



wwPDB EM Validation Summary Report ⓘ

May 12, 2025 – 01:40 PM EDT

PDB ID : 9BPB / pdb_00009bpb
EMDB ID : EMD-44770
Title : Tethered respiratory III2IV2 supercomplex from *Saccharomyces cerevisiae*
Authors : Eldeeb, M.H.; Carlstrom, A.; Berndtsson, J.; Ott, M.; Fontanesi, F.
Deposited on : 2024-05-07
Resolution : 2.57 Å (reported)
Based on initial model : 6YMX

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

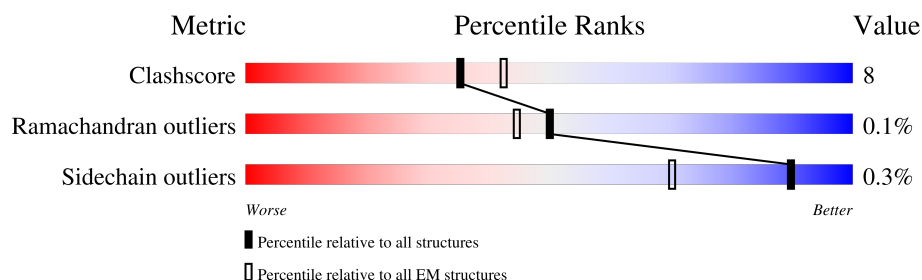
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.57 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	457	
1	K	457	
2	B	368	
2	L	368	
3	C	385	
3	M	385	
4	D	309	
4	N	309	

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Mol	Chain	Length	Quality of chain
5	E	215	
5	O	215	
6	F	147	
6	P	147	
7	G	183	
7	Q	183	
8	H	94	
8	R	94	
9	I	66	
9	S	66	
10	J	77	
10	T	77	
11	a	534	
11	m	534	
12	b	251	
12	n	251	
13	c	269	
13	o	269	
14	d	155	
14	p	155	
15	e	153	
15	q	153	
16	f	148	
16	r	148	
17	g	60	

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Mol	Chain	Length	Quality of chain
17	s	60	
18	i	59	
18	u	59	
19	j	83	
19	v	83	
20	k	129	
20	w	129	
21	l	66	
21	x	66	

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
31	FES	E	301	-	-	X	-
31	FES	O	301	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 61288 atoms, of which 460 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-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3339	2107	575	651	6		
1	K	430	Total	C	N	O	S	0	0
			3339	2107	575	651	6		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	L	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	383	Total	C	N	O	S	0	0
			3071	2071	480	499	21		
3	M	383	Total	C	N	O	S	0	0
			3071	2071	480	499	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	245	Total	C	N	O	S	0	0
			1941	1237	337	359	8		
4	N	245	Total	C	N	O	S	0	0
			1941	1237	337	359	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	O	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		
6	P	74	Total	C	N	O	S	0	0
			624	391	108	123	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial, Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	125	Total	C	N	O	S	0	0
			1008	647	171	188	2		
7	Q	125	Total	C	N	O	S	0	0
			1008	647	171	188	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	128	GLY	-	linker	UNP P00128
G	129	GLY	-	linker	UNP P00128
G	130	GLY	-	linker	UNP P00128
G	131	GLY	-	linker	UNP P00128
Q	128	GLY	-	linker	UNP P00128
Q	129	GLY	-	linker	UNP P00128
Q	130	GLY	-	linker	UNP P00128
Q	131	GLY	-	linker	UNP P00128

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	92	Total	C	N	O	S	0	0
			764	505	129	128	2		
8	R	92	Total	C	N	O	S	0	0
			764	505	129	128	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	53	Total	C	N	O	0	0
			436	291	73	72		
9	S	53	Total	C	N	O	0	0
			436	291	73	72		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	45	Total	C	N	O	S	0	0
			352	233	58	59	2		
10	T	45	Total	C	N	O	S	0	0
			352	233	58	59	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	534	Total	C	N	O	S	0	0
			4161	2778	649	712	22		
11	m	534	Total	C	N	O	S	0	0
			4161	2778	649	712	22		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	236	Total	C	N	O	S	0	0
			1888	1242	286	350	10		
12	n	236	Total	C	N	O	S	0	0
			1888	1242	286	350	10		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		
13	o	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	119	Total	C	N	O	S	0	0
			898	565	149	179	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	119	Total	C	N	O	S	0	0
			898	565	149	179	5		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	128	Total	C	N	O	S	0	0
			1008	639	175	190	4		
15	q	128	Total	C	N	O	S	0	0
			1008	639	175	190	4		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	98	Total	C	N	O	S	0	0
			819	528	133	157	1		
16	r	98	Total	C	N	O	S	0	0
			819	528	133	157	1		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	55	Total	C	N	O	0	0
			456	310	77	69		
17	s	55	Total	C	N	O	0	0
			456	310	77	69		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	i	49	Total	C	N	O	S	0	0
			404	269	68	64	3		
18	u	49	Total	C	N	O	S	0	0
			404	269	68	64	3		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	74	Total	C	N	O	S	0	0
			621	400	106	110	5		
19	v	74	Total	C	N	O	S	0	0
			621	400	106	110	5		

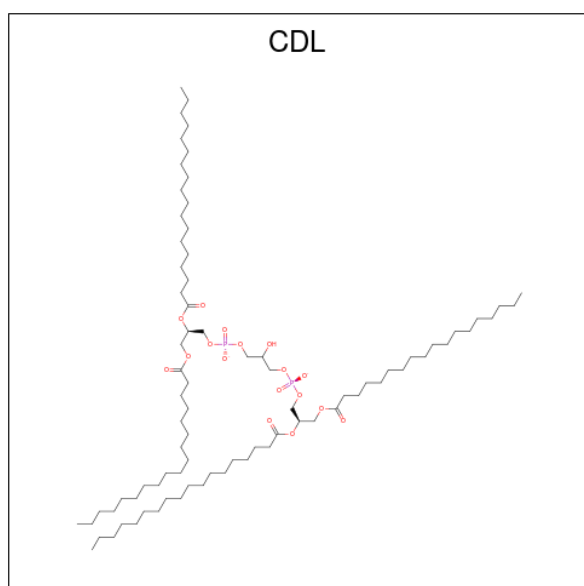
- Molecule 20 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	110	Total	C	N	O	S	0	0
			911	591	158	159	3		
20	w	110	Total	C	N	O	S	0	0
			911	591	158	159	3		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	l	36	Total	C	N	O	S	0	0
			293	199	47	46	1		
21	x	36	Total	C	N	O	S	0	0
			293	199	47	46	1		

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



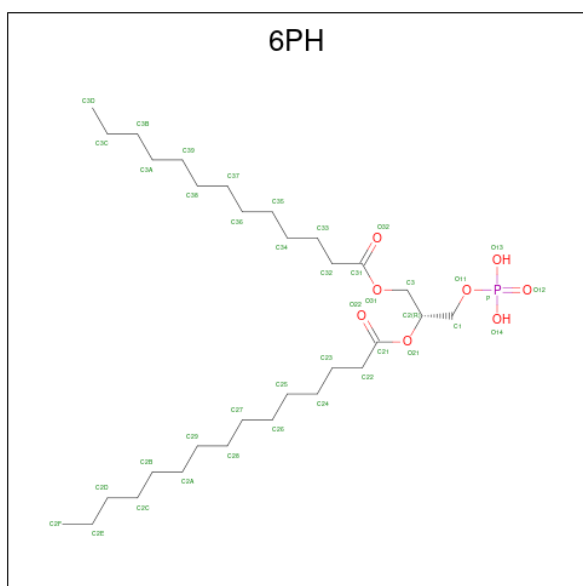
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			55	36	17	2	
22	D	1	Total	C	O	P	0
			60	41	17	2	
22	E	1	Total	C	O	P	0
			42	25	15	2	
22	H	1	Total	C	O	P	0
			53	34	17	2	
22	K	1	Total	C	O	P	0
			55	36	17	2	

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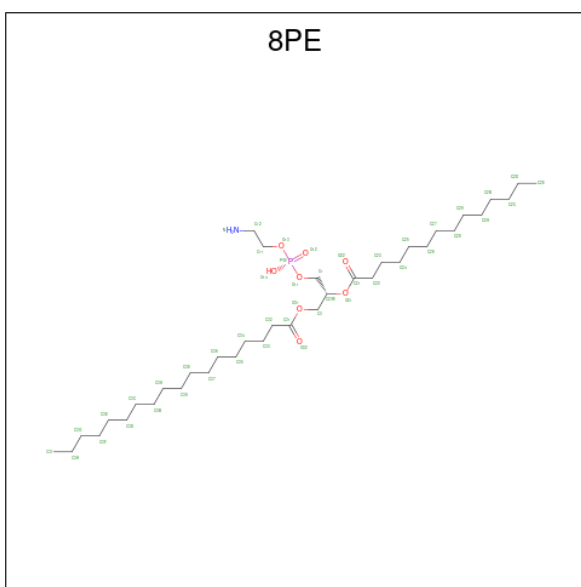
Mol	Chain	Residues	Atoms				AltConf
22	N	1	Total	C	O	P	0
			60	41	17	2	
22	O	1	Total	C	O	P	0
			42	25	15	2	
22	R	1	Total	C	O	P	0
			53	34	17	2	

- Molecule 23 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C₃₁H₆₁O₈P).



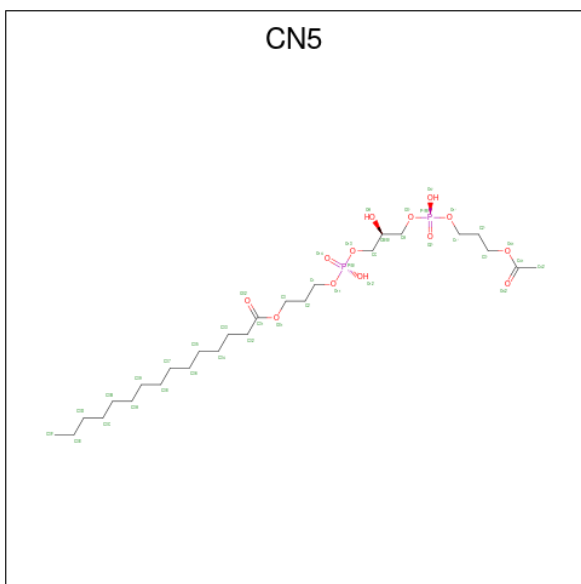
Mol	Chain	Residues	Atoms				AltConf
23	C	1	Total	C	O	P	0
			40	31	8	1	
23	M	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 24 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



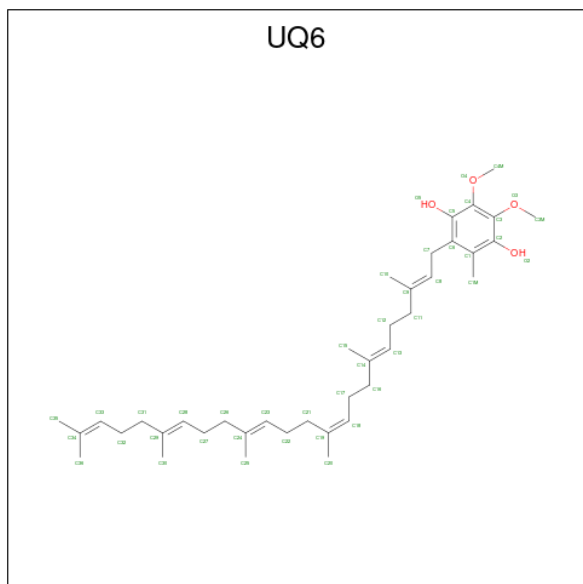
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	N	O	P	0
			26	16	1	8	1	
24	M	1	Total	C	N	O	P	0
			26	16	1	8	1	

- Molecule 25 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



Mol	Chain	Residues	Atoms				AltConf
25	C	1	Total	C	O	P	0
			32	17	13	2	

- Molecule 26 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$).



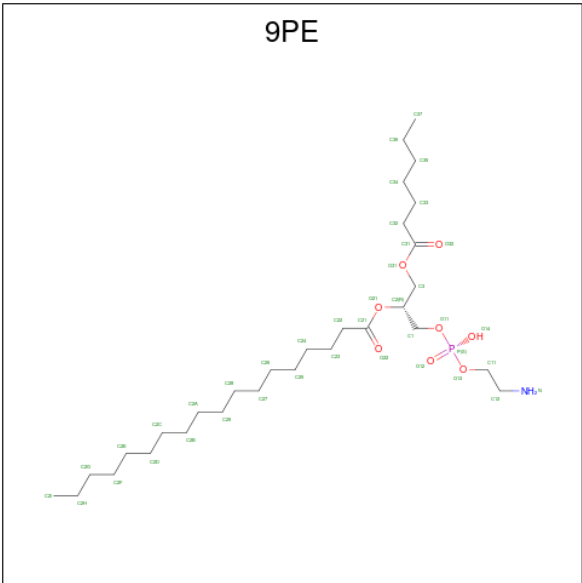
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	H	O	0
			56	22	30	4	
26	C	1	Total	C	O		0
			43	39	4		
26	M	1	Total	C	H	O	0
			56	22	30	4	
26	M	1	Total	C	O		0
			43	39	4		

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



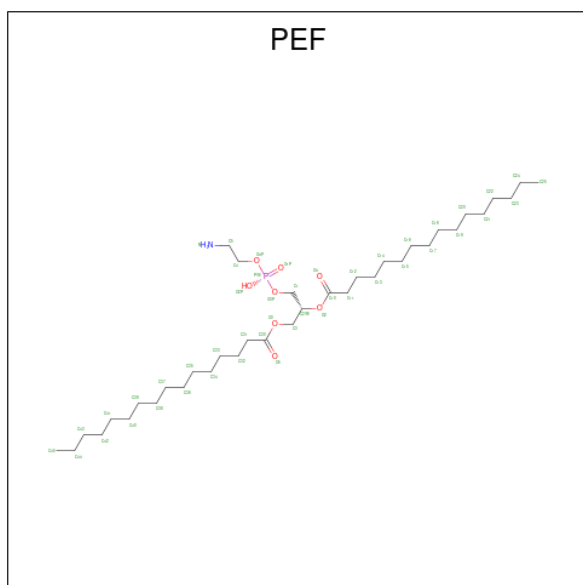
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
27	C	1	Total 73	34	1	30	4	4	0
27	C	1	Total 73	34	1	30	4	4	0
27	M	1	Total 73	34	1	30	4	4	0
27	M	1	Total 73	34	1	30	4	4	0

- Molecule 28 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P).



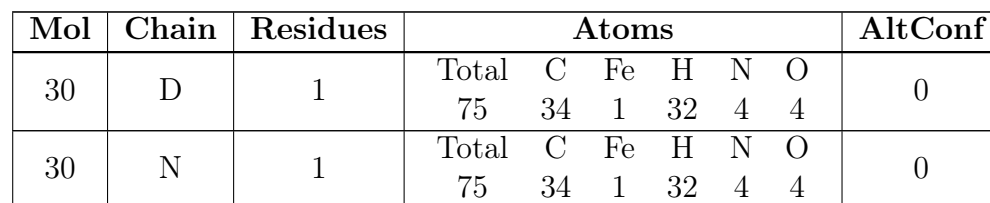
Mol	Chain	Residues	Atoms					AltConf
28	C	1	Total	C	N	O	P	0
			33	23	1	8	1	
28	M	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 29 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
29	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
29	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
29	a	1	Total	C	N	O	P	0
			43	33	1	8	1	
29	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
29	T	1	Total	C	N	O	P	0
			29	19	1	8	1	
29	m	1	Total	C	N	O	P	0
			43	33	1	8	1	

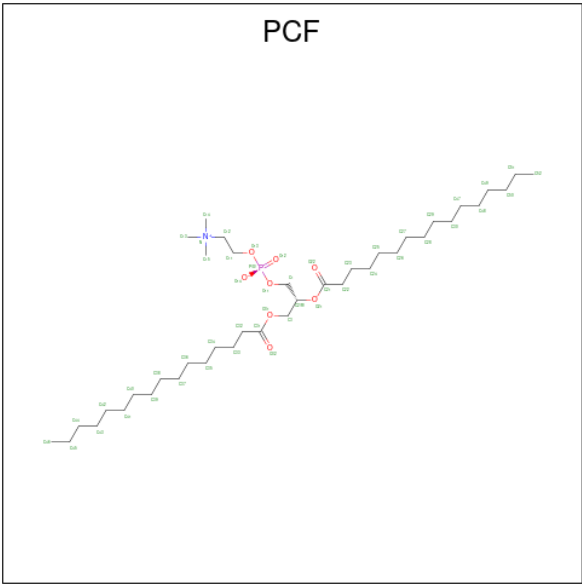
- Molecule 30 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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- Diagram illustrating the structure of a ferredoxin (FES) molecule, showing a square planar arrangement of two iron (Fe) and two sulfur (S) atoms. The atoms are labeled S1, FE2, FE1, and S2 in green text. The bonds are colored yellow and purple.

Mol	Chain	Residues	Atoms			AltConf
31	E	1	Total 4	Fe 2	S 2	0
31	O	1	Total 4	Fe 2	S 2	0

- Molecule 32 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).

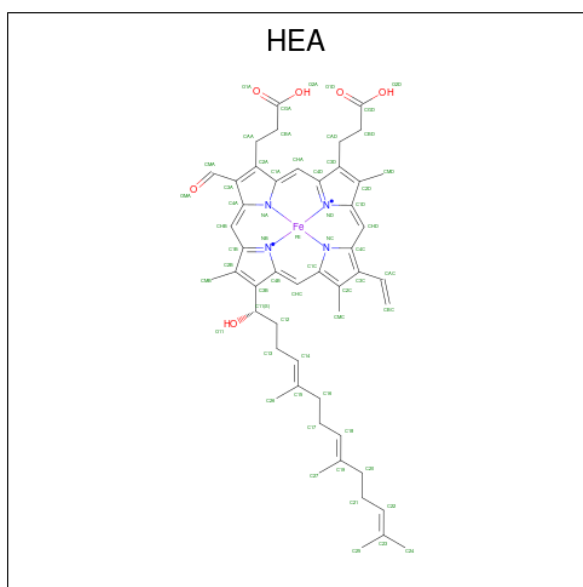


Mol	Chain	Residues	Atoms					AltConf
32	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	k	1	Total	C	N	O	P	0
			43	33	1	8	1	
32	l	1	Total	C	N	O	P	0
			37	27	1	8	1	
32	R	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	w	1	Total	C	N	O	P	0
			43	33	1	8	1	
32	x	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



- Molecule 34 is HEME-A (CCD ID: HEA) (formula: $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$).



Mol	Chain	Residues	Atoms						AltConf
34	a	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
34	a	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
34	m	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
34	m	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 35 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

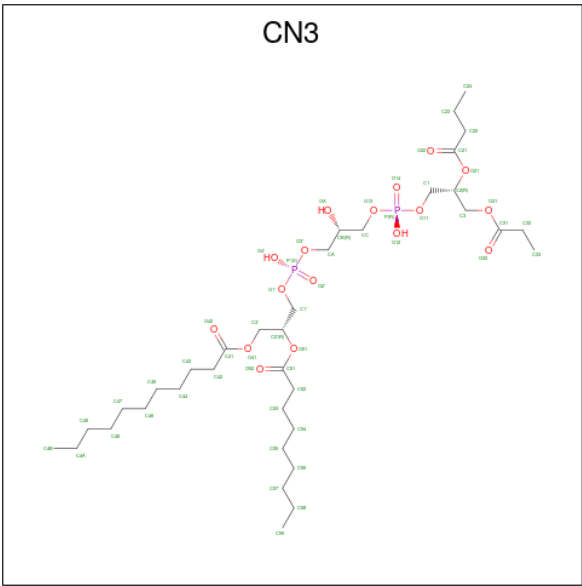
Mol	Chain	Residues	Atoms		AltConf
35	a	1	Total	Cu	0
			1	1	
35	m	1	Total	Cu	0
			1	1	

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
36	a	1	Total	Ca	0
			1	1	
36	m	1	Total	Ca	0
			1	1	

- Molecule 37 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphonadec-1-yl undecanoate

(CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).

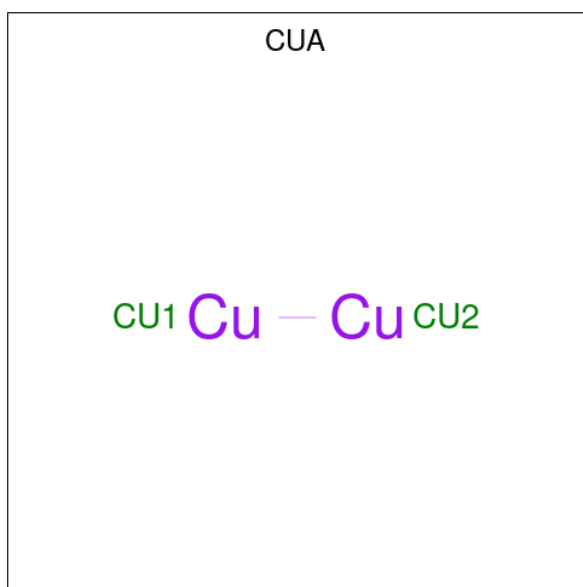


Mol	Chain	Residues	Atoms				AltConf
37	a	1	Total	C	O	P	0
			46	27	17	2	
37	m	1	Total	C	O	P	0
			46	27	17	2	

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	b	1	Total	Mg	0
			1	1	
38	n	1	Total	Mg	0
			1	1	

- Molecule 39 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
39	b	1	Total 2	Cu 2	0
39	n	1	Total 2	Cu 2	0

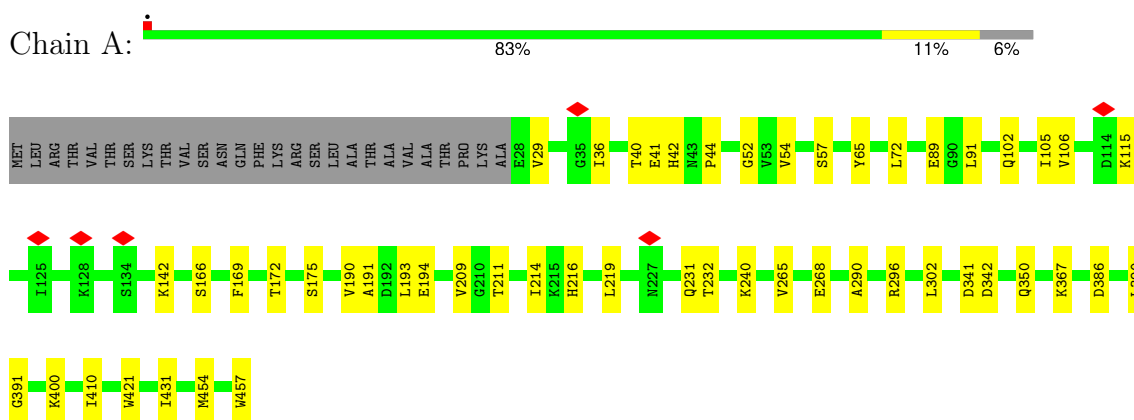
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	d	1	Total 1	Zn 1	0
40	p	1	Total 1	Zn 1	0

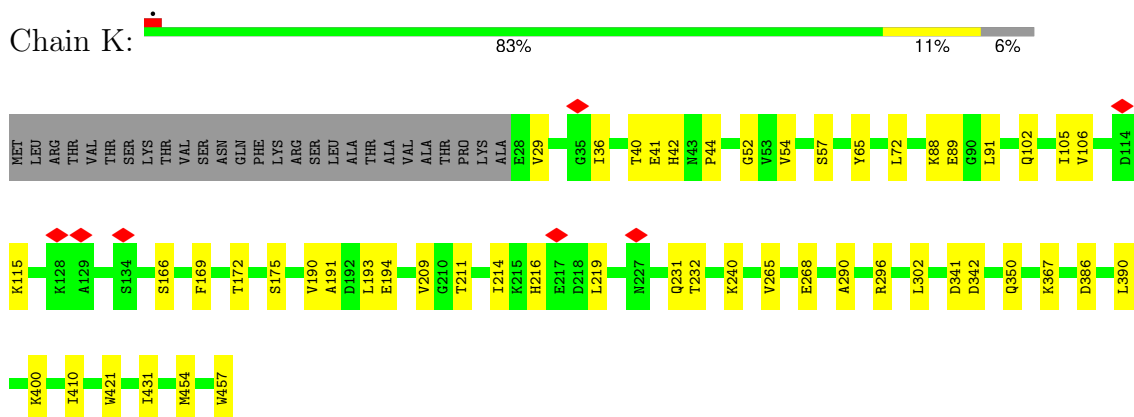
3 Residue-property plots

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.

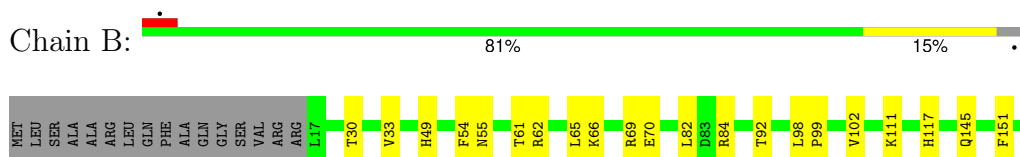
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

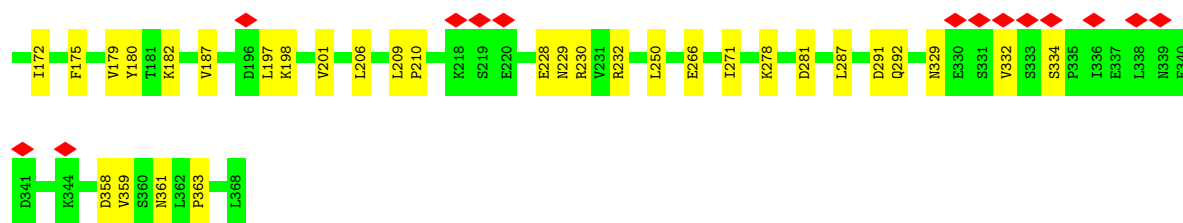


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



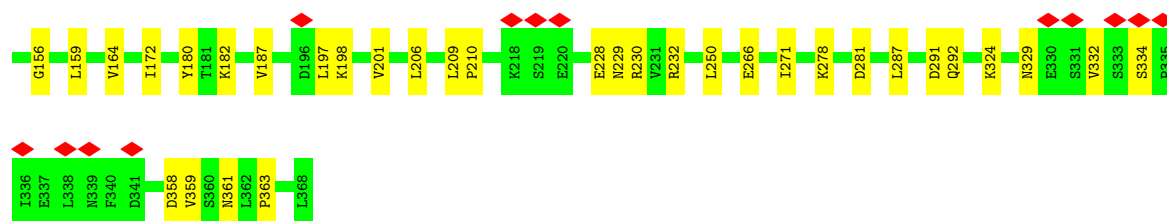
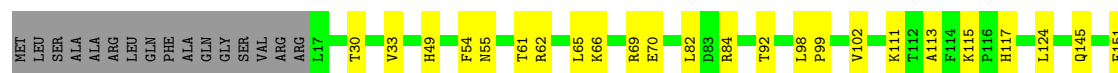
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





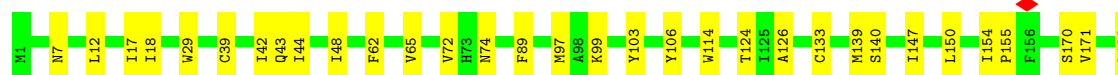
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain L: 80% 15%



- Molecule 3: Cytochrome b

Chain C: 82% 17%

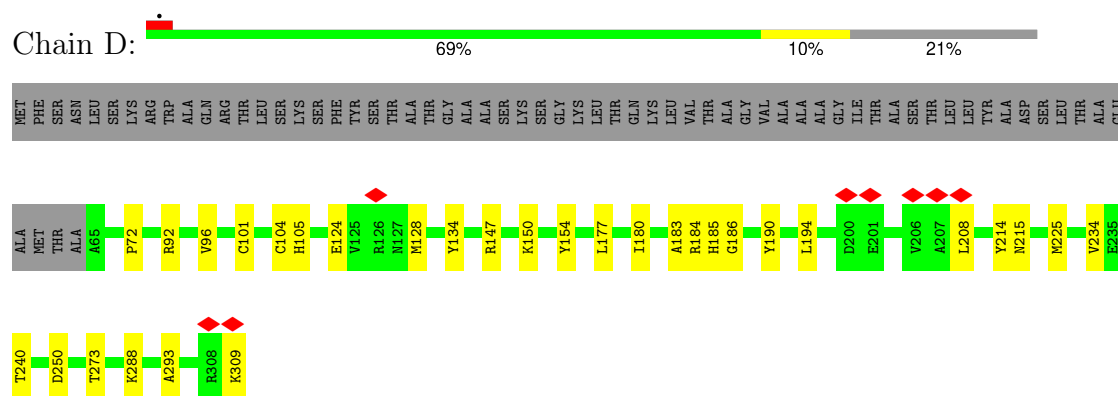


- Molecule 3: Cytochrome b

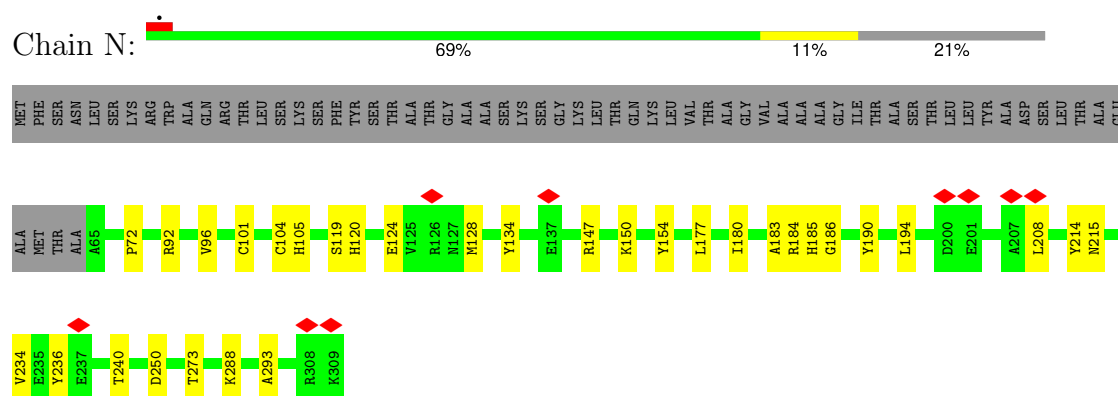
Chain M: 81% 18%



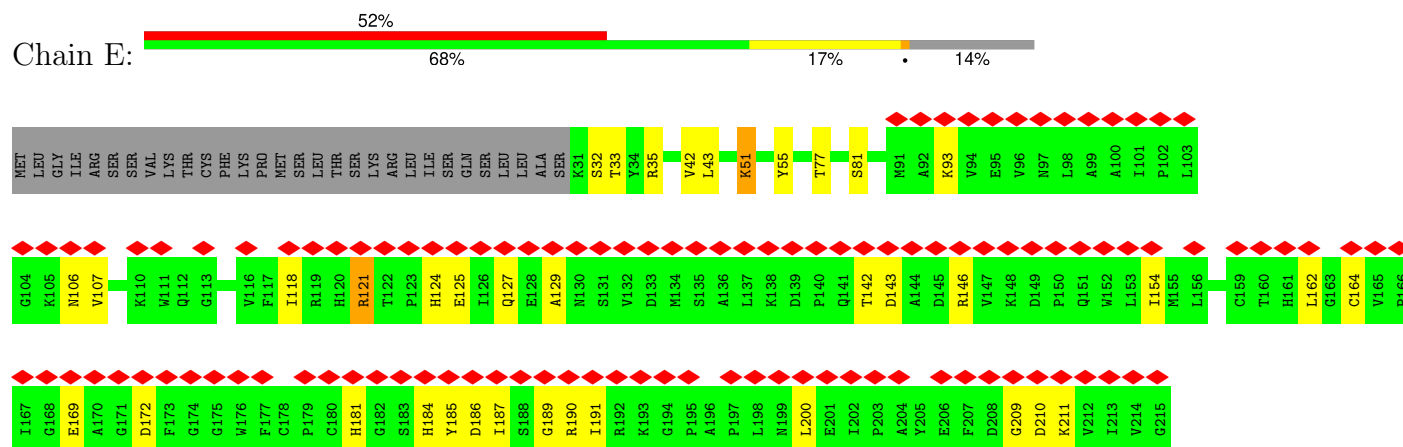
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



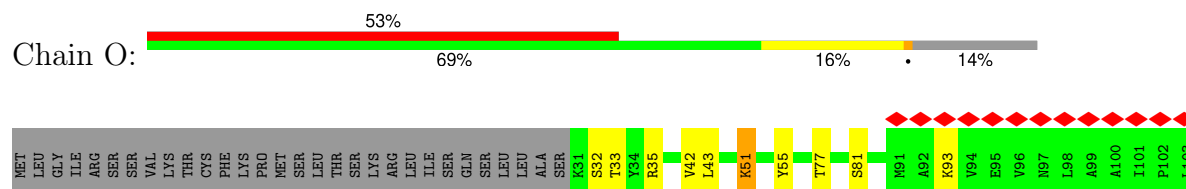
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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

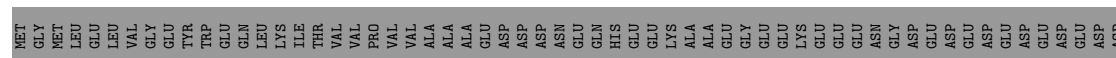
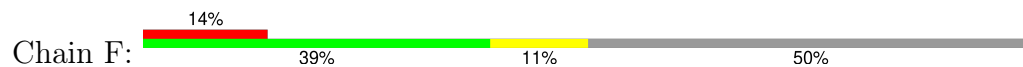


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

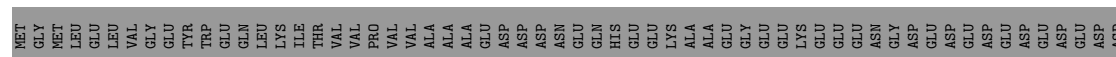
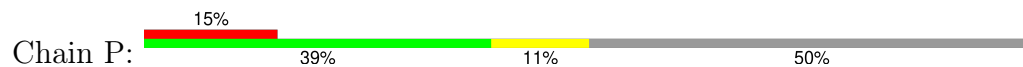




• Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



• Molecule 6: Cytochrome b-c1 complex subunit 6, mitochondrial



• Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial, Cytochrome c oxidase subunit 8, mitochondrial



• Molecule 7: Cytochrome b-c1 complex subunit 7, mitochondrial, Cytochrome c oxidase subunit 8, mitochondrial



VAL
LYS
GLY
ARG
LYS
THR
PRO
TYR
ALA
LEU
SER
HIS
PHE
GLY
PHE
PHE
PHE
ALA
ILE
GLY
PHE
ALA
VAL
PRO
PHE
VAL
VAL
ALA
CYS
TYR
VAL
GLN
LEU
LYS
LYS
SER
GLY
ALA
PHE

- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain H: 10% 81% 17%

MET G2 K7 W12 W13 Y27 A28 V29 S30 P31 Q34 F41 M47 L60 I61 P62 A63 G64 N77 E78 S82 K83 A84 G85 E88 L89 E90 R91 V92 N93 VAL

- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain R: 9% 81% 17%

MET G2 W12 W13 Y27 A28 V29 S30 P31 Q34 F41 H42 N43 L60 I61 P62 A63 G64 N77 E78 S82 K83 A84 G85 R86 E87 E88 L89 E90 R91 V92 N93 VAL

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

Chain I: 67% 14% 20%

MET SER PHE SER S5 L6 Y7 F11 K12 R13 V16 F17 I21 Q29 I36 W39 R55 I56 A57 ALA GLY ASP GLY ASP ASP ASP ASP ASP GLU

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

Chain S: 67% 14% 20%

MET SER PHE SER S5 L6 Y7 F11 K12 R13 V16 F17 I21 Q29 I36 W39 A57 ALA GLY ASP ASP ASP ASP ASP ASP GLU

- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain J: 14% 48% 9% 42%

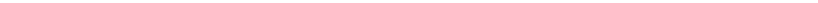
MET ALA TYR THR SER HIS LEU SER SER LYS T11 G12 L13 H14 F15 G16 R17 L20 R21 N29 V43 G47 W48 P49 K50 F51 Q52 D53 T54 L55 TYR LYS LYS ILE PRO PRO LEU LEU LEU GLY PRO THR LEU GLU ASP HIS THR PRO PRO PRO GLU ASP LYS PRO ASN

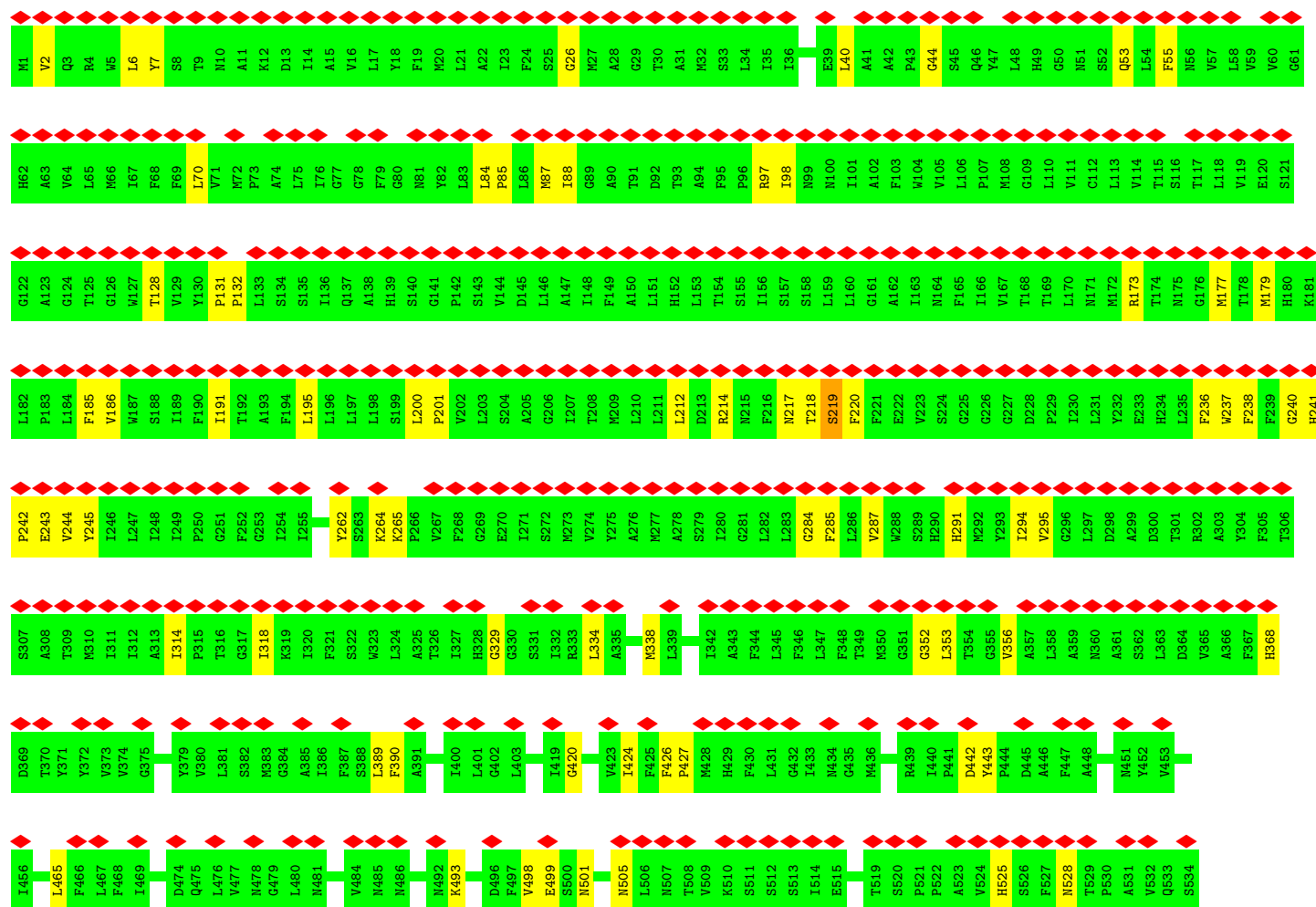
- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain T: 13% 48% 9% 42%

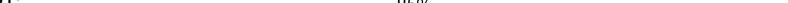
MET ALA TYR THR SER HIS LEU SER SER LYS T11 G12 L13 H14 F15 G16 R17 L20 R21 N29 V43 G47 W48 P49 K50 F51 Q52 D53 T54 L55 TYR LYS LYS ILE PRO PRO LEU LEU LEU GLY PRO THR LEU GLU ASP HIS THR PRO PRO PRO GLU ASP LYS PRO ASN

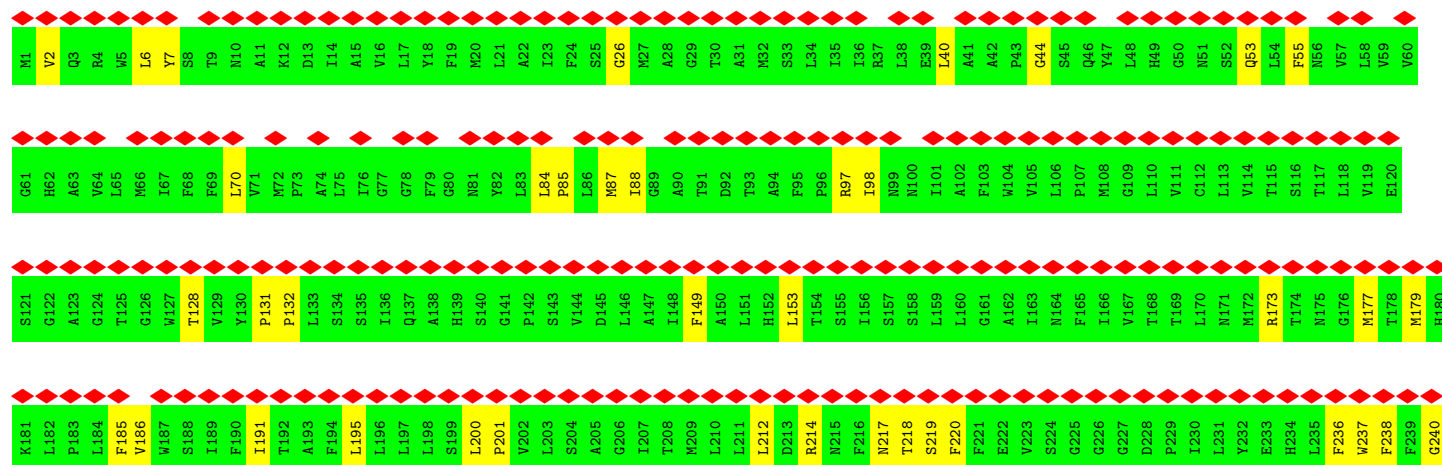
- Molecule 11: Cytochrome c oxidase subunit 1

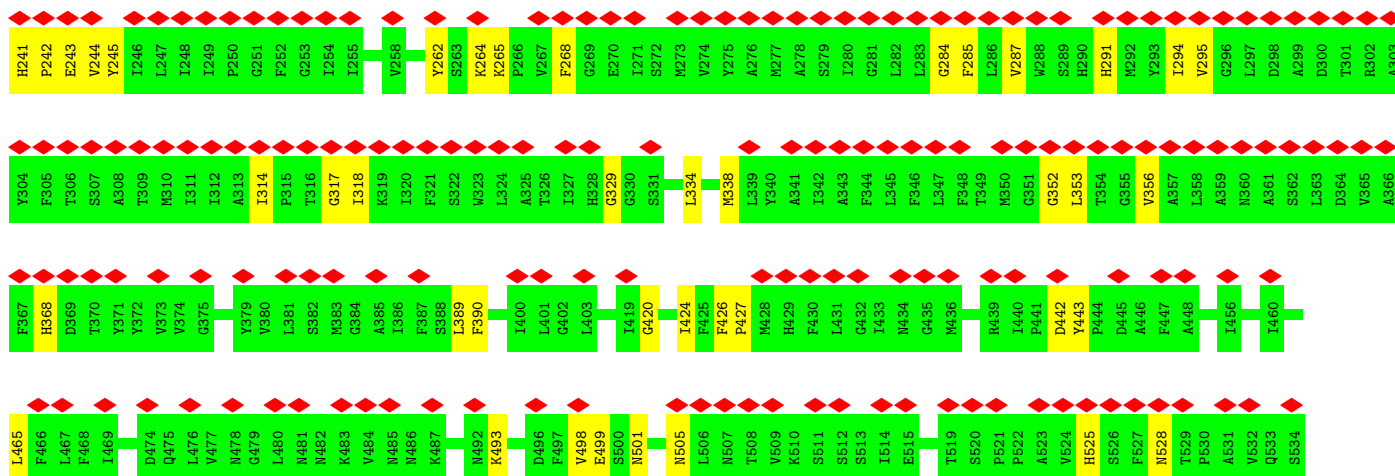
Chain a:  76% 86% 14%



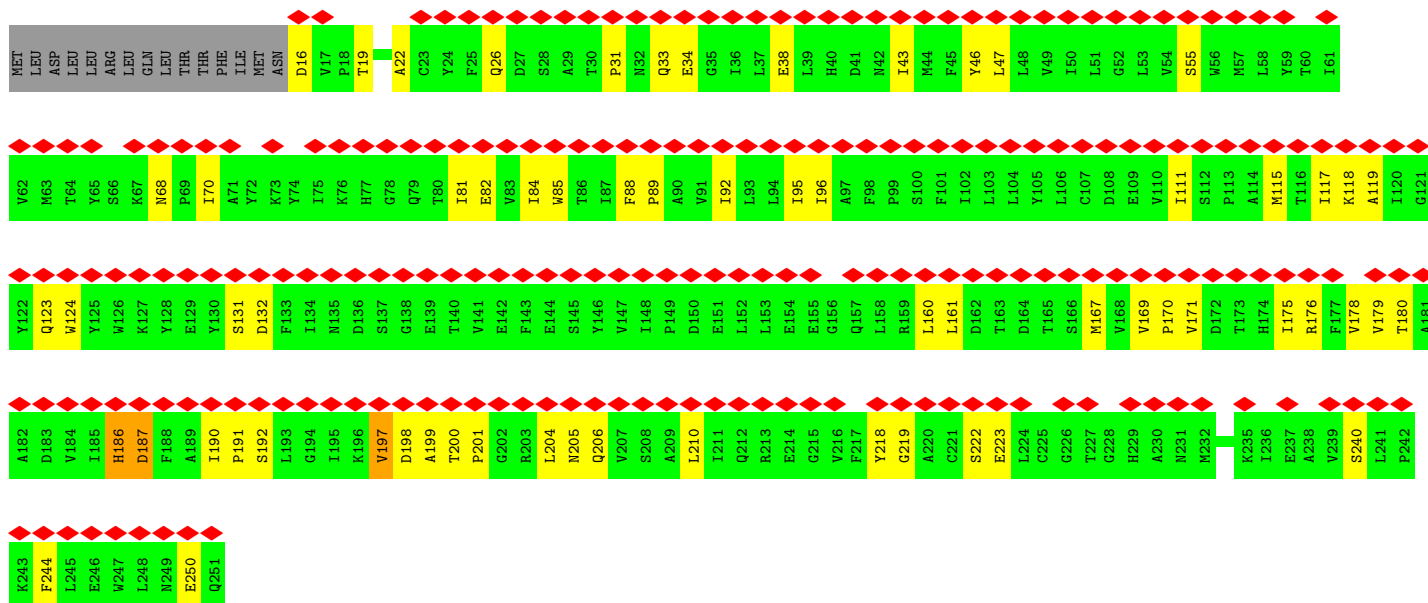
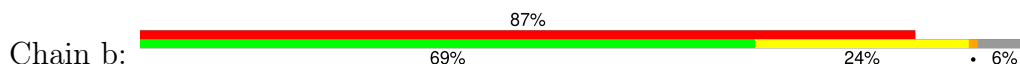
- Molecule 11: Cytochrome c oxidase subunit 1

Chain m:  74% 85% 15%

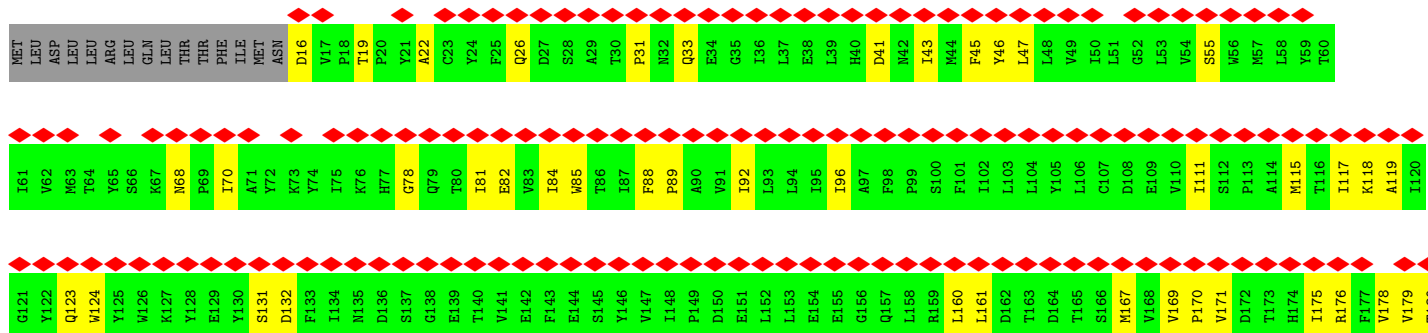
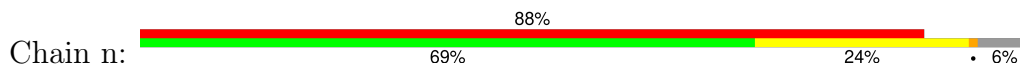


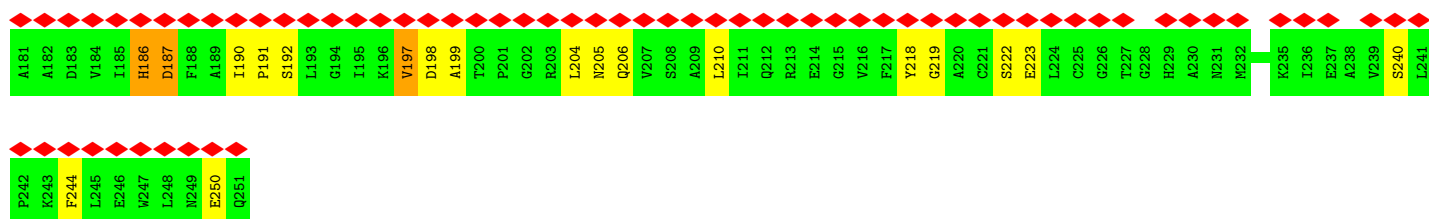


• Molecule 12: Cytochrome c oxidase subunit 2

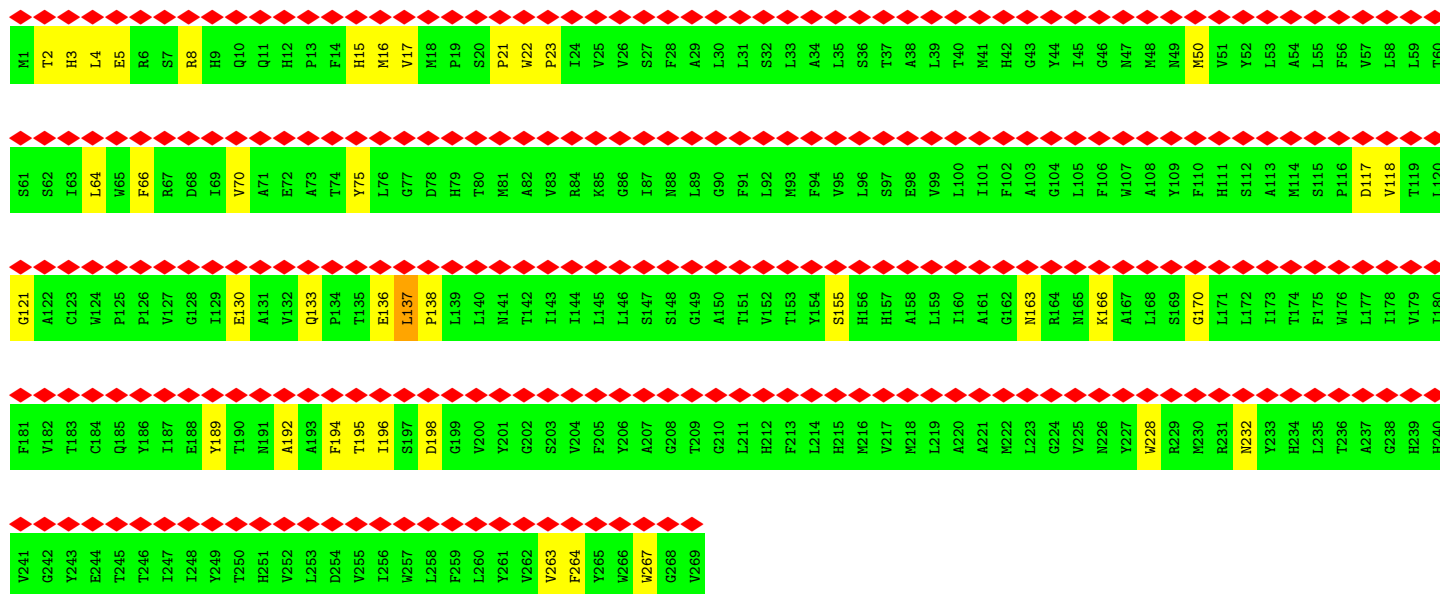
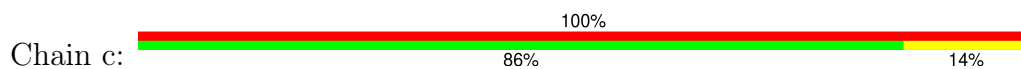


• Molecule 12: Cytochrome c oxidase subunit 2

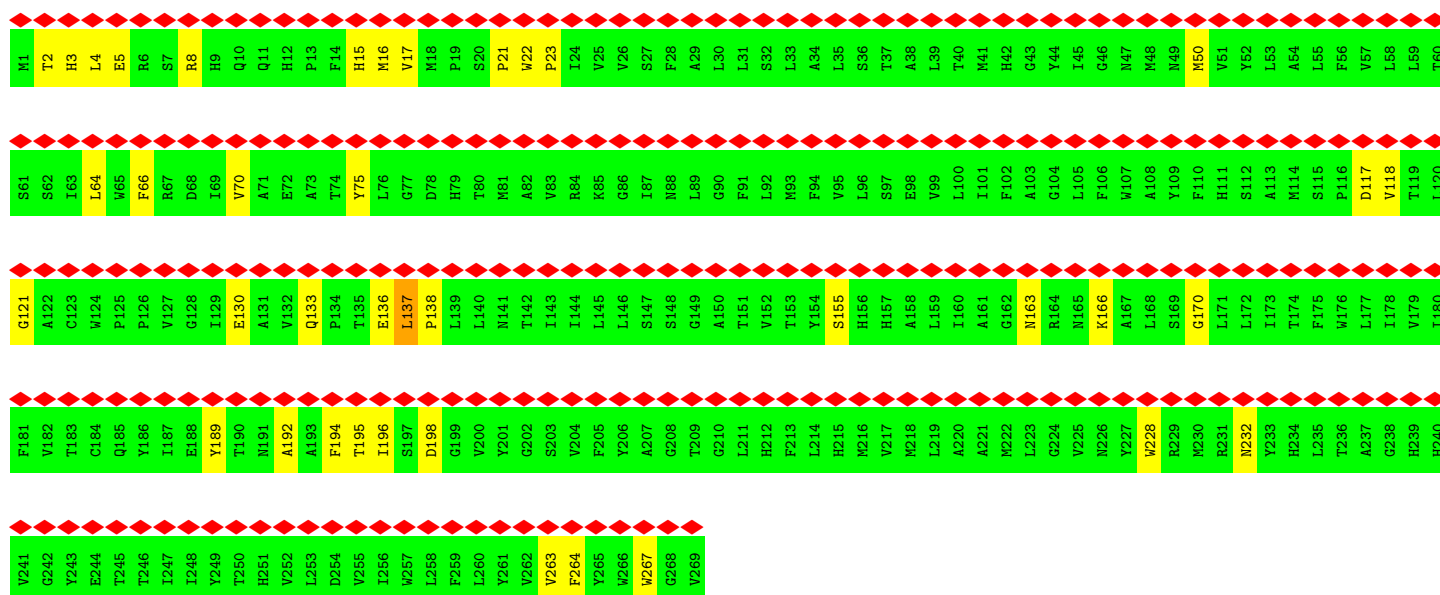
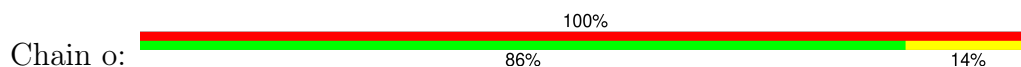




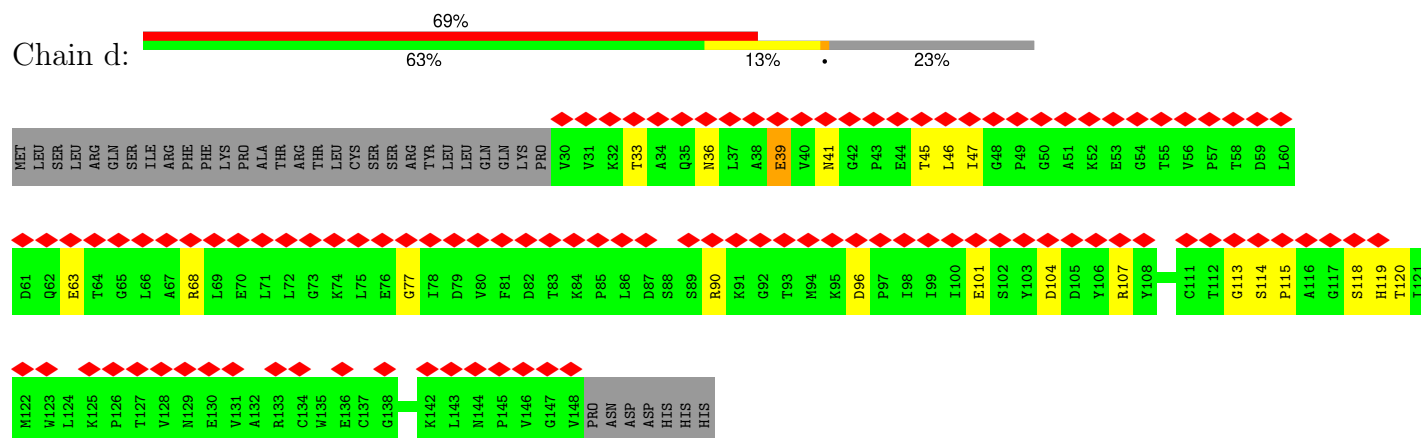
• Molecule 13: Cytochrome c oxidase subunit 3



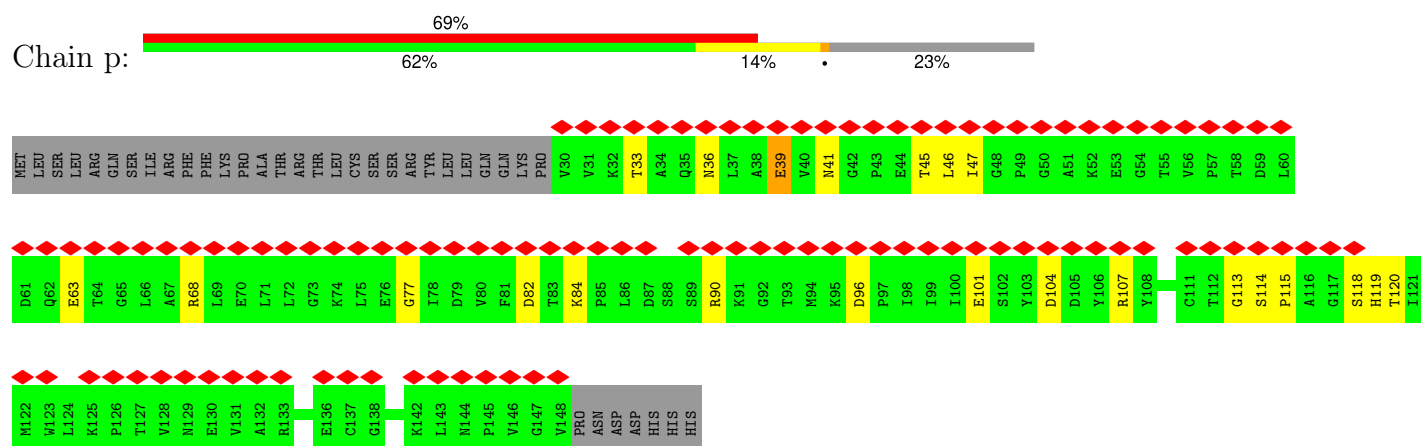
• Molecule 13: Cytochrome c oxidase subunit 3



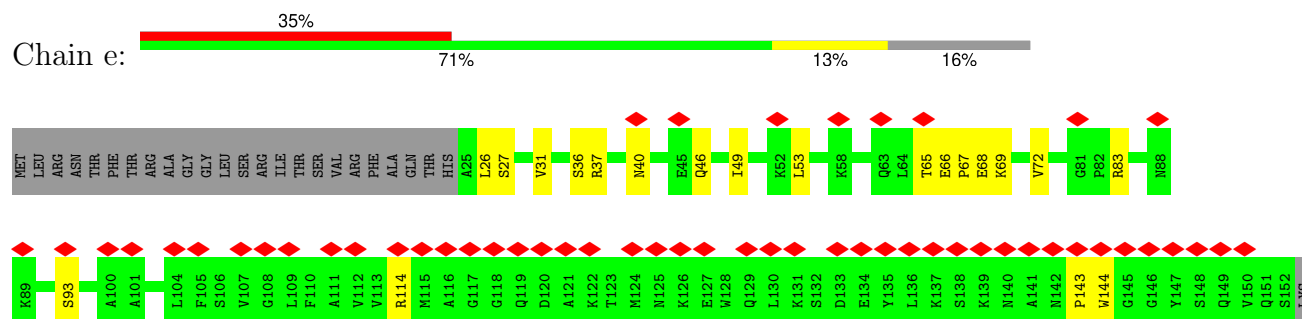
- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial



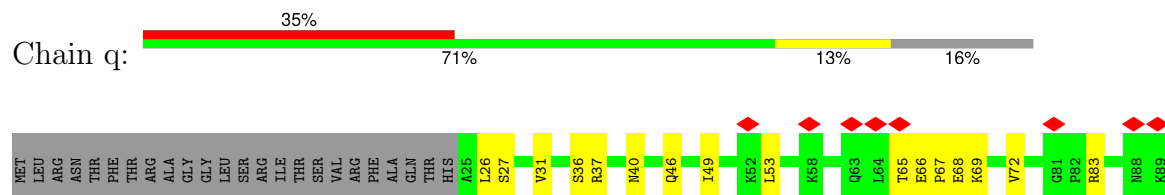
- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

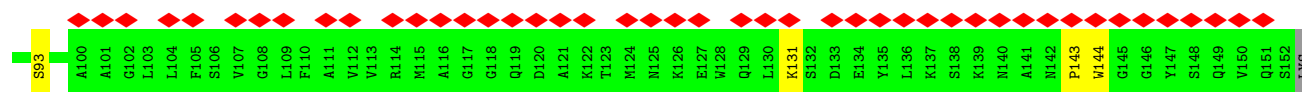


- Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial

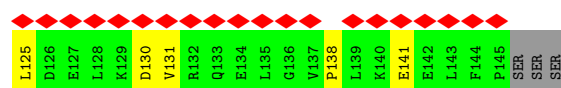
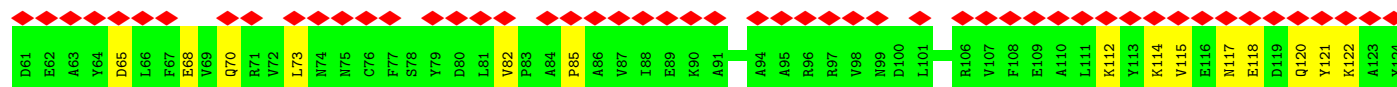
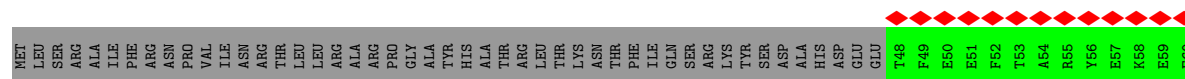


- Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial

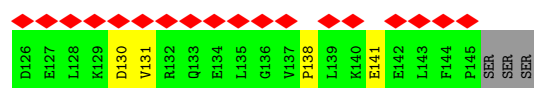
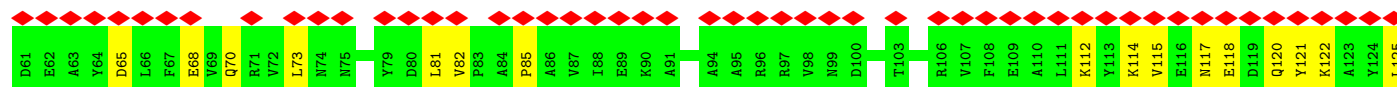
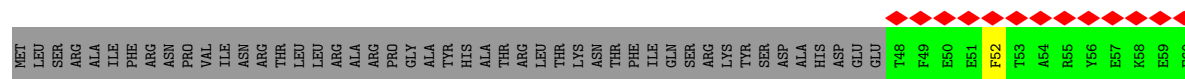




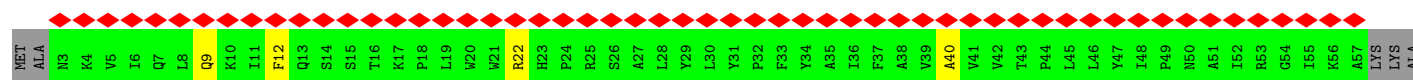
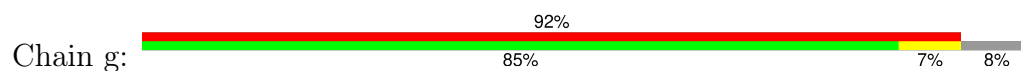
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



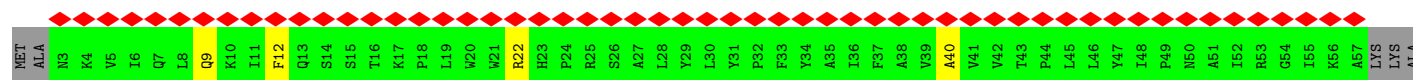
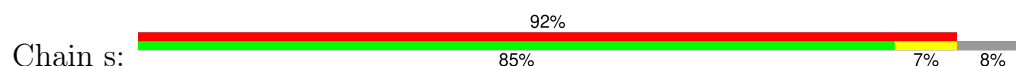
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



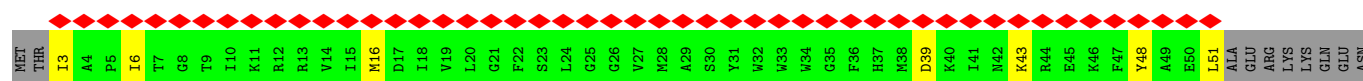
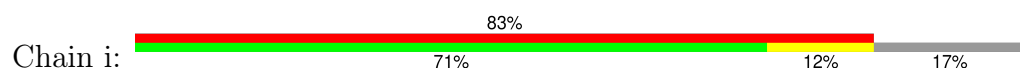
- Molecule 17: Cytochrome c oxidase subunit 7, mitochondrial



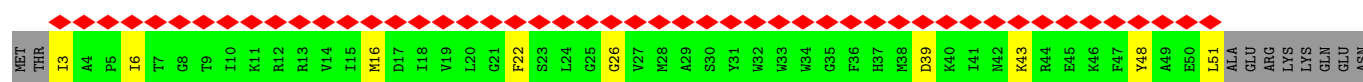
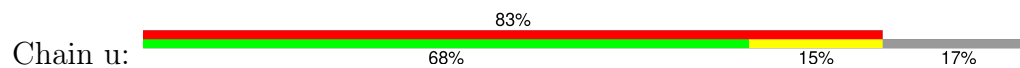
- Molecule 17: Cytochrome c oxidase subunit 7, mitochondrial



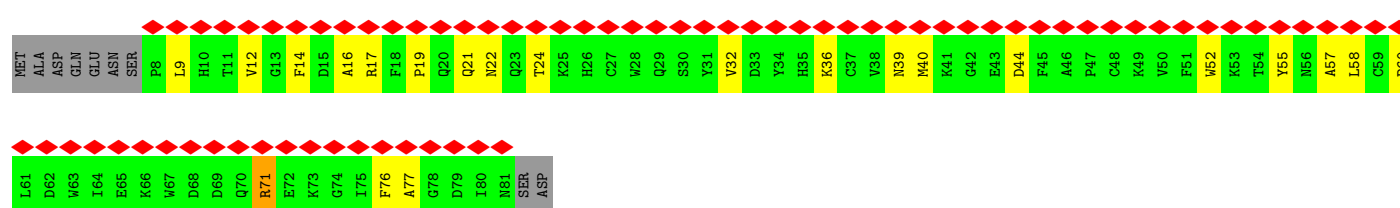
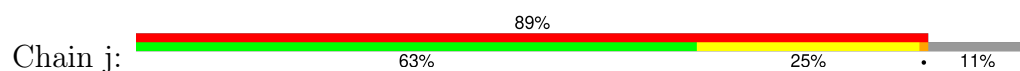
- Molecule 18: Cytochrome c oxidase subunit 9, mitochondrial



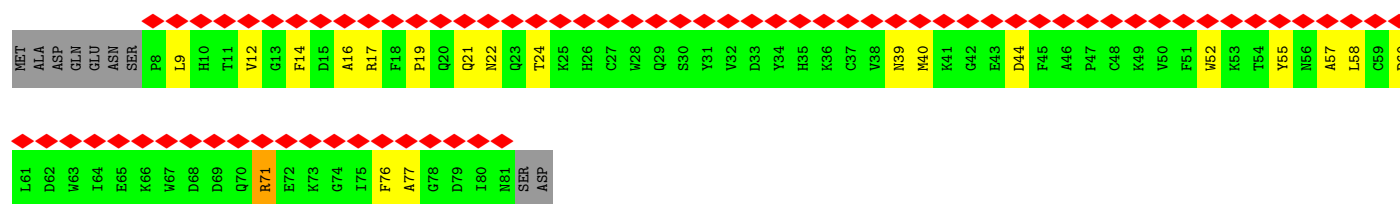
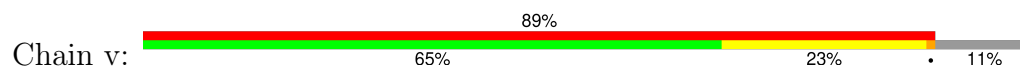
- Molecule 18: Cytochrome c oxidase subunit 9, mitochondrial



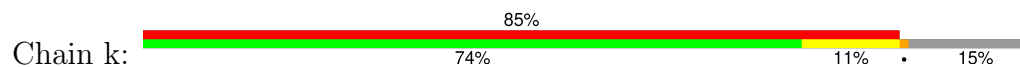
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



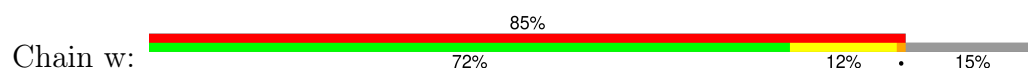
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



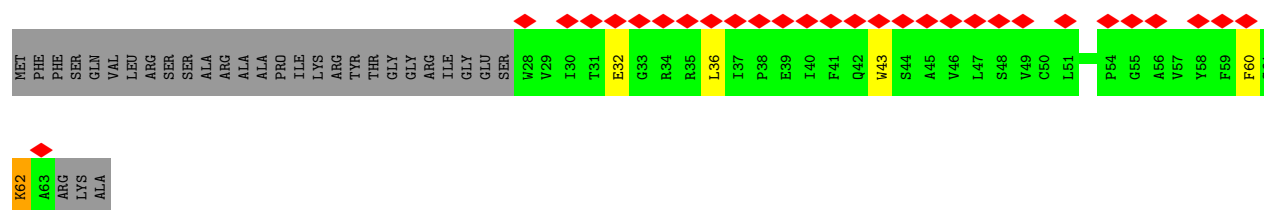
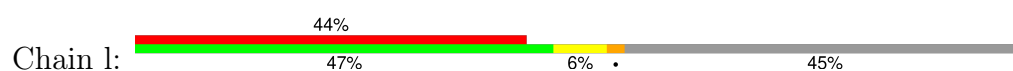
- Molecule 20: Cytochrome c oxidase subunit 13, mitochondrial



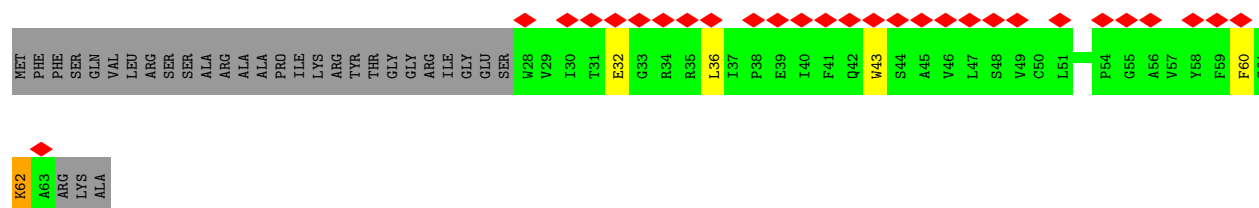
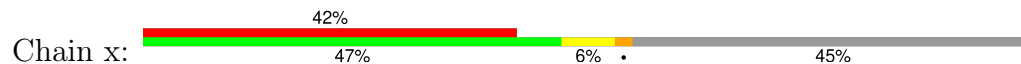
- Molecule 20: Cytochrome c oxidase subunit 13, mitochondrial



- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	47746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.452	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.231	Depositor
Minimum map value	-2.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	508.05, 508.05, 508.05	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.129, 1.129, 1.129	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, HEC, CUA, 6PH, UQ6, PTY, CA, CU, MG, 9PE, CN5, 8PE, ZN, PEF, CDL, HEA, CN3, HEM, PCF

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	0.22	0/3400	0.43	0/4608
1	K	0.22	0/3400	0.43	0/4608
2	B	0.17	0/2781	0.39	0/3764
2	L	0.17	0/2781	0.39	0/3764
3	C	0.32	0/3173	0.57	1/4330 (0.0%)
3	M	0.32	0/3173	0.57	1/4330 (0.0%)
4	D	0.27	0/2002	0.49	0/2724
4	N	0.27	0/2002	0.49	0/2724
5	E	0.58	0/1444	0.92	3/1957 (0.2%)
5	O	0.58	0/1444	0.92	3/1957 (0.2%)
6	F	0.13	0/638	0.36	0/858
6	P	0.13	0/638	0.36	0/858
7	G	0.34	0/1029	0.64	0/1396
7	Q	0.34	0/1029	0.64	0/1396
8	H	0.19	0/795	0.44	0/1076
8	R	0.19	0/795	0.44	0/1076
9	I	0.15	0/449	0.33	0/605
9	S	0.15	0/449	0.33	0/605
10	J	0.24	0/363	0.50	0/491
10	T	0.24	0/363	0.50	0/491
11	a	0.26	0/4289	0.46	1/5857 (0.0%)
11	m	0.26	0/4289	0.46	1/5857 (0.0%)
12	b	0.41	0/1940	0.59	0/2653
12	n	0.41	0/1940	0.59	0/2653
13	c	0.24	0/2218	0.40	0/3036
13	o	0.24	0/2218	0.40	0/3036
14	d	0.28	0/915	0.56	1/1244 (0.1%)
14	p	0.28	0/915	0.56	1/1244 (0.1%)
15	e	0.29	0/1032	0.50	1/1396 (0.1%)
15	q	0.29	0/1032	0.50	1/1396 (0.1%)
16	f	0.12	0/836	0.30	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	r	0.12	0/836	0.30	0/1131
17	g	0.13	0/472	0.29	0/645
17	s	0.13	0/472	0.29	0/645
18	i	0.17	0/416	0.32	0/559
18	u	0.17	0/416	0.32	0/559
19	j	0.33	0/643	0.54	0/871
19	v	0.33	0/643	0.54	0/871
20	k	0.29	0/944	0.58	0/1282
20	w	0.29	0/944	0.58	0/1282
21	l	0.44	0/304	0.90	1/415 (0.2%)
21	x	0.44	0/304	0.90	1/415 (0.2%)
All	All	0.29	0/60166	0.52	16/81796 (0.0%)

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
11	a	0	1
11	m	0	1
19	j	0	1
19	v	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	l	62	LYS	N-CA-C	-10.84	99.47	111.28
21	x	62	LYS	N-CA-C	-10.84	99.47	111.28
14	d	39	GLU	N-CA-C	-6.21	105.35	113.17
14	p	39	GLU	N-CA-C	-6.21	105.35	113.17
3	C	312	VAL	N-CA-C	-6.16	106.50	112.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	a	214	ARG	Sidechain
19	j	71	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
11	m	214	ARG	Sidechain
19	v	71	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	3339	0	3318	32	0
1	K	3339	0	3318	32	0
2	B	2735	0	2774	42	0
2	L	2735	0	2774	45	0
3	C	3071	0	3106	62	0
3	M	3071	0	3106	60	0
4	D	1941	0	1869	35	0
4	N	1941	0	1869	34	0
5	E	1411	0	1388	31	0
5	O	1411	0	1388	30	0
6	F	624	0	581	11	0
6	P	624	0	581	11	0
7	G	1008	0	1018	24	0
7	Q	1008	0	1018	23	0
8	H	764	0	725	12	0
8	R	764	0	725	12	0
9	I	436	0	431	6	0
9	S	436	0	431	6	0
10	J	352	0	346	7	0
10	T	352	0	346	7	0
11	a	4161	0	4192	71	0
11	m	4161	0	4192	72	0
12	b	1888	0	1866	58	0
12	n	1888	0	1866	56	0
13	c	2146	0	2137	37	0
13	o	2146	0	2137	37	0
14	d	898	0	891	13	0
14	p	898	0	891	14	0
15	e	1008	0	990	15	0
15	q	1008	0	990	15	0
16	f	819	0	801	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	r	819	0	801	13	0
17	g	456	0	481	3	0
17	s	456	0	481	3	0
18	i	404	0	408	5	0
18	u	404	0	408	6	0
19	j	621	0	573	18	0
19	v	621	0	573	17	0
20	k	911	0	876	16	0
20	w	911	0	876	17	0
21	l	293	0	291	5	0
21	x	293	0	291	5	0
22	A	55	0	54	2	0
22	D	60	0	64	5	0
22	E	42	0	35	6	0
22	H	53	0	50	3	0
22	K	55	0	54	2	0
22	N	60	0	64	3	0
22	O	42	0	35	6	0
22	R	53	0	50	1	0
23	C	40	0	59	2	0
23	M	40	0	59	2	0
24	C	26	0	25	0	0
24	M	26	0	25	0	0
25	C	32	0	29	0	0
26	C	69	30	89	12	0
26	M	69	30	89	12	0
27	C	86	60	60	9	0
27	M	86	60	60	9	0
28	C	33	0	42	1	0
28	M	33	0	42	1	0
29	D	40	0	53	4	0
29	J	29	0	31	1	0
29	N	40	0	53	3	0
29	T	29	0	31	1	0
29	a	43	0	62	2	0
29	m	43	0	62	1	0
30	D	43	32	32	16	0
30	N	43	32	32	16	0
31	E	4	0	0	4	0
31	O	4	0	0	4	0
32	H	32	0	38	3	0
32	I	32	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R	32	0	38	3	0
32	S	32	0	38	0	0
32	k	43	0	60	12	0
32	l	37	0	48	2	0
32	w	43	0	60	12	0
32	x	37	0	48	1	0
33	I	32	0	37	2	0
33	S	32	0	37	2	0
33	a	32	0	37	9	0
33	b	69	0	84	4	0
33	c	40	0	53	1	0
33	m	32	0	37	9	0
33	n	69	0	84	4	0
33	o	40	0	53	1	0
34	a	120	108	108	9	0
34	m	120	108	108	10	0
35	a	1	0	0	0	0
35	m	1	0	0	0	0
36	a	1	0	0	0	0
36	m	1	0	0	0	0
37	a	46	0	42	0	0
37	m	46	0	42	0	0
38	b	1	0	0	0	0
38	n	1	0	0	0	0
39	b	2	0	0	0	0
39	n	2	0	0	0	0
40	d	1	0	0	0	0
40	p	1	0	0	0	0
All	All	60828	460	60555	939	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 8.

The worst 5 of 939 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)
12:b:16:ASP:N	12:b:192:SER:HG	1.53	1.04
12:n:16:ASP:N	12:n:192:SER:HG	1.55	1.03
11:a:353:LEU:HD12	12:b:47:LEU:HD22	1.51	0.93
11:m:353:LEU:HD12	12:n:47:LEU:HD22	1.51	0.93
4:N:104:CYS:SG	30:N:402:HEC:HAC	2.09	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	428/457 (94%)	417 (97%)	11 (3%)	0	100	100
1	K	428/457 (94%)	417 (97%)	11 (3%)	0	100	100
2	B	350/368 (95%)	344 (98%)	6 (2%)	0	100	100
2	L	350/368 (95%)	344 (98%)	6 (2%)	0	100	100
3	C	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
3	M	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
4	D	243/309 (79%)	234 (96%)	9 (4%)	0	100	100
4	N	243/309 (79%)	234 (96%)	9 (4%)	0	100	100
5	E	183/215 (85%)	178 (97%)	5 (3%)	0	100	100
5	O	183/215 (85%)	178 (97%)	5 (3%)	0	100	100
6	F	72/147 (49%)	69 (96%)	3 (4%)	0	100	100
6	P	72/147 (49%)	69 (96%)	3 (4%)	0	100	100
7	G	123/183 (67%)	117 (95%)	6 (5%)	0	100	100
7	Q	123/183 (67%)	117 (95%)	6 (5%)	0	100	100
8	H	90/94 (96%)	83 (92%)	7 (8%)	0	100	100
8	R	90/94 (96%)	83 (92%)	7 (8%)	0	100	100
9	I	51/66 (77%)	50 (98%)	1 (2%)	0	100	100
9	S	51/66 (77%)	50 (98%)	1 (2%)	0	100	100
10	J	43/77 (56%)	41 (95%)	2 (5%)	0	100	100
10	T	43/77 (56%)	41 (95%)	2 (5%)	0	100	100
11	a	532/534 (100%)	506 (95%)	25 (5%)	1 (0%)	44	64
11	m	532/534 (100%)	506 (95%)	25 (5%)	1 (0%)	44	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	b	234/251 (93%)	221 (94%)	13 (6%)	0	100	100
12	n	234/251 (93%)	221 (94%)	13 (6%)	0	100	100
13	c	267/269 (99%)	261 (98%)	5 (2%)	1 (0%)	30	50
13	o	267/269 (99%)	261 (98%)	5 (2%)	1 (0%)	30	50
14	d	117/155 (76%)	108 (92%)	9 (8%)	0	100	100
14	p	117/155 (76%)	108 (92%)	9 (8%)	0	100	100
15	e	126/153 (82%)	120 (95%)	6 (5%)	0	100	100
15	q	126/153 (82%)	120 (95%)	6 (5%)	0	100	100
16	f	96/148 (65%)	95 (99%)	1 (1%)	0	100	100
16	r	96/148 (65%)	95 (99%)	1 (1%)	0	100	100
17	g	53/60 (88%)	53 (100%)	0	0	100	100
17	s	53/60 (88%)	53 (100%)	0	0	100	100
18	i	47/59 (80%)	44 (94%)	3 (6%)	0	100	100
18	u	47/59 (80%)	44 (94%)	3 (6%)	0	100	100
19	j	72/83 (87%)	68 (94%)	4 (6%)	0	100	100
19	v	72/83 (87%)	68 (94%)	4 (6%)	0	100	100
20	k	108/129 (84%)	98 (91%)	10 (9%)	0	100	100
20	w	108/129 (84%)	98 (91%)	10 (9%)	0	100	100
21	l	34/66 (52%)	32 (94%)	2 (6%)	0	100	100
21	x	34/66 (52%)	32 (94%)	2 (6%)	0	100	100
All	All	7300/8416 (87%)	7024 (96%)	272 (4%)	4 (0%)	50	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	c	137	LEU
13	o	137	LEU
11	a	219	SER
11	m	219	SER

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	370/393 (94%)	370 (100%)	0	100	100
1	K	370/393 (94%)	370 (100%)	0	100	100
2	B	301/313 (96%)	301 (100%)	0	100	100
2	L	301/313 (96%)	301 (100%)	0	100	100
3	C	335/338 (99%)	335 (100%)	0	100	100
3	M	336/338 (99%)	336 (100%)	0	100	100
4	D	204/251 (81%)	204 (100%)	0	100	100
4	N	204/251 (81%)	204 (100%)	0	100	100
5	E	151/179 (84%)	150 (99%)	1 (1%)	81	92
5	O	151/179 (84%)	150 (99%)	1 (1%)	81	92
6	F	67/131 (51%)	67 (100%)	0	100	100
6	P	67/131 (51%)	67 (100%)	0	100	100
7	G	108/153 (71%)	107 (99%)	1 (1%)	75	89
7	Q	108/153 (71%)	107 (99%)	1 (1%)	75	89
8	H	76/78 (97%)	76 (100%)	0	100	100
8	R	76/78 (97%)	76 (100%)	0	100	100
9	I	44/54 (82%)	44 (100%)	0	100	100
9	S	44/54 (82%)	44 (100%)	0	100	100
10	J	36/66 (54%)	35 (97%)	1 (3%)	38	63
10	T	35/66 (53%)	34 (97%)	1 (3%)	37	62
11	a	447/447 (100%)	447 (100%)	0	100	100
11	m	447/447 (100%)	447 (100%)	0	100	100
12	b	209/224 (93%)	205 (98%)	4 (2%)	52	74
12	n	209/224 (93%)	205 (98%)	4 (2%)	52	74
13	c	228/228 (100%)	228 (100%)	0	100	100
13	o	228/228 (100%)	228 (100%)	0	100	100
14	d	100/135 (74%)	100 (100%)	0	100	100
14	p	100/135 (74%)	100 (100%)	0	100	100
15	e	106/127 (84%)	106 (100%)	0	100	100
15	q	106/127 (84%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	f	87/131 (66%)	87 (100%)	0	100	100
16	r	87/131 (66%)	87 (100%)	0	100	100
17	g	48/51 (94%)	48 (100%)	0	100	100
17	s	48/51 (94%)	48 (100%)	0	100	100
18	i	41/50 (82%)	41 (100%)	0	100	100
18	u	41/50 (82%)	41 (100%)	0	100	100
19	j	66/74 (89%)	66 (100%)	0	100	100
19	v	66/74 (89%)	66 (100%)	0	100	100
20	k	97/113 (86%)	96 (99%)	1 (1%)	73	87
20	w	97/113 (86%)	96 (99%)	1 (1%)	73	87
21	l	30/53 (57%)	29 (97%)	1 (3%)	33	57
21	x	30/53 (57%)	29 (97%)	1 (3%)	33	57
All	All	6302/7178 (88%)	6284 (100%)	18 (0%)	90	97

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	n	190	ILE
21	x	62	LYS
20	w	19	LYS
21	l	62	LYS
12	n	187	ASP

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

Mol	Chain	Res	Type
4	N	122	ASN
12	n	205	ASN
5	O	151	GLN
8	R	43	ASN
13	o	226	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 8 are monoatomic - leaving 59 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	$\# Z > 2$
22	CDL	O	302	-	41,41,99	0.37	0	46,51,111	0.50	0
39	CUA	n	303	12	0,1,1	-	-	-		
33	PTY	b	304	-	34,34,49	0.33	0	37,39,54	0.39	0
22	CDL	D	403	-	59,59,99	0.36	0	65,71,111	0.47	0
33	PTY	a	604	-	31,31,49	0.39	0	34,36,54	0.49	0
22	CDL	H	101	-	52,52,99	0.37	0	58,64,111	0.47	0
27	HEM	C	407	3	42,50,50	1.35	6 (14%)	46,82,82	1.84	12 (26%)
33	PTY	o	301	-	39,39,49	0.34	0	42,44,54	0.39	0
34	HEA	a	603	-	58,67,67	2.12	18 (31%)	63,103,103	2.42	26 (41%)
29	PEF	a	607	-	42,42,46	0.31	0	45,47,51	0.34	0
33	PTY	b	302	-	33,33,49	0.36	0	36,38,54	0.52	0
22	CDL	K	501	-	54,54,99	0.37	0	60,66,111	0.49	0
30	HEC	D	402	4	32,50,50	1.94	5 (15%)	30,82,82	2.91	11 (36%)
23	6PH	M	401	-	39,39,39	0.38	0	42,44,44	0.29	0
27	HEM	C	405	3	42,50,50	1.41	7 (16%)	46,82,82	1.71	11 (23%)
22	CDL	R	101	-	52,52,99	0.37	0	58,64,111	0.47	0
33	PTY	n	302	-	33,33,49	0.36	0	36,38,54	0.52	0
33	PTY	c	301	-	39,39,49	0.34	0	42,44,54	0.39	0
22	CDL	E	302	-	41,41,99	0.37	0	46,51,111	0.50	0
32	PCF	I	102	-	31,31,49	0.39	0	37,39,57	0.37	0
26	UQ6	C	408	-	43,43,43	0.24	0	54,55,55	0.62	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PCF	x	101	-	36,36,49	0.36	0	42,44,57	0.42	0
34	HEA	m	601	11	58,67,67	2.22	20 (34%)	63,103,103	2.27	20 (31%)
26	UQ6	M	407	-	43,43,43	0.24	0	54,55,55	0.62	1 (1%)
27	HEM	M	406	3	42,50,50	1.35	6 (14%)	46,82,82	1.84	12 (26%)
32	PCF	S	102	-	31,31,49	0.39	0	37,39,57	0.37	0
34	HEA	m	603	-	58,67,67	2.12	18 (31%)	63,103,103	2.42	26 (41%)
33	PTY	S	101	-	31,31,49	0.36	0	34,36,54	0.37	0
25	CN5	C	403	-	31,31,40	0.36	0	35,39,48	0.44	0
29	PEF	D	401	-	39,39,46	0.34	0	42,44,51	0.37	0
27	HEM	M	404	3	42,50,50	1.41	7 (16%)	46,82,82	1.71	11 (23%)
30	HEC	N	402	4	32,50,50	1.94	5 (15%)	30,82,82	2.91	11 (36%)
31	FES	E	301	-	0,4,4	-	-	-	-	-
37	CN3	a	606	-	45,45,54	0.38	0	51,57,66	0.43	0
32	PCF	l	101	-	36,36,49	0.36	0	42,44,57	0.42	0
23	6PH	C	401	-	39,39,39	0.38	0	42,44,44	0.29	0
32	PCF	k	201	-	42,42,49	0.37	0	48,50,57	0.38	0
29	PEF	m	607	-	42,42,46	0.31	0	45,47,51	0.34	0
33	PTY	m	604	-	31,31,49	0.39	0	34,36,54	0.49	0
29	PEF	J	101	-	28,28,46	0.39	0	31,33,51	0.50	0
33	PTY	n	304	-	34,34,49	0.33	0	37,39,54	0.39	0
34	HEA	a	601	11	58,67,67	2.22	20 (34%)	63,103,103	2.27	20 (31%)
26	UQ6	C	404	-	26,26,43	0.37	0	33,34,55	0.64	0
37	CN3	m	606	-	45,45,54	0.38	0	51,57,66	0.43	0
29	PEF	T	101	-	28,28,46	0.39	0	31,33,51	0.50	0
28	9PE	M	405	-	32,32,39	0.36	0	35,37,44	0.42	0
22	CDL	A	501	-	54,54,99	0.37	0	60,66,111	0.49	0
24	8PE	M	402	-	25,25,46	0.40	0	28,30,51	0.51	0
32	PCF	w	201	-	42,42,49	0.37	0	48,50,57	0.38	0
28	9PE	C	406	-	32,32,39	0.36	0	35,37,44	0.42	0
33	PTY	I	101	-	31,31,49	0.36	0	34,36,54	0.37	0
32	PCF	H	102	-	31,31,49	0.37	0	37,39,57	0.37	0
22	CDL	N	403	-	59,59,99	0.36	0	65,71,111	0.47	0
31	FES	O	301	-	0,4,4	-	-	-	-	-
39	CUA	b	303	12	0,1,1	-	-	-	-	-
24	8PE	C	402	-	25,25,46	0.40	0	28,30,51	0.51	0
29	PEF	N	401	-	39,39,46	0.34	0	42,44,51	0.37	0
32	PCF	R	102	-	31,31,49	0.37	0	37,39,57	0.37	0
26	UQ6	M	403	-	26,26,43	0.37	0	33,34,55	0.64	0

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
22	CDL	O	302	-	-	16/49/49/110	-
33	PTY	b	304	-	-	12/38/38/53	-
22	CDL	D	403	-	-	25/70/70/110	-
33	PTY	a	604	-	-	11/35/35/53	-
22	CDL	H	101	-	-	13/63/63/110	-
27	HEM	C	407	3	-	5/12/54/54	-
33	PTY	o	301	-	-	10/43/43/53	-
34	HEA	a	603	-	-	8/32/76/76	-
29	PEF	a	607	-	-	12/46/46/50	-
33	PTY	b	302	-	-	7/37/37/53	-
22	CDL	K	501	-	-	10/64/64/110	-
30	HEC	D	402	4	-	1/10/54/54	-
23	6PH	M	401	-	-	26/41/41/41	-
27	HEM	C	405	3	-	0/12/54/54	-
22	CDL	R	101	-	-	13/63/63/110	-
33	PTY	n	302	-	-	7/37/37/53	-
33	PTY	c	301	-	-	10/43/43/53	-
22	CDL	E	302	-	-	16/49/49/110	-
32	PCF	I	102	-	-	4/35/35/53	-
26	UQ6	C	408	-	-	16/39/39/39	0/1/1/1
32	PCF	x	101	-	-	6/40/40/53	-
34	HEA	m	601	11	-	6/32/76/76	-
26	UQ6	M	407	-	-	16/39/39/39	0/1/1/1
27	HEM	M	406	3	-	5/12/54/54	-
32	PCF	S	102	-	-	4/35/35/53	-
34	HEA	m	603	-	-	8/32/76/76	-
33	PTY	S	101	-	-	6/35/35/53	-
25	CN5	C	403	-	-	7/35/35/44	-
29	PEF	D	401	-	-	12/43/43/50	-
27	HEM	M	404	3	-	0/12/54/54	-
30	HEC	N	402	4	-	1/10/54/54	-
37	CN3	a	606	-	-	10/56/56/65	-
31	FES	E	301	-	-	-	0/1/1/1
32	PCF	l	101	-	-	6/40/40/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	6PH	C	401	-	-	26/41/41/41	-
32	PCF	k	201	-	-	12/46/46/53	-
29	PEF	m	607	-	-	12/46/46/50	-
33	PTY	m	604	-	-	11/35/35/53	-
29	PEF	J	101	-	-	6/32/32/50	-
33	PTY	n	304	-	-	12/38/38/53	-
34	HEA	a	601	11	-	6/32/76/76	-
26	UQ6	C	404	-	-	9/19/19/39	0/1/1/1
37	CN3	m	606	-	-	10/56/56/65	-
29	PEF	T	101	-	-	6/32/32/50	-
28	9PE	M	405	-	-	4/36/36/43	-
22	CDL	A	501	-	-	10/64/64/110	-
24	8PE	M	402	-	-	6/29/29/50	-
32	PCF	w	201	-	-	12/46/46/53	-
28	9PE	C	406	-	-	4/36/36/43	-
33	PTY	I	101	-	-	6/35/35/53	-
32	PCF	H	102	-	-	11/35/35/53	-
22	CDL	N	403	-	-	25/70/70/110	-
31	FES	O	301	-	-	-	0/1/1/1
24	8PE	C	402	-	-	6/29/29/50	-
29	PEF	N	401	-	-	12/43/43/50	-
32	PCF	R	102	-	-	11/35/35/53	-
26	UQ6	M	403	-	-	9/19/19/39	0/1/1/1

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	402	HEC	C3C-C2C	-6.52	1.33	1.40
30	N	402	HEC	C3C-C2C	-6.52	1.33	1.40
34	a	601	HEA	C3B-C2B	5.56	1.47	1.34
34	m	601	HEA	C3B-C2B	5.56	1.47	1.34
34	a	603	HEA	CHC-C4B	5.53	1.48	1.34

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	402	HEC	CMB-C2B-C3B	6.99	134.04	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	402	HEC	CMB-C2B-C3B	6.99	134.04	125.82
30	D	402	HEC	CBC-CAC-C3C	-6.70	111.81	127.49
30	N	402	HEC	CBC-CAC-C3C	-6.70	111.81	127.49
34	a	601	HEA	C3D-C4D-ND	6.63	116.76	110.35

There are no chirality outliers.

5 of 535 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	501	CDL	CB3-OB5-PB2-OB2
22	A	501	CDL	CB3-OB5-PB2-OB4
22	D	403	CDL	CA2-OA2-PA1-OA3
22	D	403	CDL	CA2-OA2-PA1-OA5
22	D	403	CDL	CA3-OA5-PA1-OA2

There are no ring outliers.

50 monomers are involved in 207 short contacts:

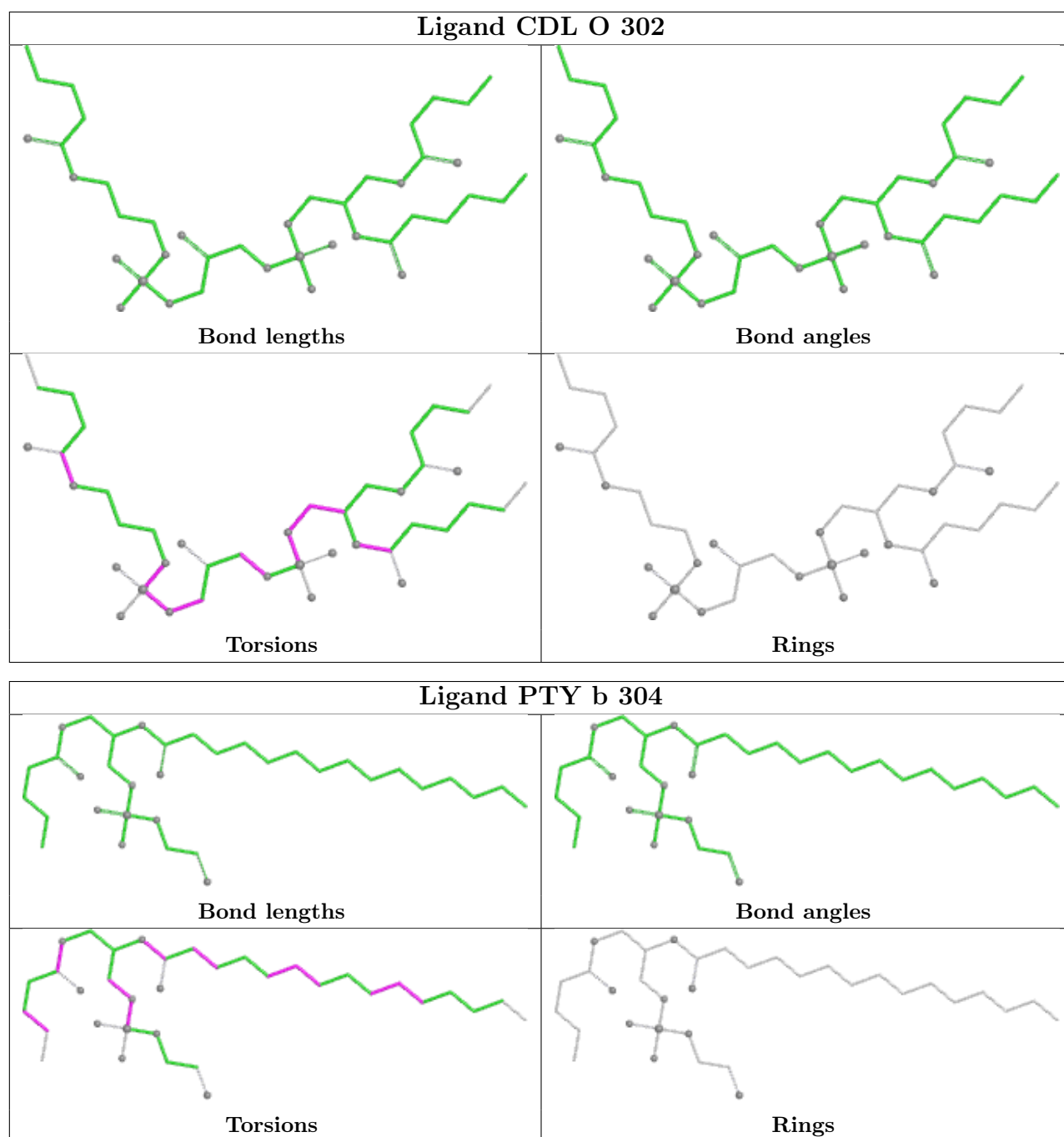
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	302	CDL	6	0
33	b	304	PTY	2	0
22	D	403	CDL	5	0
33	a	604	PTY	9	0
22	H	101	CDL	3	0
27	C	407	HEM	3	0
33	o	301	PTY	1	0
34	a	603	HEA	2	0
29	a	607	PEF	2	0
33	b	302	PTY	2	0
22	K	501	CDL	2	0
30	D	402	HEC	16	0
23	M	401	6PH	2	0
27	C	405	HEM	6	0
22	R	101	CDL	1	0
33	n	302	PTY	2	0
33	c	301	PTY	1	0
22	E	302	CDL	6	0
26	C	408	UQ6	9	0
32	x	101	PCF	1	0
34	m	601	HEA	7	0
26	M	407	UQ6	9	0

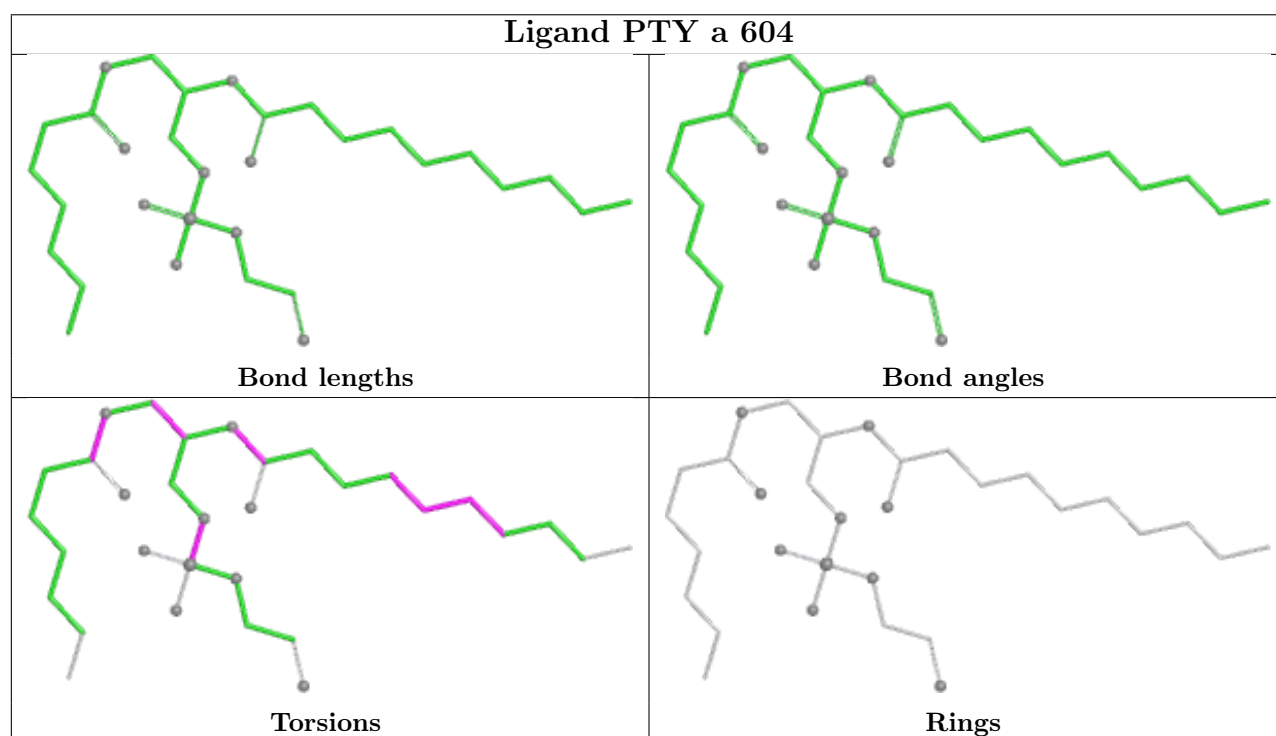
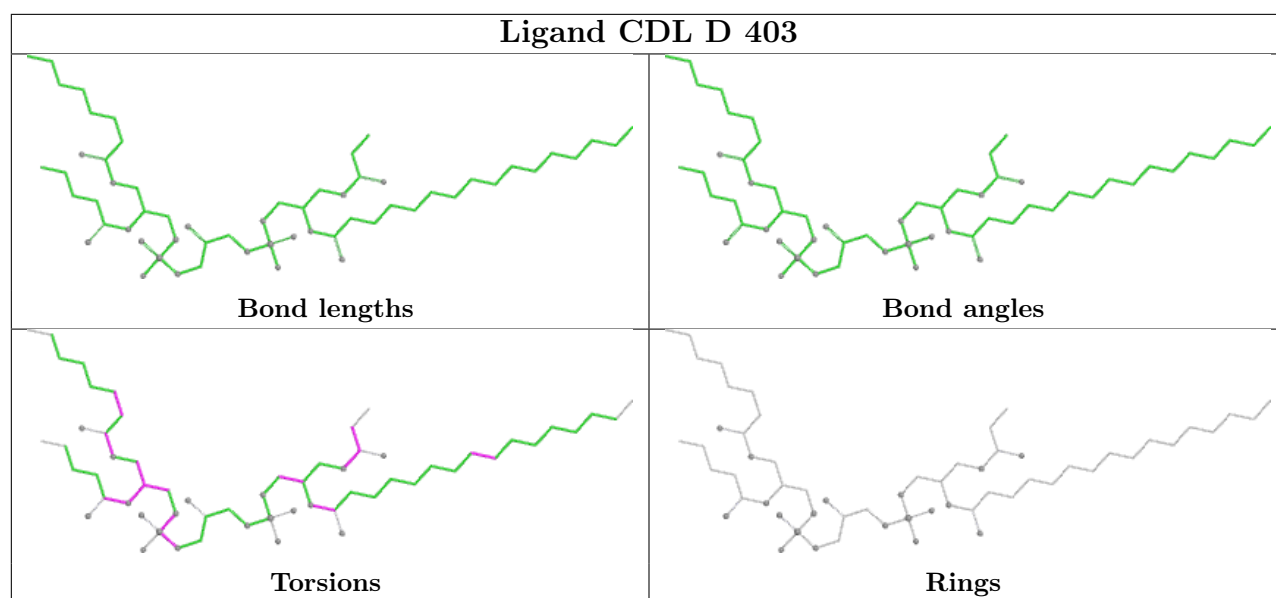
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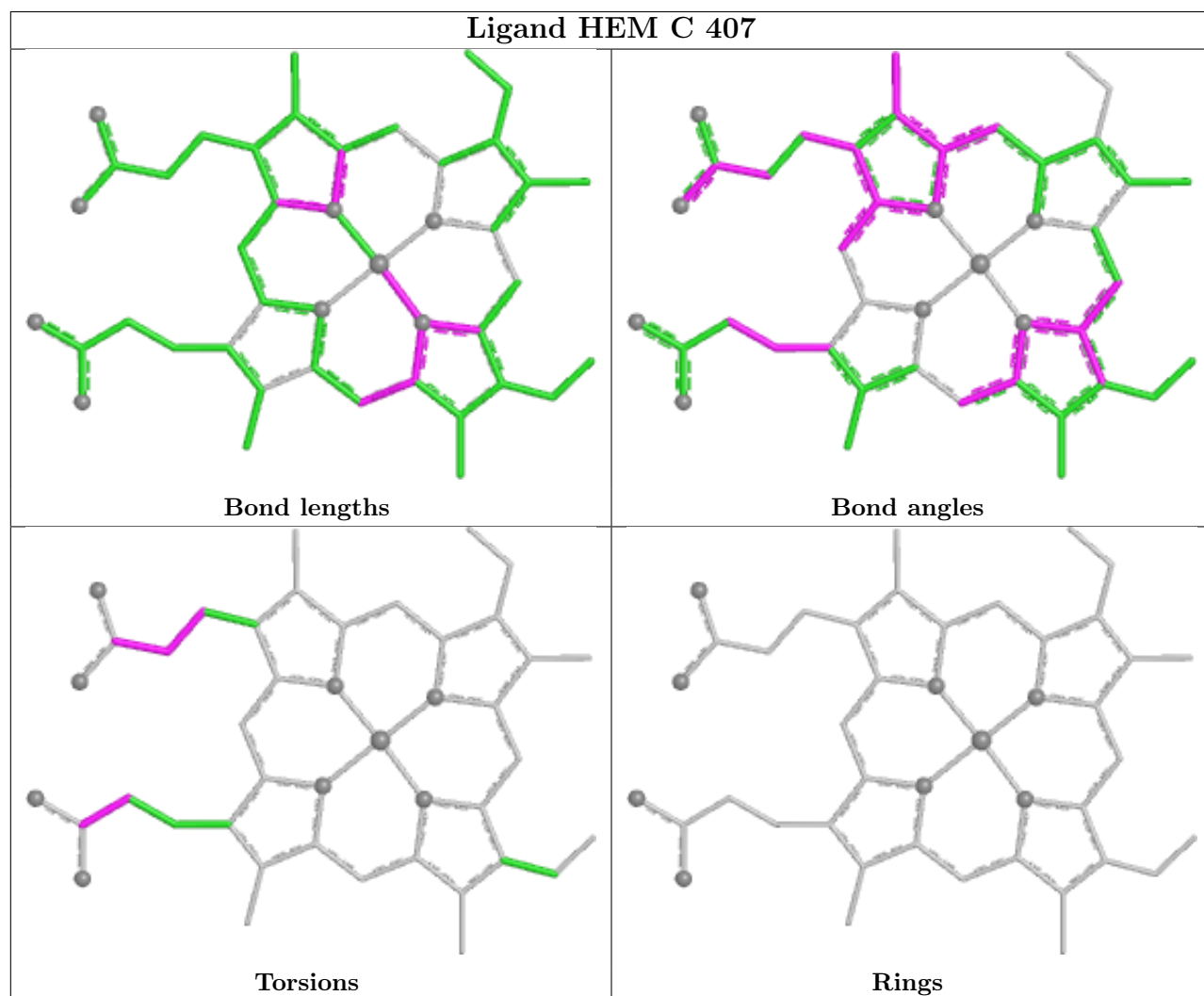
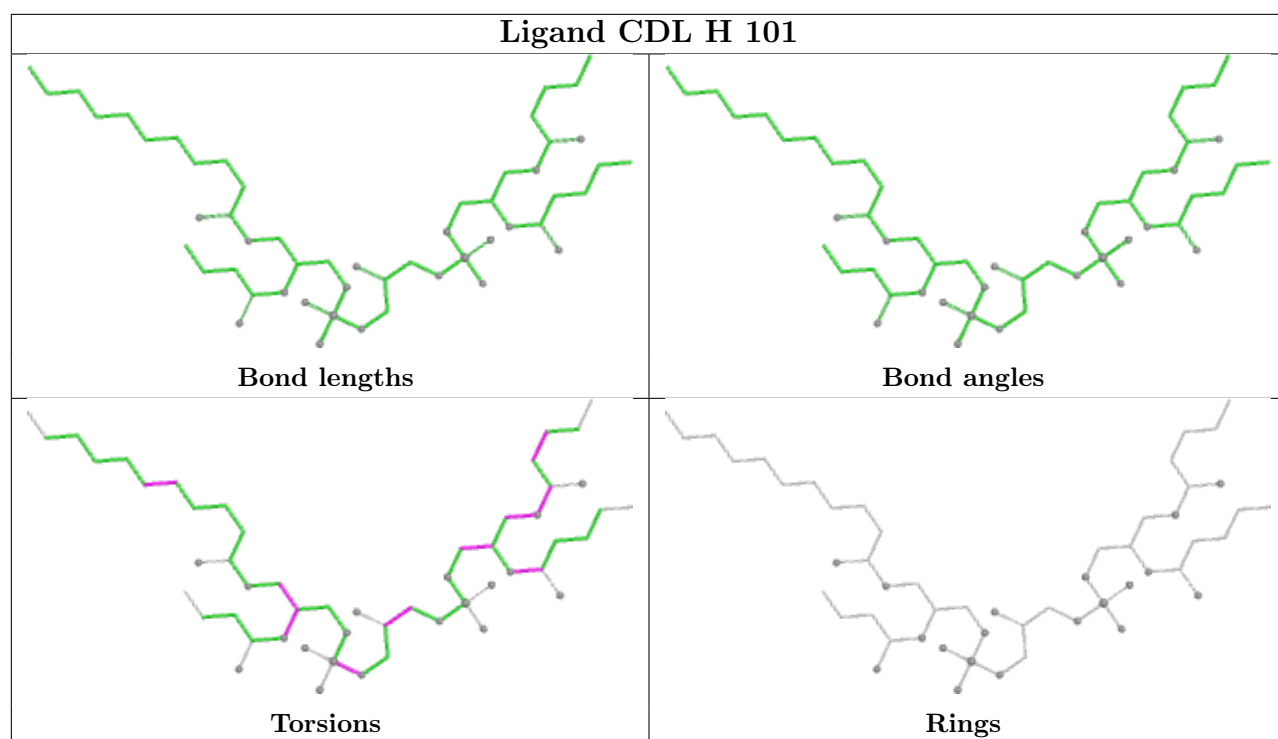
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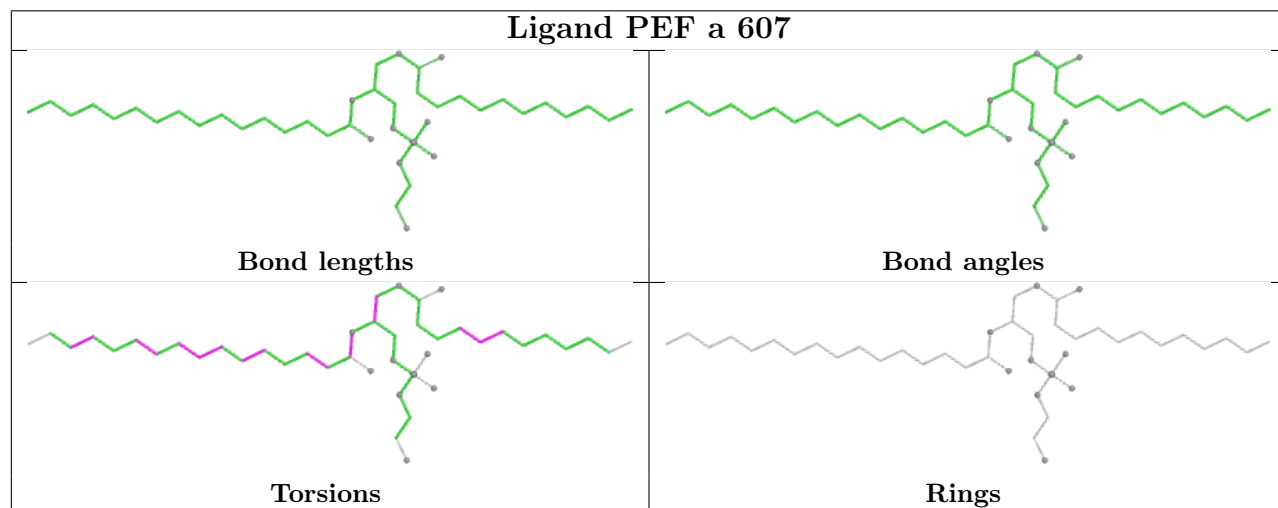
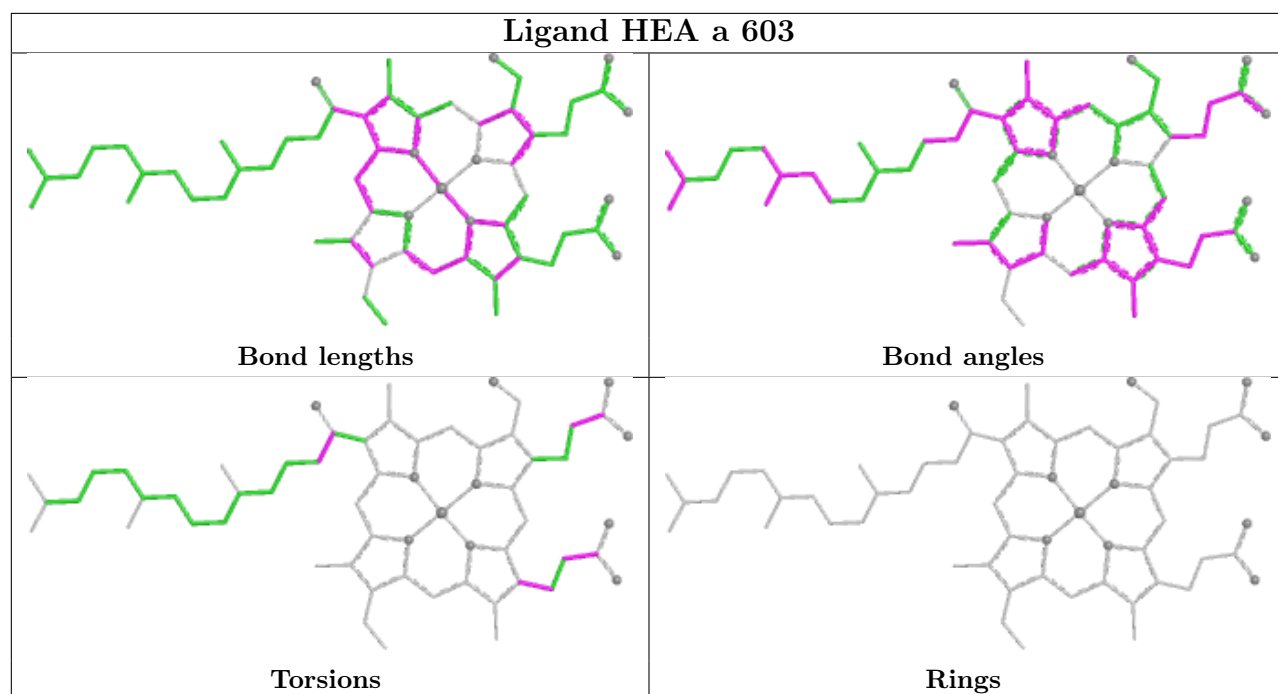
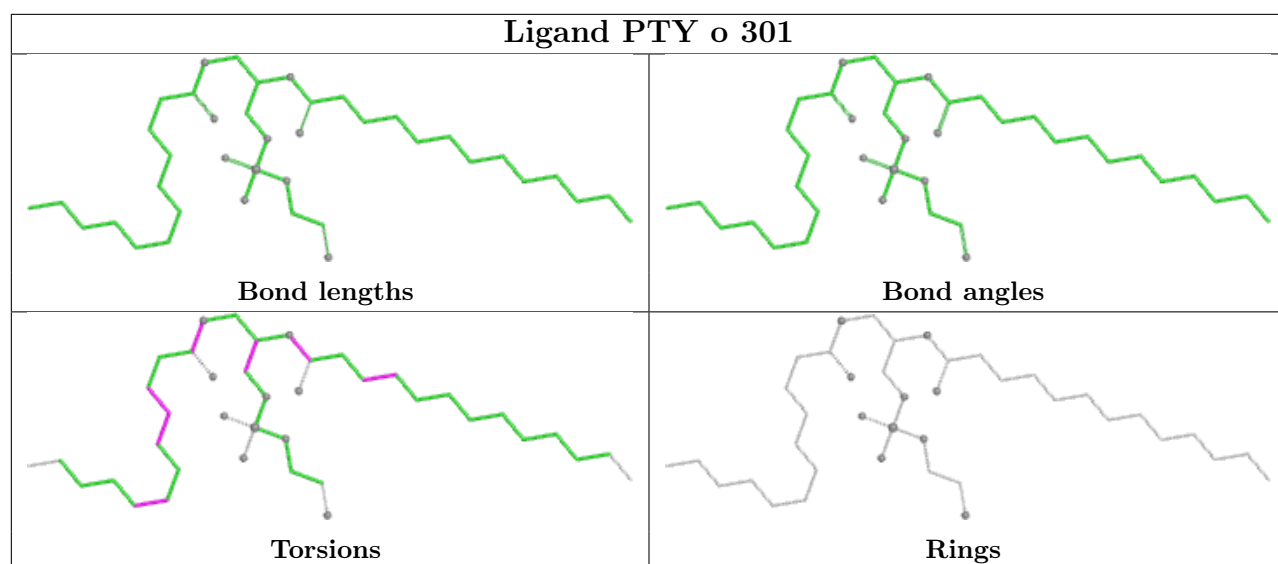
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	M	406	HEM	3	0
34	m	603	HEA	3	0
33	S	101	PTY	2	0
29	D	401	PEF	4	0
27	M	404	HEM	6	0
30	N	402	HEC	16	0
31	E	301	FES	4	0
32	l	101	PCF	2	0
23	C	401	6PH	2	0
32	k	201	PCF	12	0
29	m	607	PEF	1	0
33	m	604	PTY	9	0
29	J	101	PEF	1	0
33	n	304	PTY	2	0
34	a	601	HEA	7	0
26	C	404	UQ6	3	0
29	T	101	PEF	1	0
28	M	405	9PE	1	0
22	A	501	CDL	2	0
32	w	201	PCF	12	0
28	C	406	9PE	1	0
33	I	101	PTY	2	0
32	H	102	PCF	3	0
22	N	403	CDL	3	0
31	O	301	FES	4	0
29	N	401	PEF	3	0
32	R	102	PCF	3	0
26	M	403	UQ6	3	0

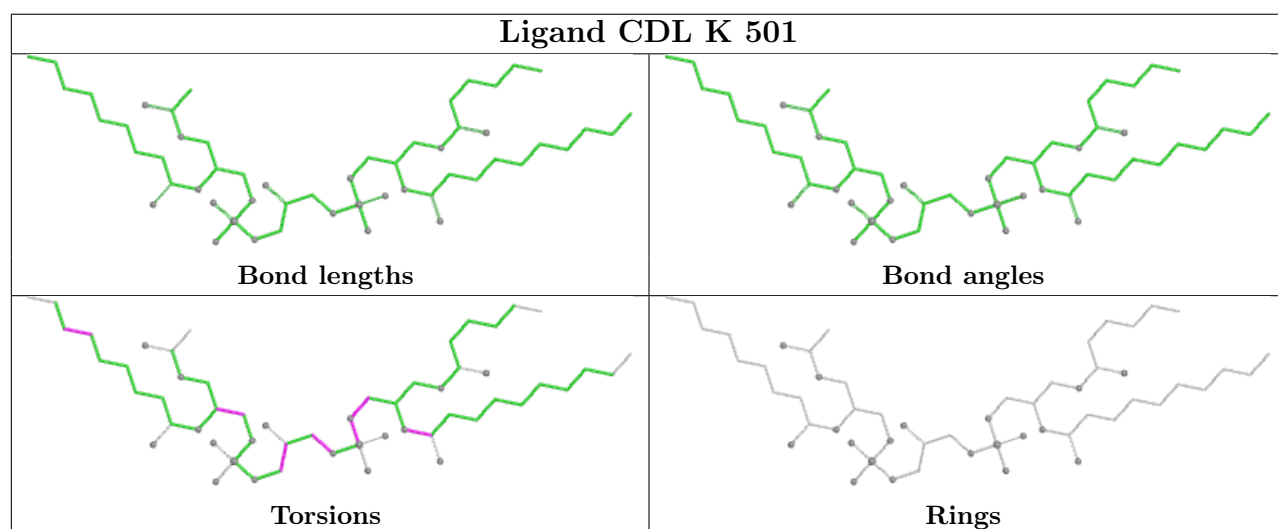
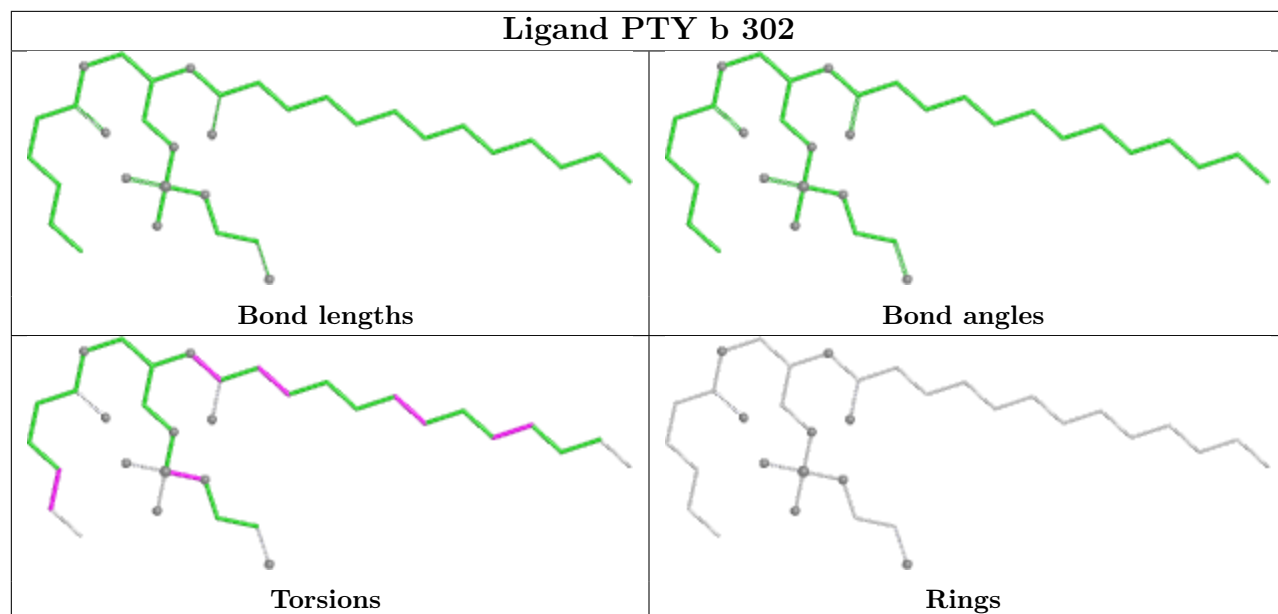
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

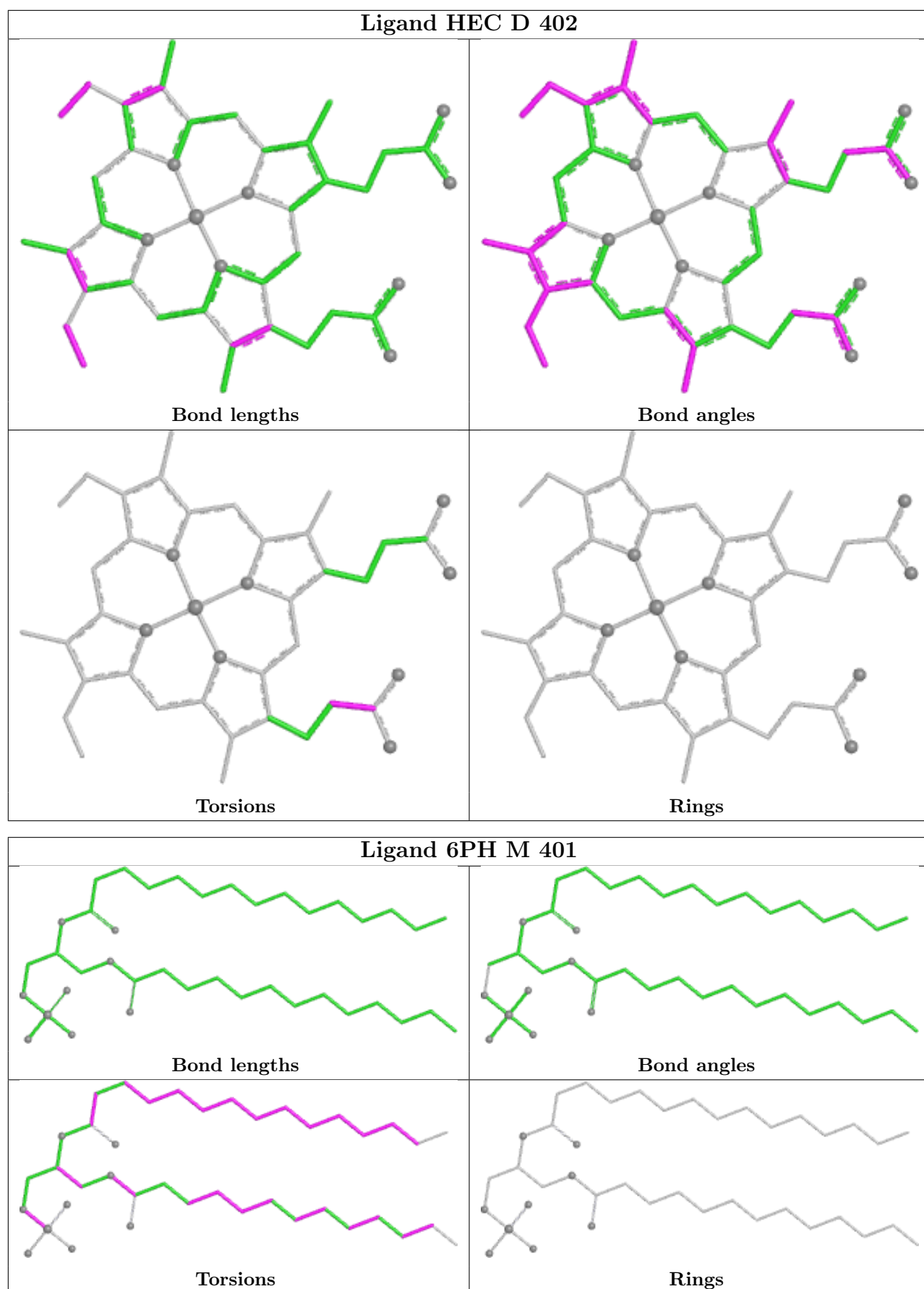


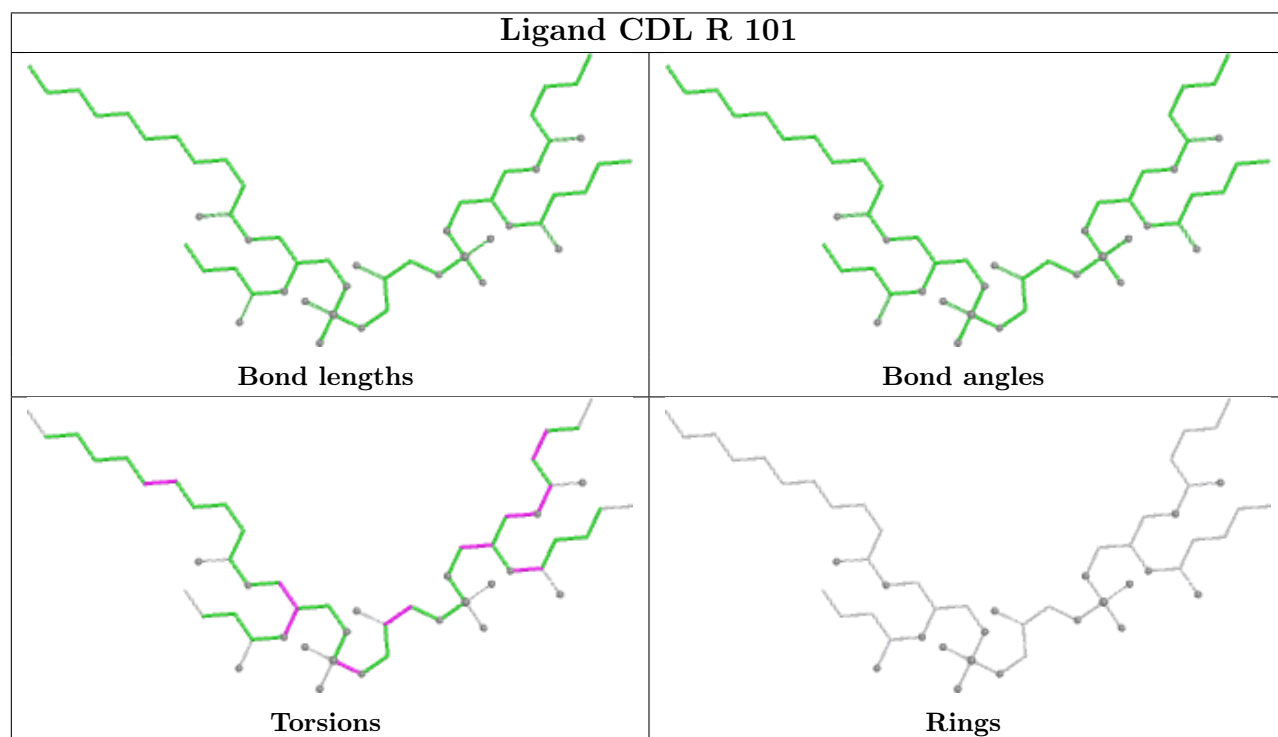
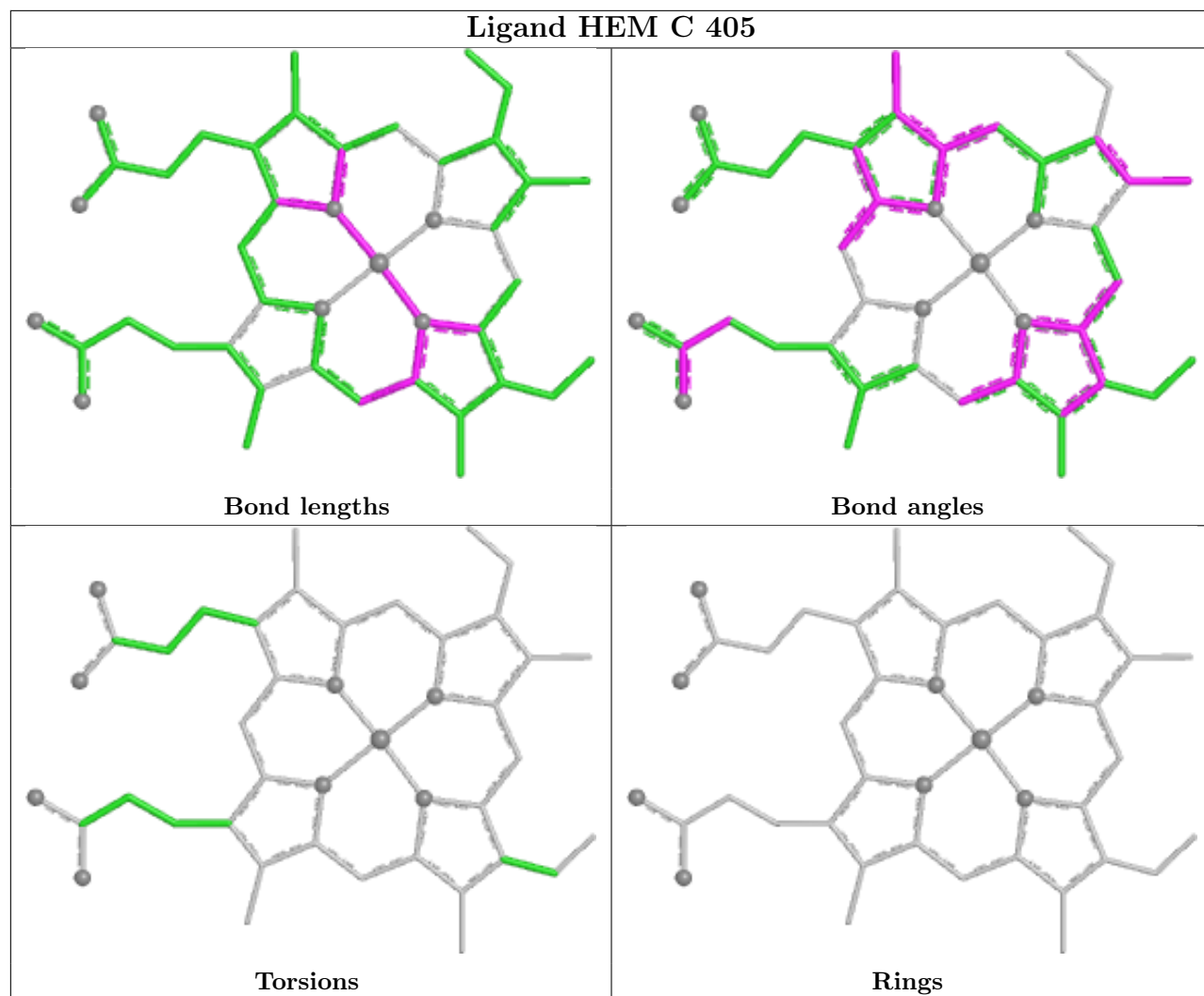


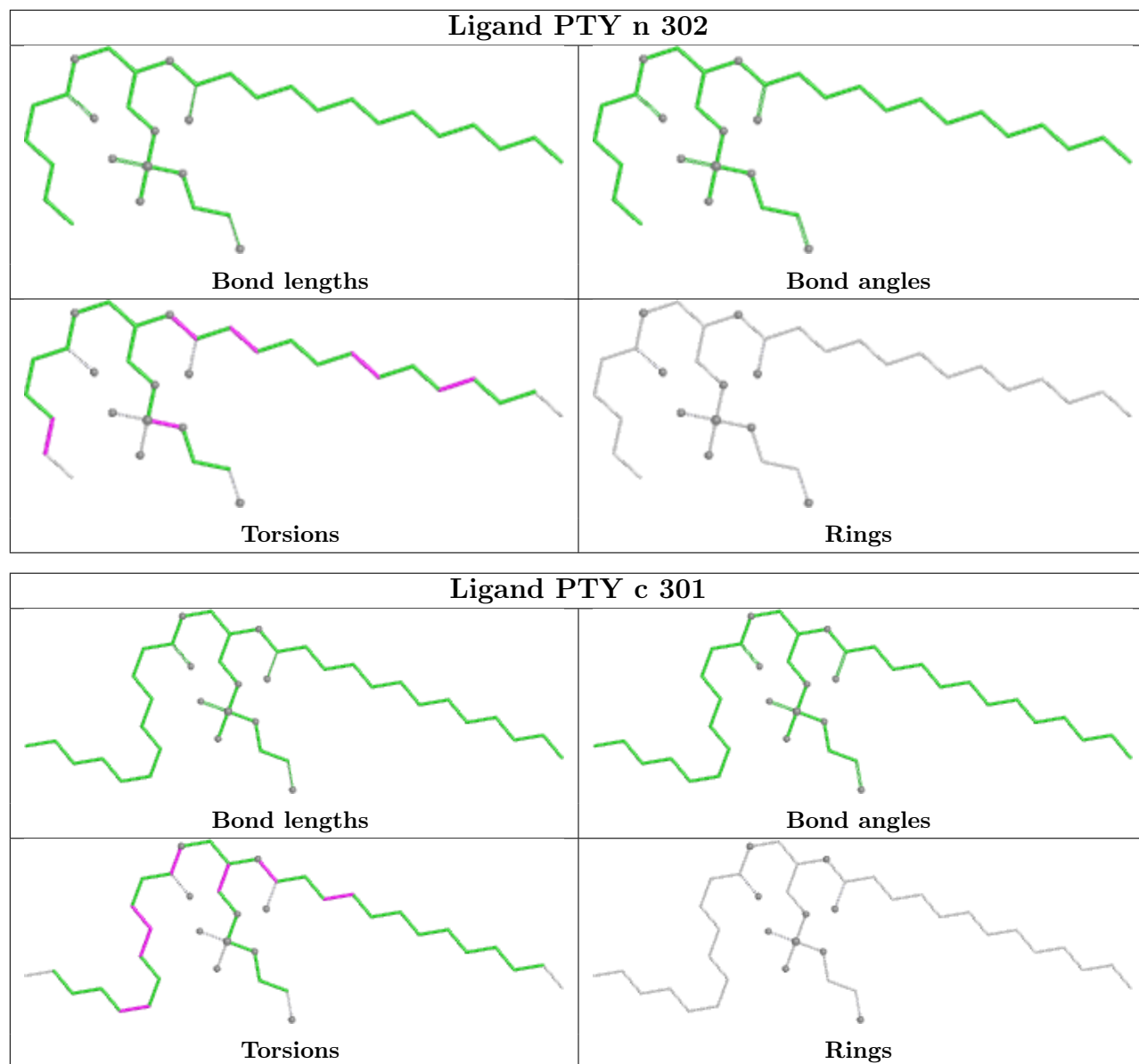


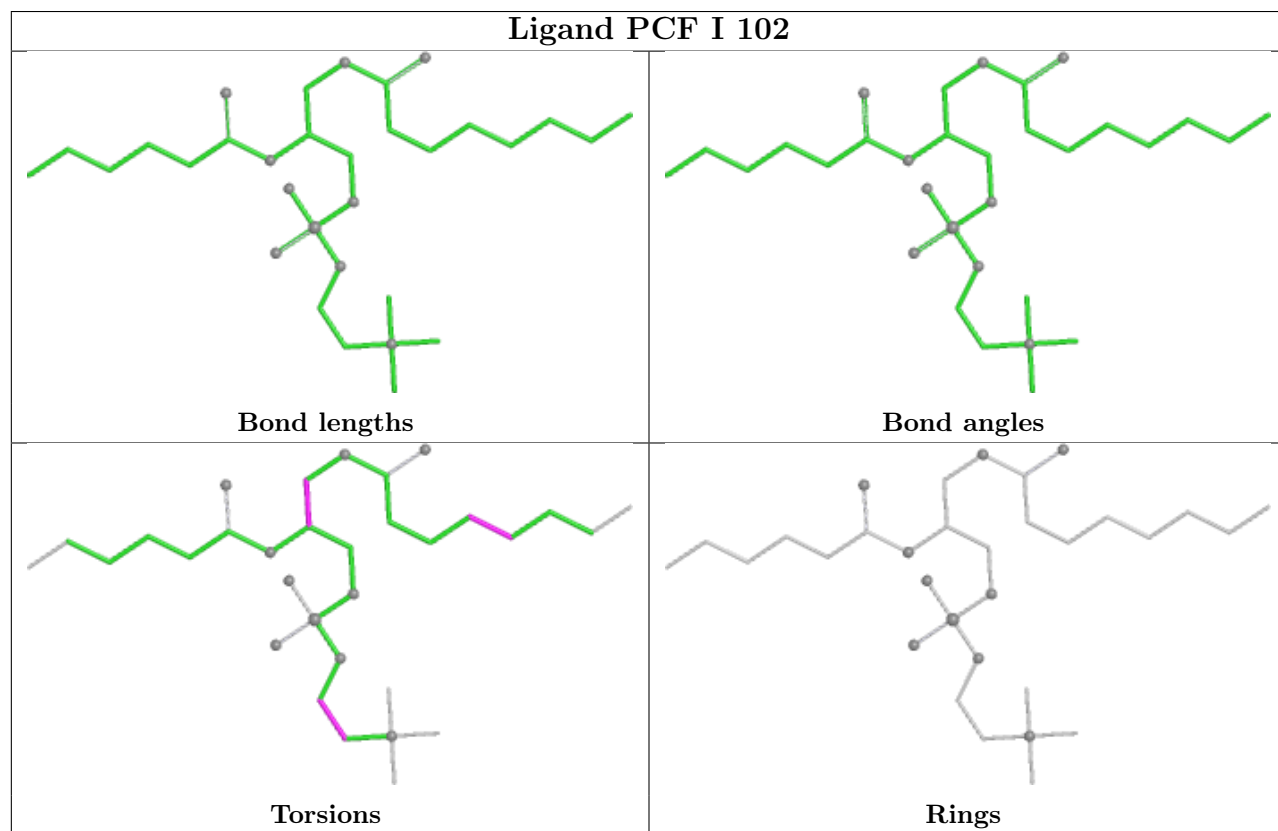
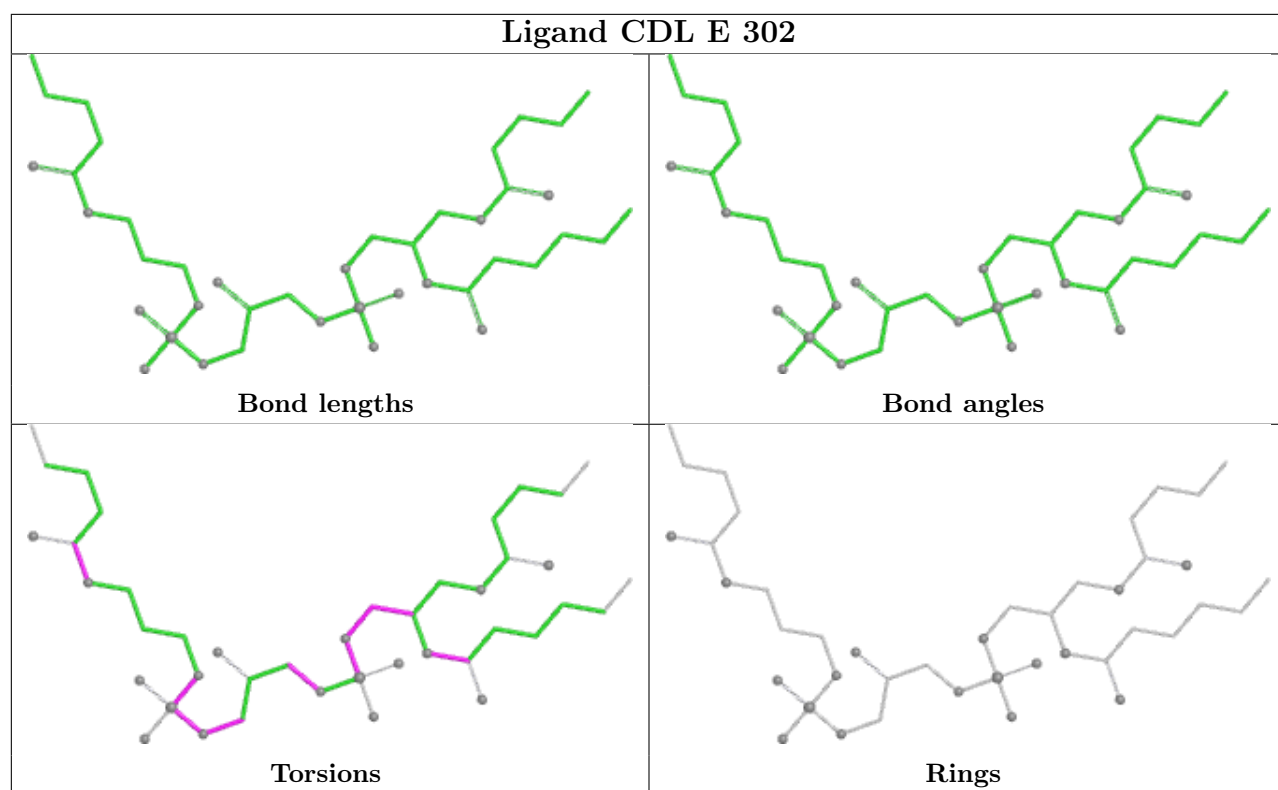


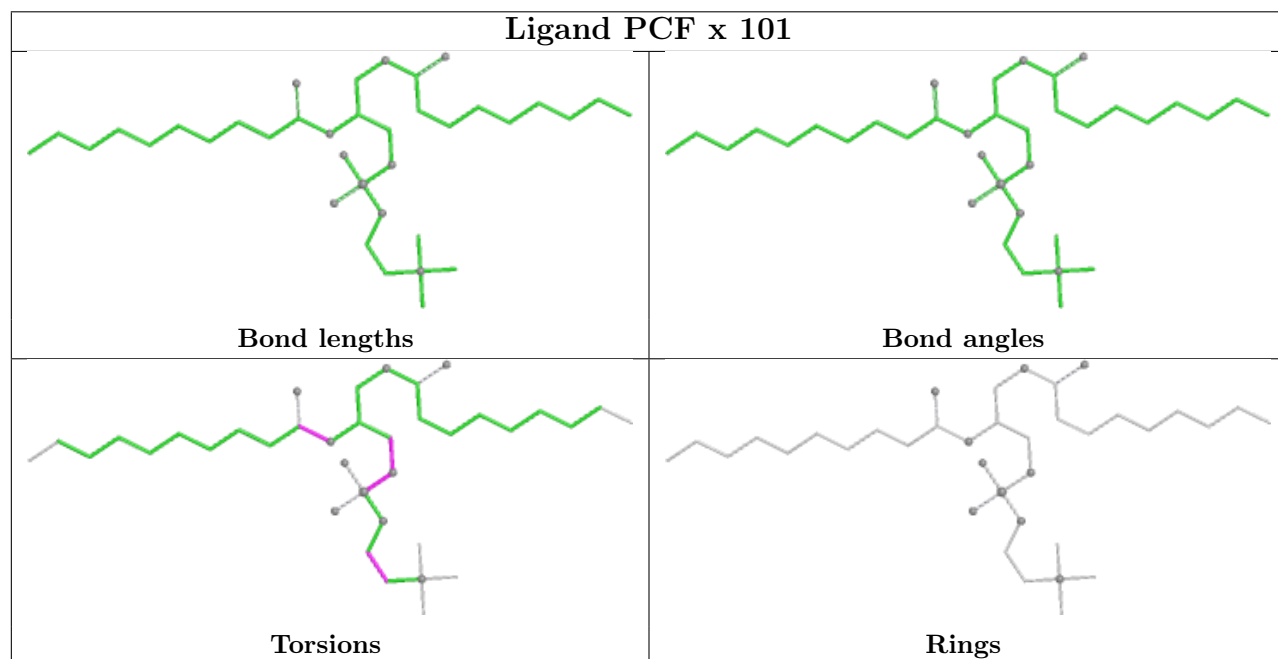
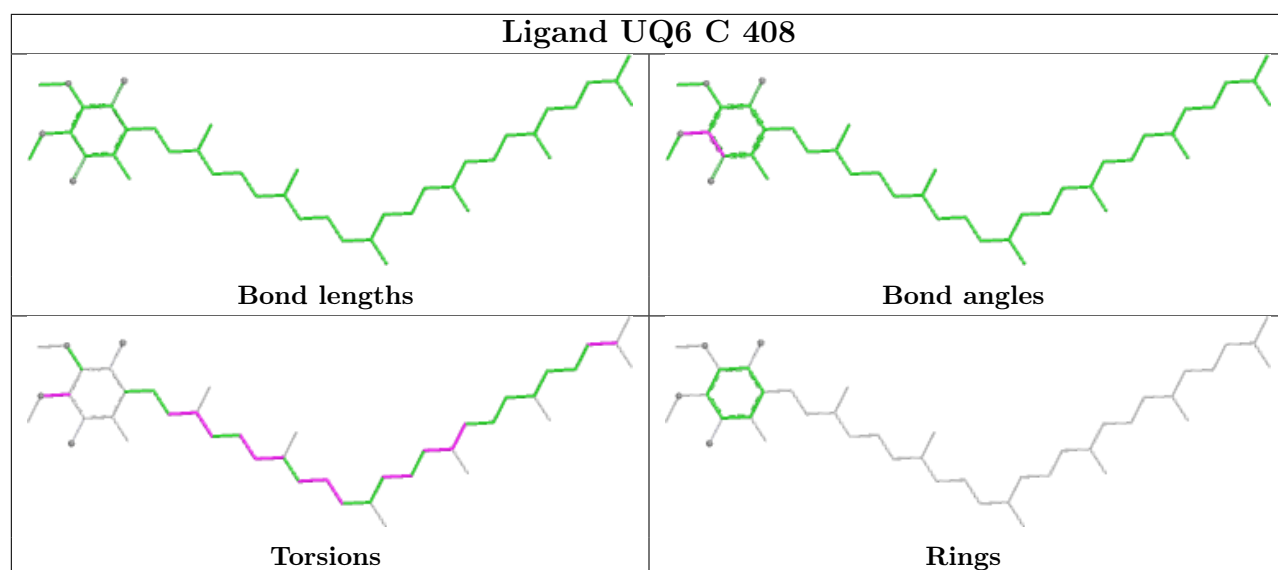


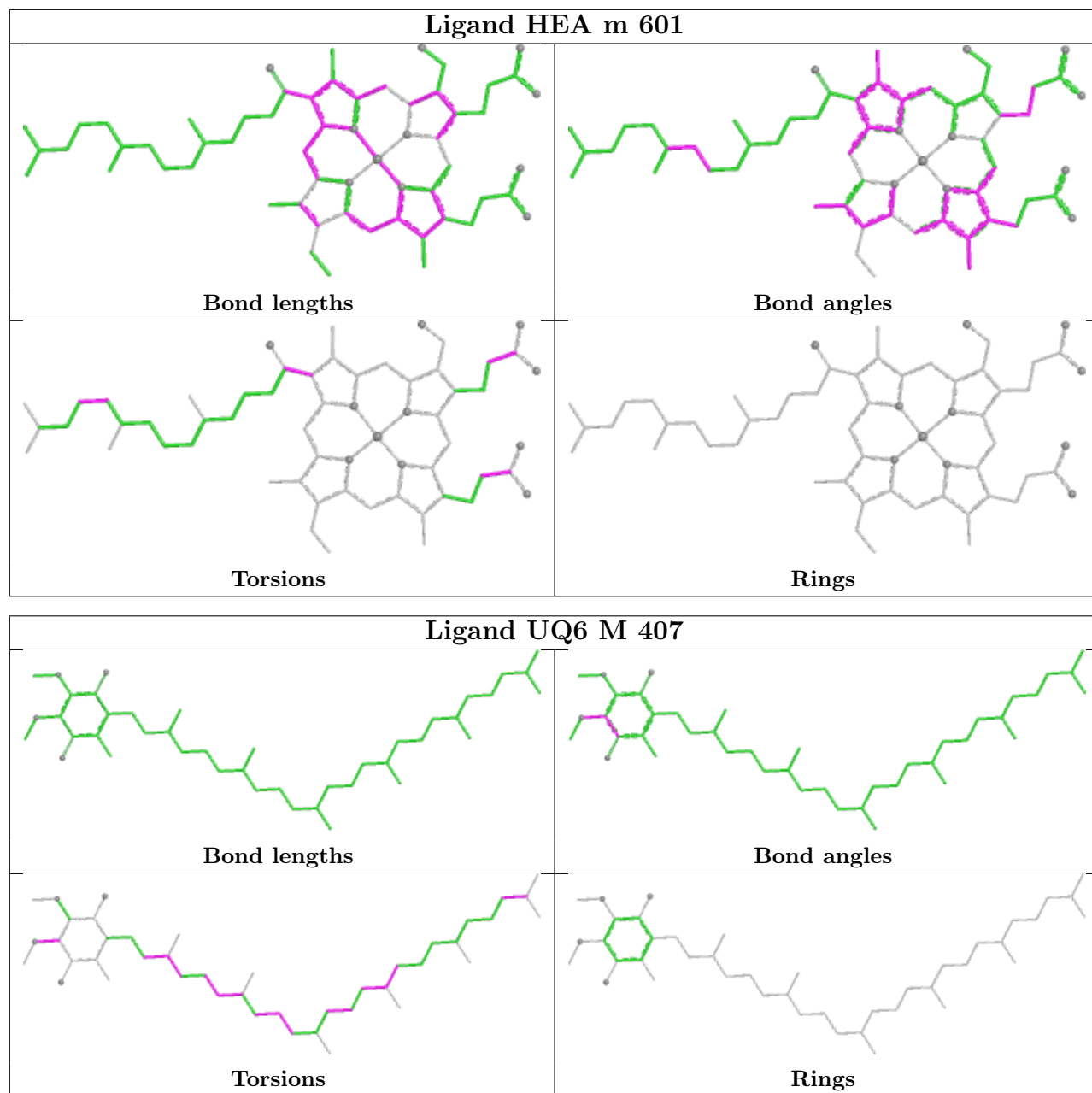




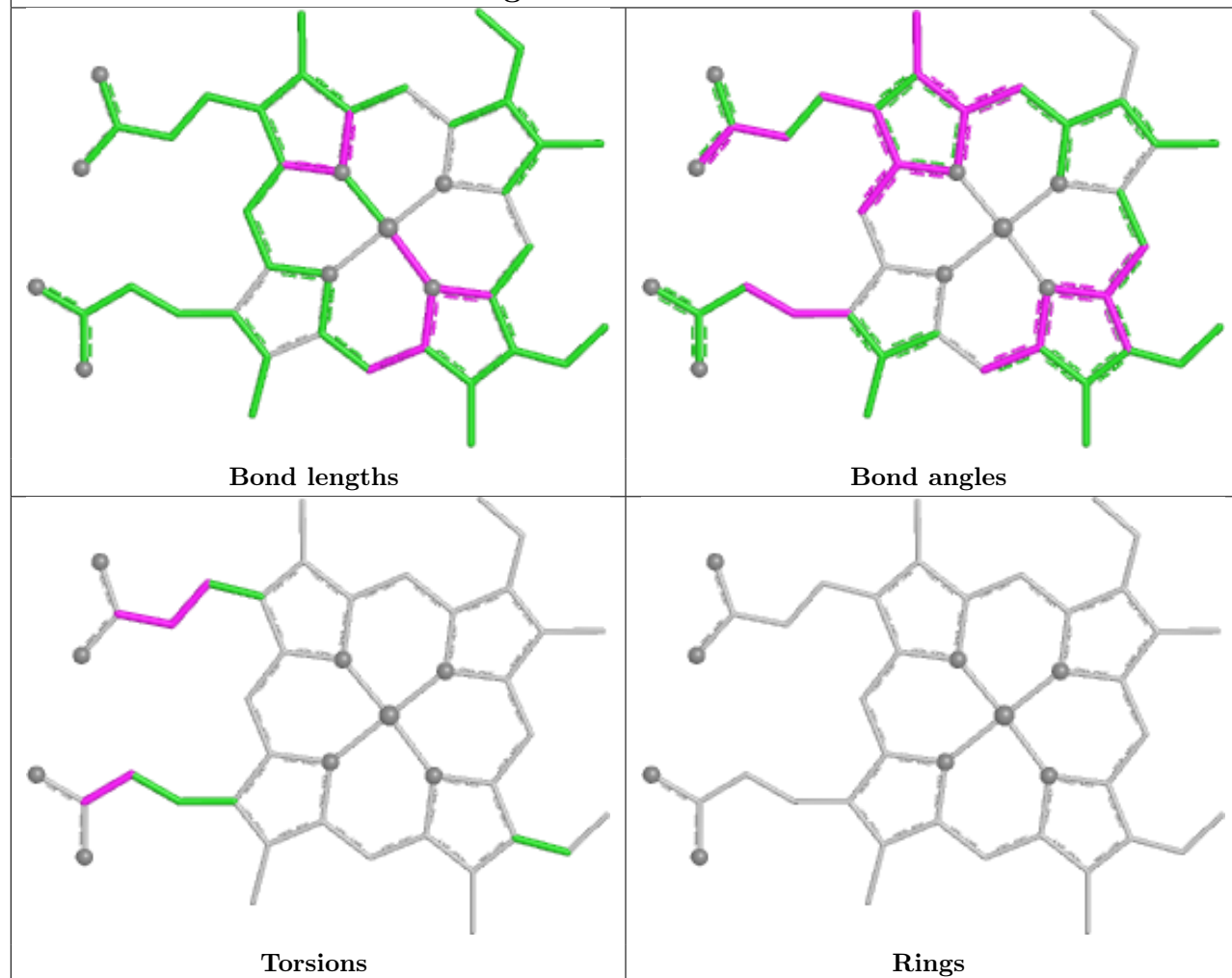


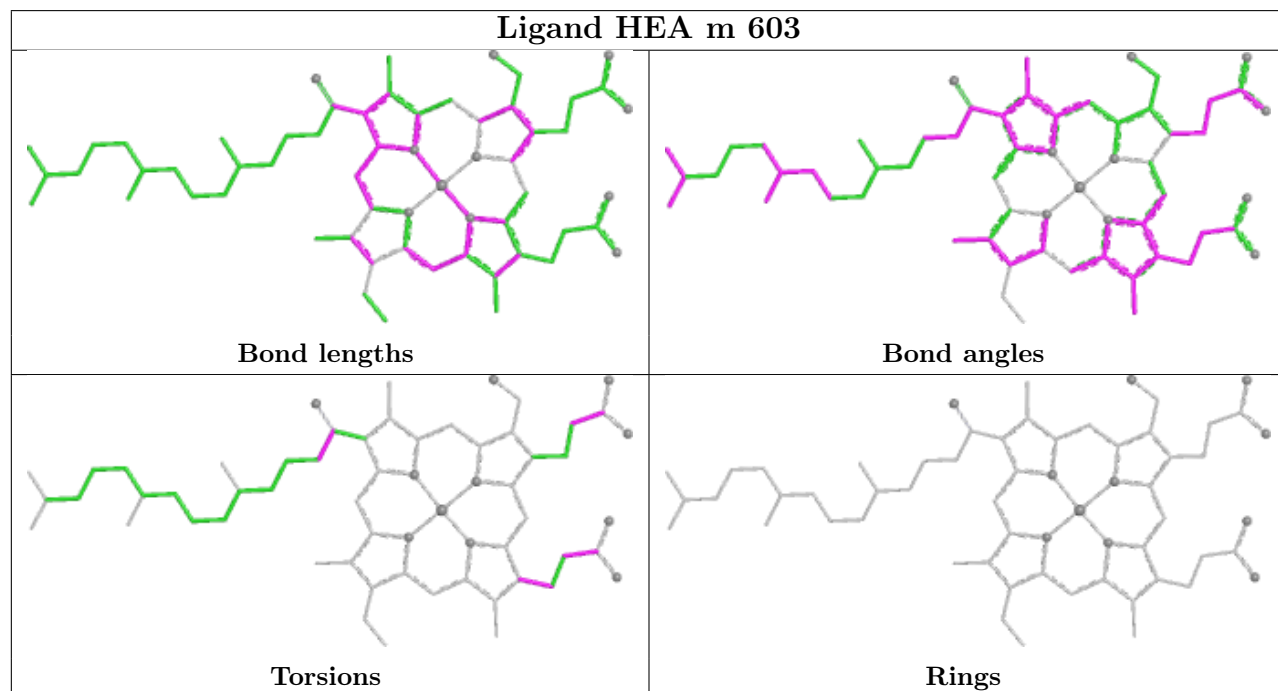
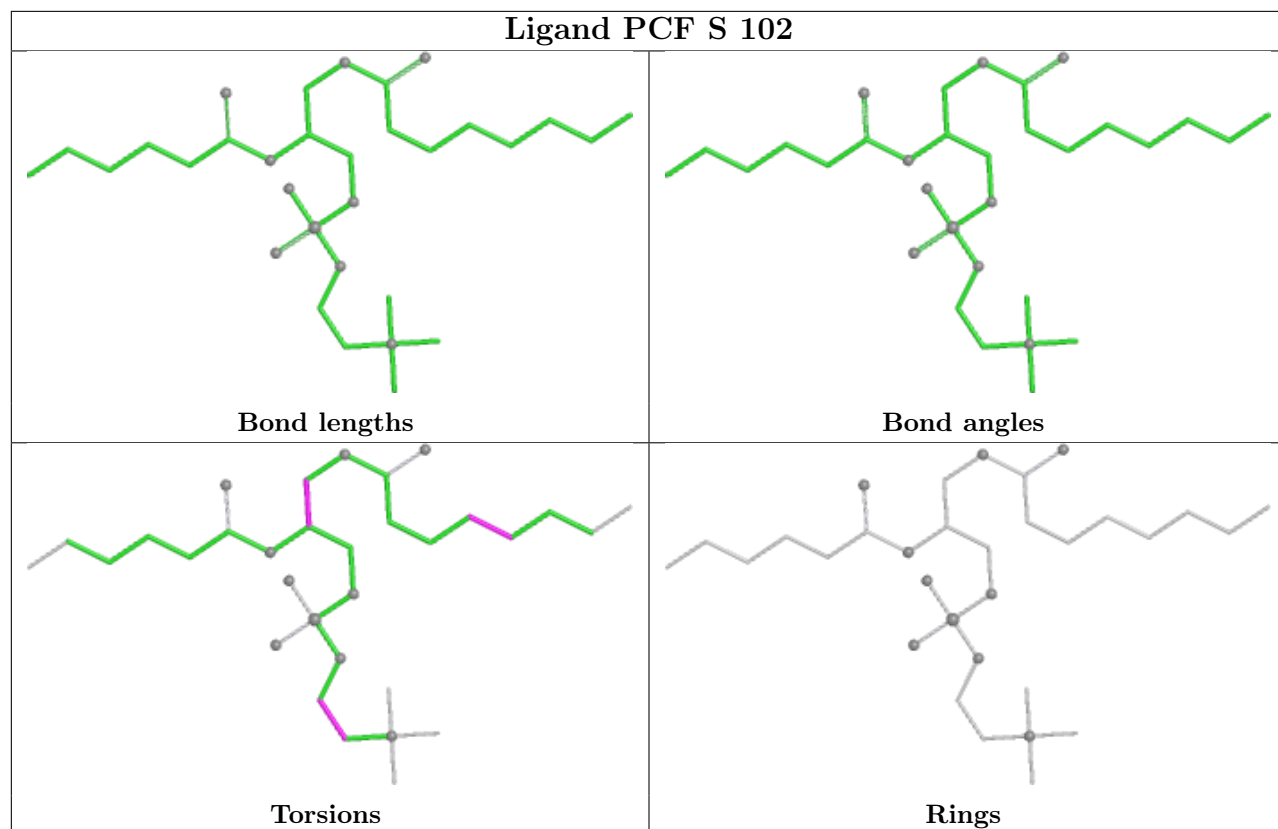


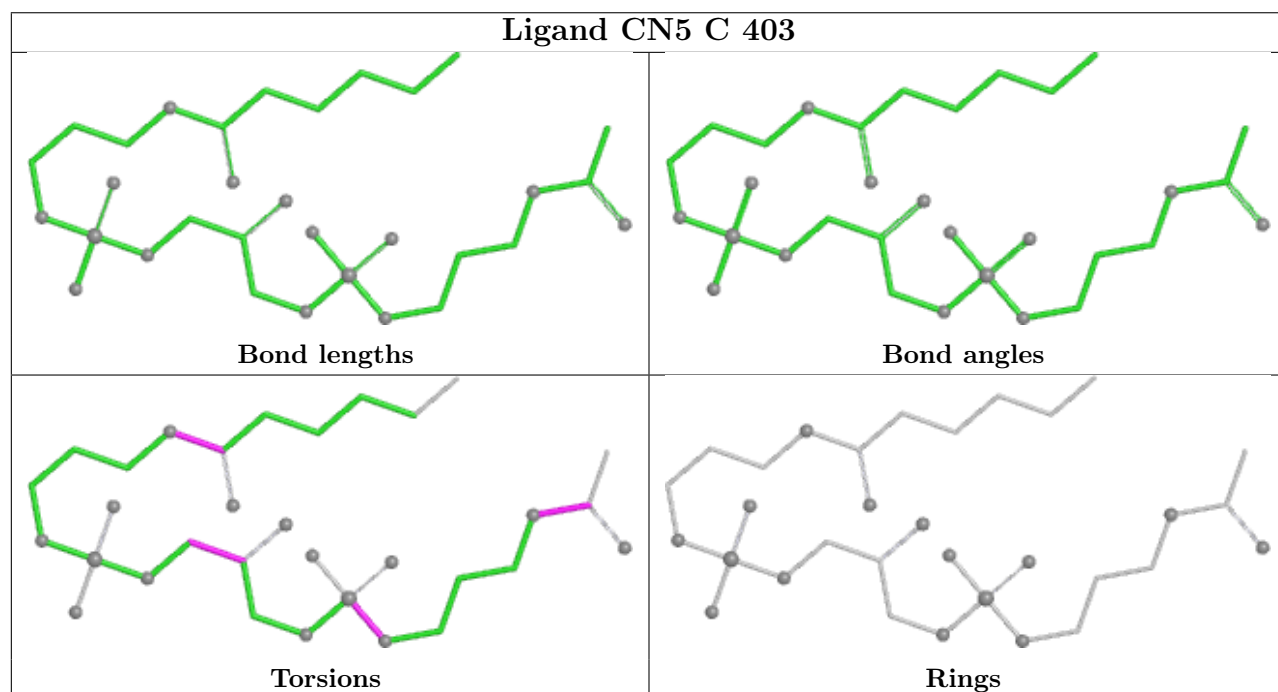
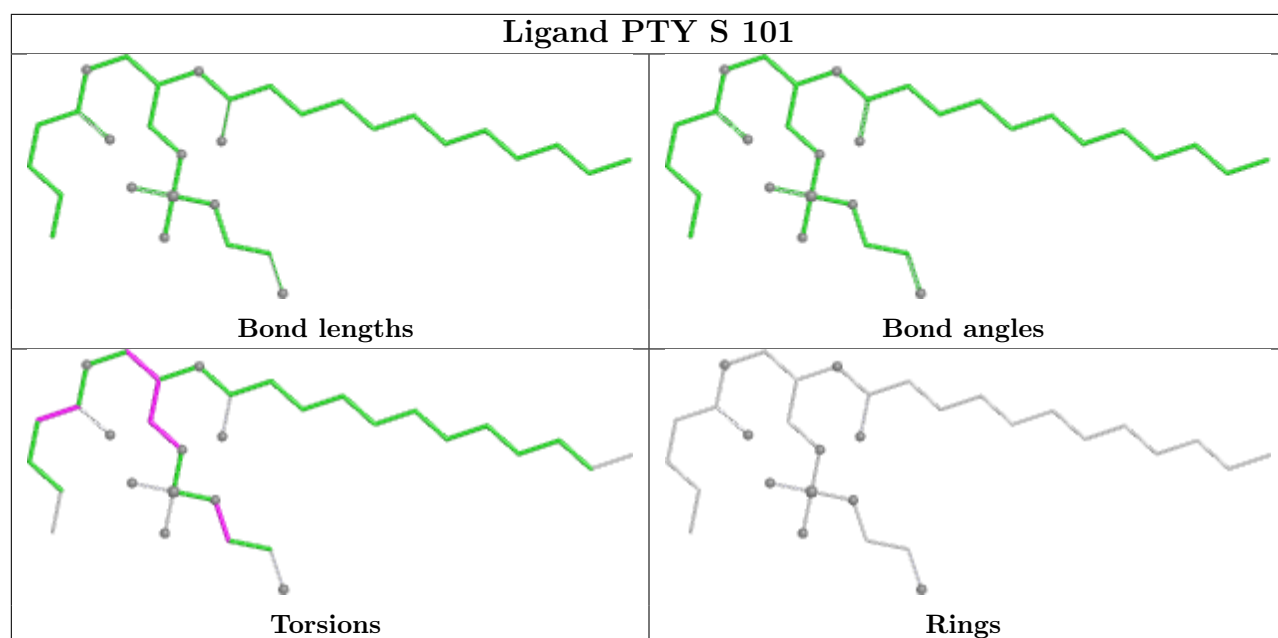


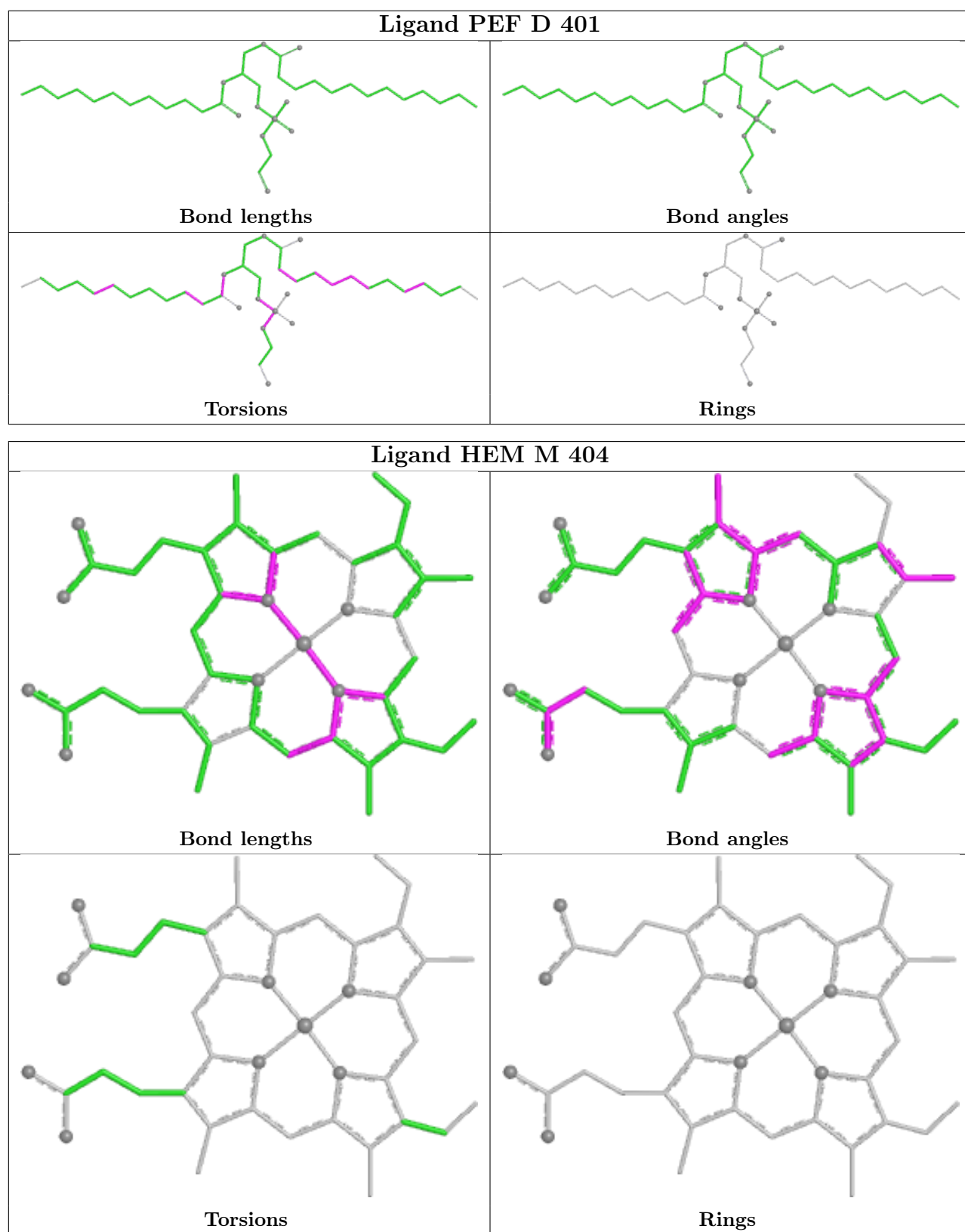


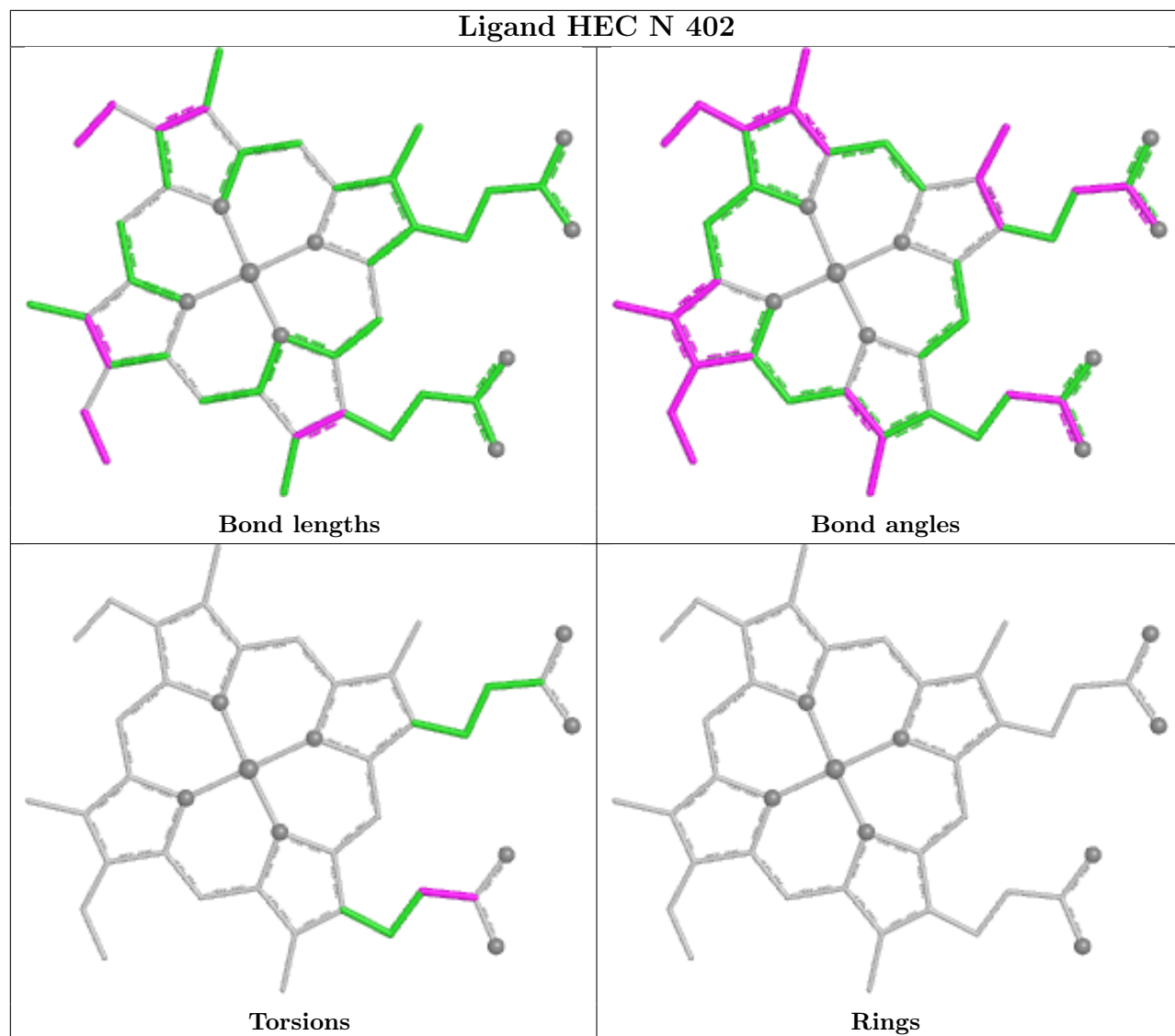
Ligand HEM M 406

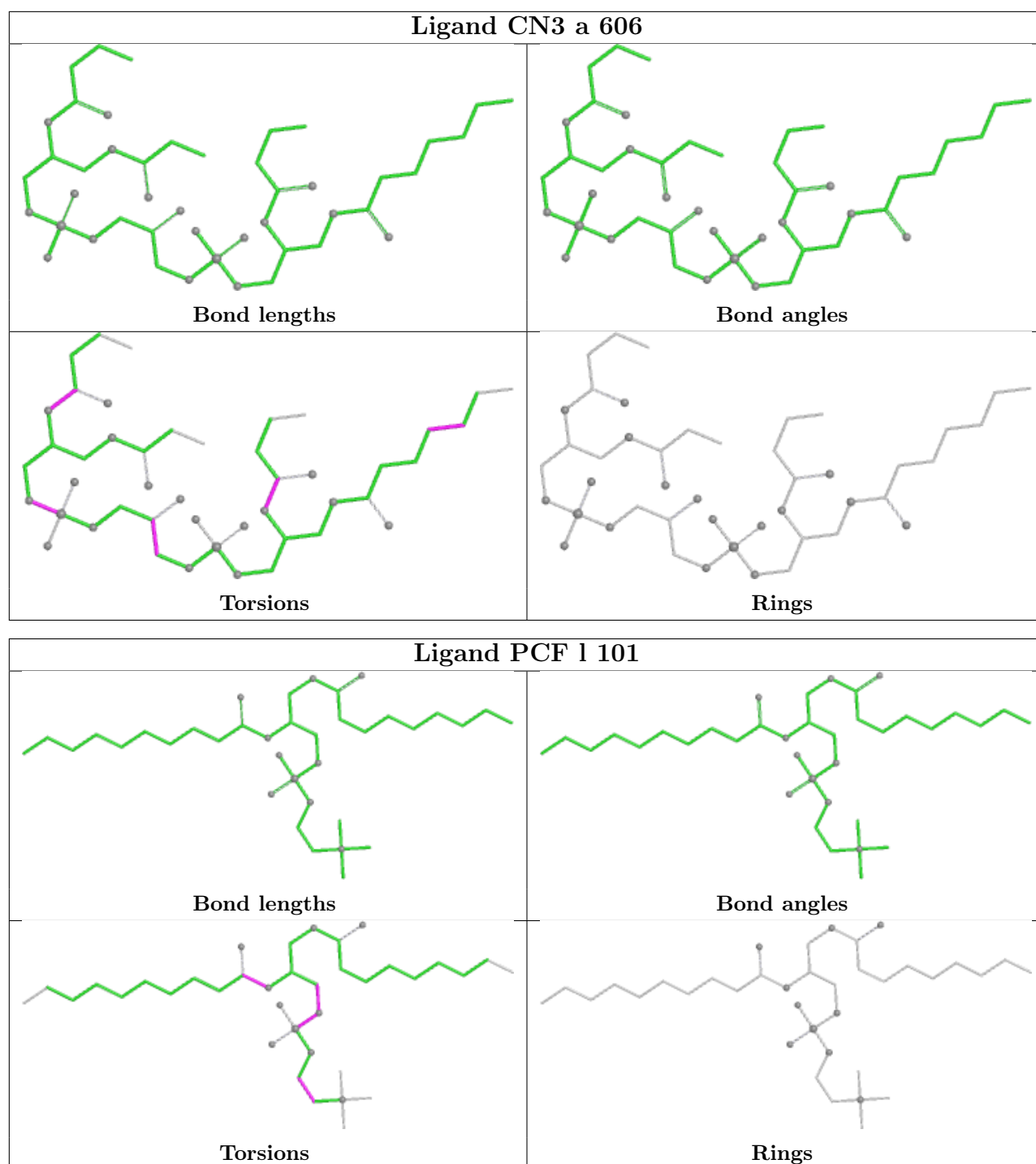


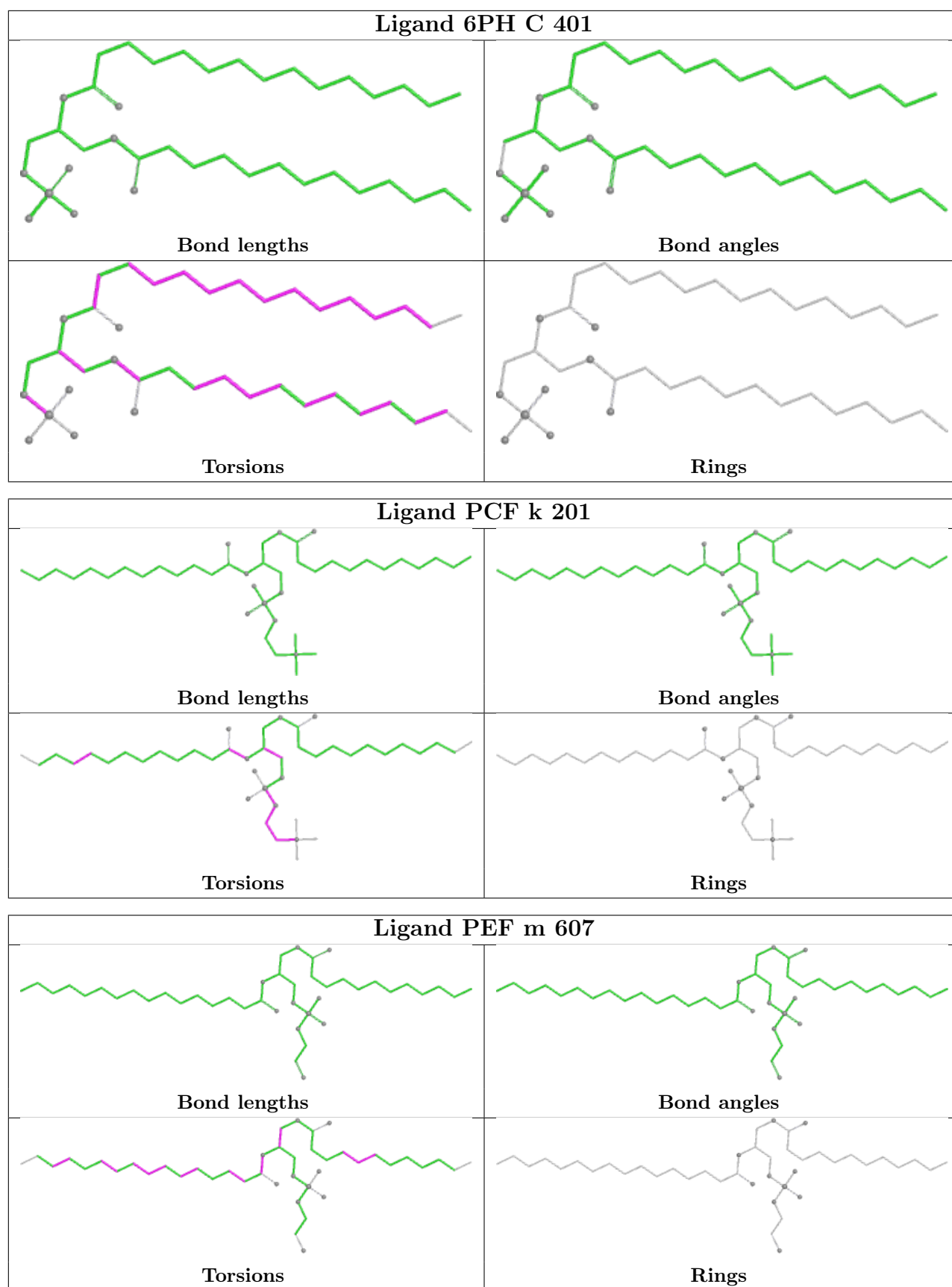


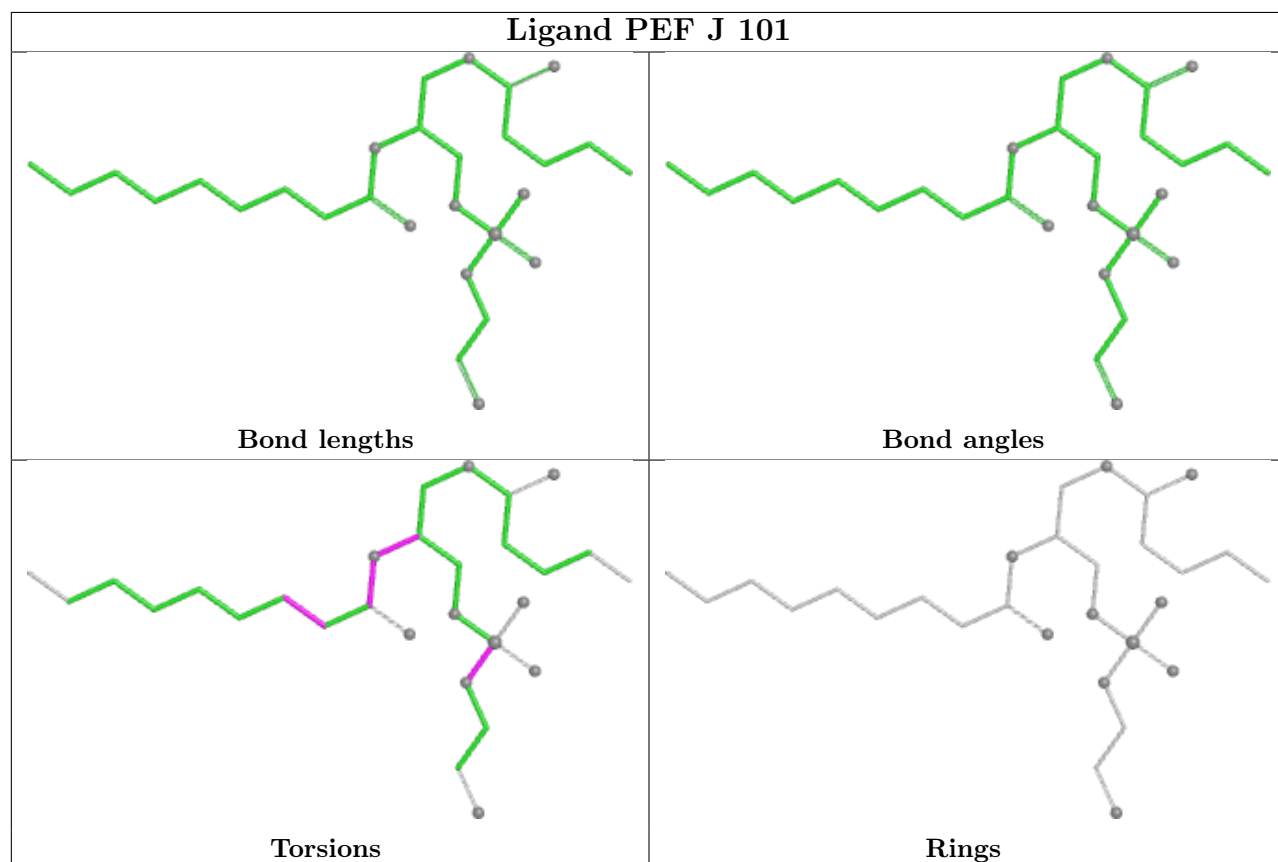
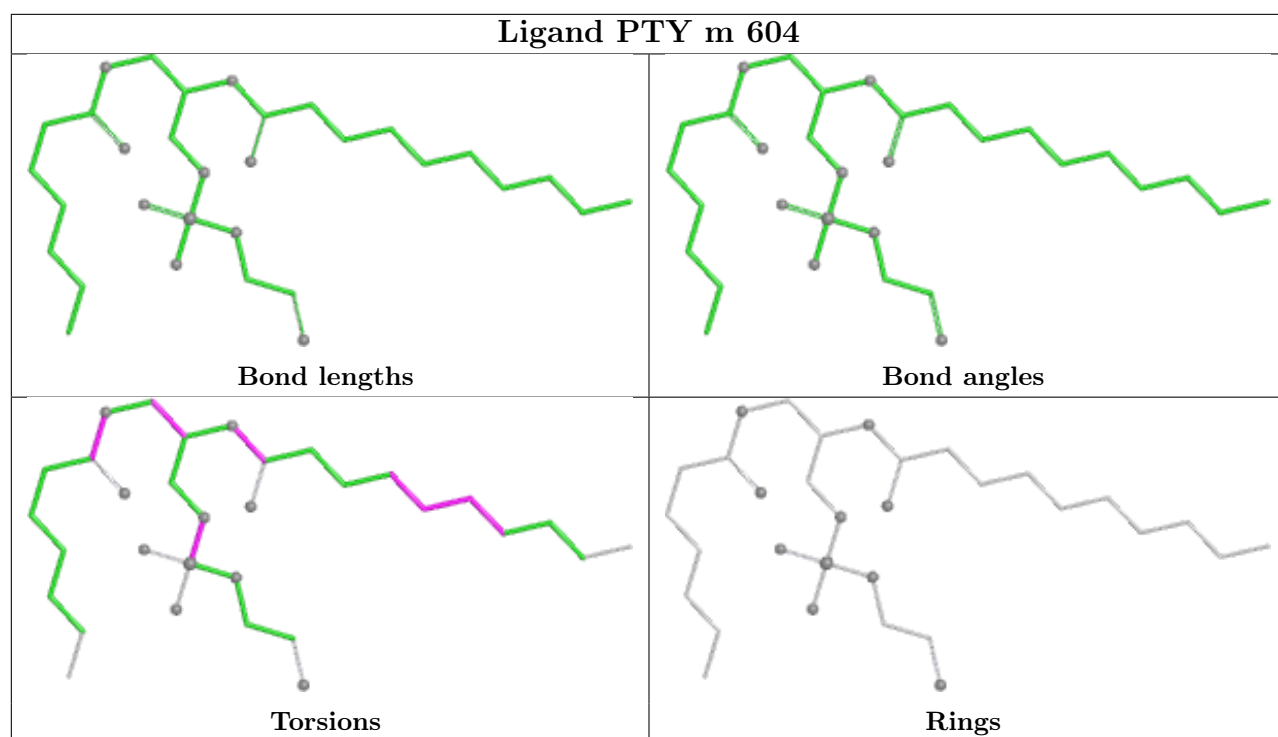


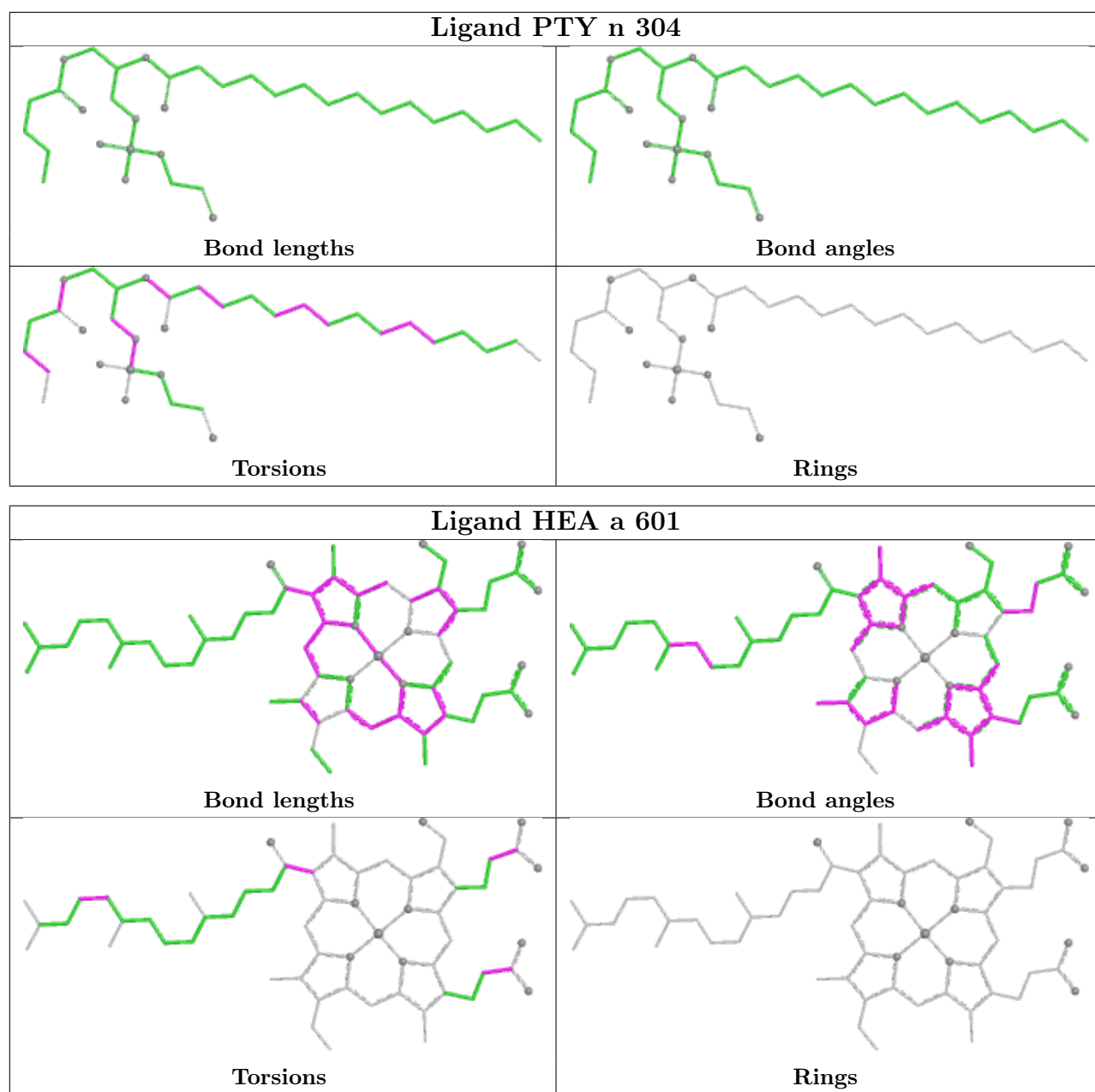


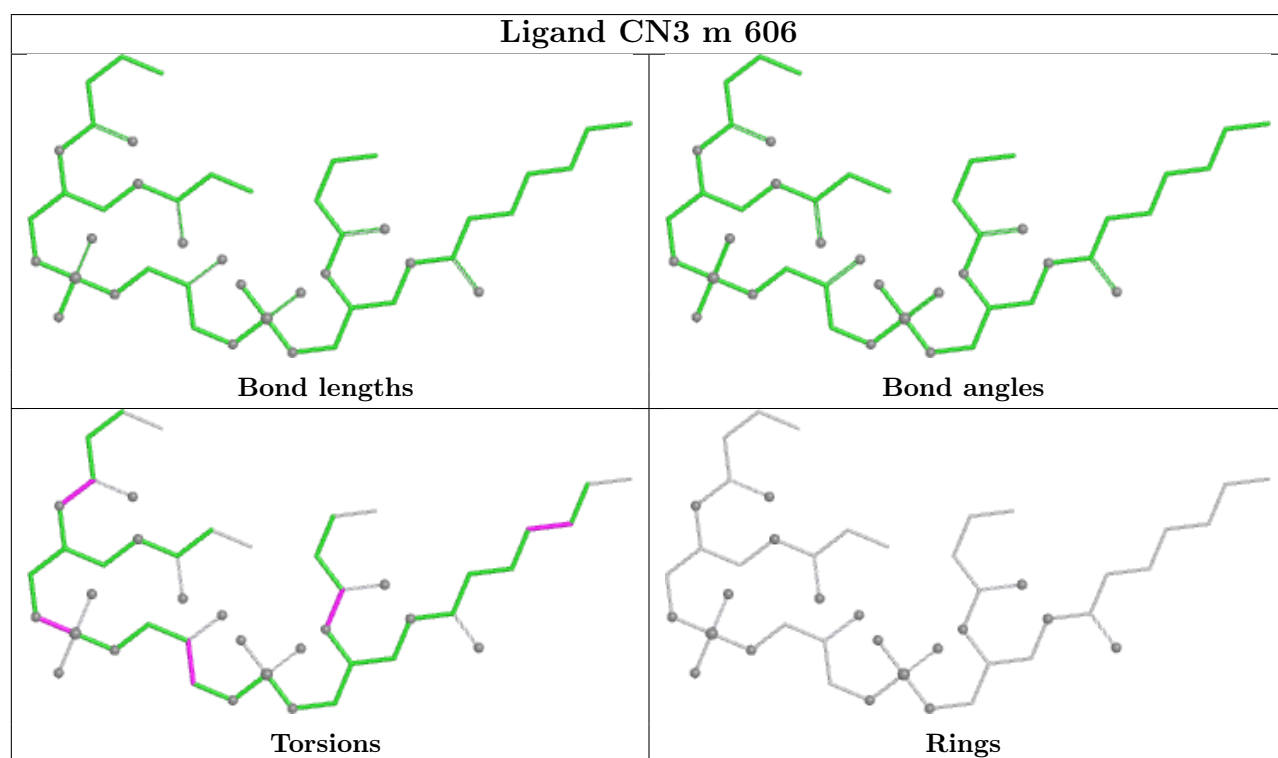
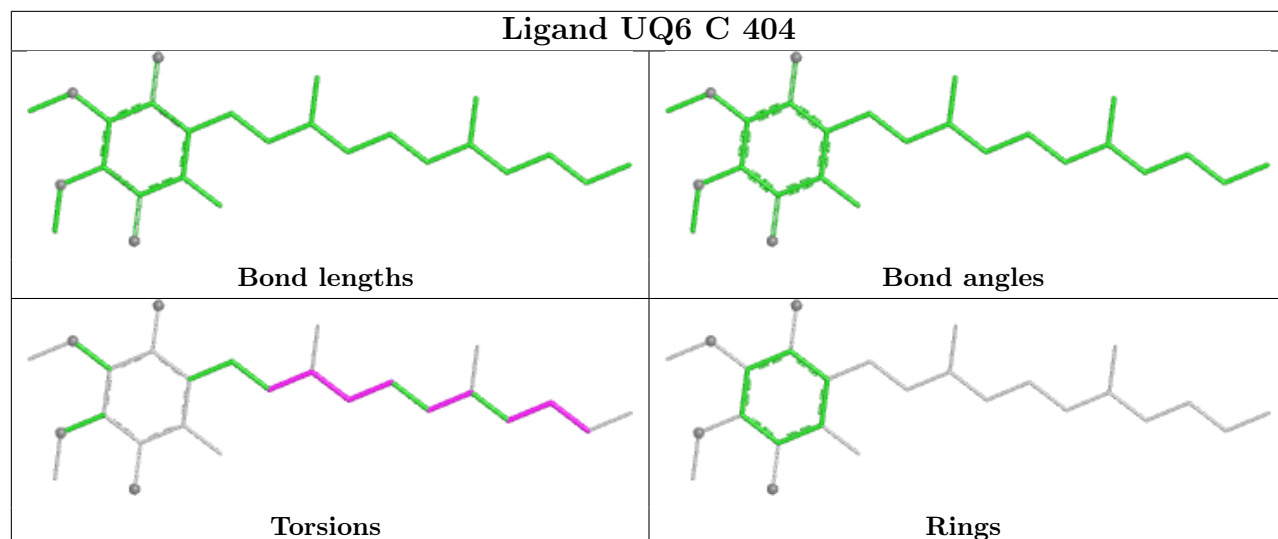


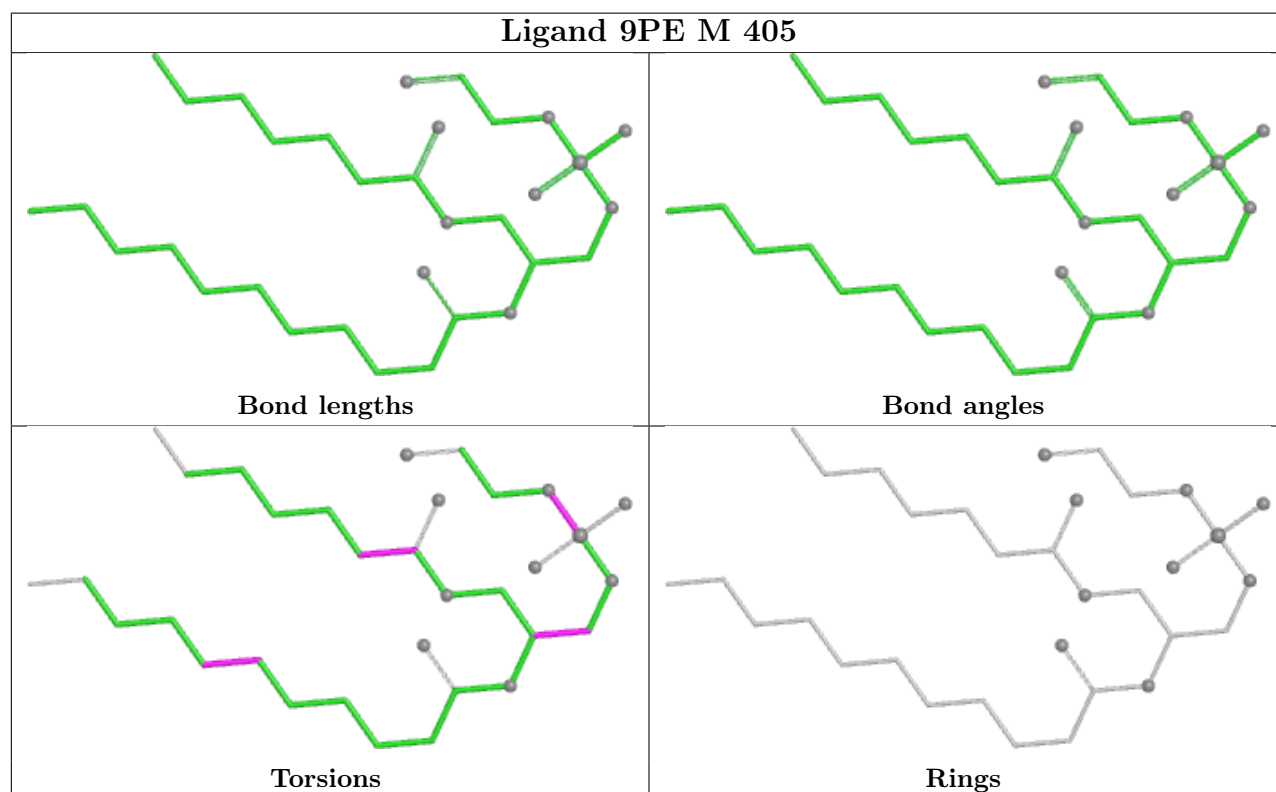
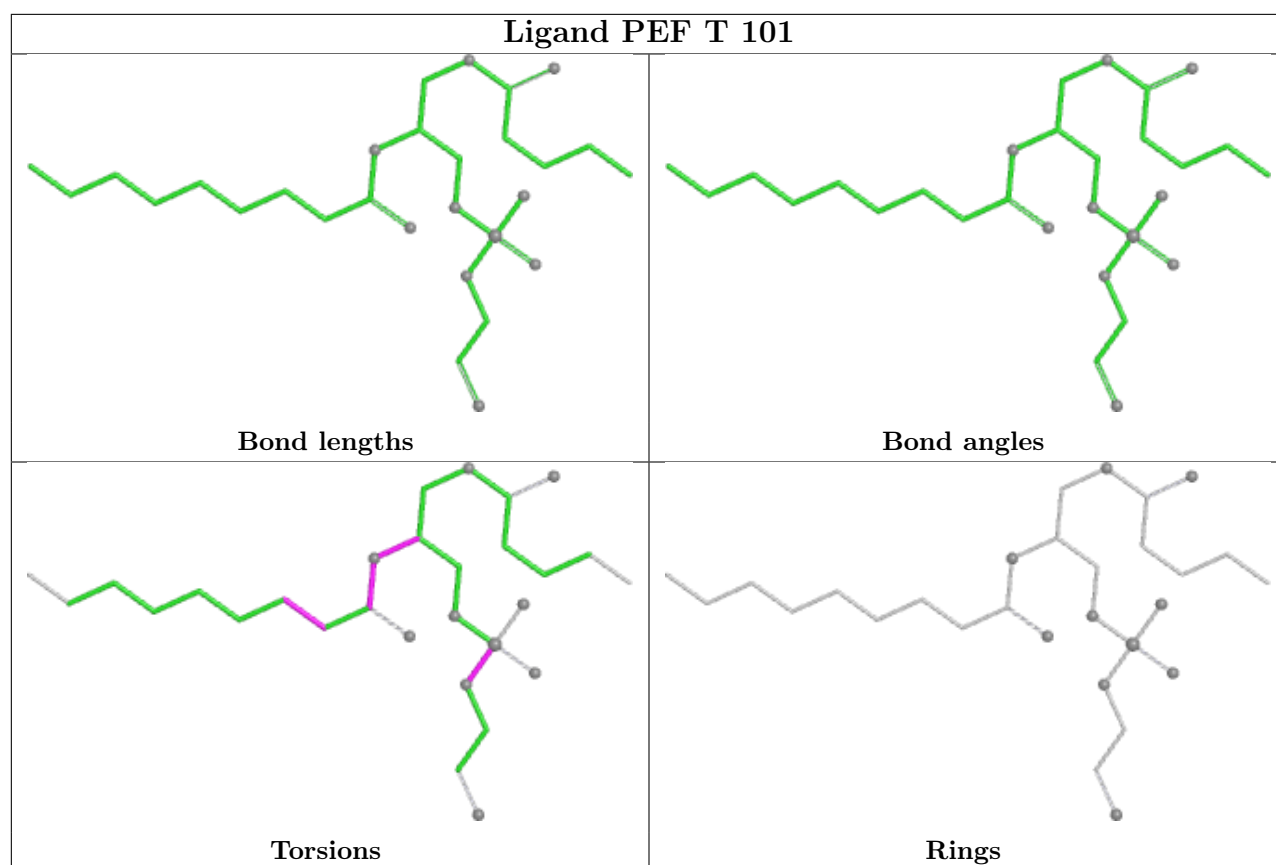


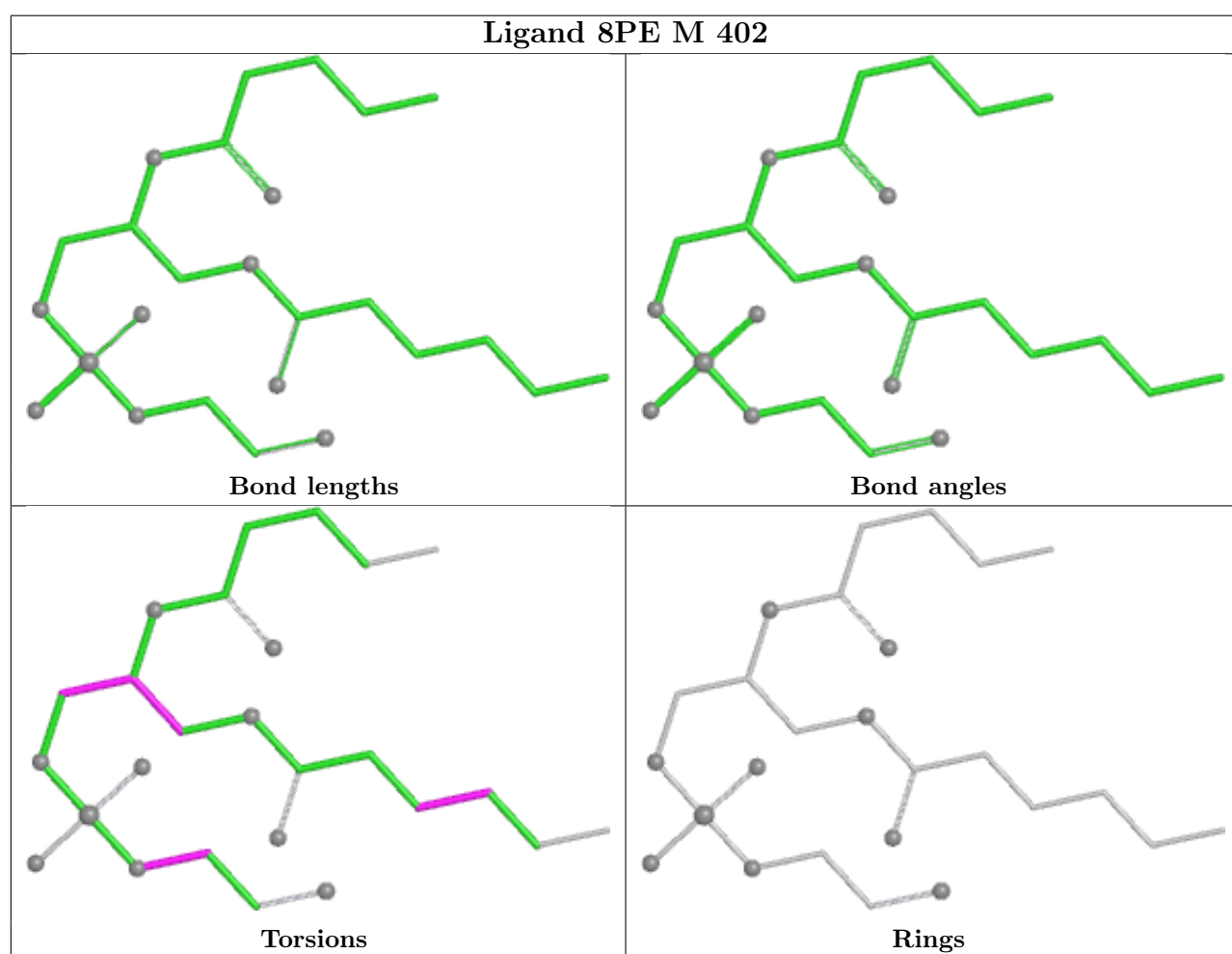
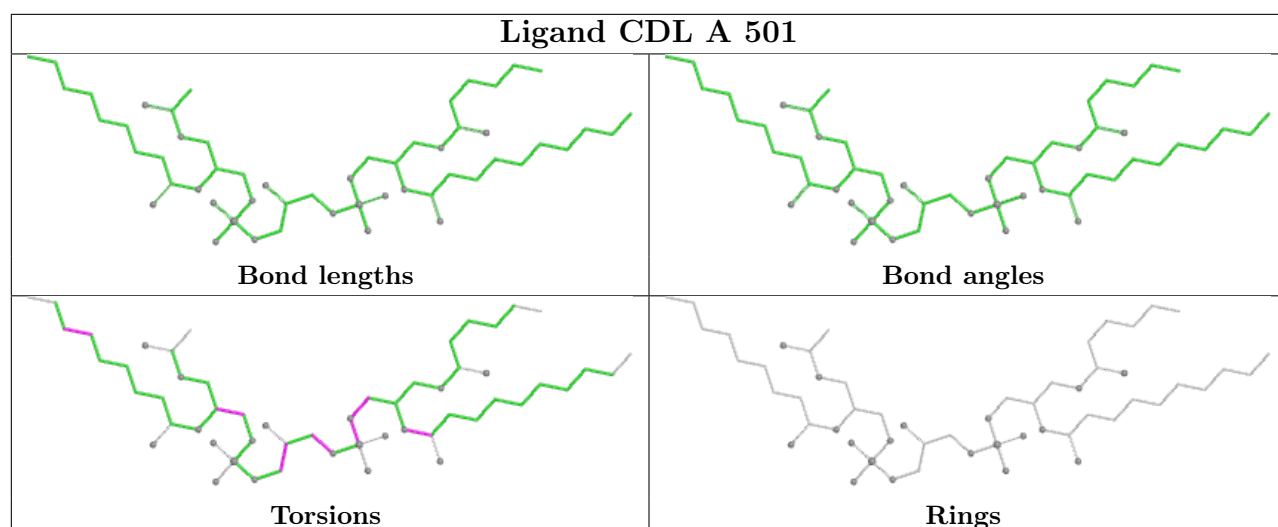


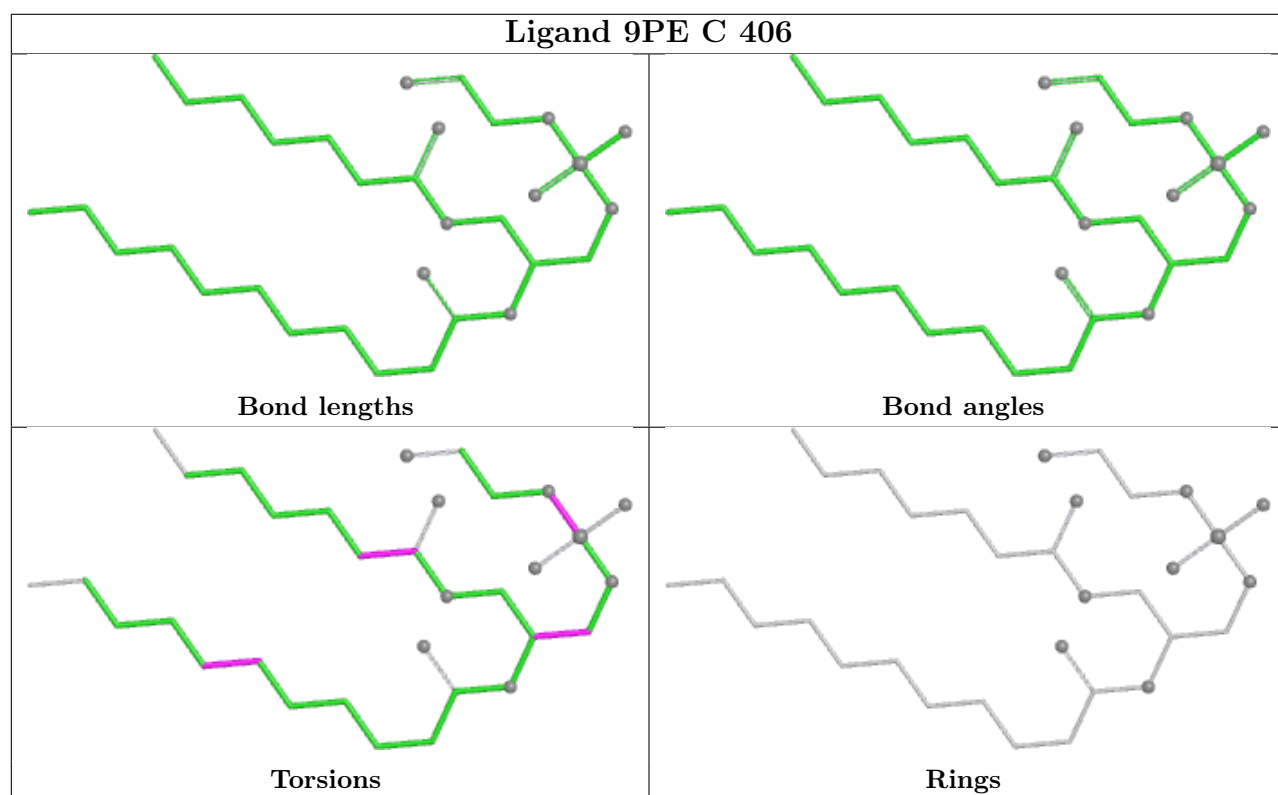
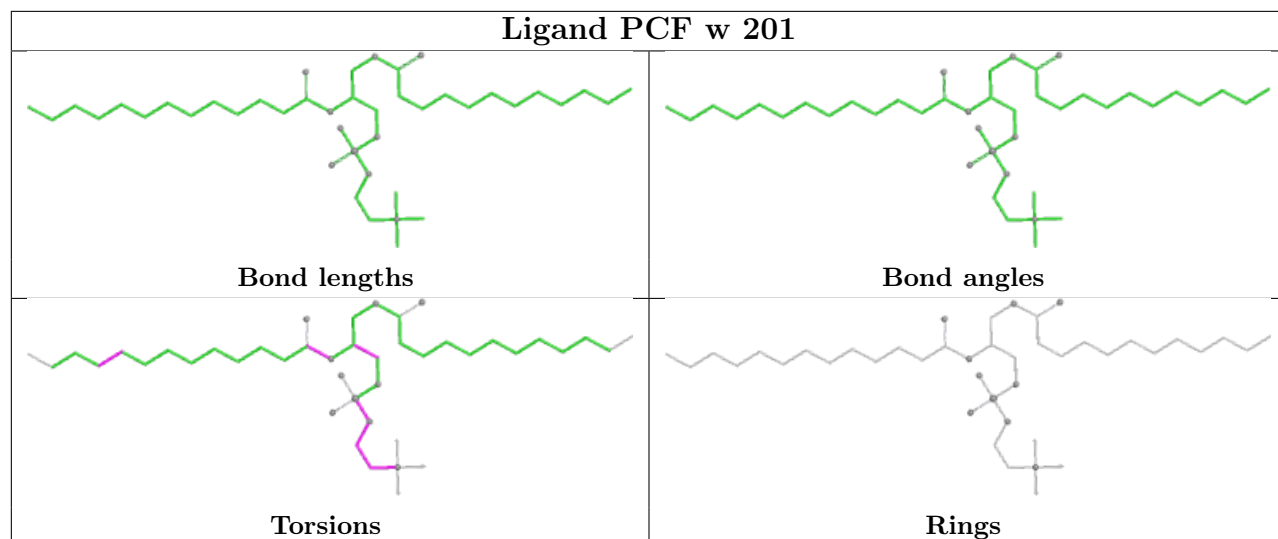


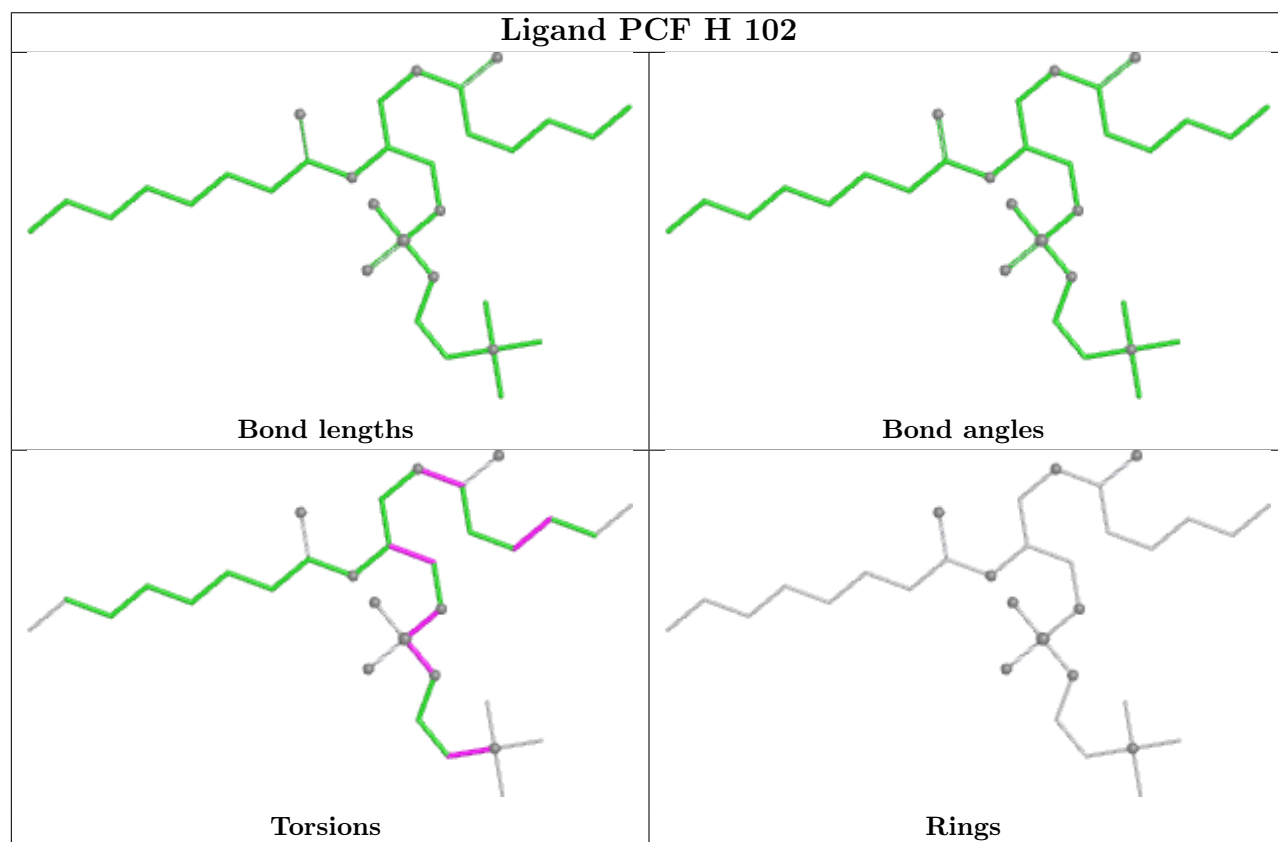
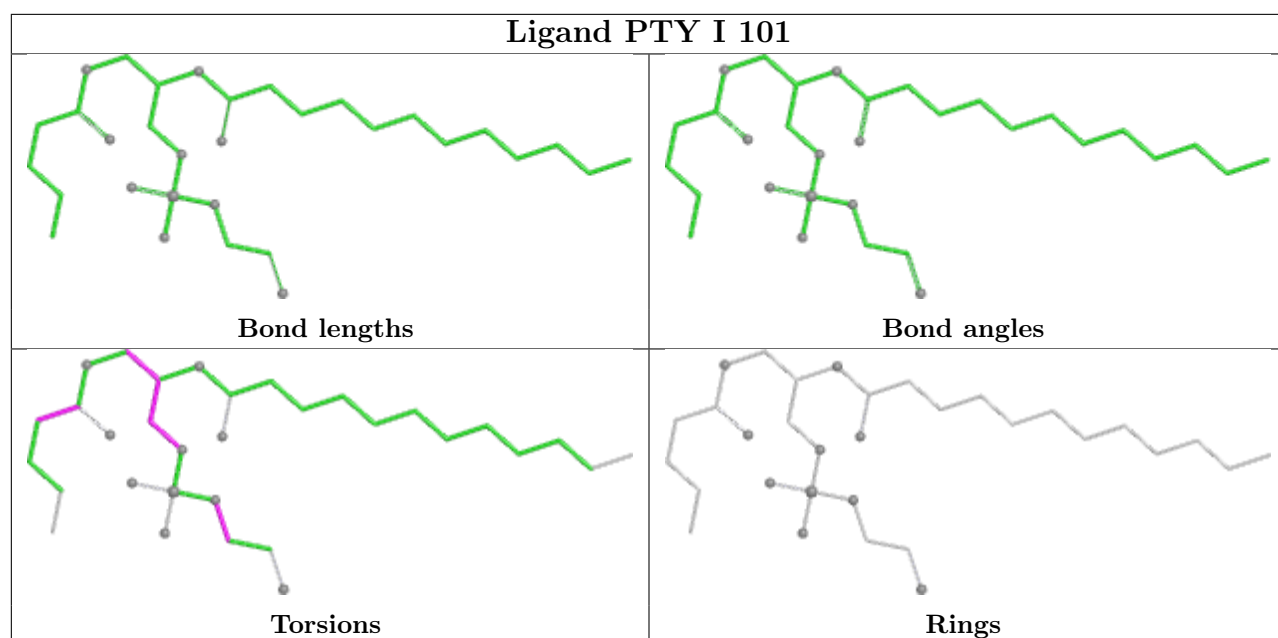


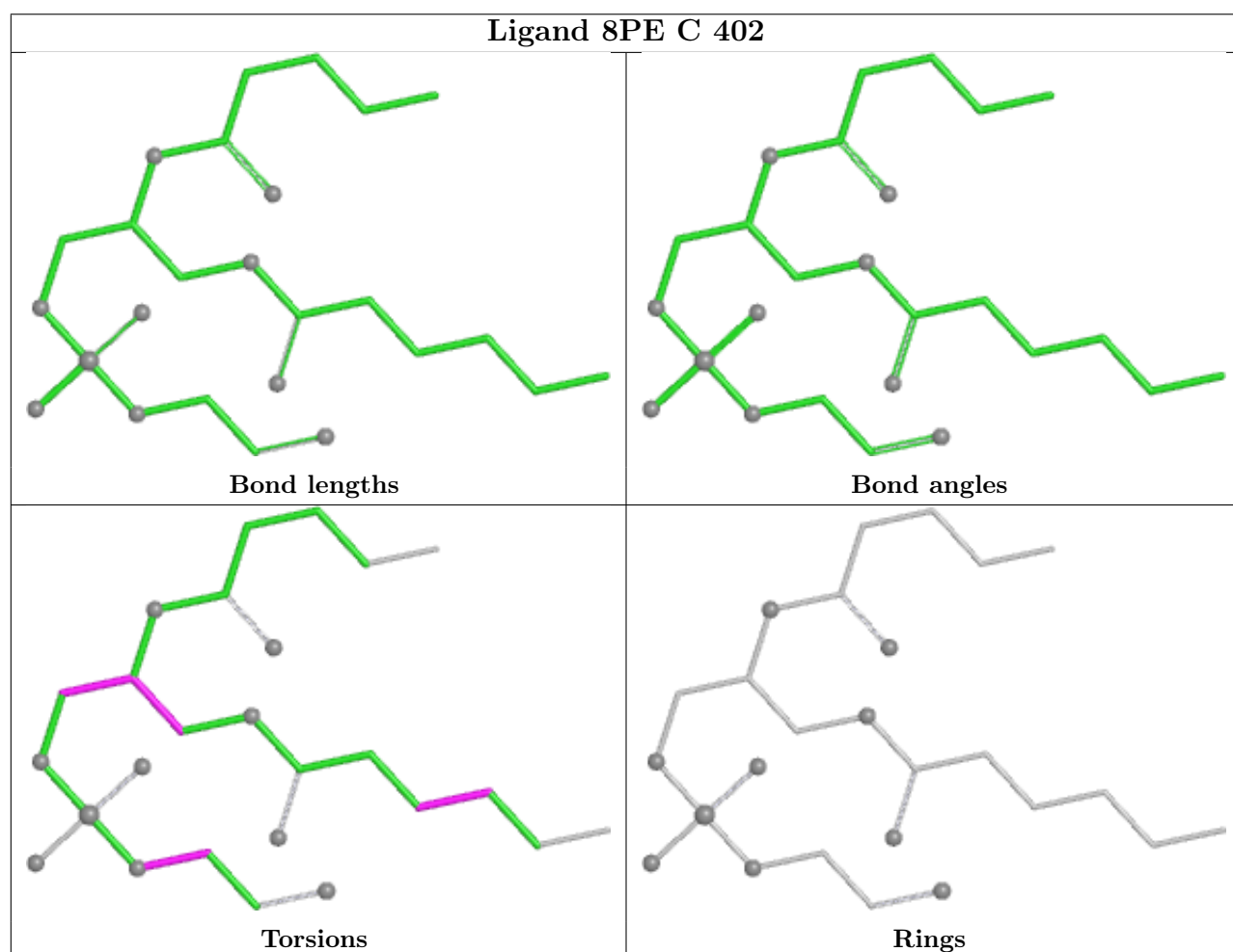
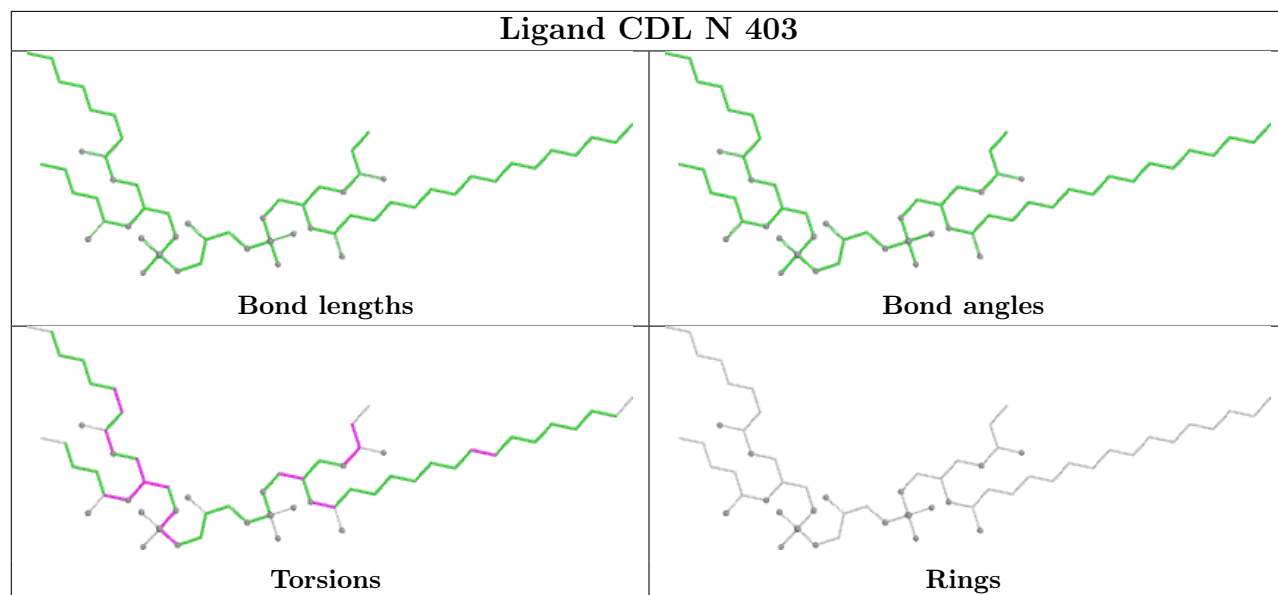


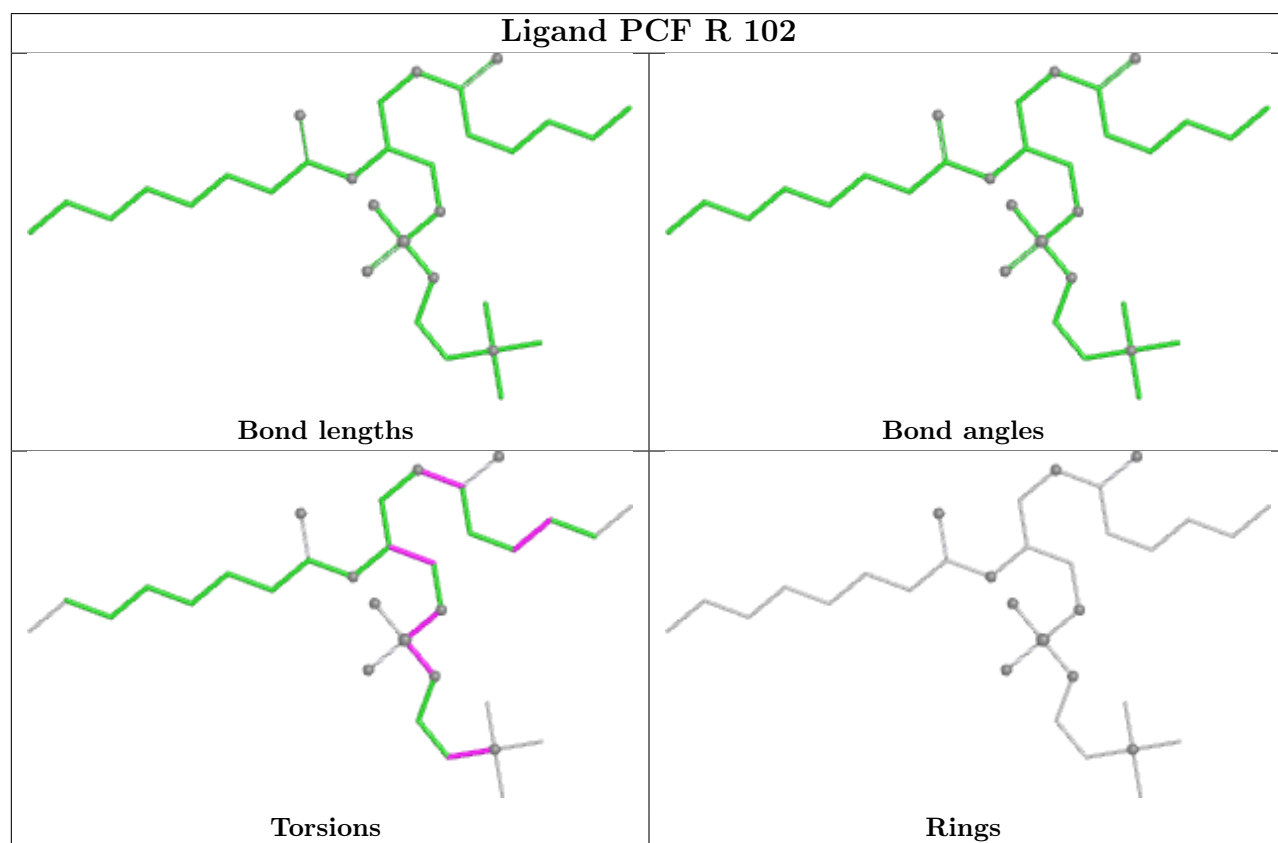
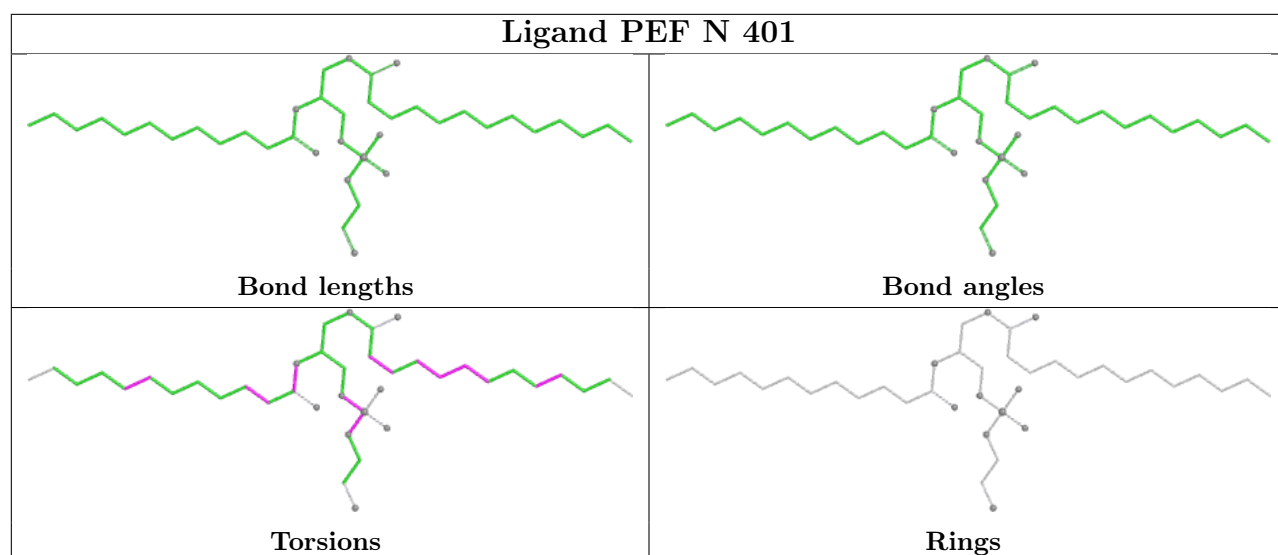


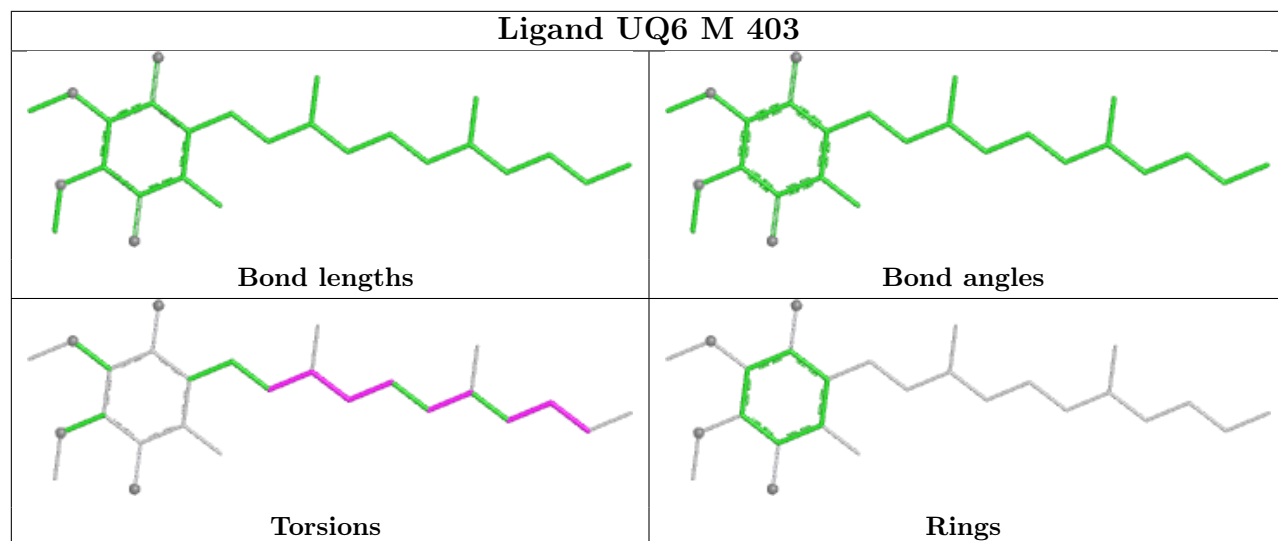












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

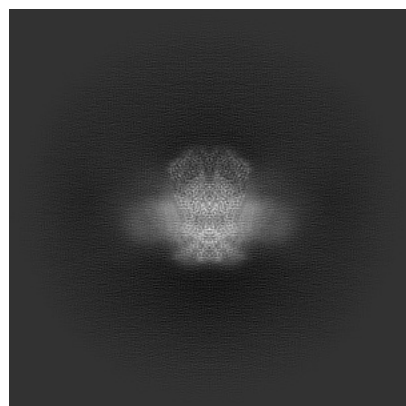
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44770. These allow visual inspection of the internal detail of the map and identification of artifacts.

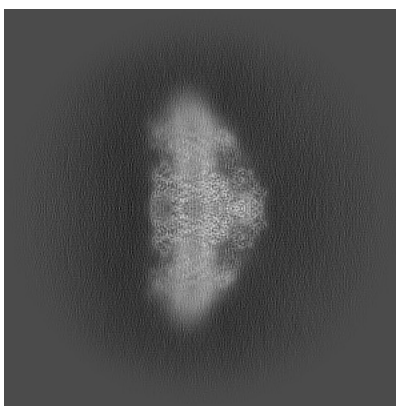
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

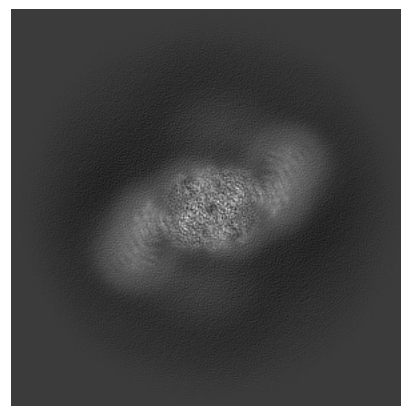
6.1.1 Primary map



X

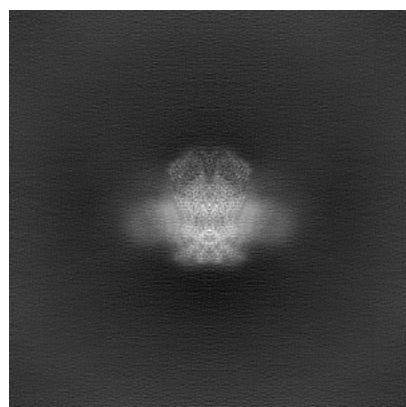


Y

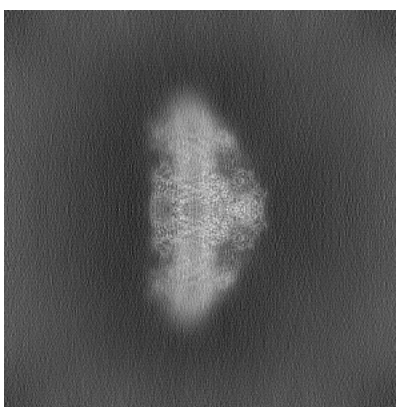


Z

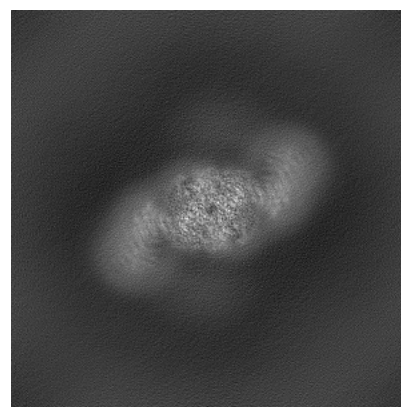
6.1.2 Raw map



X



Y

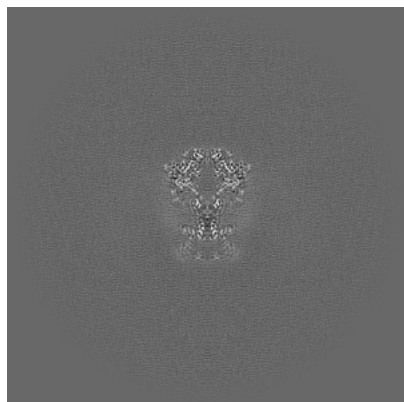


Z

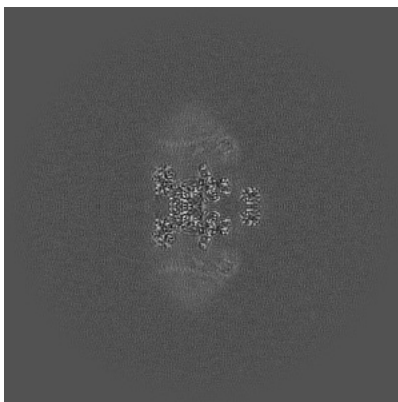
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

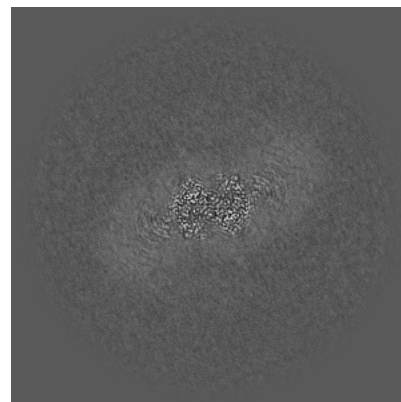
6.2.1 Primary map



X Index: 225

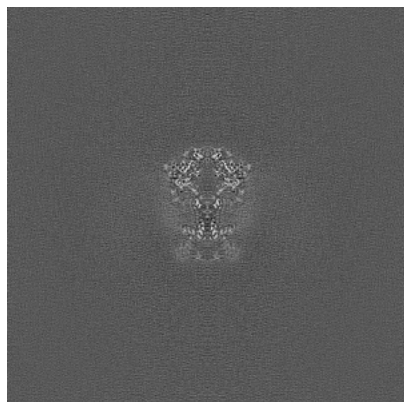


Y Index: 225

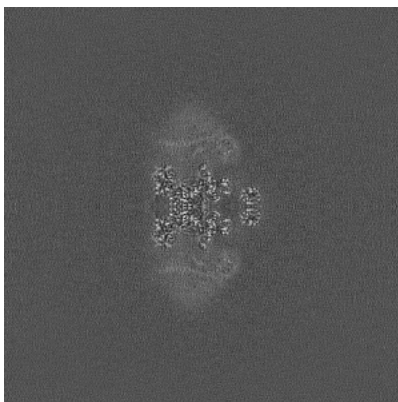


Z Index: 225

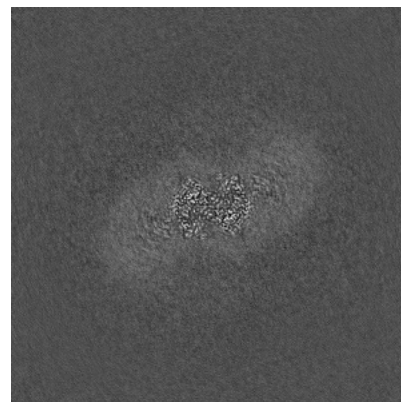
6.2.2 Raw map



X Index: 225



Y Index: 225

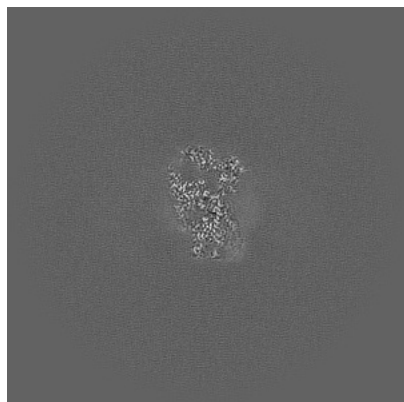


Z Index: 225

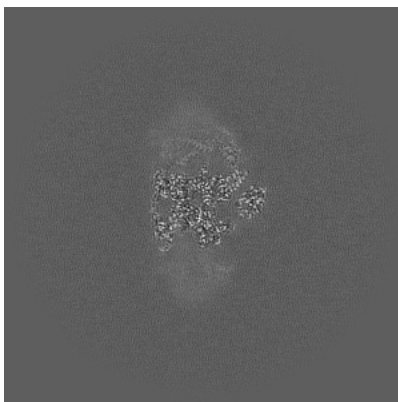
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

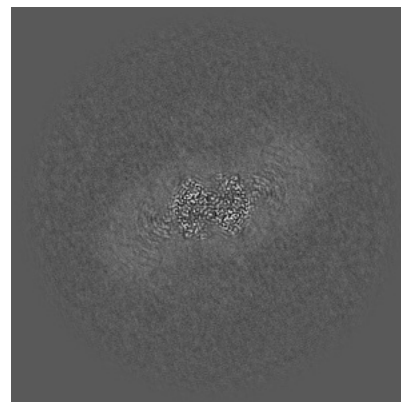
6.3.1 Primary map



X Index: 214

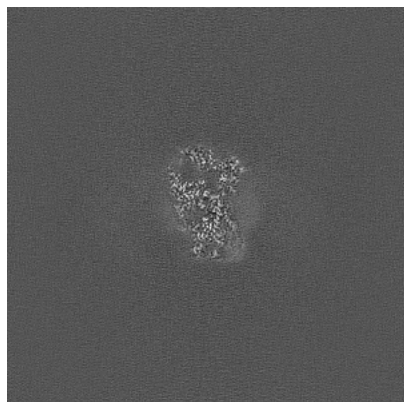


Y Index: 232

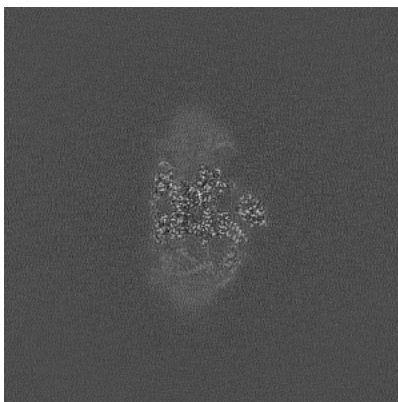


Z Index: 225

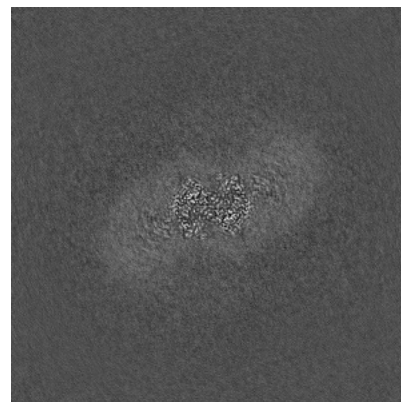
6.3.2 Raw map



X Index: 214



Y Index: 218

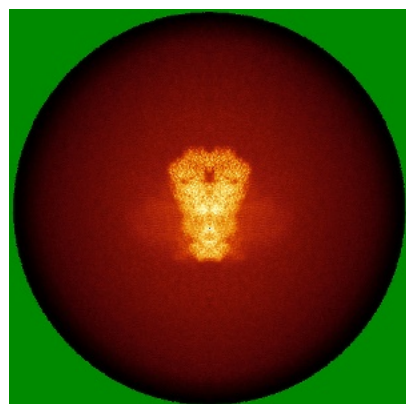


Z Index: 225

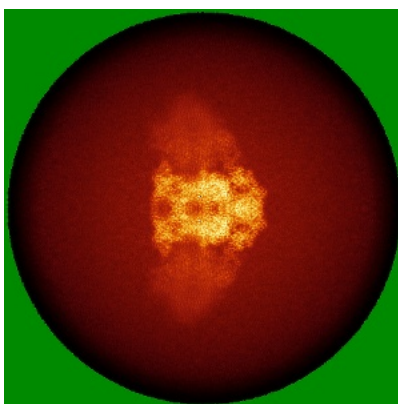
The images above show the largest variance slices of the map in three orthogonal directions.

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

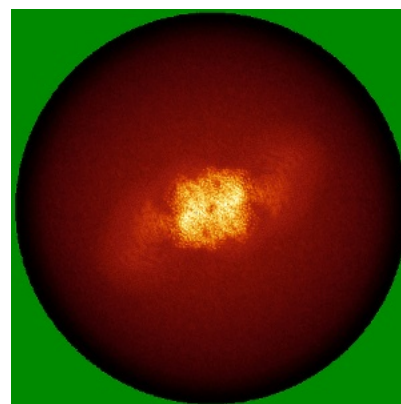
6.4.1 Primary map



X

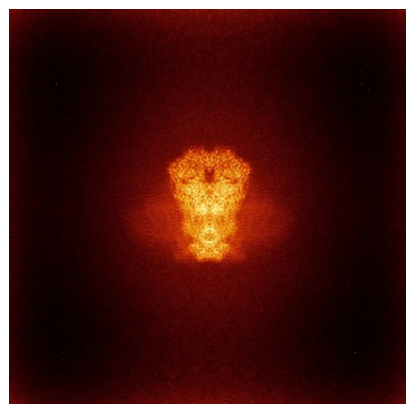


Y

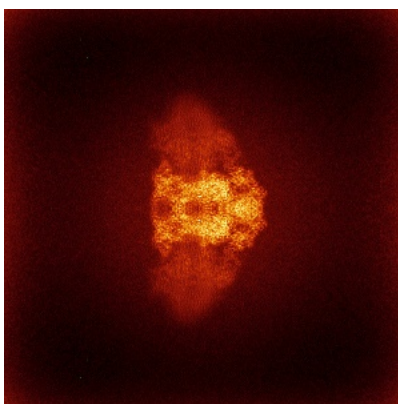


Z

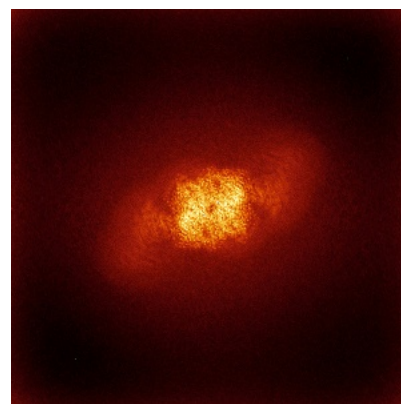
6.4.2 Raw map



X



Y

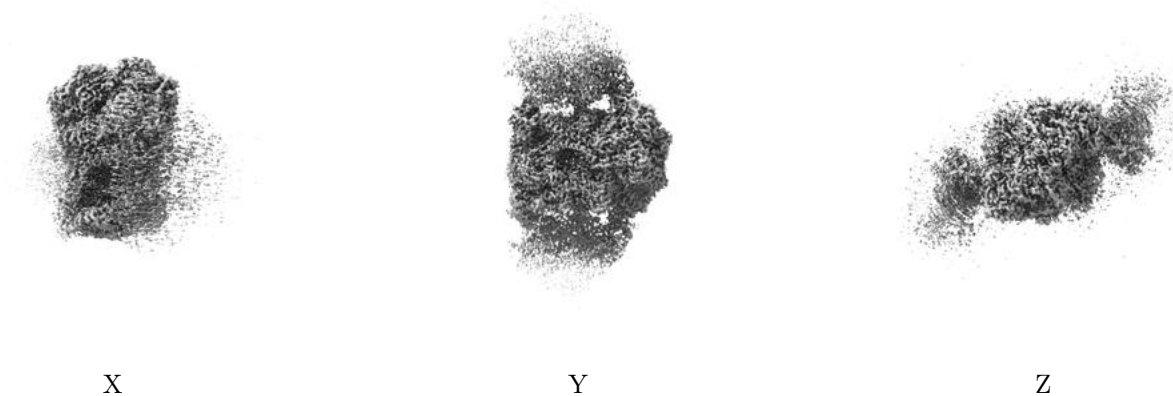


Z

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.

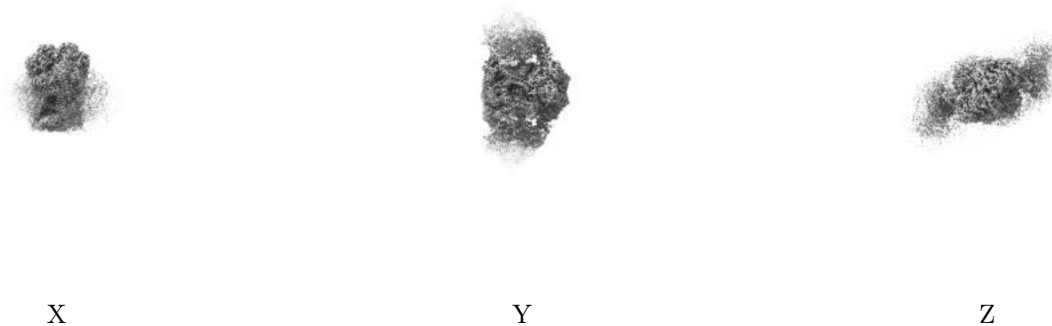
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

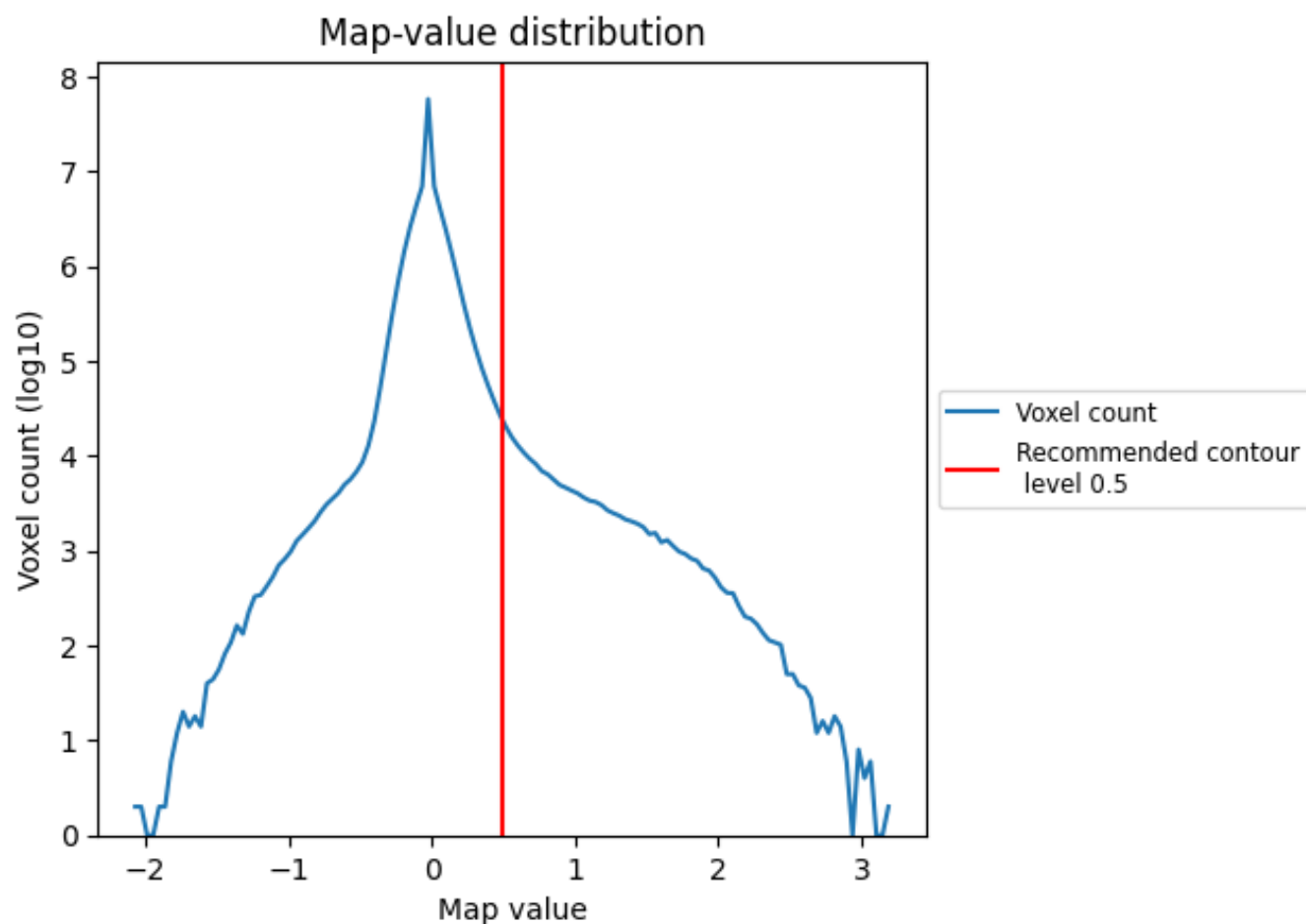
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

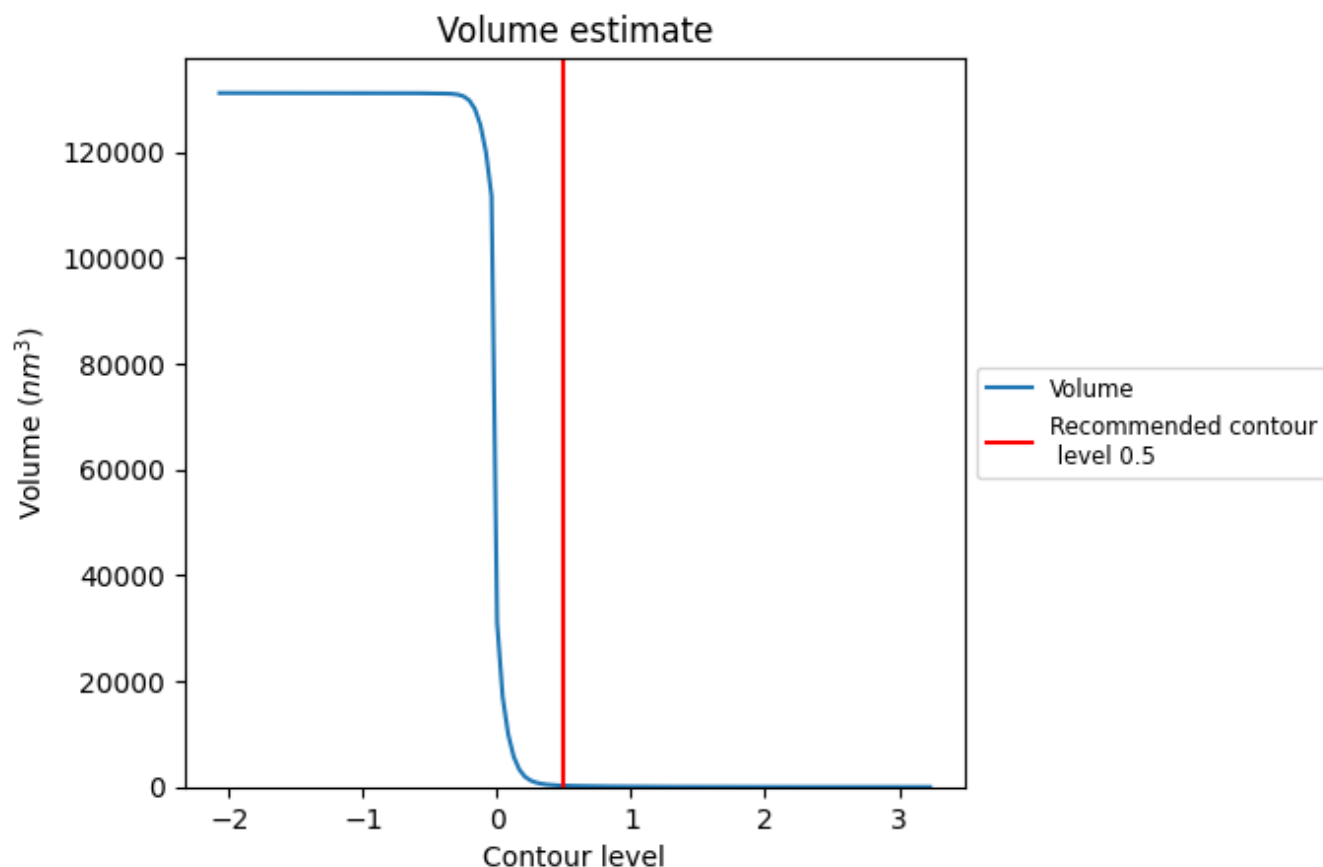
This section contains the results of statistical analysis of the map.

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.

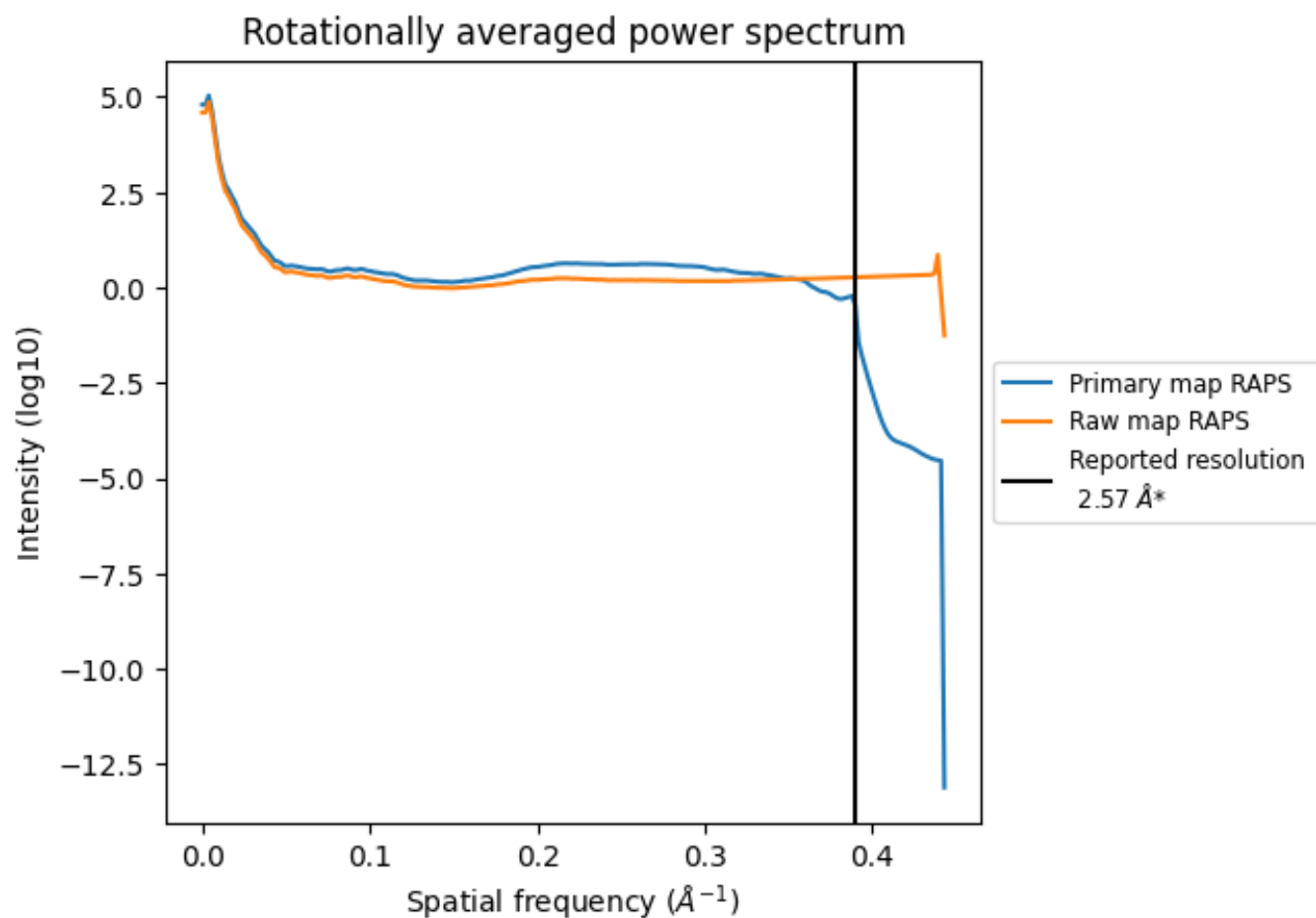
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 219 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 ⓘ

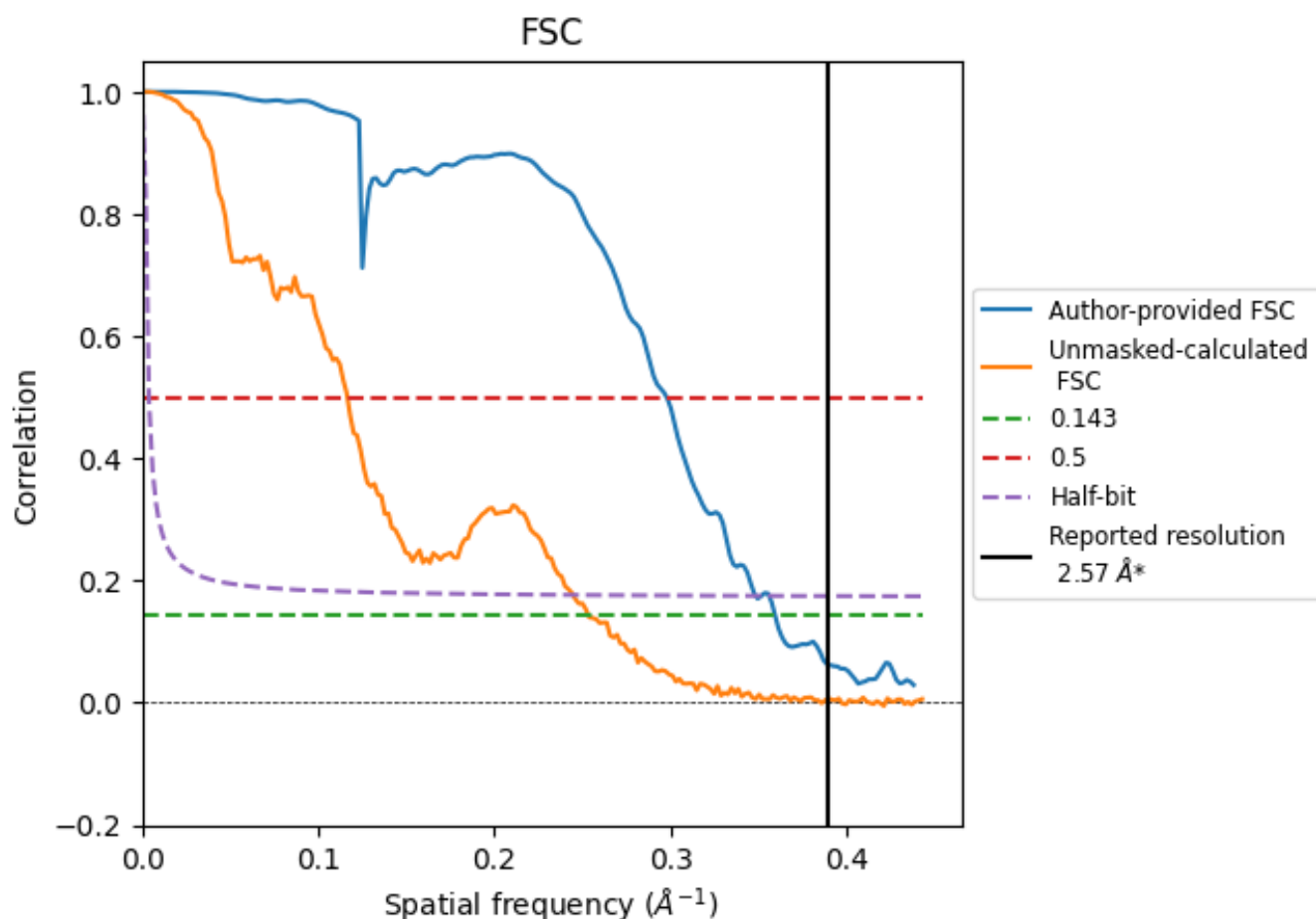


*Reported resolution corresponds to spatial frequency of 0.389 Å⁻¹

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 0.389 Å⁻¹

8.2 Resolution estimates

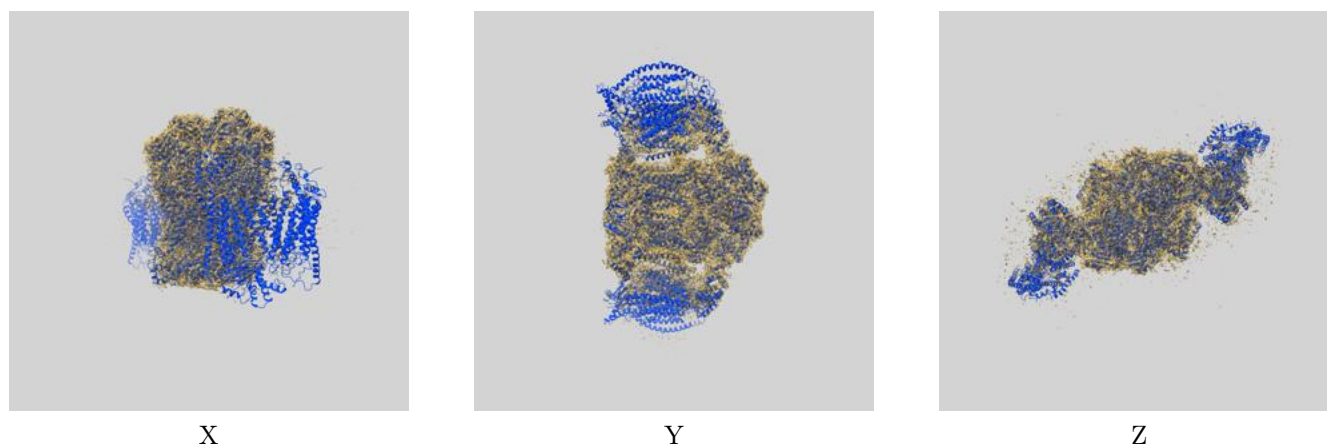
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.78	3.36	2.87
Unmasked-calculated*	3.95	8.58	4.09

*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 3.95 differs from the reported value 2.57 by more than 10 %

9 Map-model fit [i](#)

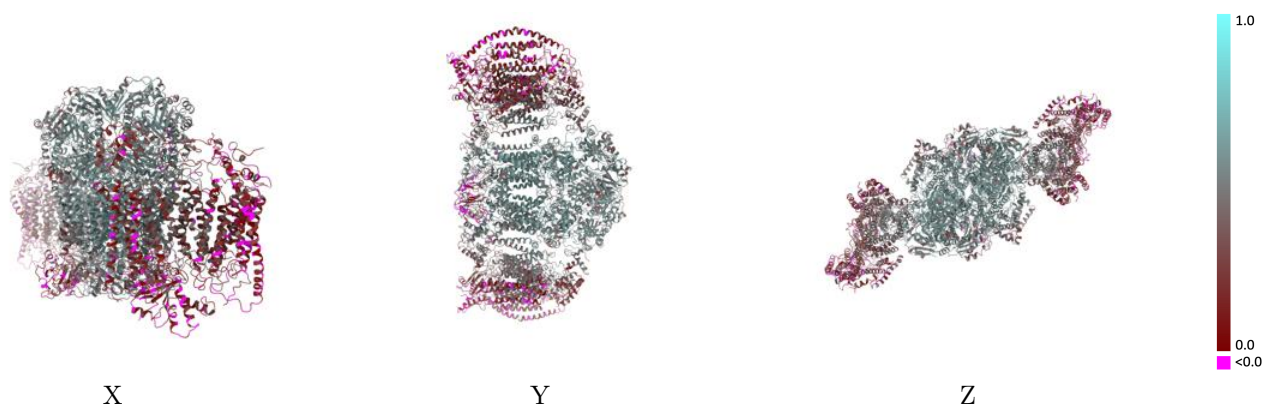
This section contains information regarding the fit between EMDB map EMD-44770 and PDB model 9BPB. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



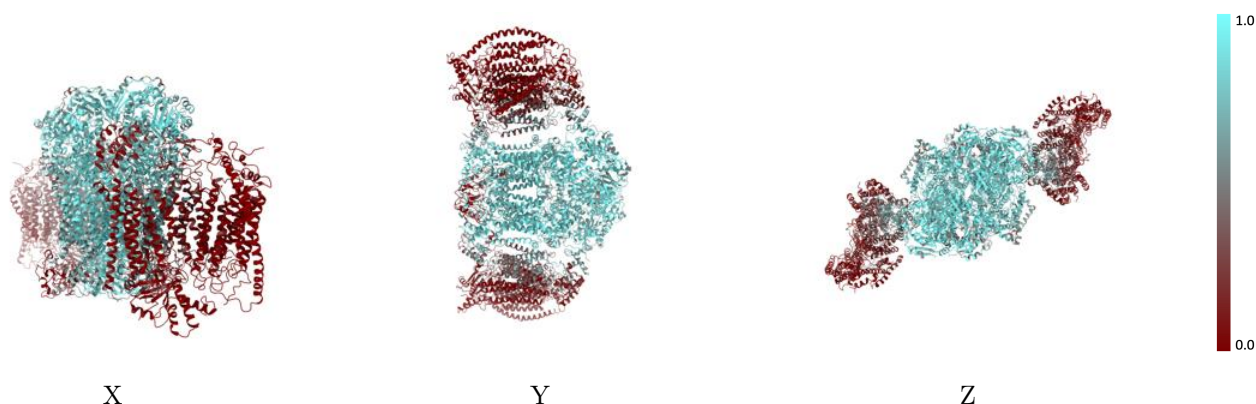
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



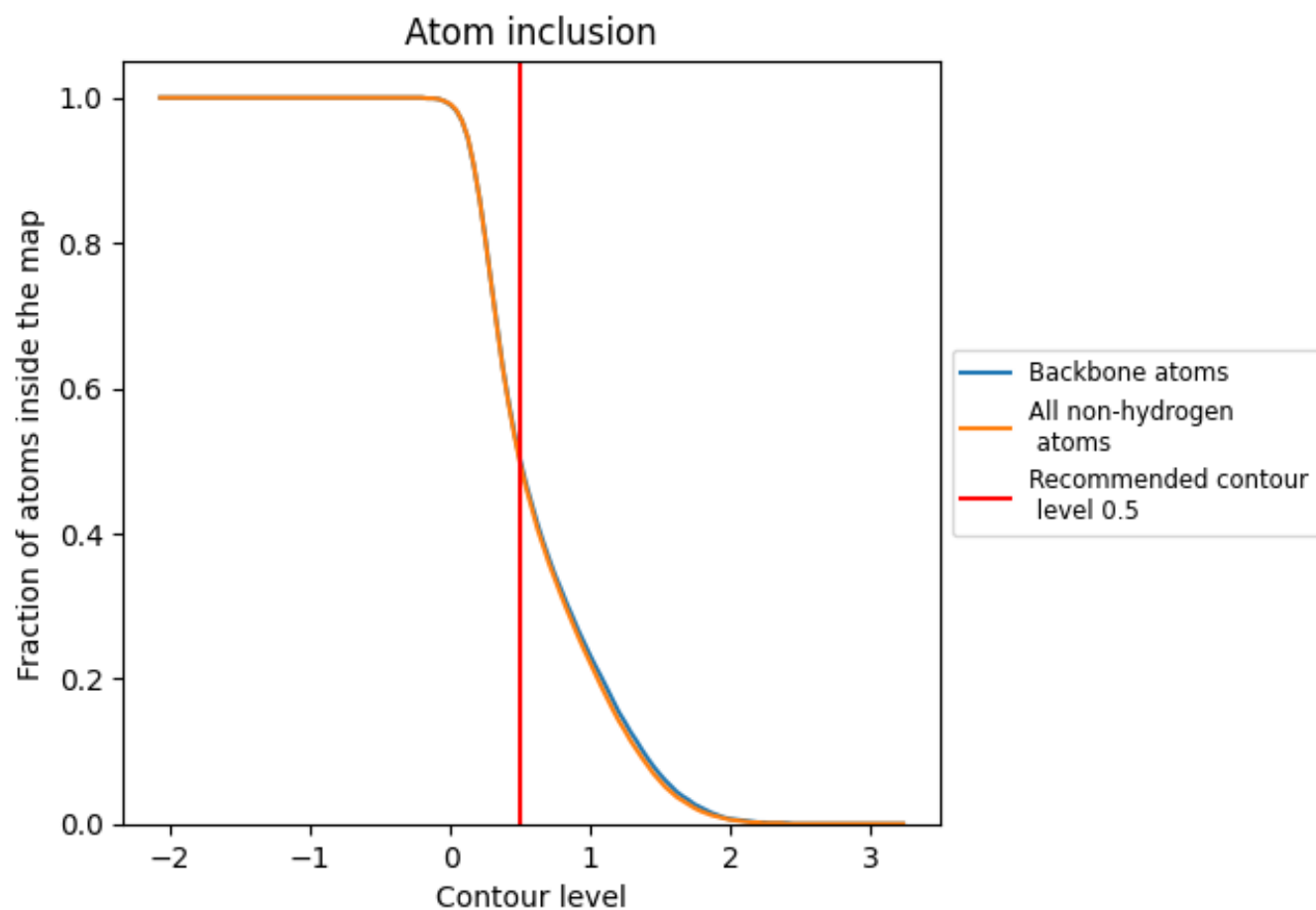
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4950	 0.4000
A	 0.8630	 0.5680
B	 0.8230	 0.5170
C	 0.8730	 0.5730
D	 0.8460	 0.5330
E	 0.3640	 0.2620
F	 0.5450	 0.3850
G	 0.7980	 0.5160
H	 0.7770	 0.5180
I	 0.8170	 0.5720
J	 0.5880	 0.4820
K	 0.8640	 0.5700
L	 0.8160	 0.5160
M	 0.8840	 0.5790
N	 0.8490	 0.5420
O	 0.3690	 0.2690
P	 0.5410	 0.3910
Q	 0.8220	 0.5310
R	 0.7870	 0.5240
S	 0.8250	 0.5750
T	 0.6020	 0.4800
a	 0.2470	 0.3670
b	 0.1120	 0.2250
c	 0.0190	 0.1780
d	 0.1220	 0.2240
e	 0.4680	 0.3950
f	 0.2000	 0.2730
g	 0.0090	 0.1430
i	 0.0710	 0.1490
j	 0.0050	 0.1020
k	 0.0030	 0.0890
l	 0.1890	 0.3040
m	 0.2580	 0.3800
n	 0.1080	 0.2310
o	 0.0190	 0.1870



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Chain	Atom inclusion	Q-score
p	 0.1300	 0.2430
q	 0.4700	 0.4030
r	 0.2250	 0.2850
s	 0.0070	 0.1450
u	 0.0460	 0.1510
v	 0.0050	 0.1070
w	 0.0020	 0.0900
x	 0.2140	 0.3120