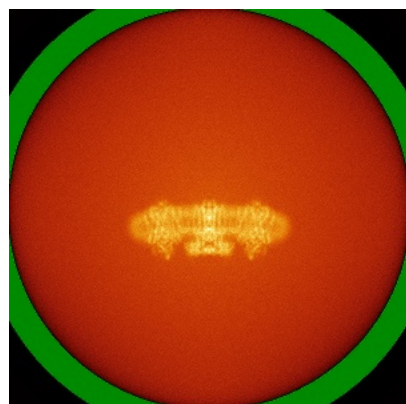


Y

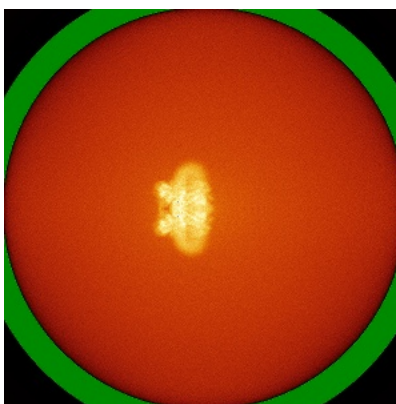


Z

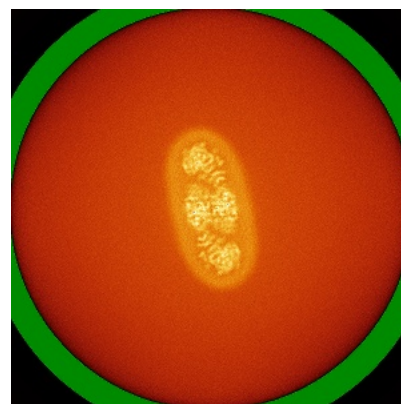
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

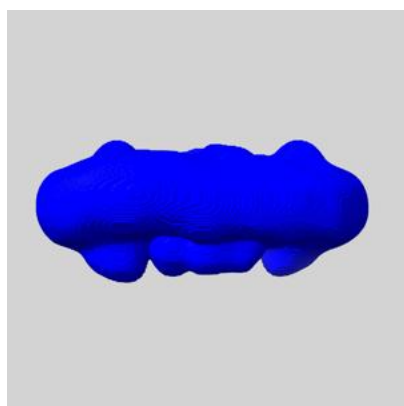
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

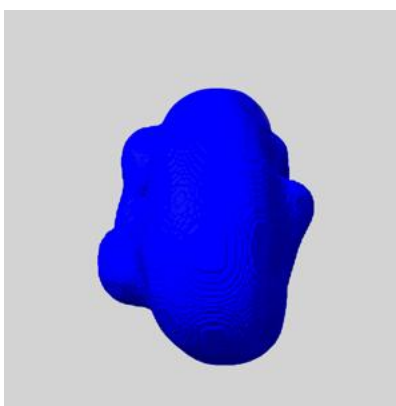
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

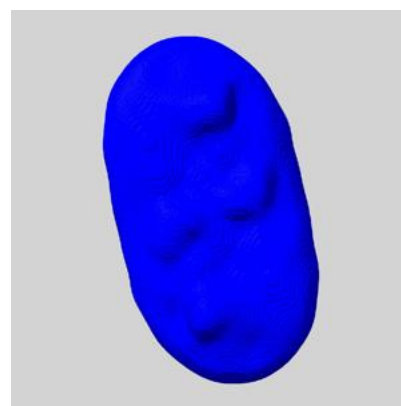
6.6.1 emd_50526_msk_1.map [i](#)



X



Y

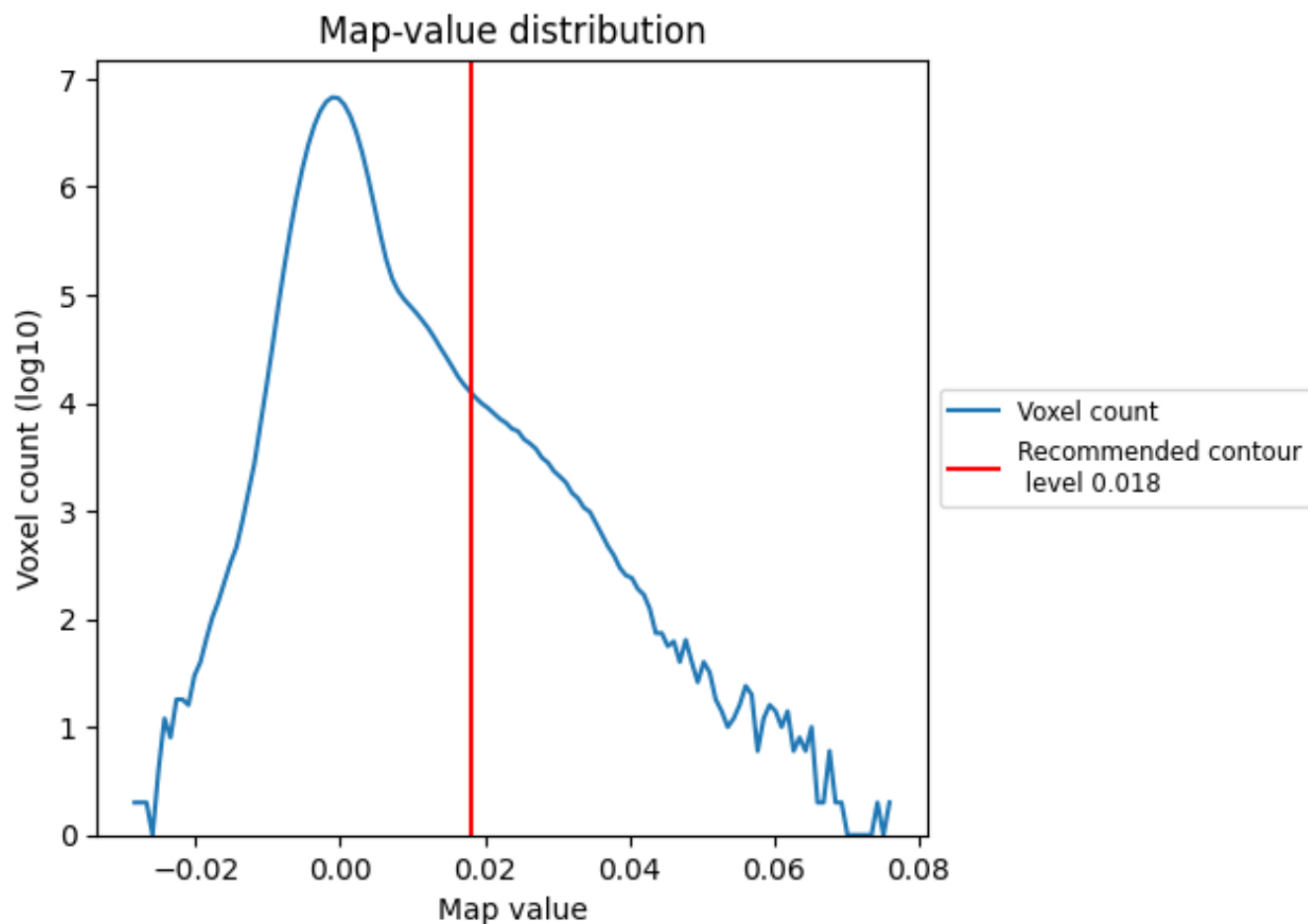


Z

7 Map analysis [i](#)

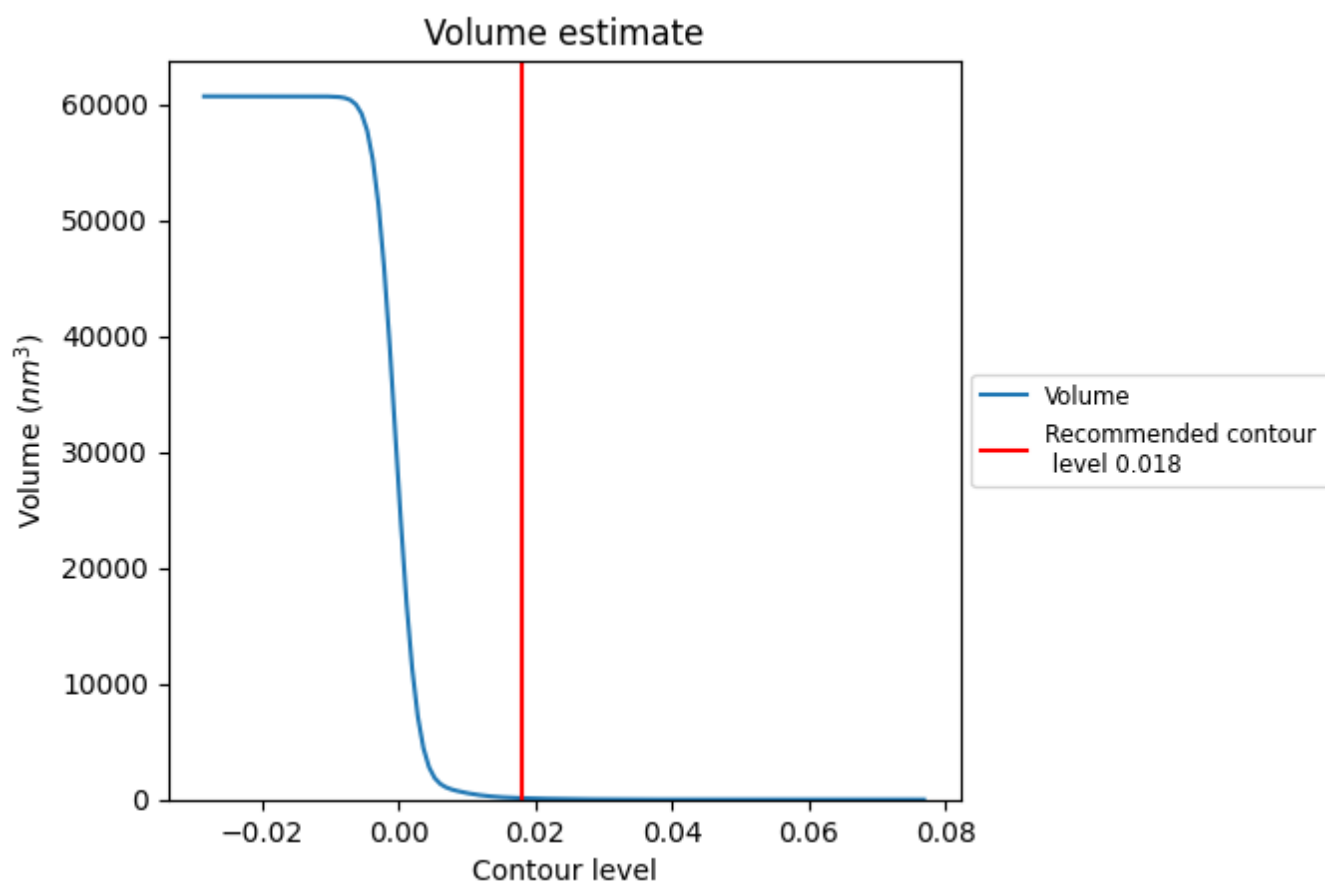
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

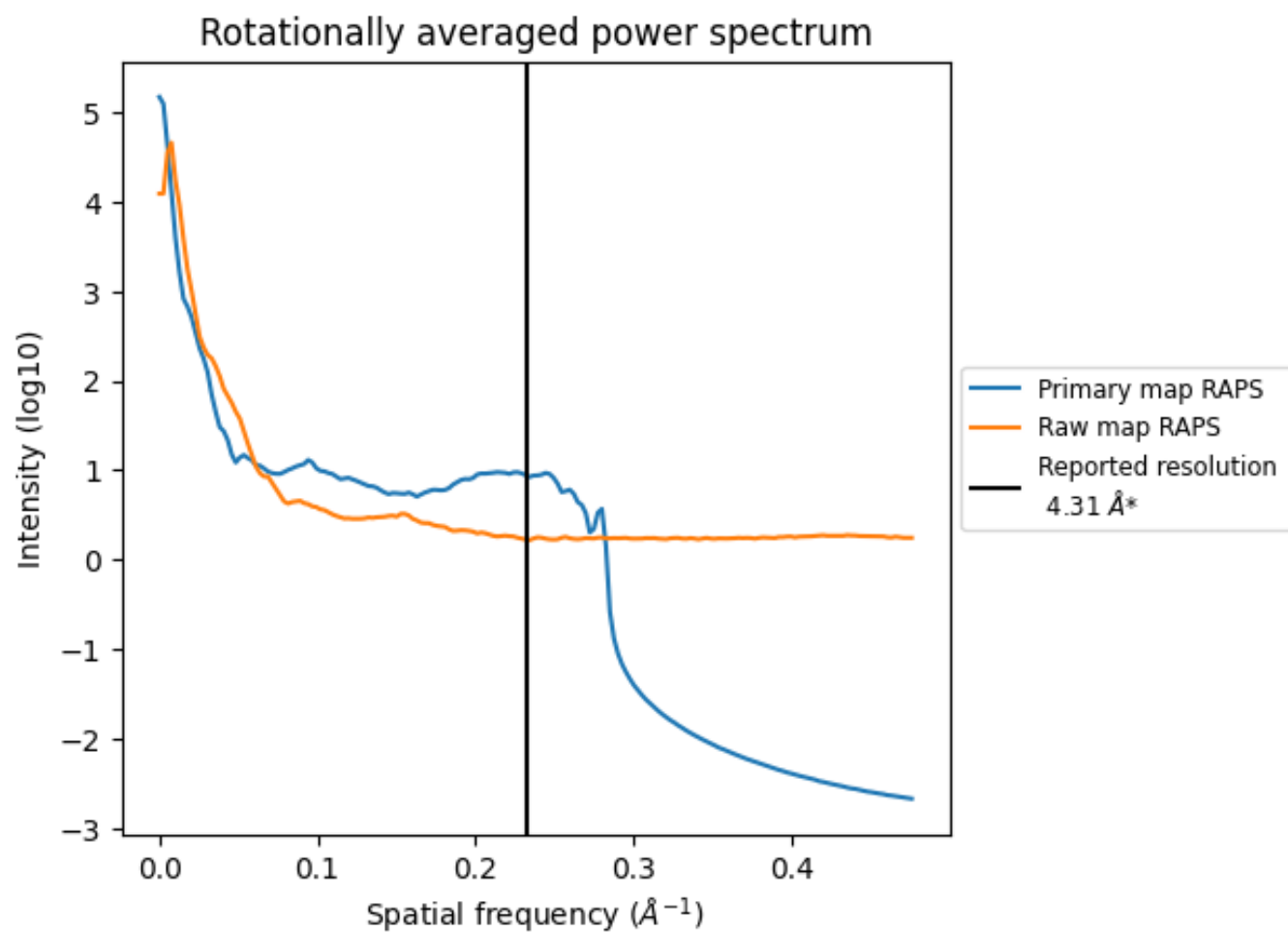
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm³; this corresponds to an approximate mass of 113 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

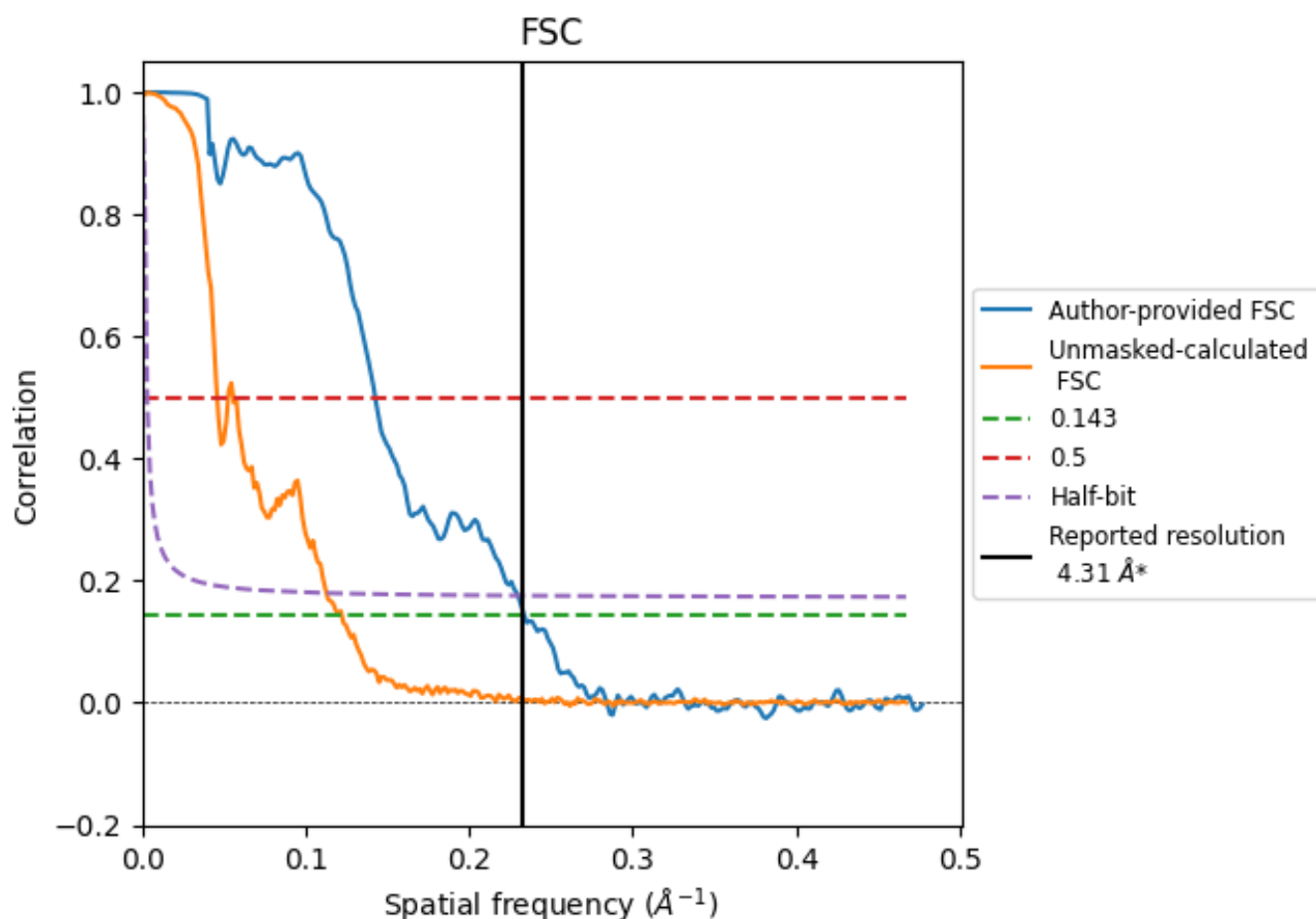


*Reported resolution corresponds to spatial frequency of 0.232 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.232 Å⁻¹

8.2 Resolution estimates [i](#)

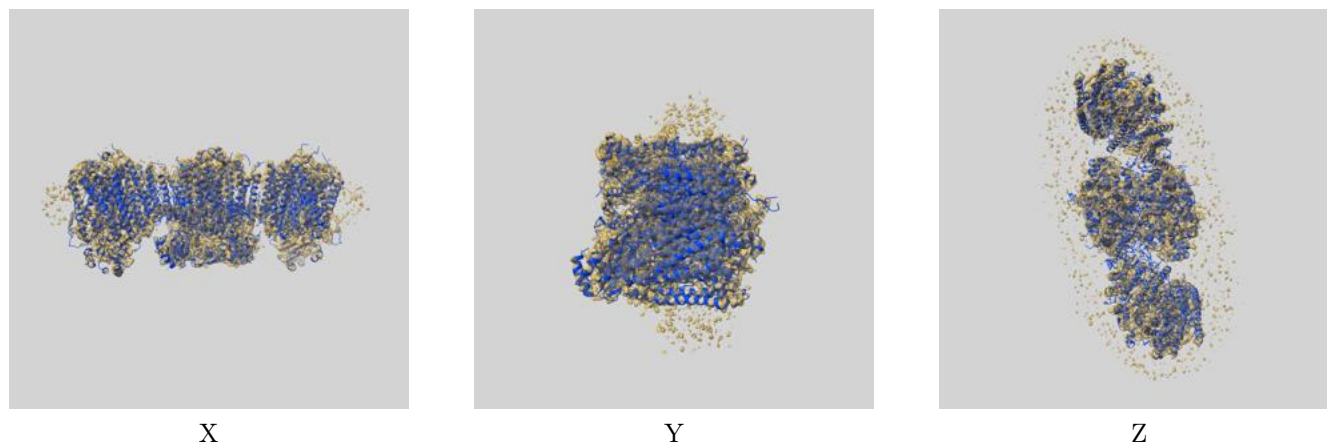
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.31	-	-
Author-provided FSC curve	4.28	7.01	4.35
Unmasked-calculated*	8.19	21.83	8.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.19 differs from the reported value 4.31 by more than 10 %

9 Map-model fit [i](#)

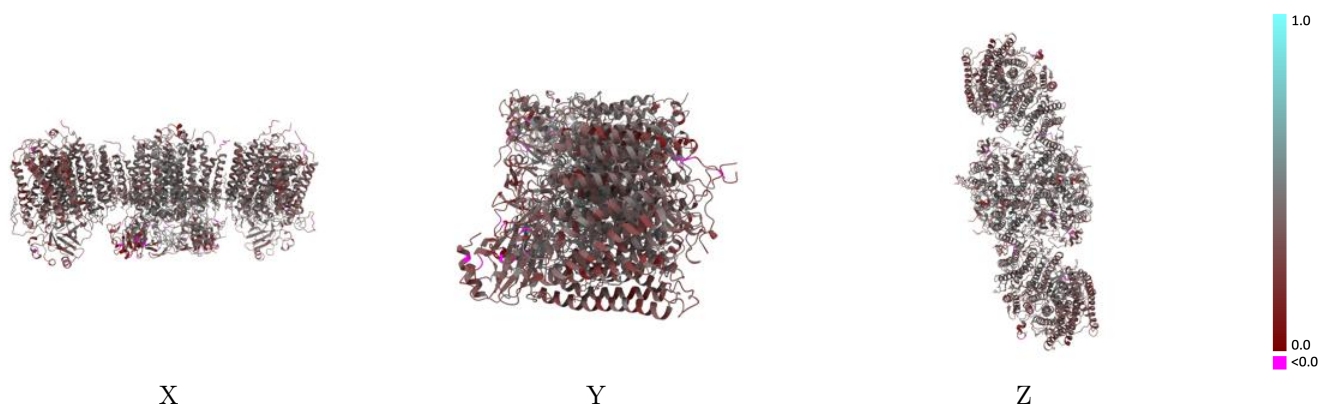
This section contains information regarding the fit between EMDB map EMD-50526 and PDB model 9FKS. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



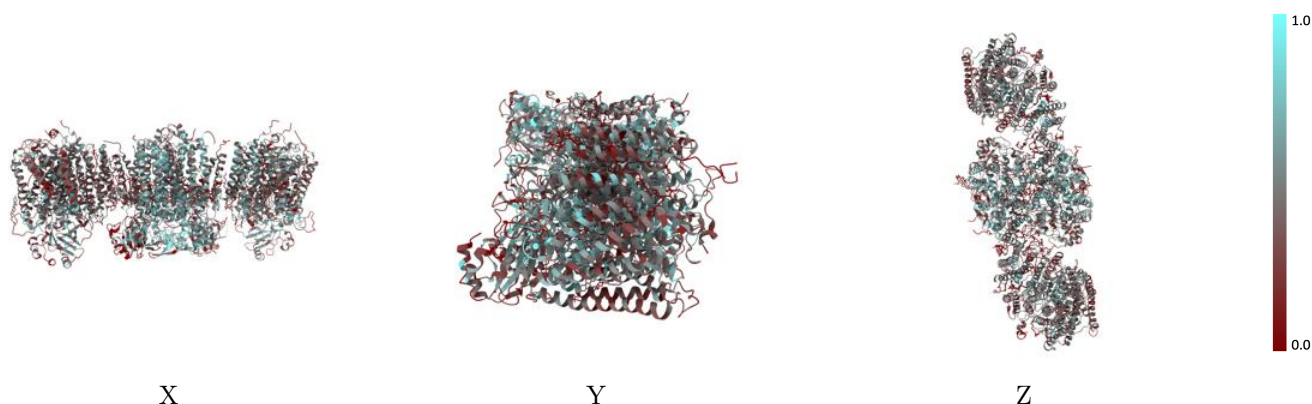
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



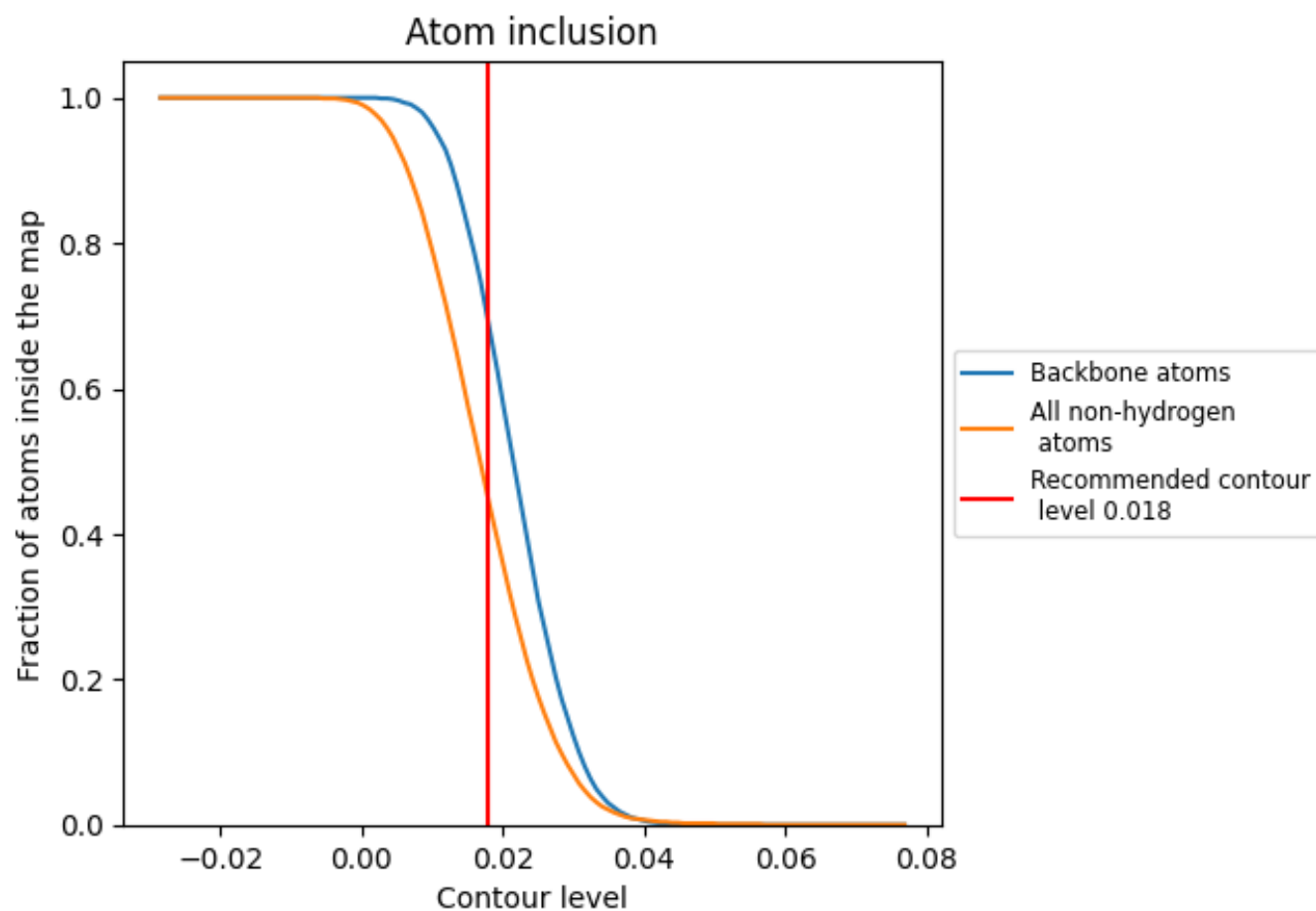
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4440	<div></div> 0.3780
a	<div></div> 0.5320	<div></div> 0.4210
b	<div></div> 0.5390	<div></div> 0.4010
c	<div></div> 0.3150	<div></div> 0.3070
d	<div></div> 0.5090	<div></div> 0.4190
e	<div></div> 0.5360	<div></div> 0.4060
f	<div></div> 0.3200	<div></div> 0.2990
g	<div></div> 0.4480	<div></div> 0.3670
h	<div></div> 0.3910	<div></div> 0.3430
i	<div></div> 0.4260	<div></div> 0.3910
j	<div></div> 0.2760	<div></div> 0.3450
k	<div></div> 0.4430	<div></div> 0.3680
l	<div></div> 0.3950	<div></div> 0.3370
m	<div></div> 0.3890	<div></div> 0.3850
n	<div></div> 0.2670	<div></div> 0.3390
o	<div></div> 0.3960	<div></div> 0.3840
p	<div></div> 0.3800	<div></div> 0.3950

1.0

0.0

<0.0