



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 04:06 PM EST

PDB ID : 8E7S
EMDB ID : EMD-27940
Title : III2IV2 respiratory supercomplex from *Saccharomyces cerevisiae* with 4 bound UQ6
Authors : Hryc, C.F.; Mileykovskaya, E.; Baker, M.; Dowhan, W.
Deposited on : 2022-08-24
Resolution : 3.20 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:

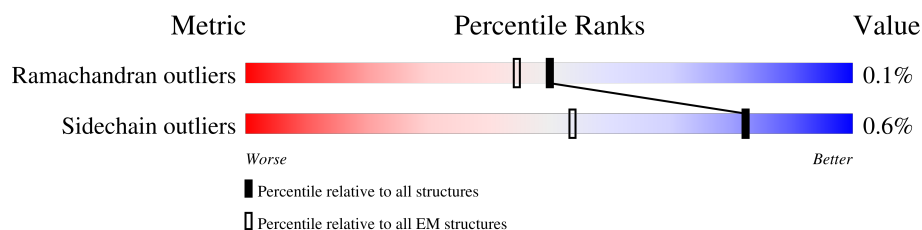
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.20 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.




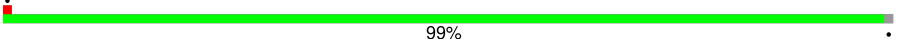
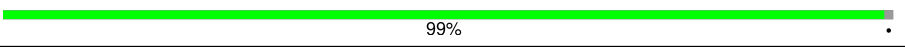

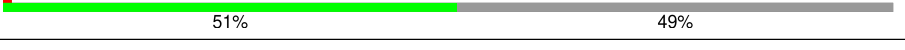
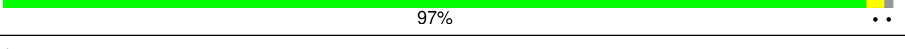
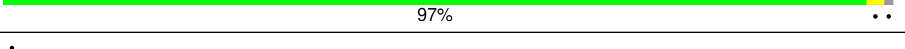
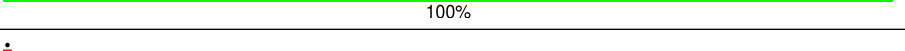
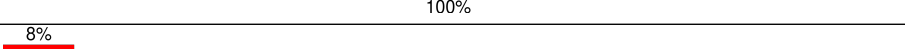
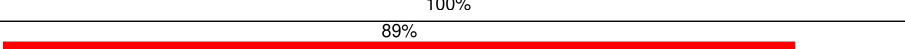
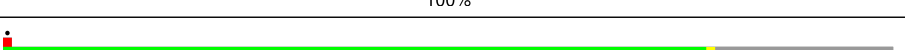

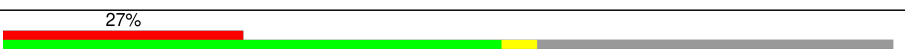

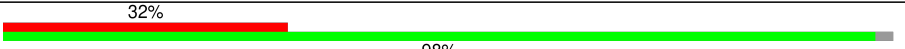
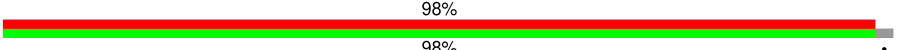

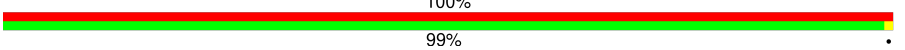
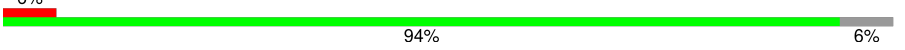
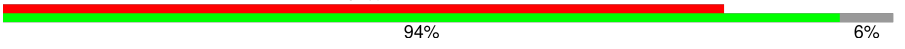
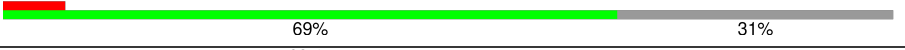




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 94% • 6%
1	a	457	 94% • 6%
2	B	368	 95% •
2	b	368	 96% •
3	C	215	 10% 86% 14%
3	c	215	 16% 86% 14%
4	D	77	 8% 86% 14%
4	d	77	 25% 86% 14%
5	E	66	 86% 14%

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Mol	Chain	Length	Quality of chain
5	e	66	
6	F	127	
6	f	127	
7	G	147	
7	g	147	
8	H	94	
8	h	94	
9	J	385	
9	j	385	
10	K	534	
10	k	534	
11	L	309	
11	l	309	
12	M	78	
12	m	78	
13	N	60	
13	n	60	
14	O	269	
14	o	269	
15	P	251	
15	p	251	
16	Q	148	
16	q	148	
17	R	59	
17	r	59	

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Mol	Chain	Length	Quality of chain
18	S	129	
18	s	129	
19	T	155	
19	t	155	
20	U	83	
20	u	83	
21	V	66	
21	v	66	
22	W	153	
22	w	153	

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
25	CDL	C	302	X	-	-	-
25	CDL	H	601	X	-	-	-
25	CDL	J	403	X	-	-	-
25	CDL	K	603	X	-	-	-
25	CDL	L	402	X	-	-	-
25	CDL	c	302	X	-	-	-
25	CDL	h	601	X	-	-	-
25	CDL	h	602	X	-	-	-
25	CDL	j	402	X	-	-	-
25	CDL	k	602	X	-	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 62847 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-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	a	431	Total	C	N	O	S	0	0
			3345	2110	576	653	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	b	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	66	Total	C	N	O	S	0	0
			521	344	84	91	2		
4	d	66	Total	C	N	O	S	0	0
			521	344	84	91	2		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	57	Total	C	N	O	0	0
			465	310	77	78		
5	e	57	Total	C	N	O	0	0
			465	310	77	78		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
6	f	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
7	g	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	h	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 9 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
9	j	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

- Molecule 11 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
11	l	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	47	Total	C	N	O	S	0	0
			382	261	62	58	1		
12	m	47	Total	C	N	O	S	0	0
			382	261	62	58	1		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	59	Total	C	N	O		0	0
			484	328	83	73			
13	n	59	Total	C	N	O		0	0
			484	328	83	73			

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		
15	p	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	102	Total	C	N	O	S	0	0
			851	545	137	168	1		
16	q	102	Total	C	N	O	S	0	0
			851	545	137	168	1		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	55	Total	C	N	O	S	0	0
			455	300	79	73	3		
17	r	55	Total	C	N	O	S	0	0
			455	300	79	73	3		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	113	Total	C	N	O	S	0	0
			928	605	160	160	3		
18	s	113	Total	C	N	O	S	0	0
			928	605	160	160	3		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	121	Total	C	N	O	S	0	0
			913	576	151	181	5		
19	t	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	77	Total	C	N	O	S	0	0
			642	410	109	118	5		
20	u	77	Total	C	N	O	S	0	0
			642	410	109	118	5		

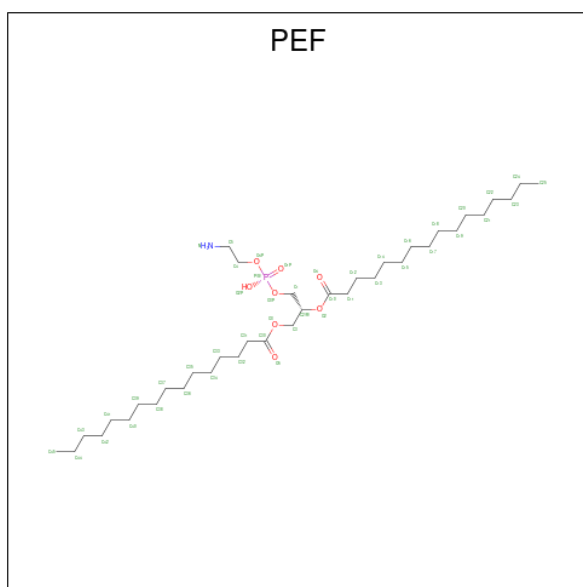
- Molecule 21 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	45	Total	C	N	O	S	0	0
			361	238	63	59	1		
21	v	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		
22	w	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		

- Molecule 23 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$) (labeled as "Ligand of Interest" by depositor).



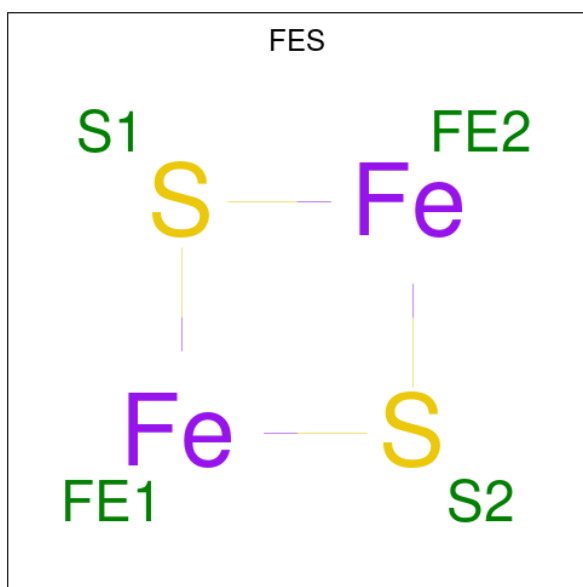
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
23	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	C	1	Total	C	N	O	P	0
			32	22	1	8	1	

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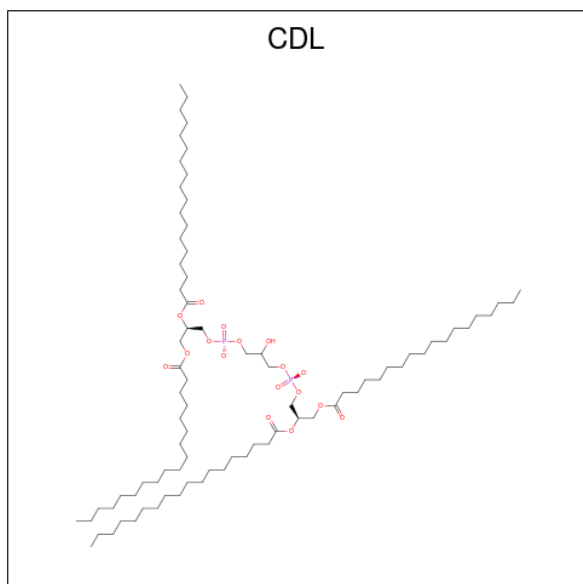
Mol	Chain	Residues	Atoms					AltConf
23	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	J	1	Total	C	N	O	P	0
			45	35	1	8	1	
23	J	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	V	1	Total	C	N	O	P	0
			33	23	1	8	1	
23	W	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
23	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	a	1	Total	C	N	O	P	0
			31	21	1	8	1	
23	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	c	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	c	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	e	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	j	1	Total	C	N	O	P	0
			45	35	1	8	1	
23	j	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	j	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	v	1	Total	C	N	O	P	0
			33	23	1	8	1	
23	w	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	w	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	Fe	S	0
			4	2	2	
24	c	1	Total	Fe	S	0
			4	2	2	

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



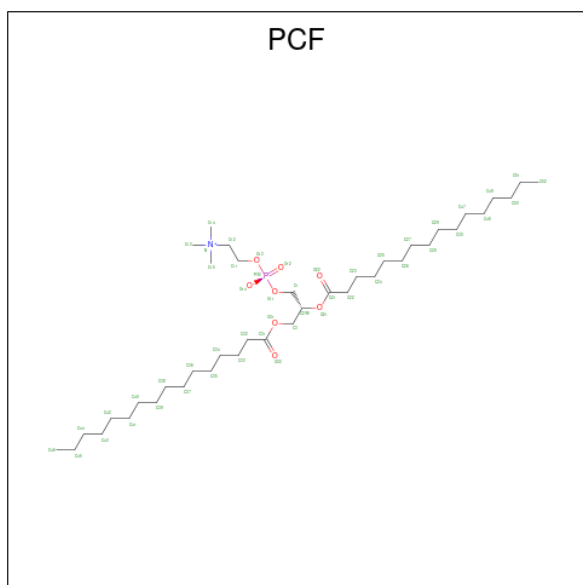
Mol	Chain	Residues	Atoms				AltConf
25	C	1	Total	C	O	P	0
			53	34	17	2	

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Mol	Chain	Residues	Atoms				AltConf
25	H	1	Total	C	O	P	0
			53	34	17	2	
25	J	1	Total	C	O	P	0
			56	37	17	2	
25	K	1	Total	C	O	P	0
			67	48	17	2	
25	L	1	Total	C	O	P	0
			67	48	17	2	
25	c	1	Total	C	O	P	0
			48	29	17	2	
25	h	1	Total	C	O	P	0
			53	34	17	2	
25	h	1	Total	C	O	P	0
			67	48	17	2	
25	j	1	Total	C	O	P	0
			56	37	17	2	
25	k	1	Total	C	O	P	0
			67	48	17	2	

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



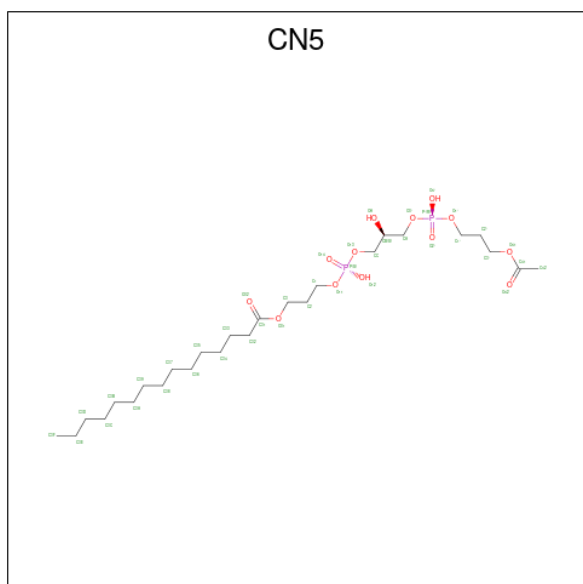
Mol	Chain	Residues	Atoms					AltConf
26	E	1	Total	C	N	O	P	0
			47	37	1	8	1	
26	H	1	Total	C	N	O	P	0
			50	40	1	8	1	

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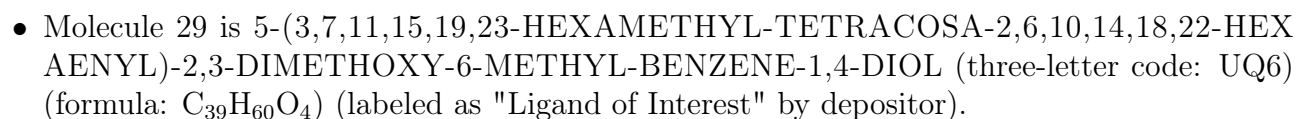
Mol	Chain	Residues	Atoms					AltConf
26	W	1	Total	C	N	O	P	0
			36	26	1	8	1	
26	a	1	Total	C	N	O	P	0
			47	37	1	8	1	
26	k	1	Total	C	N	O	P	0
			36	26	1	8	1	
26	w	1	Total	C	N	O	P	0
			50	40	1	8	1	

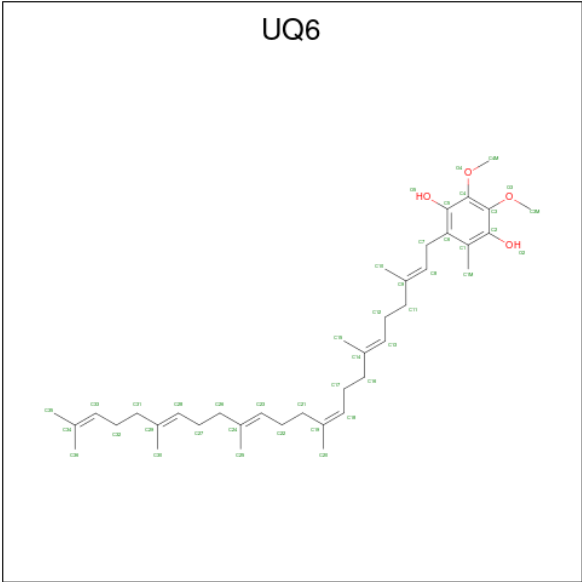
- Molecule 27 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (three-letter code: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



Mol	Chain	Residues	Atoms				AltConf
27	J	1	Total	C	O	P	0
			41	26	13	2	

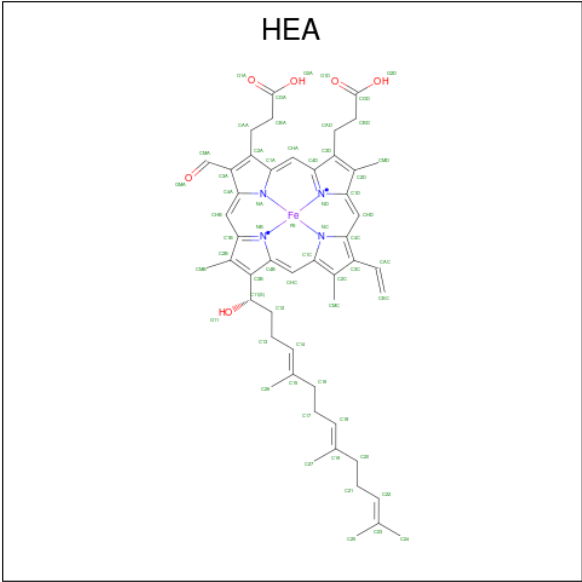
- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			43	39	4	
29	J	1	Total	C	O	0
			20	16	4	
29	j	1	Total	C	O	0
			43	39	4	
29	j	1	Total	C	O	0
			43	39	4	

- Molecule 30 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).

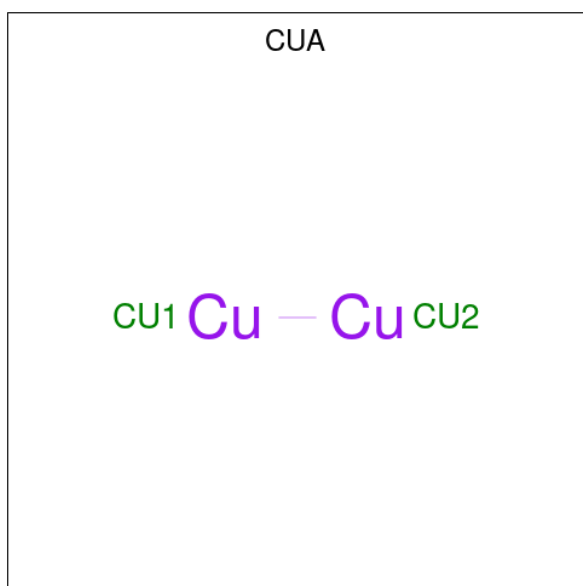


Mol	Chain	Residues	Atoms					AltConf
30	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	K	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
30	k	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 31 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
31	K	1	Total	Cu	0
			1	1	
31	k	1	Total	Cu	0
			1	1	

- Molecule 32 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



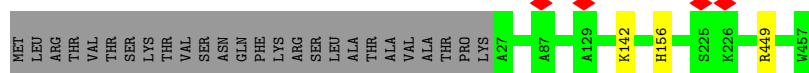
Mol	Chain	Residues	Atoms		AltConf
32	P	1	Total	Cu	0
			1	1	
32	P	1	Total	Cu	0
			1	1	
32	p	1	Total	Cu	0
			1	1	
32	p	1	Total	Cu	0
			1	1	

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.

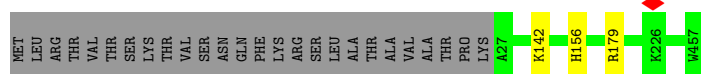
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A: 



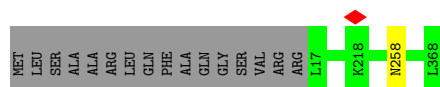
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain a: 



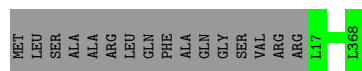
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 




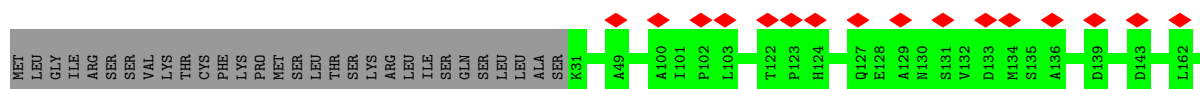
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

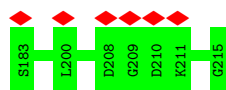
Chain b: 



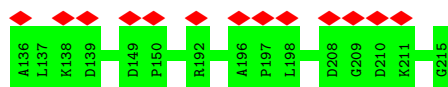
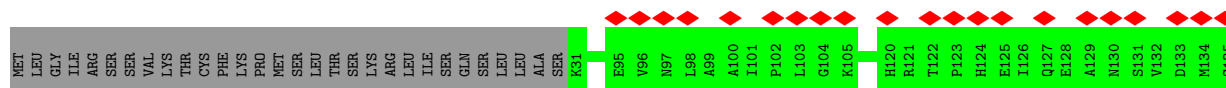
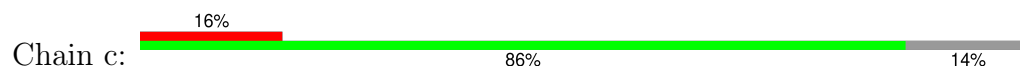
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain C: 

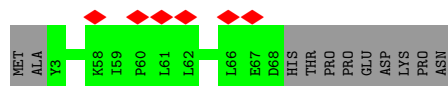
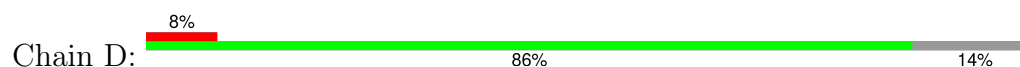




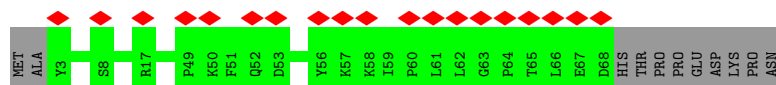
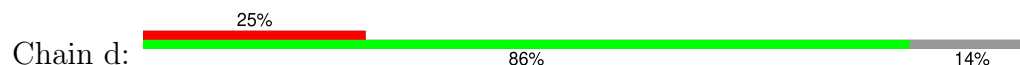
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



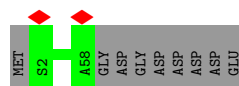
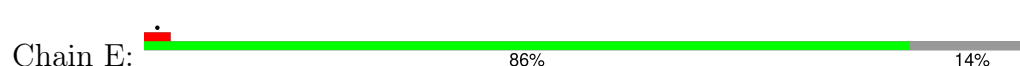
- Molecule 4: Cytochrome b-c1 complex subunit 10, mitochondrial



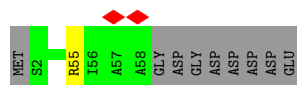
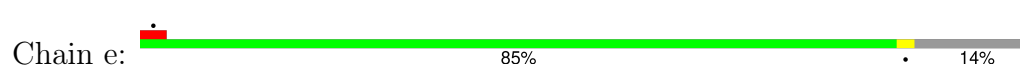
- Molecule 4: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 7, mitochondrial





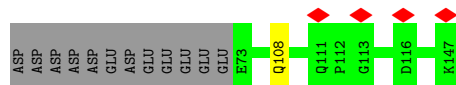
- Molecule 6: Cytochrome b-c1 complex subunit 7, mitochondrial

Chain f: 99%



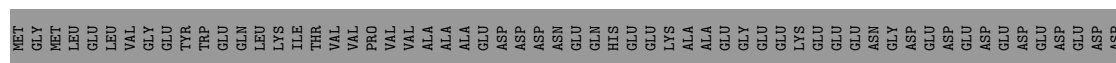
- Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain G: 50%



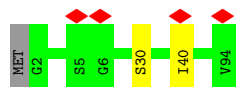
- Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain g: 51%



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

Chain H: 97%



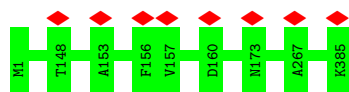
- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain h: 97%



- Molecule 9: Cytochrome b

Chain J: 100%



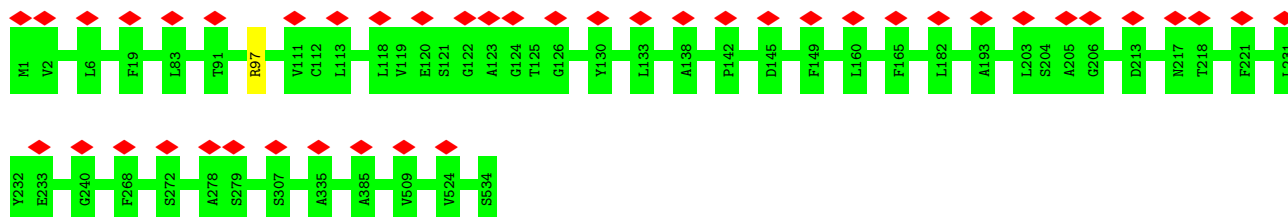
- Molecule 9: Cytochrome b

Chain j: 100%



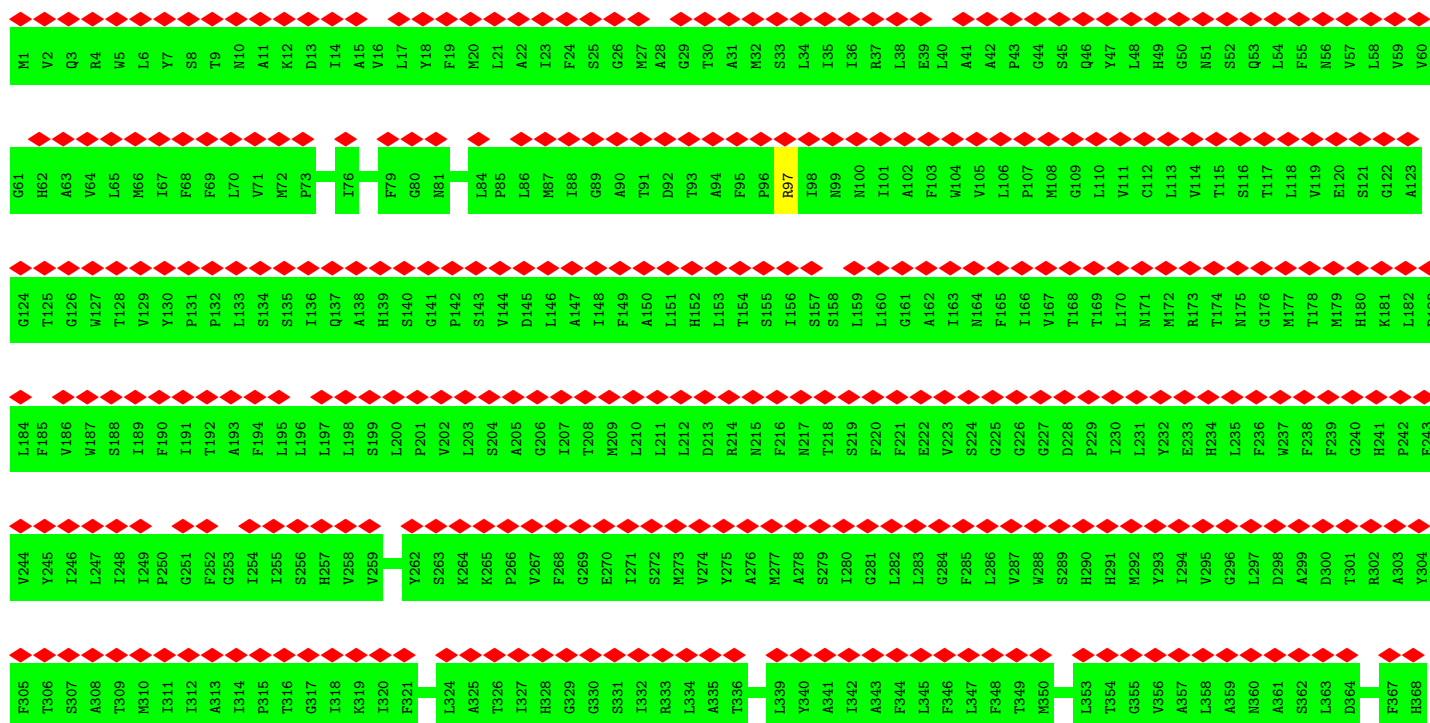
- Molecule 10: Cytochrome c oxidase subunit 1

Chain K: 8% 100%



- Molecule 10: Cytochrome c oxidase subunit 1

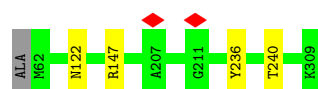
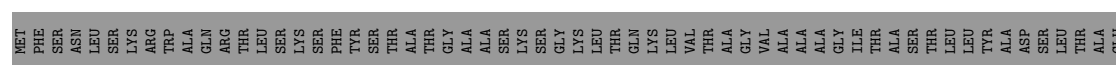
Chain k: 89% 100%





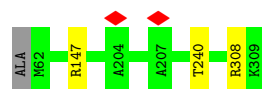
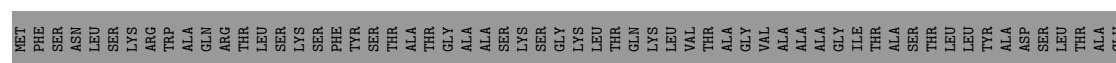
- Molecule 11: Cytochrome c1, heme protein, mitochondrial

Chain L: 79% 20%



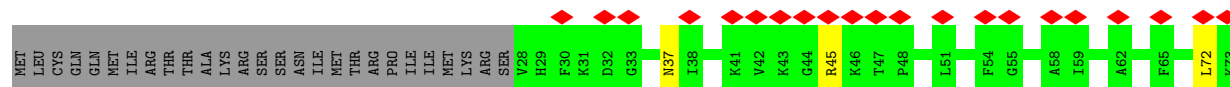
- Molecule 11: Cytochrome c1, heme protein, mitochondrial

Chain l: 79% 20%



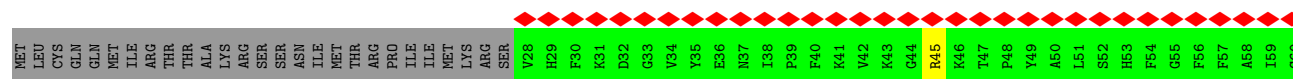
- Molecule 12: Cytochrome c oxidase subunit 8, mitochondrial

Chain M: 27% 56% 40%



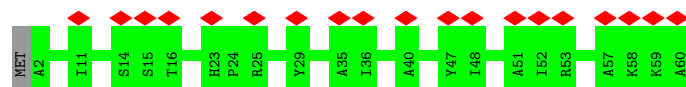
- Molecule 12: Cytochrome c oxidase subunit 8, mitochondrial

Chain m: 60% 58% 40%





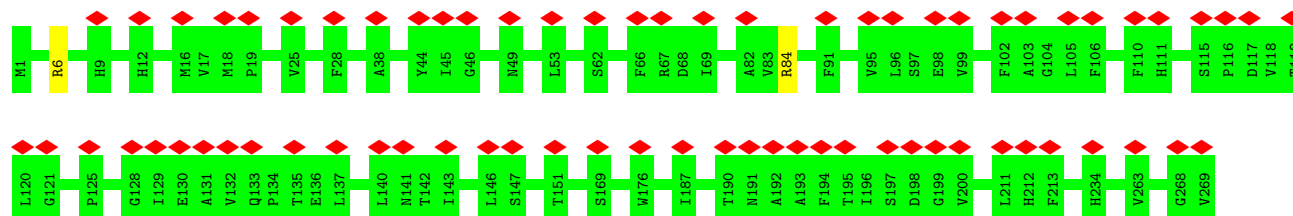
- Molecule 13: Cytochrome c oxidase subunit 7, mitochondrial



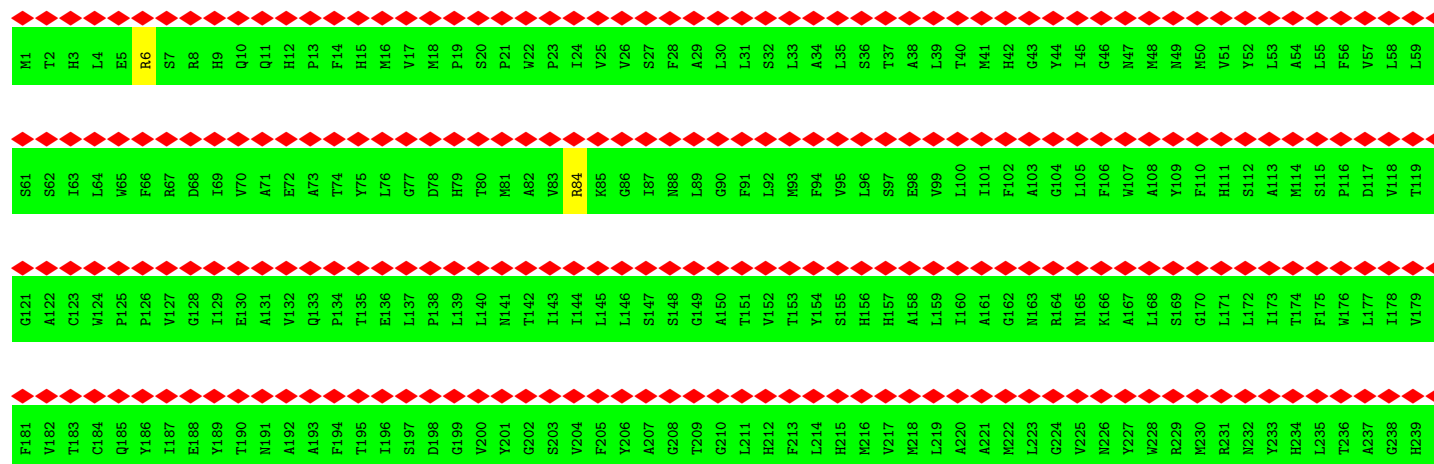
- Molecule 13: Cytochrome c oxidase subunit 7, mitochondrial

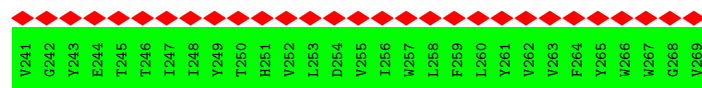


- Molecule 14: Cytochrome c oxidase subunit 3

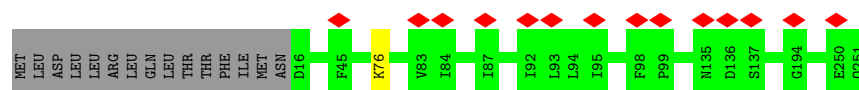


- Molecule 14: Cytochrome c oxidase subunit 3

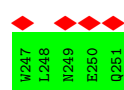
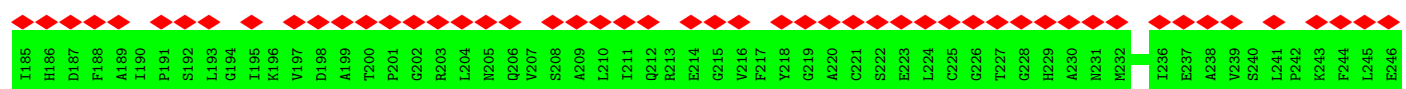
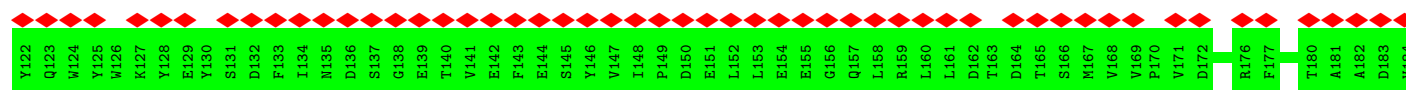
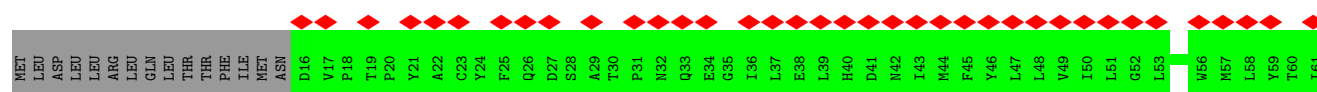
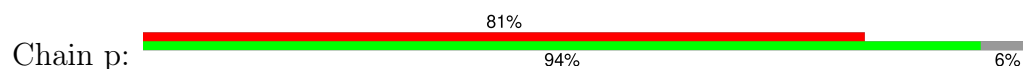




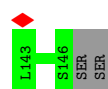
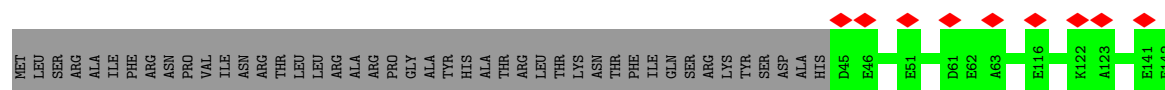
• Molecule 15: Cytochrome c oxidase subunit 2



• Molecule 15: Cytochrome c oxidase subunit 2

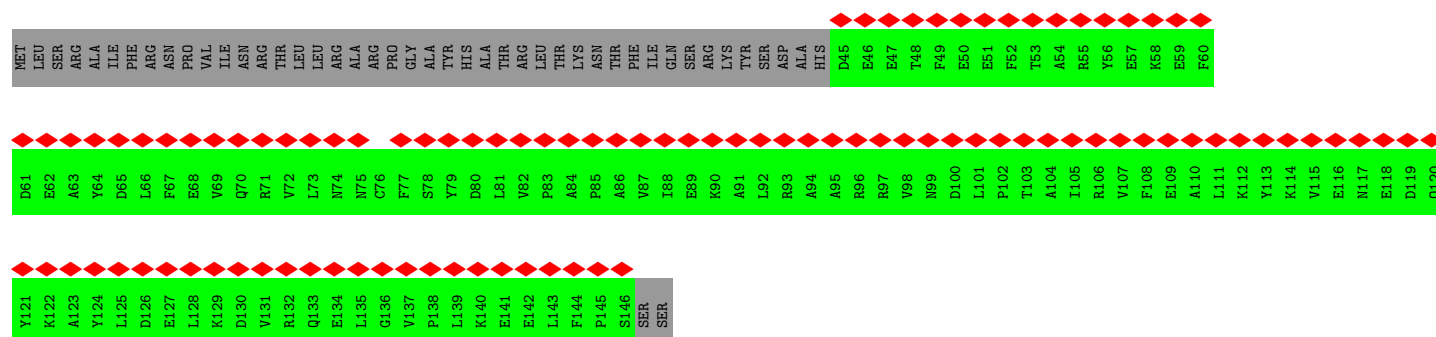


• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

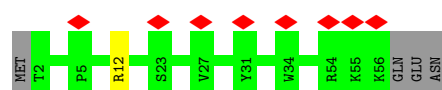
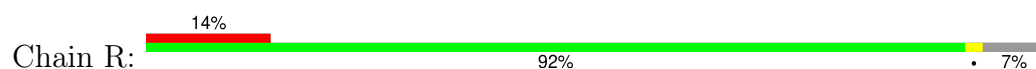


• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

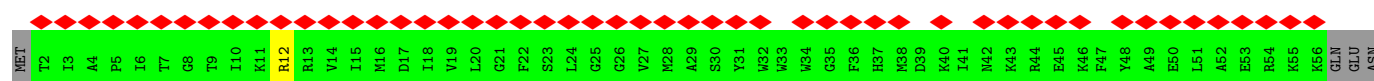
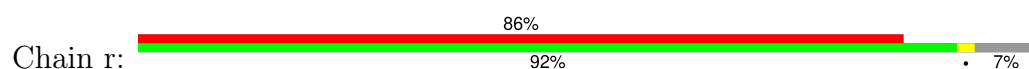




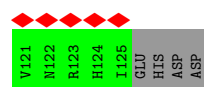
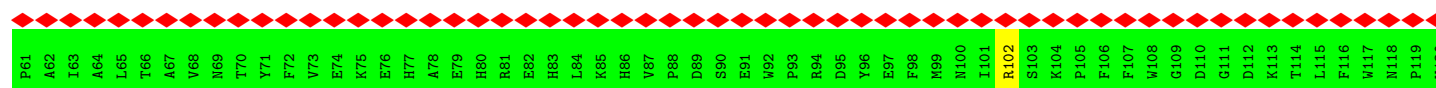
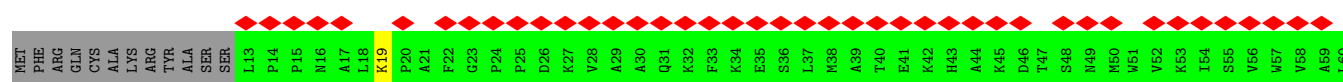
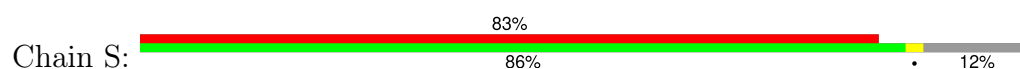
- Molecule 17: Cytochrome c oxidase subunit 9, mitochondrial



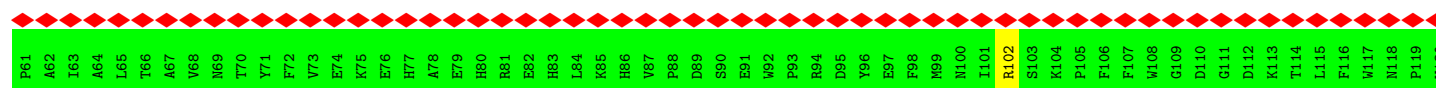
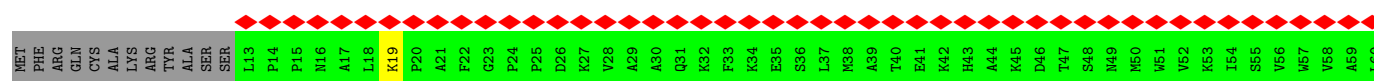
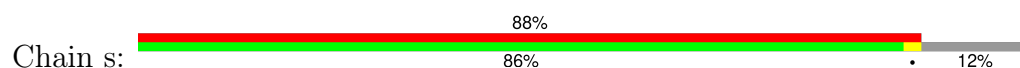
- Molecule 17: Cytochrome c oxidase subunit 9, mitochondrial

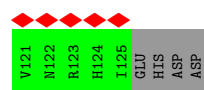


- Molecule 18: Cytochrome c oxidase subunit 13, mitochondrial

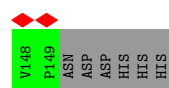
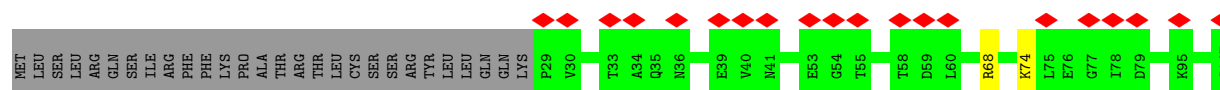
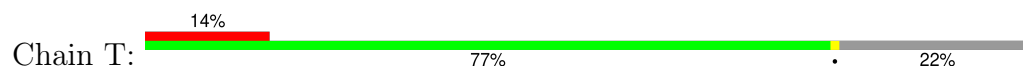


- Molecule 18: Cytochrome c oxidase subunit 13, mitochondrial

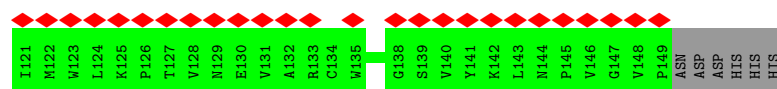
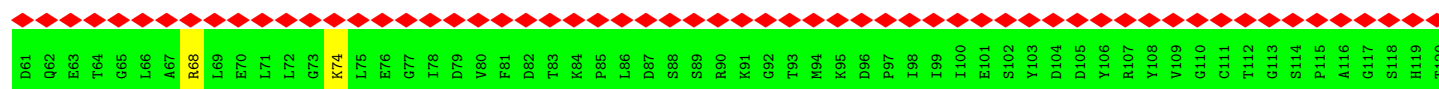
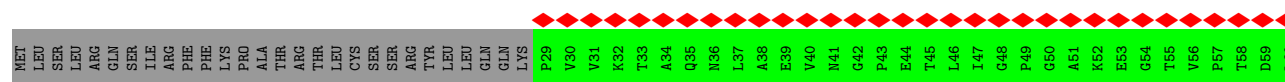
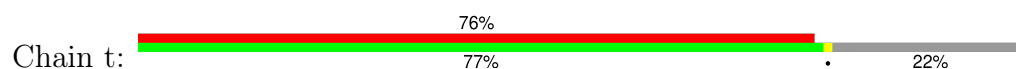




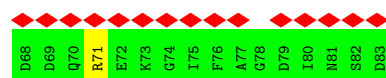
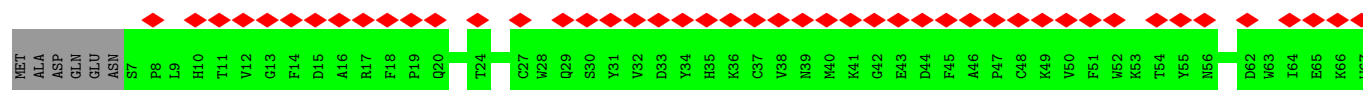
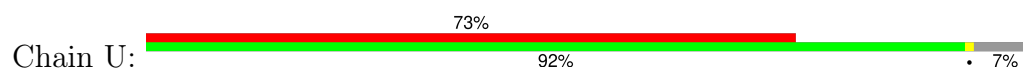
- Molecule 19: Cytochrome c oxidase subunit 4, mitochondrial



- Molecule 19: Cytochrome c oxidase subunit 4, mitochondrial



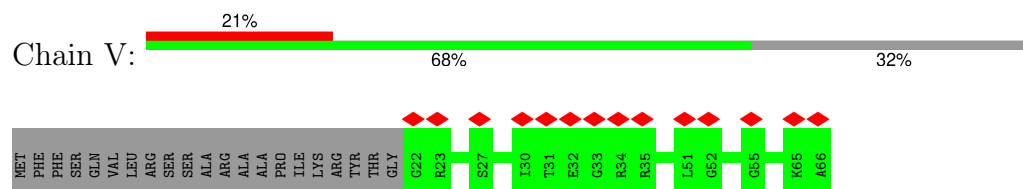
- Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial



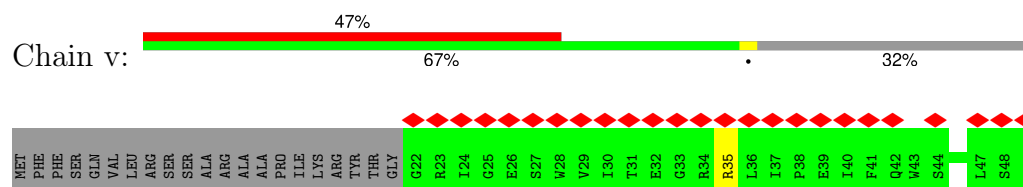
- Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial



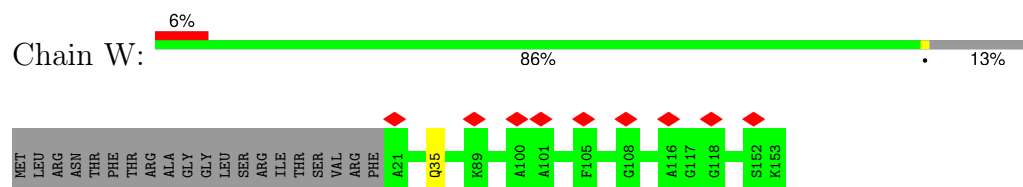
- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



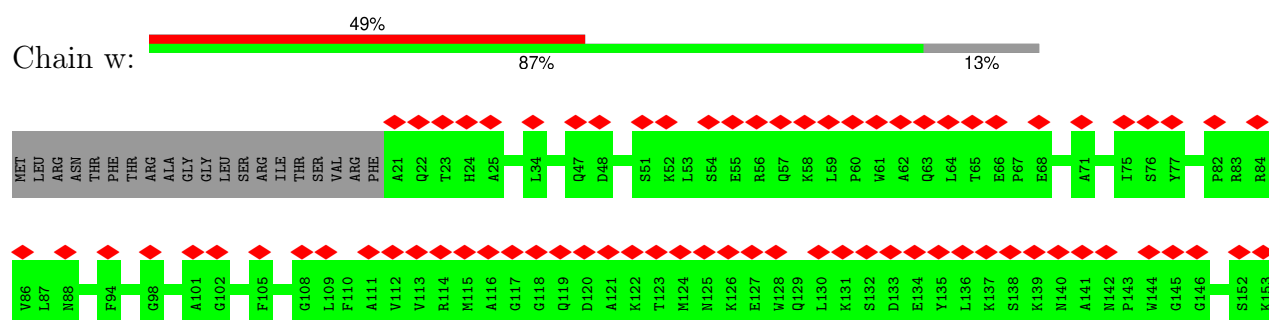
- Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



- Molecule 22: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 22: Cytochrome c oxidase subunit 5A, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	493055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.844	Depositor
Minimum map value	-0.873	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.245	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEA, CN5, PCF, CDL, CUA, PEF, HEM, UQ6, FES

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	0.32	0/3406	0.52	0/4615
1	a	0.33	0/3406	0.53	0/4615
2	B	0.36	0/2781	0.53	0/3764
2	b	0.35	0/2781	0.52	0/3764
3	C	0.27	0/1444	0.50	0/1957
3	c	0.28	0/1444	0.50	0/1957
4	D	0.27	0/537	0.54	0/728
4	d	0.26	0/537	0.54	0/728
5	E	0.31	0/479	0.44	0/646
5	e	0.32	0/479	0.51	0/646
6	F	0.31	0/1040	0.53	0/1408
6	f	0.31	0/1040	0.52	0/1408
7	G	0.28	0/647	0.49	0/870
7	g	0.29	0/647	0.50	0/870
8	H	0.33	0/804	0.46	0/1088
8	h	0.36	0/804	0.49	0/1088
9	J	0.37	0/3192	0.52	0/4354
9	j	0.36	0/3192	0.51	0/4354
10	K	0.28	0/4290	0.47	0/5857
10	k	0.26	0/4290	0.47	0/5857
11	L	0.34	0/2022	0.51	0/2751
11	l	0.35	0/2022	0.54	0/2751
12	M	0.29	0/396	0.53	1/533 (0.2%)
12	m	0.27	0/396	0.54	1/533 (0.2%)
13	N	0.25	0/500	0.47	0/681
13	n	0.24	0/500	0.46	0/681
14	O	0.24	0/2218	0.47	0/3036
14	o	0.24	0/2218	0.48	0/3036
15	P	0.26	0/1941	0.47	0/2653
15	p	0.25	0/1941	0.47	0/2653
16	Q	0.28	0/868	0.52	0/1174
16	q	0.26	0/868	0.51	0/1174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.24	0/467	0.51	0/626
17	r	0.24	0/467	0.52	0/626
18	S	0.24	0/962	0.44	0/1310
18	s	0.24	0/962	0.43	0/1310
19	T	0.25	0/932	0.50	0/1269
19	t	0.24	0/932	0.49	0/1269
20	U	0.24	0/664	0.41	0/899
20	u	0.24	0/664	0.44	0/899
21	V	0.27	0/372	0.53	0/502
21	v	0.26	0/372	0.54	0/502
22	W	0.26	0/1074	0.51	0/1451
22	w	0.26	0/1074	0.48	0/1451
All	All	0.30	0/62072	0.50	2/84344 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	72	LEU	CA-CB-CG	5.32	127.54	115.30
12	m	72	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	429/457 (94%)	368 (86%)	60 (14%)	1 (0%)	44	75
1	a	429/457 (94%)	366 (85%)	62 (14%)	1 (0%)	44	75
2	B	350/368 (95%)	324 (93%)	26 (7%)	0	100	100
2	b	350/368 (95%)	319 (91%)	31 (9%)	0	100	100
3	C	183/215 (85%)	166 (91%)	17 (9%)	0	100	100
3	c	183/215 (85%)	167 (91%)	16 (9%)	0	100	100
4	D	64/77 (83%)	59 (92%)	5 (8%)	0	100	100
4	d	64/77 (83%)	61 (95%)	3 (5%)	0	100	100
5	E	55/66 (83%)	55 (100%)	0	0	100	100
5	e	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
6	F	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
6	f	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
7	G	73/147 (50%)	72 (99%)	1 (1%)	0	100	100
7	g	73/147 (50%)	71 (97%)	2 (3%)	0	100	100
8	H	91/94 (97%)	84 (92%)	5 (6%)	2 (2%)	5	30
8	h	91/94 (97%)	82 (90%)	8 (9%)	1 (1%)	12	44
9	J	383/385 (100%)	352 (92%)	31 (8%)	0	100	100
9	j	383/385 (100%)	363 (95%)	20 (5%)	0	100	100
10	K	532/534 (100%)	493 (93%)	39 (7%)	0	100	100
10	k	532/534 (100%)	506 (95%)	26 (5%)	0	100	100
11	L	246/309 (80%)	210 (85%)	33 (13%)	3 (1%)	11	43
11	l	246/309 (80%)	211 (86%)	34 (14%)	1 (0%)	30	64
12	M	45/78 (58%)	43 (96%)	2 (4%)	0	100	100
12	m	45/78 (58%)	40 (89%)	5 (11%)	0	100	100
13	N	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
13	n	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
14	O	267/269 (99%)	245 (92%)	22 (8%)	0	100	100
14	o	267/269 (99%)	246 (92%)	21 (8%)	0	100	100
15	P	234/251 (93%)	218 (93%)	16 (7%)	0	100	100
15	p	234/251 (93%)	222 (95%)	12 (5%)	0	100	100
16	Q	100/148 (68%)	92 (92%)	8 (8%)	0	100	100
16	q	100/148 (68%)	92 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	53/59 (90%)	50 (94%)	3 (6%)	0	100	100
17	r	53/59 (90%)	52 (98%)	1 (2%)	0	100	100
18	S	111/129 (86%)	103 (93%)	8 (7%)	0	100	100
18	s	111/129 (86%)	102 (92%)	9 (8%)	0	100	100
19	T	119/155 (77%)	109 (92%)	10 (8%)	0	100	100
19	t	119/155 (77%)	110 (92%)	9 (8%)	0	100	100
20	U	75/83 (90%)	72 (96%)	3 (4%)	0	100	100
20	u	75/83 (90%)	72 (96%)	3 (4%)	0	100	100
21	V	43/66 (65%)	41 (95%)	2 (5%)	0	100	100
21	v	43/66 (65%)	39 (91%)	4 (9%)	0	100	100
22	W	131/153 (86%)	115 (88%)	16 (12%)	0	100	100
22	w	131/153 (86%)	119 (91%)	12 (9%)	0	100	100
All	All	7530/8460 (89%)	6898 (92%)	623 (8%)	9 (0%)	50	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	40	ILE
11	L	240	THR
11	l	240	THR
11	L	122	ASN
1	A	156	HIS

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%)	368 (100%)	2 (0%)	86	93
1	a	370/393 (94%)	368 (100%)	2 (0%)	86	93
2	B	301/313 (96%)	300 (100%)	1 (0%)	91	96
2	b	301/313 (96%)	301 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	151/179 (84%)	151 (100%)	0	100	100
3	c	151/179 (84%)	151 (100%)	0	100	100
4	D	56/66 (85%)	56 (100%)	0	100	100
4	d	56/66 (85%)	56 (100%)	0	100	100
5	E	47/54 (87%)	47 (100%)	0	100	100
5	e	47/54 (87%)	46 (98%)	1 (2%)	48	74
6	F	110/111 (99%)	110 (100%)	0	100	100
6	f	110/111 (99%)	110 (100%)	0	100	100
7	G	68/131 (52%)	67 (98%)	1 (2%)	60	81
7	g	68/131 (52%)	68 (100%)	0	100	100
8	H	77/78 (99%)	77 (100%)	0	100	100
8	h	77/78 (99%)	76 (99%)	1 (1%)	65	83
9	J	338/338 (100%)	338 (100%)	0	100	100
9	j	338/338 (100%)	337 (100%)	1 (0%)	91	96
10	K	447/447 (100%)	446 (100%)	1 (0%)	92	97
10	k	447/447 (100%)	446 (100%)	1 (0%)	92	97
11	L	206/251 (82%)	205 (100%)	1 (0%)	86	93
11	l	206/251 (82%)	204 (99%)	2 (1%)	73	87
12	M	39/67 (58%)	37 (95%)	2 (5%)	20	53
12	m	39/67 (58%)	38 (97%)	1 (3%)	41	70
13	N	50/51 (98%)	50 (100%)	0	100	100
13	n	50/51 (98%)	50 (100%)	0	100	100
14	O	228/228 (100%)	226 (99%)	2 (1%)	75	89
14	o	228/228 (100%)	226 (99%)	2 (1%)	75	89
15	P	209/224 (93%)	208 (100%)	1 (0%)	86	93
15	p	209/224 (93%)	208 (100%)	1 (0%)	86	93
16	Q	91/131 (70%)	91 (100%)	0	100	100
16	q	91/131 (70%)	91 (100%)	0	100	100
17	R	46/50 (92%)	45 (98%)	1 (2%)	47	73
17	r	46/50 (92%)	45 (98%)	1 (2%)	47	73
18	S	99/113 (88%)	97 (98%)	2 (2%)	50	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	s	99/113 (88%)	97 (98%)	2 (2%)	50	75
19	T	102/135 (76%)	100 (98%)	2 (2%)	50	75
19	t	102/135 (76%)	100 (98%)	2 (2%)	50	75
20	U	69/74 (93%)	68 (99%)	1 (1%)	62	82
20	u	69/74 (93%)	68 (99%)	1 (1%)	62	82
21	V	36/53 (68%)	36 (100%)	0	100	100
21	v	36/53 (68%)	35 (97%)	1 (3%)	38	68
22	W	110/127 (87%)	109 (99%)	1 (1%)	75	89
22	w	110/127 (87%)	110 (100%)	0	100	100
All	All	6500/7228 (90%)	6463 (99%)	37 (1%)	82	92

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	o	84	ARG
20	u	71	ARG
15	p	76	LYS
18	s	102	ARG
18	S	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
9	j	332	ASN
15	p	229	HIS
11	l	169	ASN
16	q	70	GLN
10	K	485	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 2 are monoatomic and 4 are modelled with single atom - leaving 57 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	$\# Z > 2$
23	PEF	J	401	-	44,44,46	0.45	0	47,49,51	1.21	4 (8%)
29	UQ6	J	406	-	43,43,43	0.50	0	54,55,55	1.70	13 (24%)
23	PEF	a	501	-	39,39,46	0.46	0	42,44,51	1.36	5 (11%)
25	CDL	H	601	-	52,52,99	1.22	6 (11%)	58,64,111	0.96	4 (6%)
23	PEF	c	303	-	28,28,46	0.49	0	31,33,51	1.33	4 (12%)
26	PCF	W	203	-	35,35,49	0.71	0	41,43,57	0.55	0
28	HEM	J	404	9	42,50,50	1.52	7 (16%)	46,82,82	2.06	13 (28%)
25	CDL	j	402	-	55,55,99	1.20	6 (10%)	61,67,111	0.93	4 (6%)
28	HEM	L	401	11	42,50,50	1.46	6 (14%)	46,82,82	1.99	12 (26%)
23	PEF	a	504	-	39,39,46	0.45	0	42,44,51	1.24	4 (9%)
26	PCF	a	502	-	46,46,49	0.63	0	52,54,57	0.58	0
23	PEF	C	304	-	31,31,46	0.48	0	34,36,51	1.32	4 (11%)
25	CDL	c	302	-	47,47,99	1.28	6 (12%)	53,59,111	1.02	5 (9%)
29	UQ6	j	407	-	43,43,43	0.47	0	54,55,55	1.57	13 (24%)
23	PEF	A	503	-	39,39,46	0.44	0	42,44,51	1.28	4 (9%)
25	CDL	C	302	-	52,52,99	1.22	6 (11%)	58,64,111	0.94	3 (5%)
28	HEM	j	403	9	42,50,50	1.51	6 (14%)	46,82,82	2.07	13 (28%)
23	PEF	A	502	-	30,30,46	0.48	0	33,35,51	1.38	4 (12%)
23	PEF	e	101	-	31,31,46	0.51	0	34,36,51	1.33	5 (14%)
30	HEA	K	604	10	58,67,67	2.02	14 (24%)	63,103,103	2.57	31 (49%)
26	PCF	H	602	-	49,49,49	0.62	0	55,57,57	0.50	0
23	PEF	w	202	-	40,40,46	0.46	0	43,45,51	1.24	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PEF	J	407	-	42,42,46	0.46	0	45,47,51	1.30	5 (11%)
25	CDL	K	603	-	66,66,99	1.08	6 (9%)	72,78,111	0.89	2 (2%)
27	CN5	J	402	-	40,40,40	0.50	0	44,48,48	0.92	1 (2%)
24	FES	c	301	3	0,4,4	-	-	-		
23	PEF	a	503	-	30,30,46	0.49	0	33,35,51	1.32	4 (12%)
23	PEF	w	201	-	35,35,46	0.48	0	38,40,51	1.32	4 (10%)
23	PEF	W	201	-	35,35,46	0.46	0	38,40,51	1.32	4 (10%)
25	CDL	L	402	-	66,66,99	1.09	6 (9%)	72,78,111	0.89	4 (5%)
25	CDL	h	601	-	52,52,99	1.23	6 (11%)	58,64,111	0.97	4 (6%)
26	PCF	E	101	-	46,46,49	0.63	0	52,54,57	0.62	1 (1%)
26	PCF	k	605	-	35,35,49	0.71	0	41,43,57	0.54	0
25	CDL	J	403	-	55,55,99	1.19	6 (10%)	61,67,111	0.97	4 (6%)
23	PEF	c	304	-	31,31,46	0.47	0	34,36,51	1.34	4 (11%)
29	UQ6	j	405	-	43,43,43	0.46	0	54,55,55	1.60	14 (25%)
23	PEF	j	406	-	42,42,46	0.44	0	45,47,51	1.29	4 (8%)
23	PEF	W	202	-	40,40,46	0.45	0	43,45,51	1.27	4 (9%)
23	PEF	E	102	-	31,31,46	0.49	0	34,36,51	1.34	5 (14%)
23	PEF	J	409	-	28,28,46	0.50	0	31,33,51	1.39	4 (12%)
23	PEF	j	401	-	44,44,46	0.44	0	47,49,51	1.20	4 (8%)
30	HEA	k	604	10	58,67,67	2.03	17 (29%)	63,103,103	2.59	32 (50%)
28	HEM	j	404	9	42,50,50	1.51	6 (14%)	46,82,82	2.12	12 (26%)
23	PEF	v	101	-	32,32,46	0.48	0	35,37,51	1.31	5 (14%)
26	PCF	w	203	-	49,49,49	0.63	0	55,57,57	0.53	0
23	PEF	V	101	-	32,32,46	0.49	0	35,37,51	1.34	5 (14%)
30	HEA	K	601	10	58,67,67	2.03	16 (27%)	63,103,103	2.60	33 (52%)
25	CDL	h	602	-	66,66,99	1.09	6 (9%)	72,78,111	0.89	4 (5%)
30	HEA	k	603	10	58,67,67	2.06	18 (31%)	63,103,103	2.50	32 (50%)
28	HEM	l	401	11	42,50,50	1.48	7 (16%)	46,82,82	1.91	12 (26%)
29	UQ6	J	408	-	20,20,43	0.59	0	25,27,55	1.67	5 (20%)
23	PEF	A	501	-	39,39,46	0.45	0	42,44,51	1.27	4 (9%)
24	FES	C	301	3	0,4,4	-	-	-		
25	CDL	k	602	-	66,66,99	1.09	6 (9%)	72,78,111	0.87	2 (2%)
23	PEF	j	408	-	28,28,46	0.51	0	31,33,51	1.32	4 (12%)
28	HEM	J	405	9	42,50,50	1.51	6 (14%)	46,82,82	2.14	12 (26%)
23	PEF	C	303	-	28,28,46	0.52	0	31,33,51	1.38	5 (16%)

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
23	PEF	J	401	-	-	16/48/48/50	-
29	UQ6	J	406	-	-	11/39/39/39	0/1/1/1
25	CDL	H	601	-	1/1/9/9	28/63/63/110	-
23	PEF	a	501	-	-	9/43/43/50	-
23	PEF	c	303	-	-	8/32/32/50	-
26	PCF	W	203	-	-	10/39/39/53	-
28	HEM	J	404	9	-	5/12/54/54	-
25	CDL	j	402	-	1/1/9/9	23/66/66/110	-
28	HEM	L	401	11	-	6/12/54/54	-
23	PEF	a	504	-	-	7/43/43/50	-
26	PCF	a	502	-	-	13/50/50/53	-
23	PEF	C	304	-	-	8/35/35/50	-
25	CDL	c	302	-	1/1/9/9	22/58/58/110	-
29	UQ6	j	407	-	-	9/39/39/39	0/1/1/1
23	PEF	A	503	-	-	11/43/43/50	-
25	CDL	C	302	-	1/1/9/9	27/63/63/110	-
28	HEM	j	403	9	-	10/12/54/54	-
23	PEF	A	502	-	-	1/34/34/50	-
23	PEF	e	101	-	-	6/35/35/50	-
30	HEA	K	604	10	-	16/32/76/76	-
26	PCF	H	602	-	-	16/53/53/53	-
23	PEF	w	202	-	-	6/44/44/50	-
23	PEF	J	407	-	-	10/46/46/50	-
25	CDL	K	603	-	1/1/9/9	34/77/77/110	-
27	CN5	J	402	-	-	8/44/44/44	-
24	FES	c	301	3	-	-	0/1/1/1
23	PEF	a	503	-	-	6/34/34/50	-
25	CDL	L	402	-	1/1/9/9	33/77/77/110	-
25	CDL	h	601	-	1/1/9/9	26/63/63/110	-
23	PEF	W	201	-	-	7/39/39/50	-
23	PEF	w	201	-	-	10/39/39/50	-
26	PCF	E	101	-	-	12/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PCF	k	605	-	-	7/39/39/53	-
25	CDL	J	403	-	1/1/9/9	27/66/66/110	-
23	PEF	c	304	-	-	10/35/35/50	-
29	UQ6	j	405	-	-	7/39/39/39	0/1/1/1
23	PEF	j	406	-	-	14/46/46/50	-
23	PEF	W	202	-	-	8/44/44/50	-
23	PEF	E	102	-	-	8/35/35/50	-
23	PEF	J	409	-	-	11/32/32/50	-
23	PEF	j	401	-	-	11/48/48/50	-
30	HEA	k	604	10	-	14/32/76/76	-
28	HEM	j	404	9	-	6/12/54/54	-
23	PEF	v	101	-	-	7/36/36/50	-
26	PCF	w	203	-	-	15/53/53/53	-
23	PEF	V	101	-	-	9/36/36/50	-
30	HEA	K	601	10	-	14/32/76/76	-
25	CDL	h	602	-	1/1/9/9	26/77/77/110	-
30	HEA	k	603	10	-	15/32/76/76	-
28	HEM	l	401	11	-	4/12/54/54	-
29	UQ6	J	408	-	-	2/12/12/39	0/1/1/1
23	PEF	A	501	-	-	8/43/43/50	-
24	FES	C	301	3	-	-	0/1/1/1
25	CDL	k	602	-	1/1/9/9	33/77/77/110	-
23	PEF	j	408	-	-	5/32/32/50	-
28	HEM	J	405	9	-	7/12/54/54	-
23	PEF	C	303	-	-	9/32/32/50	-

The worst 5 of 163 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	k	603	HEA	C3A-C2A	5.19	1.47	1.40
30	k	604	HEA	C3A-C2A	5.18	1.47	1.40
30	K	604	HEA	C3A-C2A	5.02	1.47	1.40
30	K	601	HEA	C3A-C2A	5.02	1.47	1.40
30	k	603	HEA	CHC-C4B	4.97	1.46	1.34

The worst 5 of 388 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	601	HEA	C3D-C4D-ND	6.70	116.82	110.35
30	k	603	HEA	C3D-C4D-ND	6.60	116.73	110.35
30	k	604	HEA	C3D-C4D-ND	6.50	116.63	110.35
28	j	404	HEM	CAD-C3D-C4D	6.45	135.95	124.70
30	K	604	HEA	C3D-C4D-ND	6.42	116.56	110.35

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	C	302	CDL	CA4
25	H	601	CDL	CA4
25	J	403	CDL	CA4
25	K	603	CDL	CA4
25	L	402	CDL	CA4

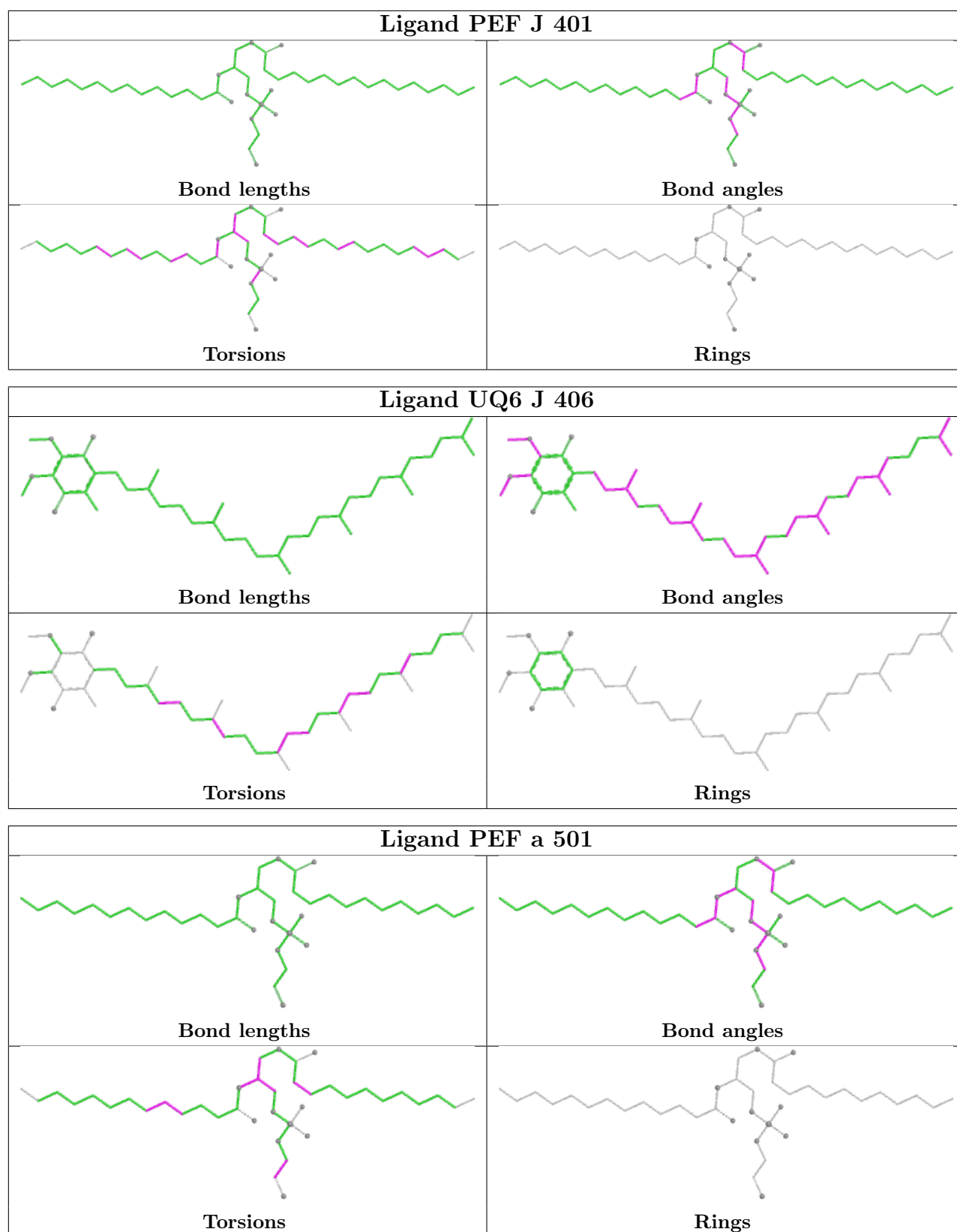
5 of 691 torsion outliers are listed below:

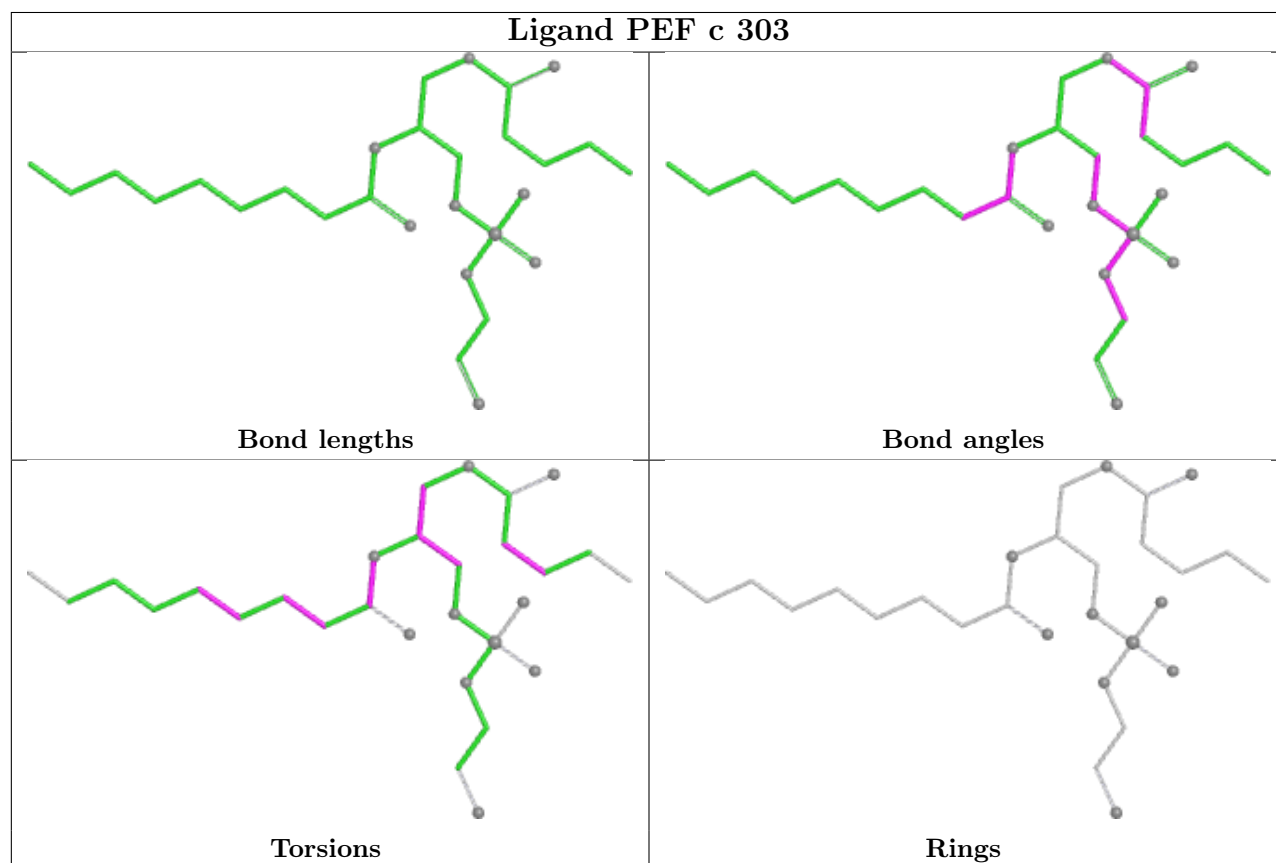
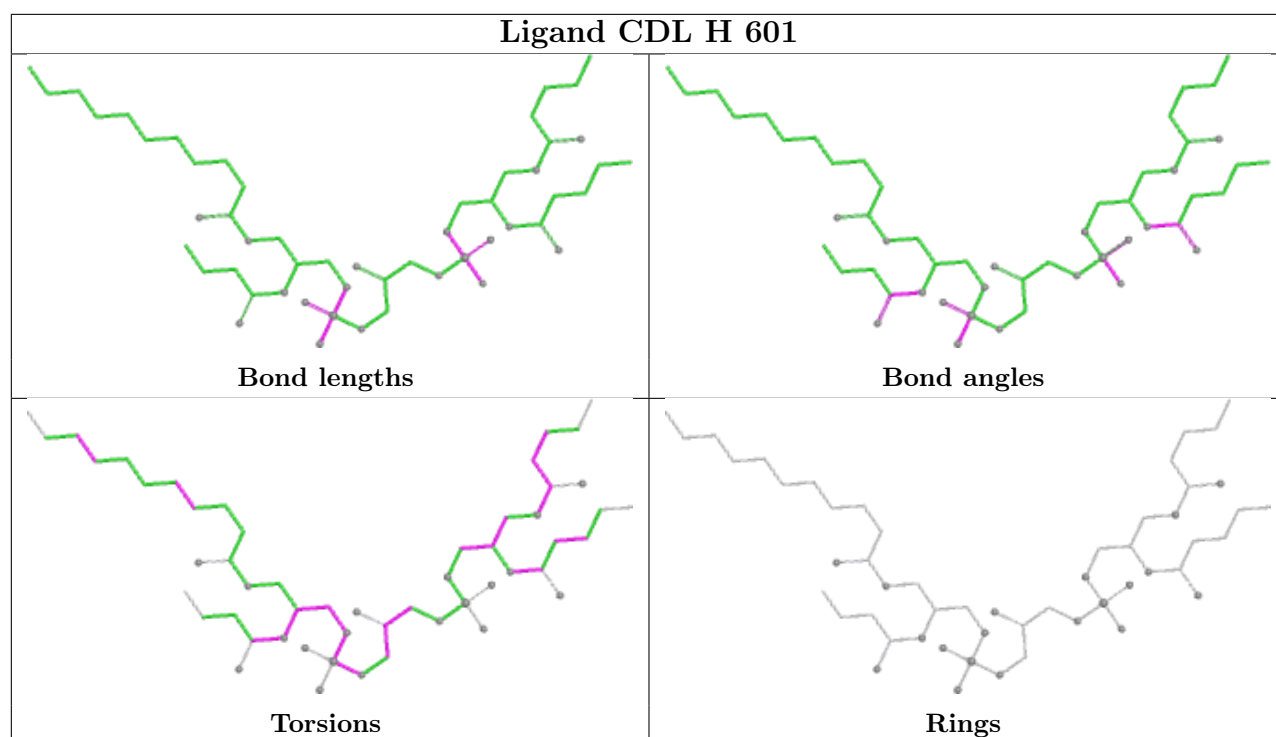
Mol	Chain	Res	Type	Atoms
23	A	501	PEF	O2-C2-C3-O3
23	A	503	PEF	O4P-C4-C5-N
23	A	503	PEF	C4-O4P-P-O3P
23	C	303	PEF	C11-C10-O2-C2
23	E	102	PEF	C1-O3P-P-O1P

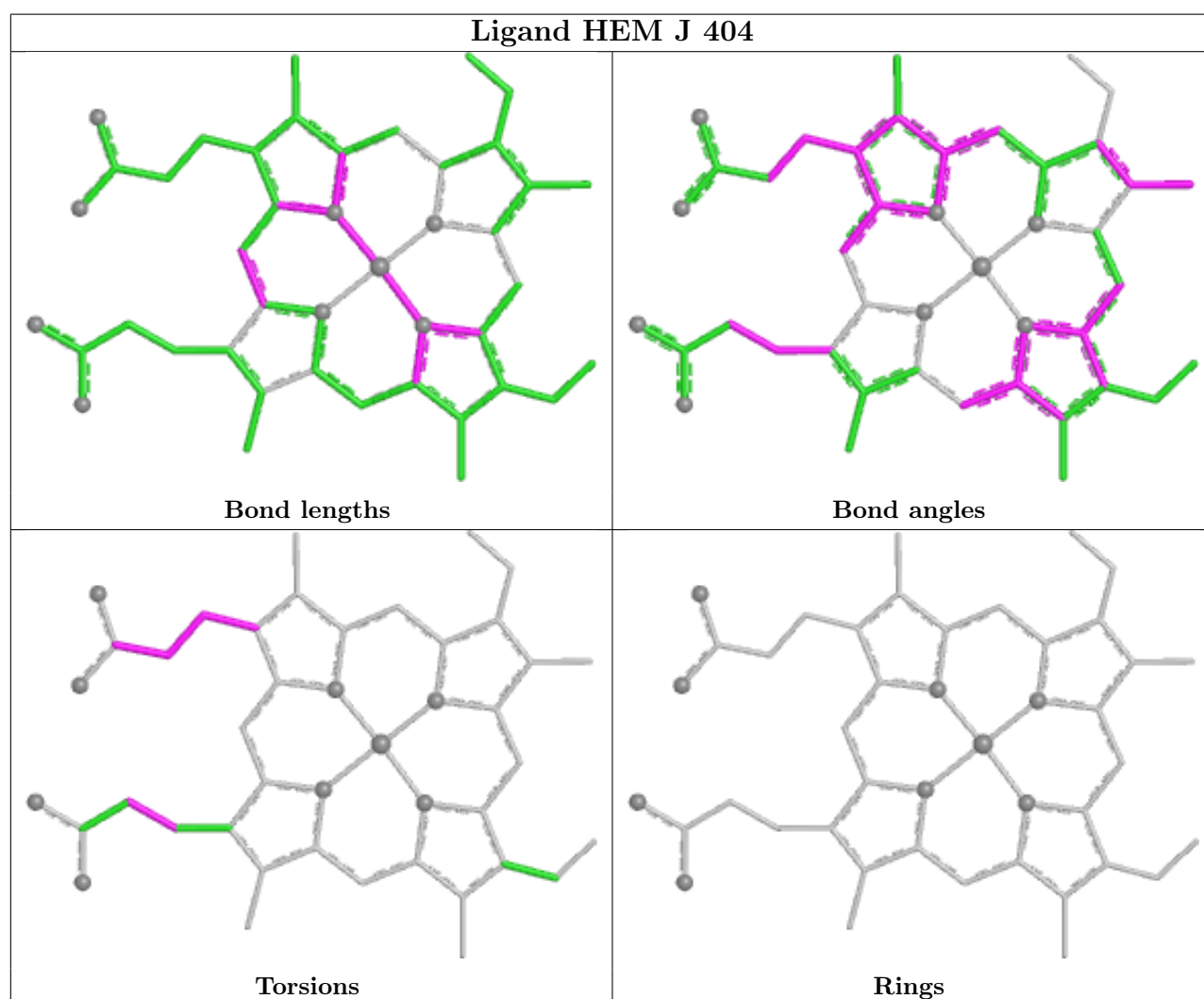
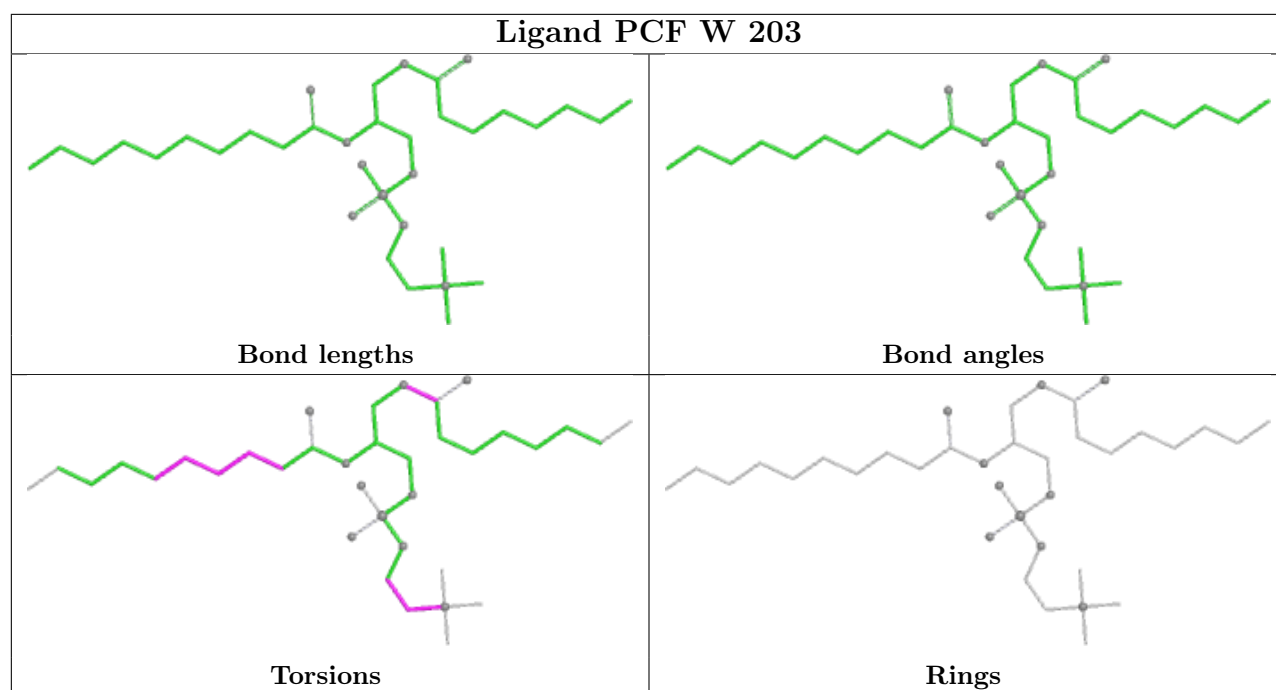
There are no ring outliers.

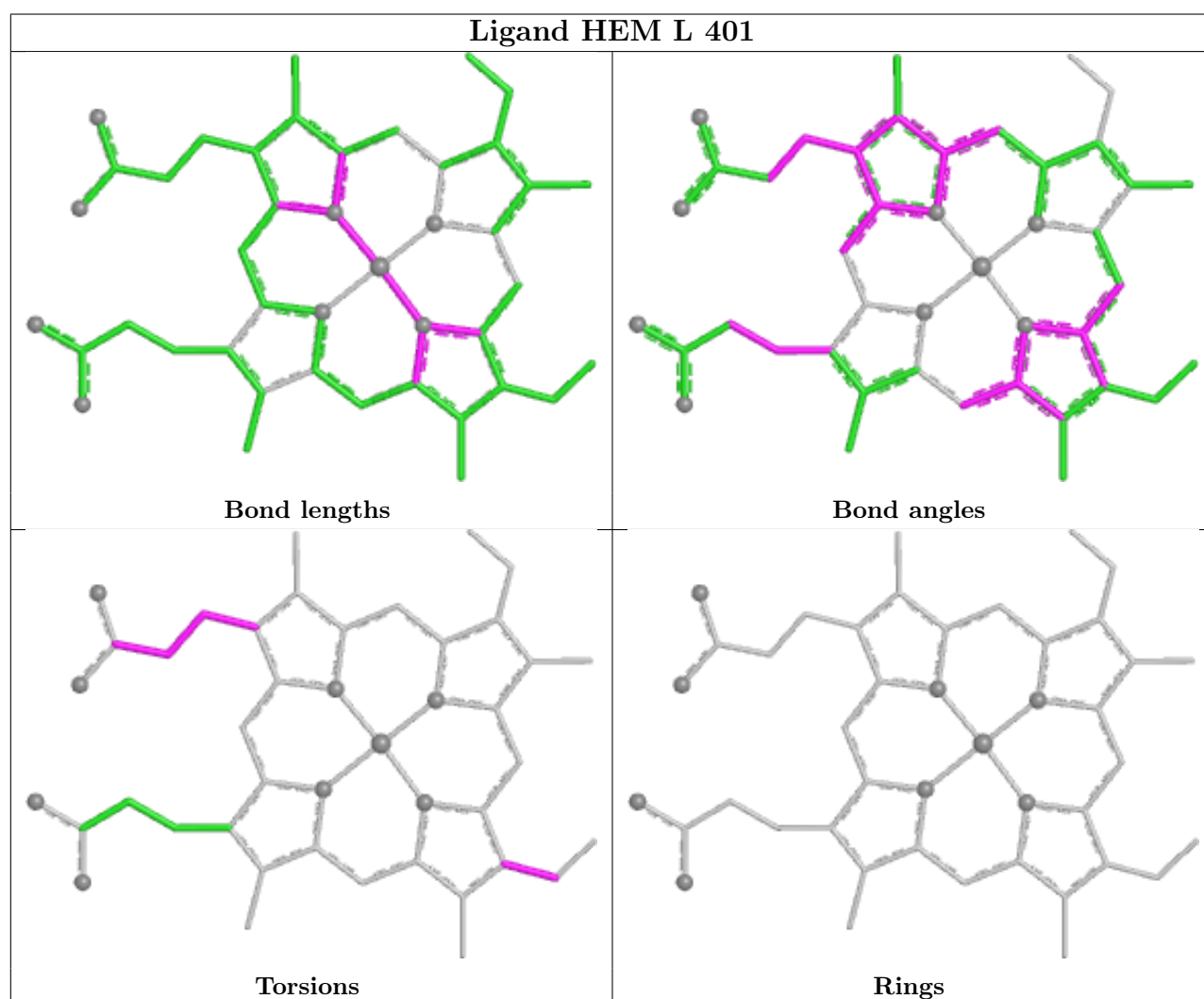
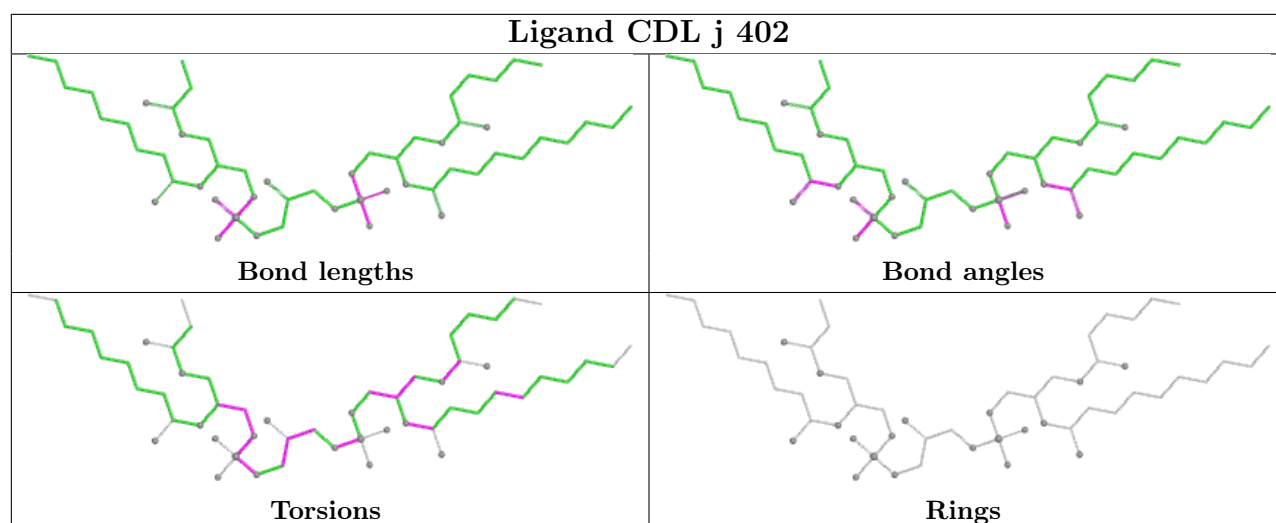
No monomer is involved in short contacts.

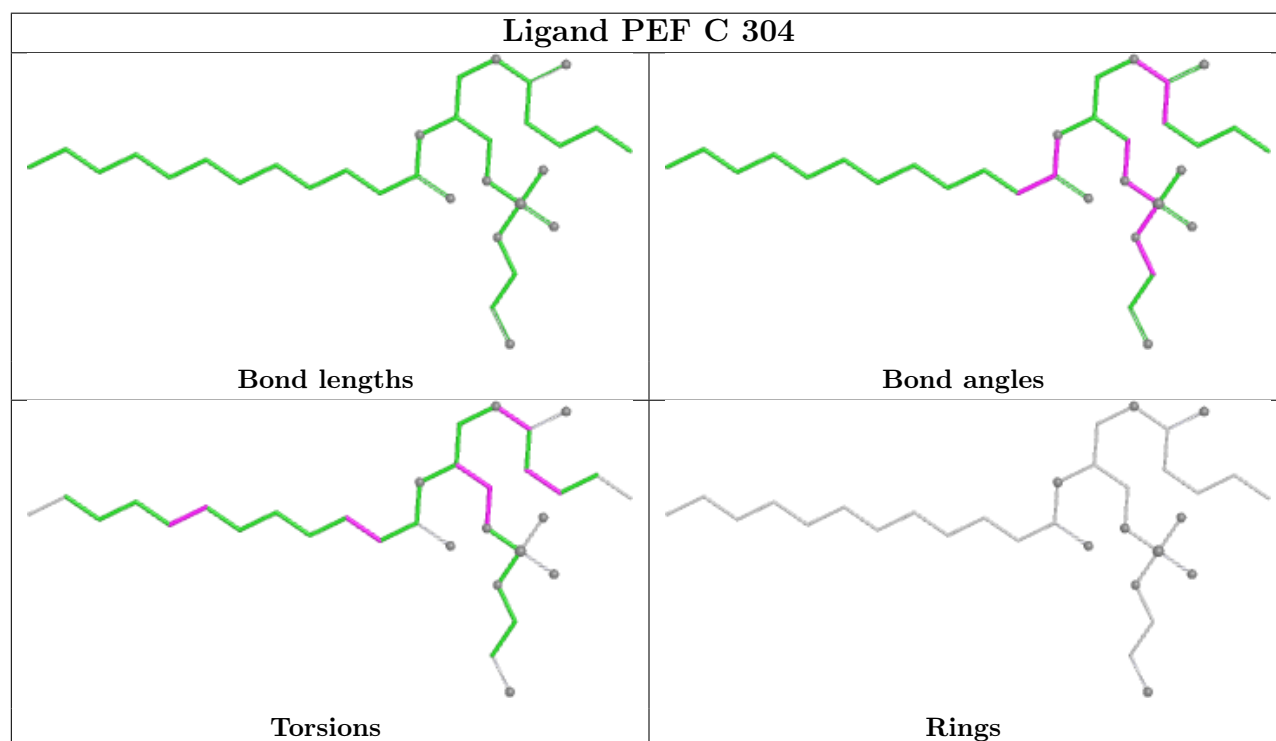
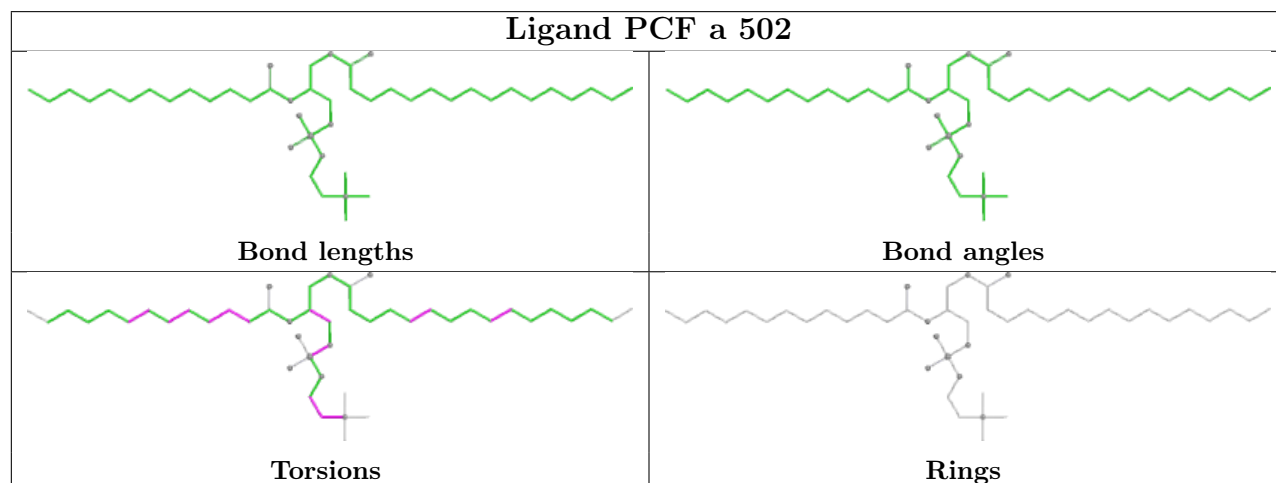
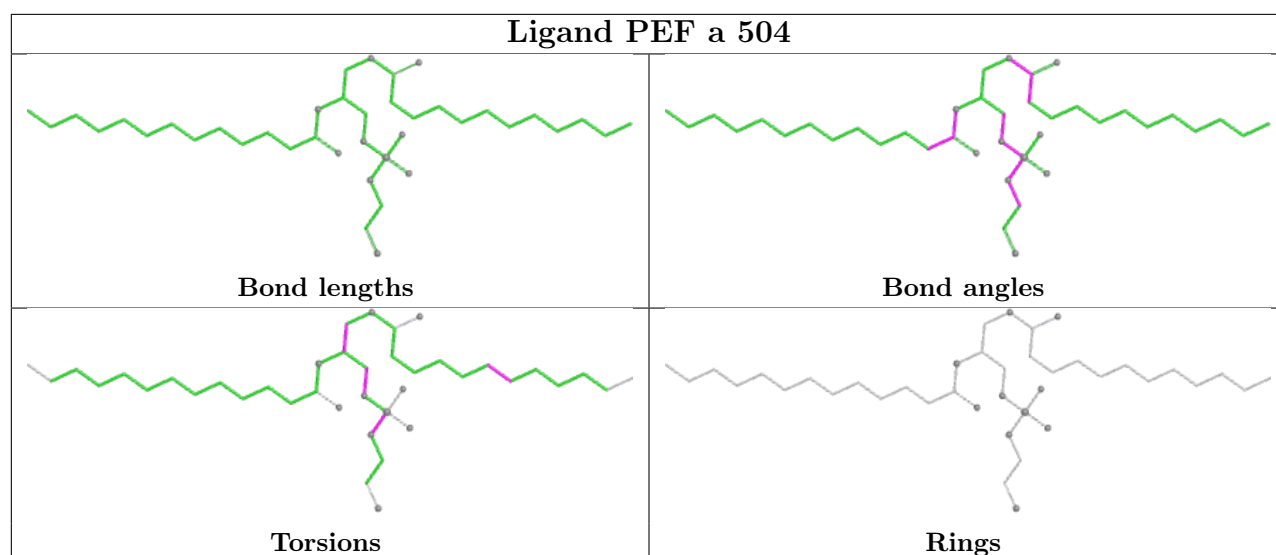
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

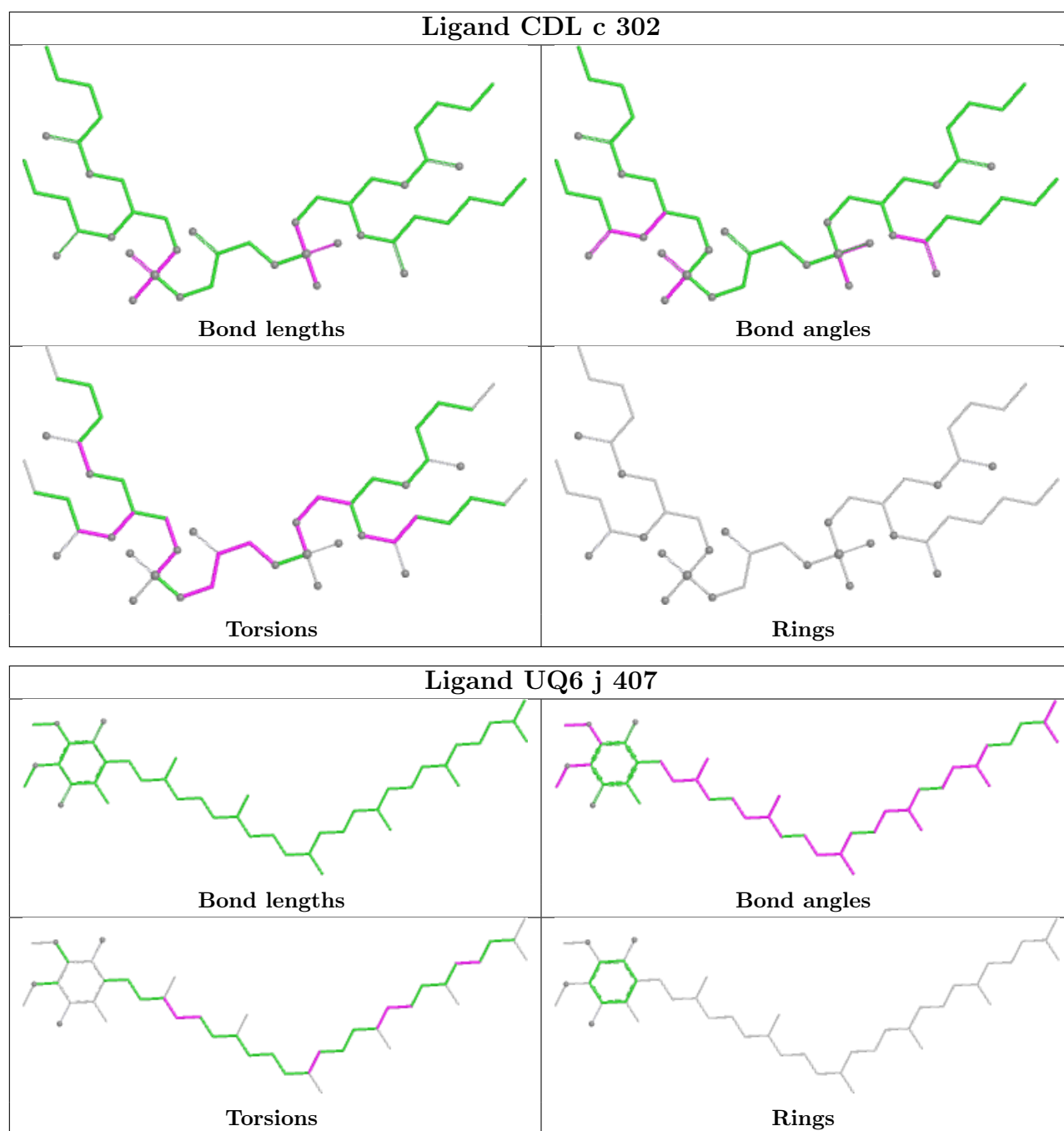


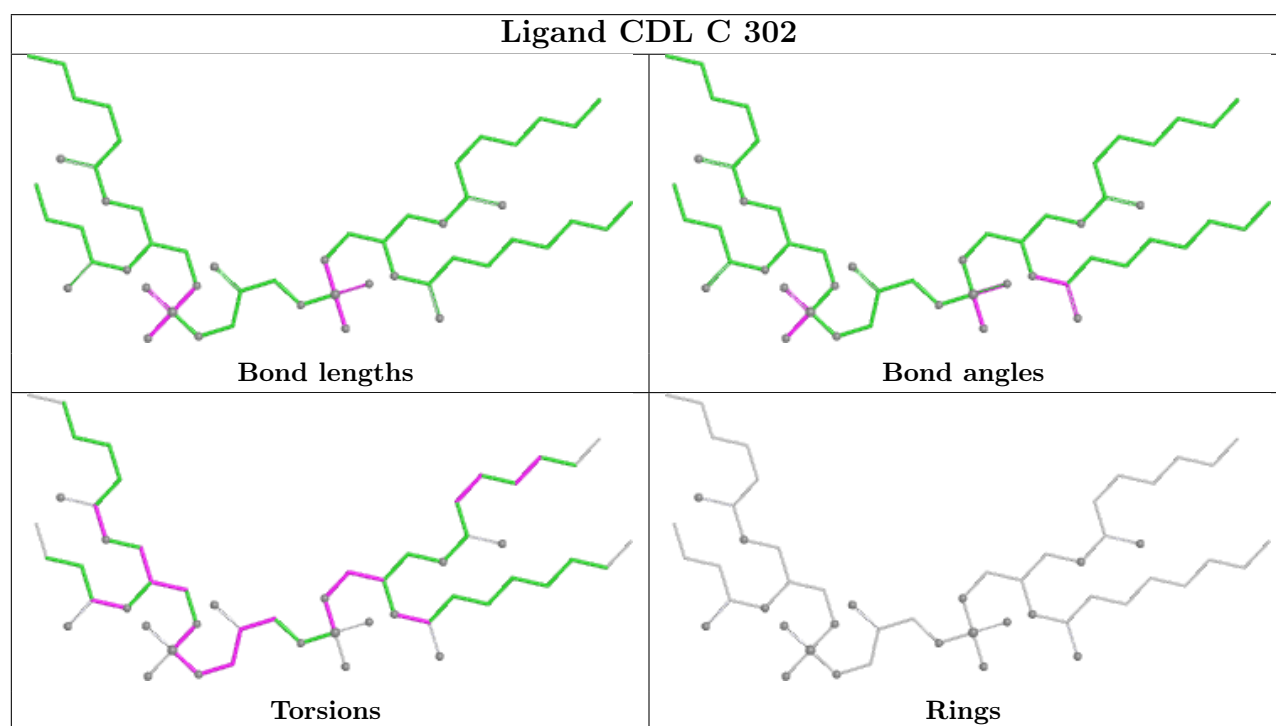
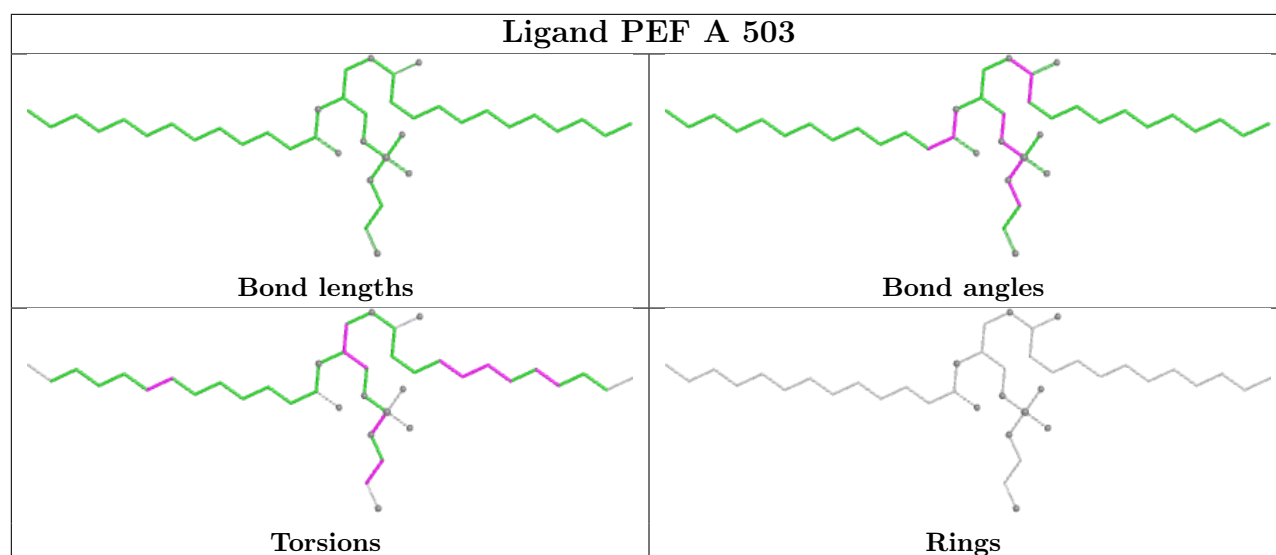


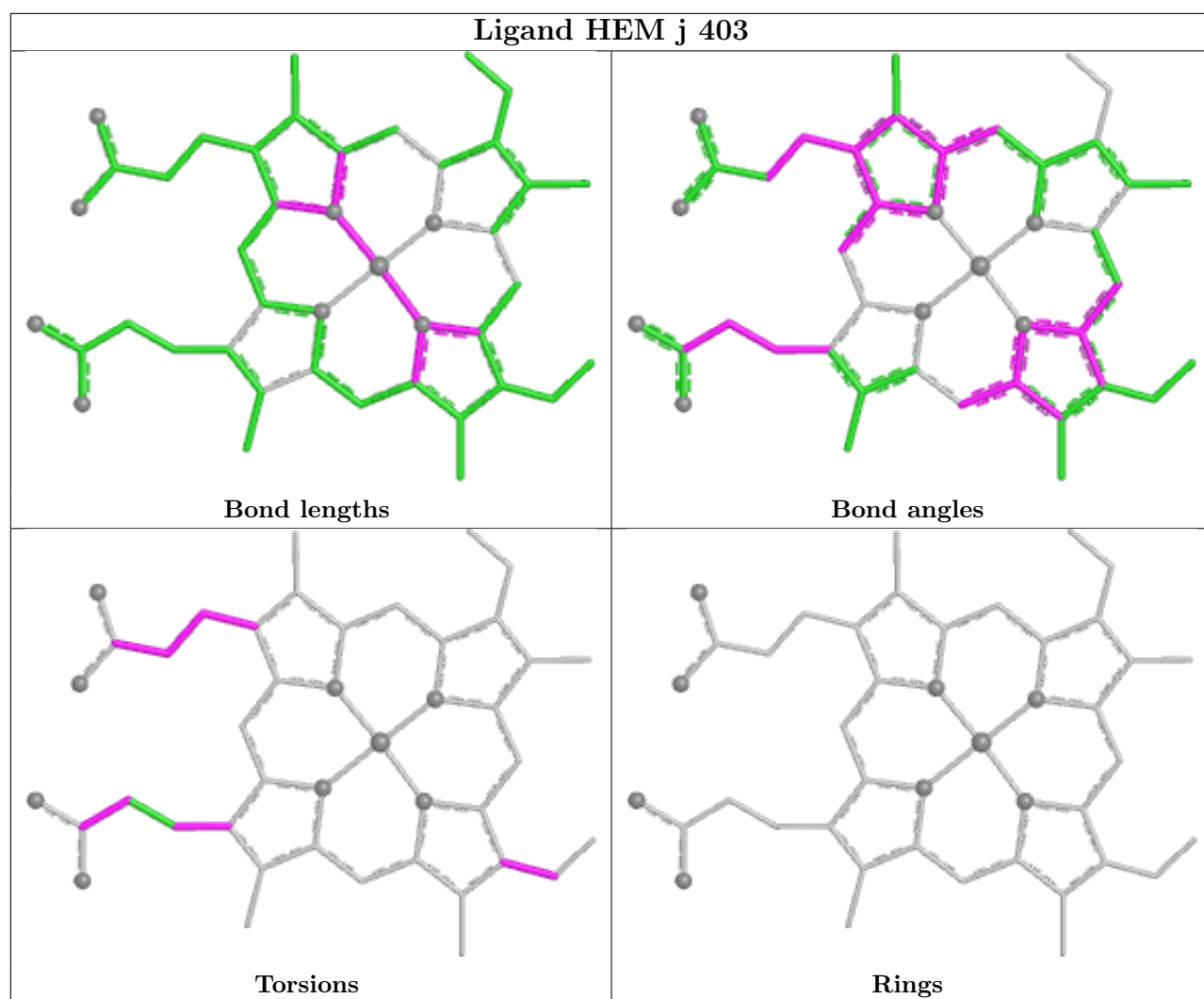


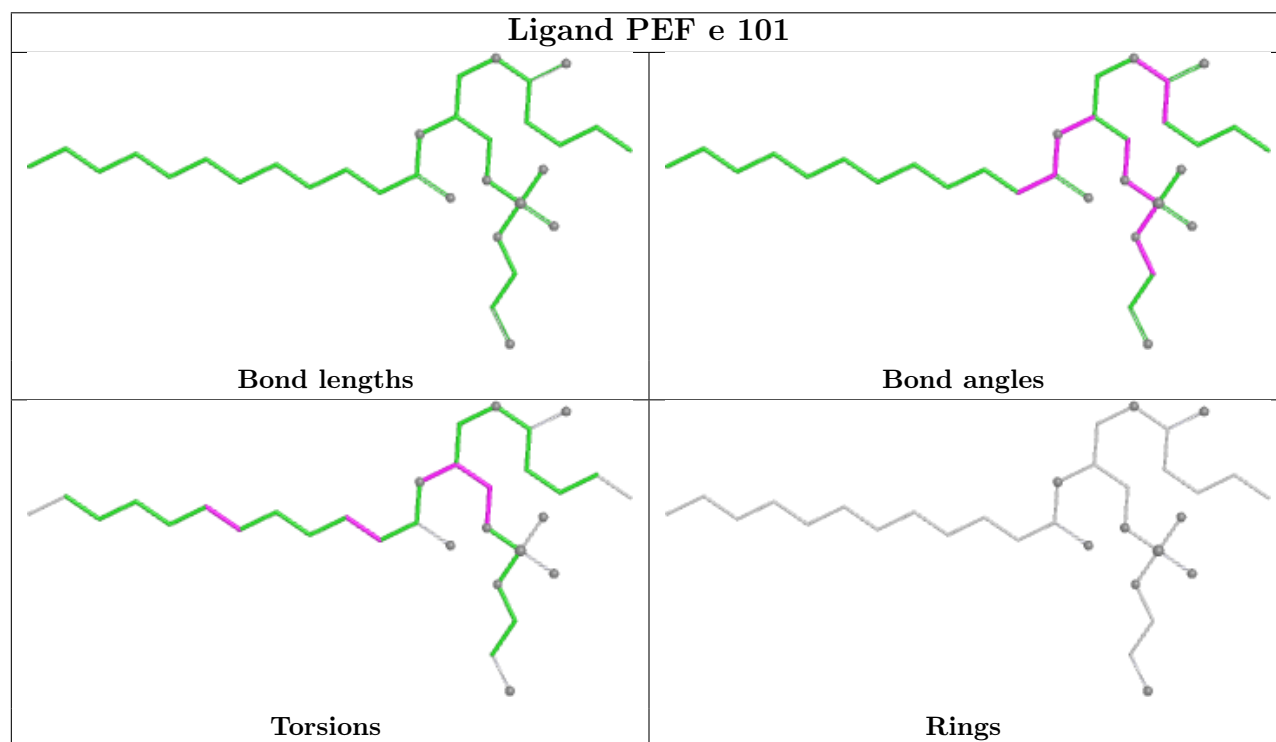
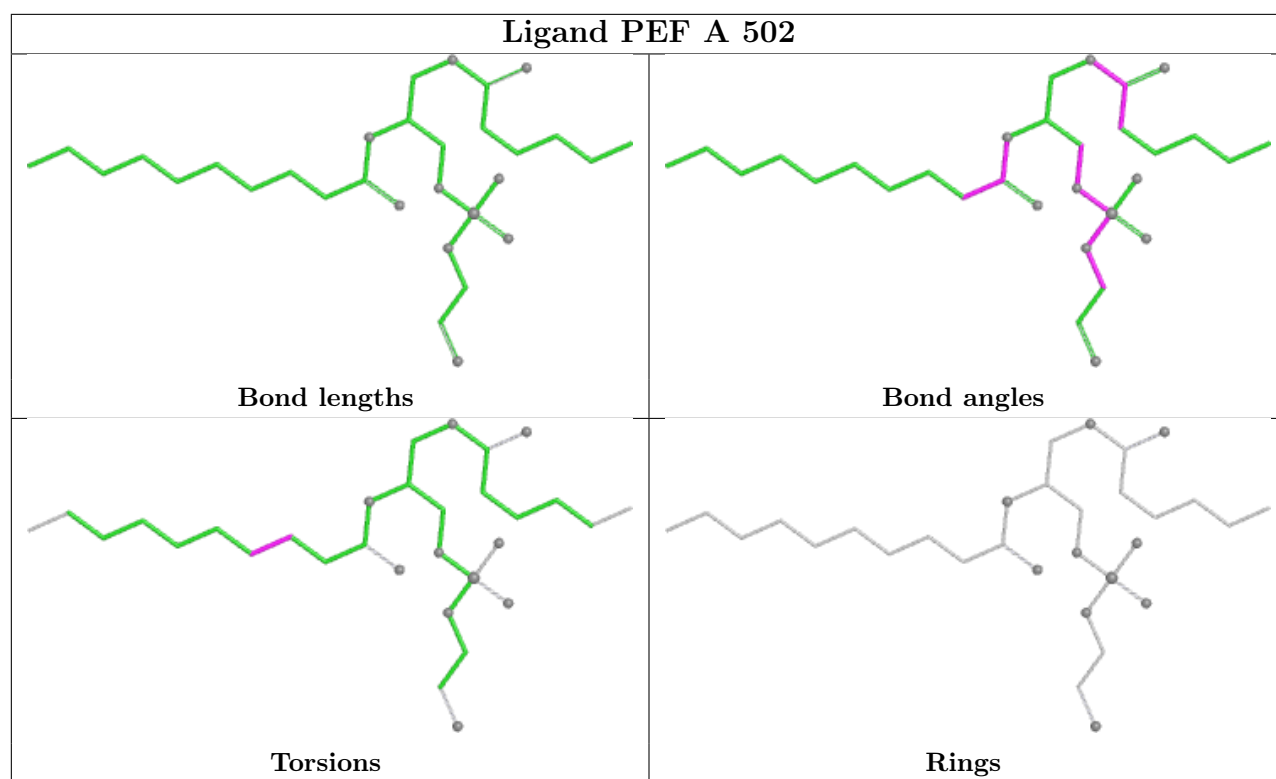


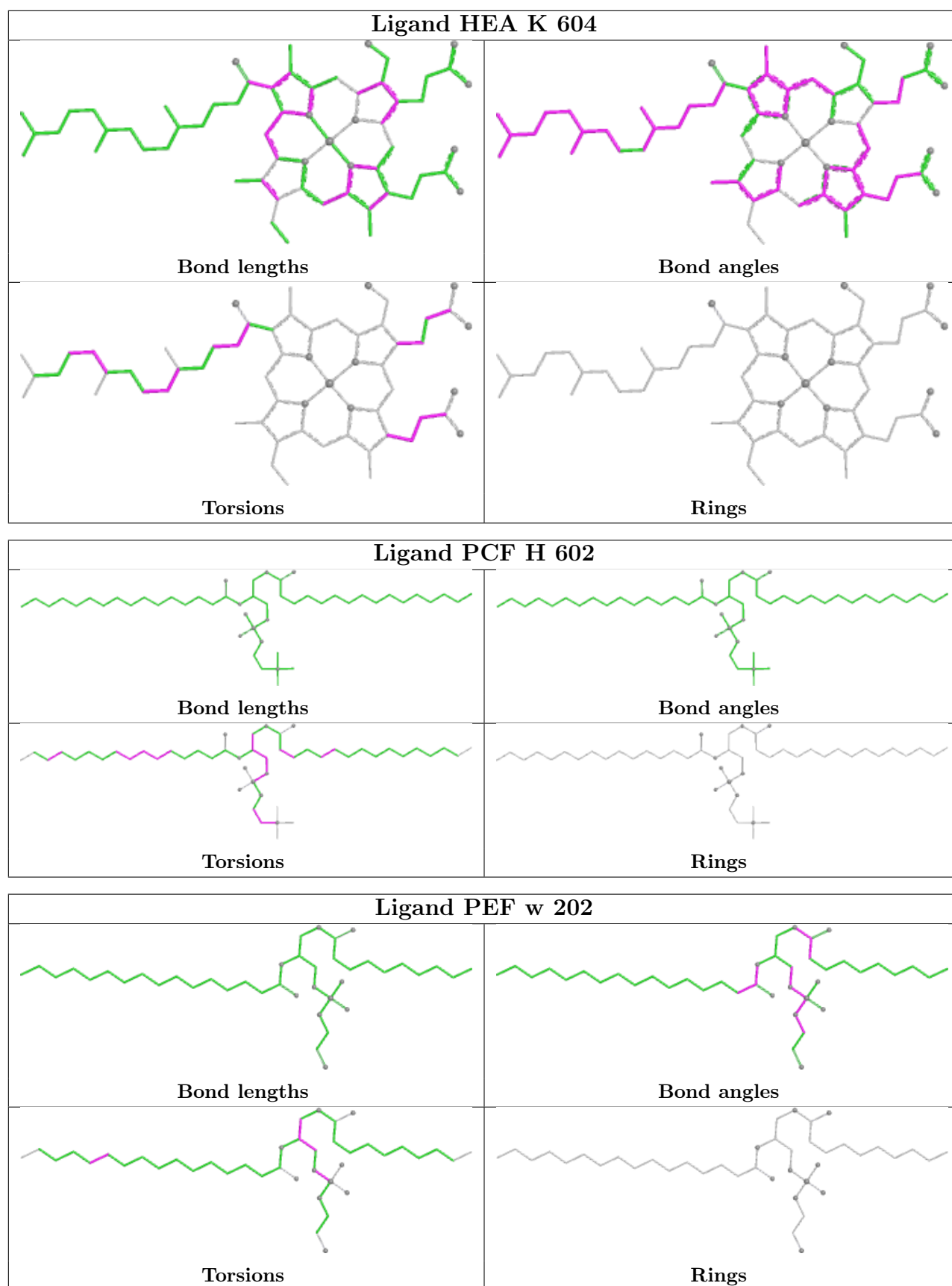


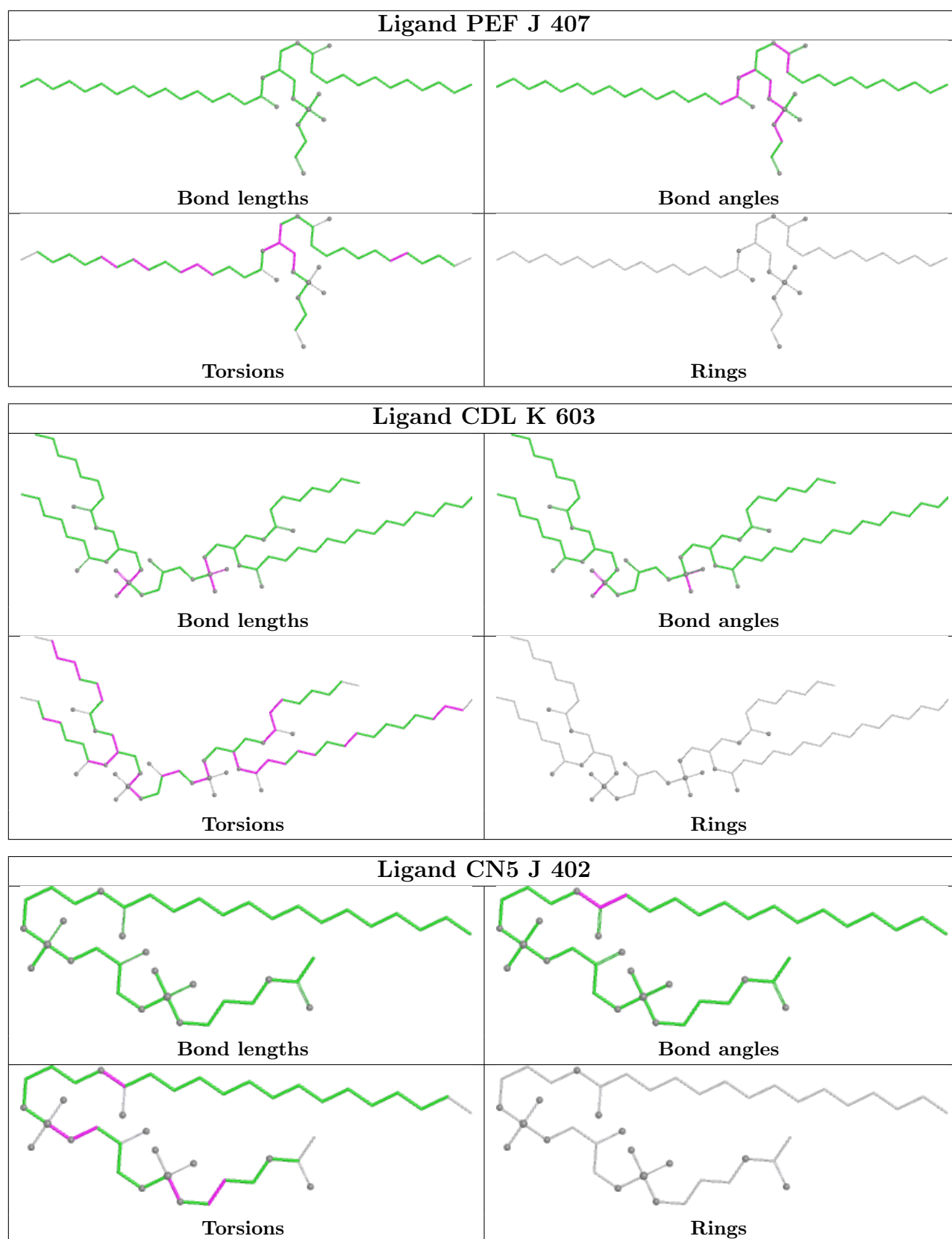


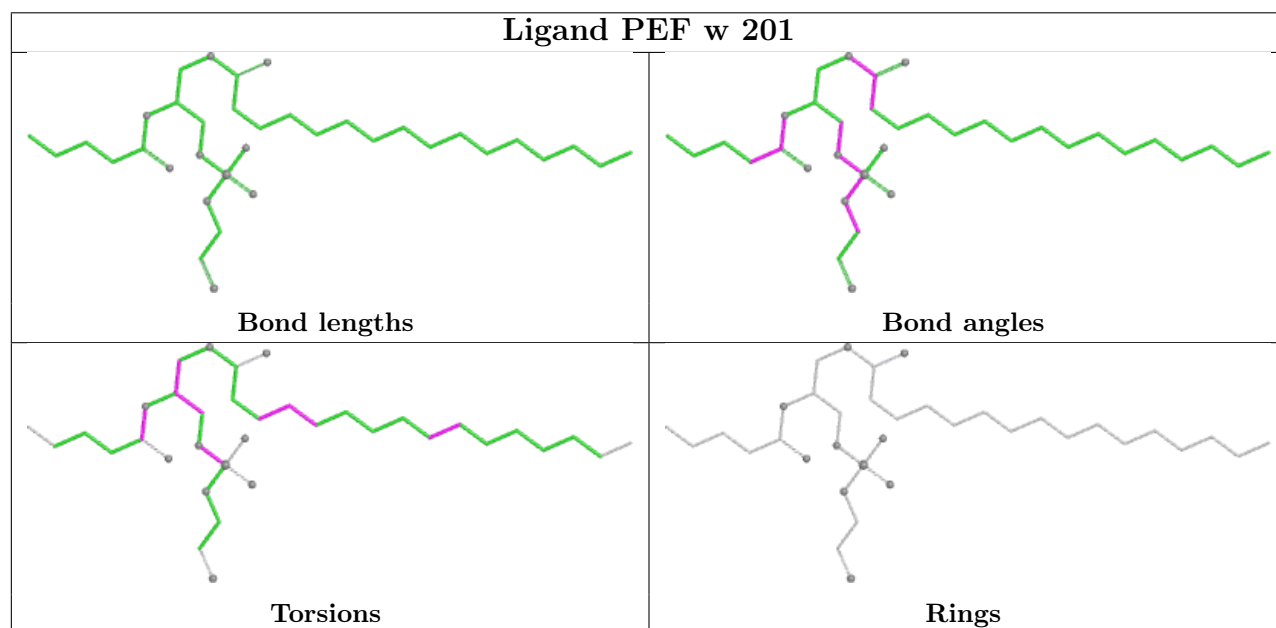
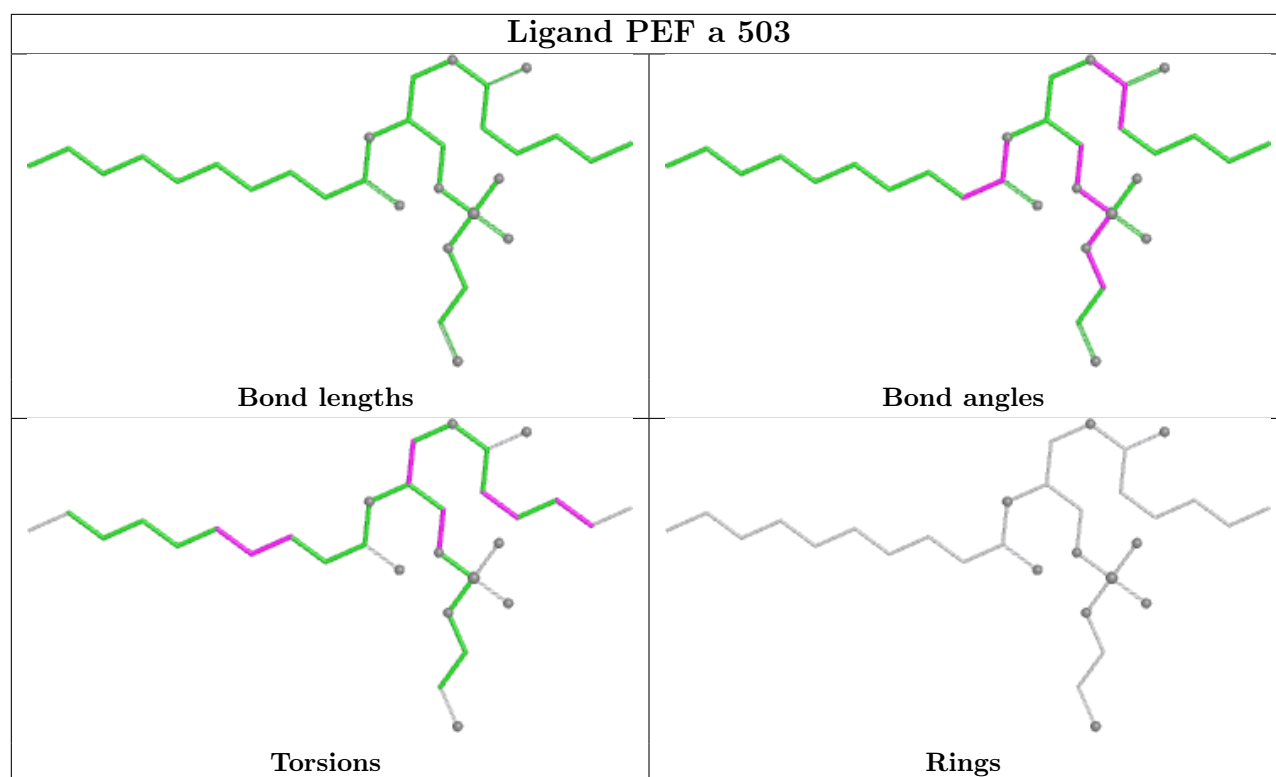


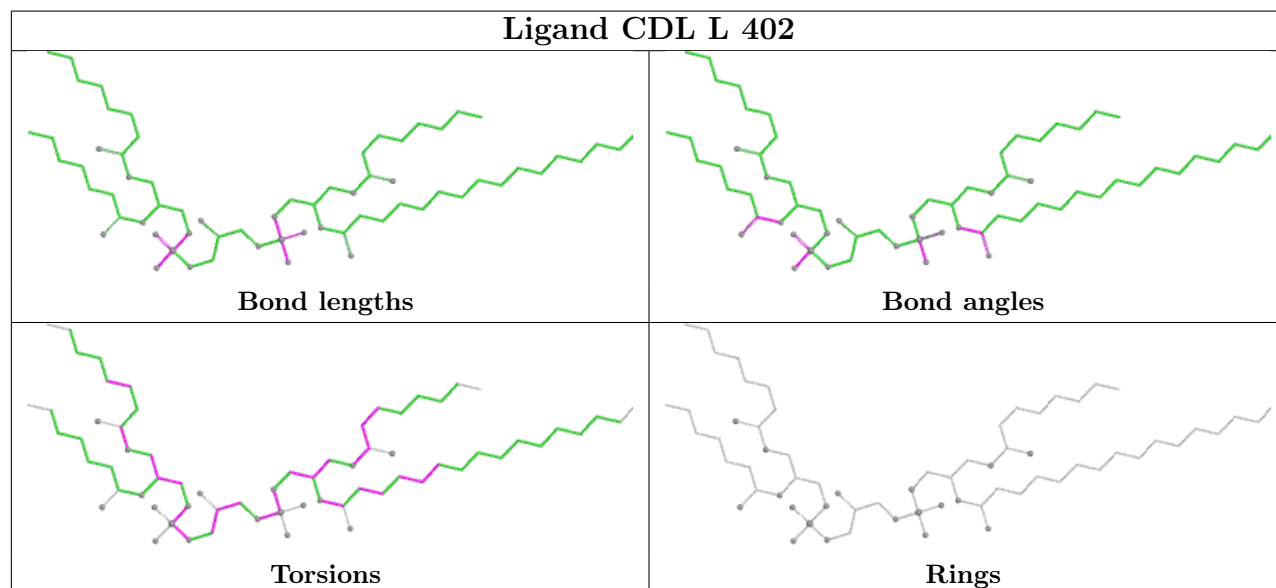
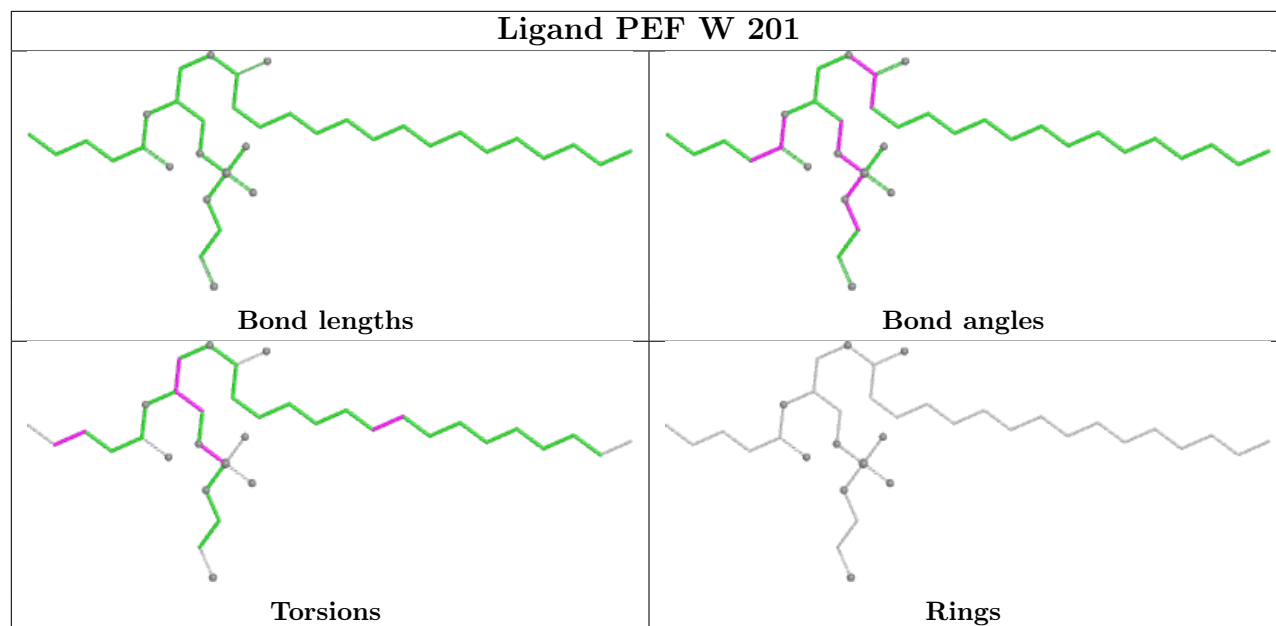


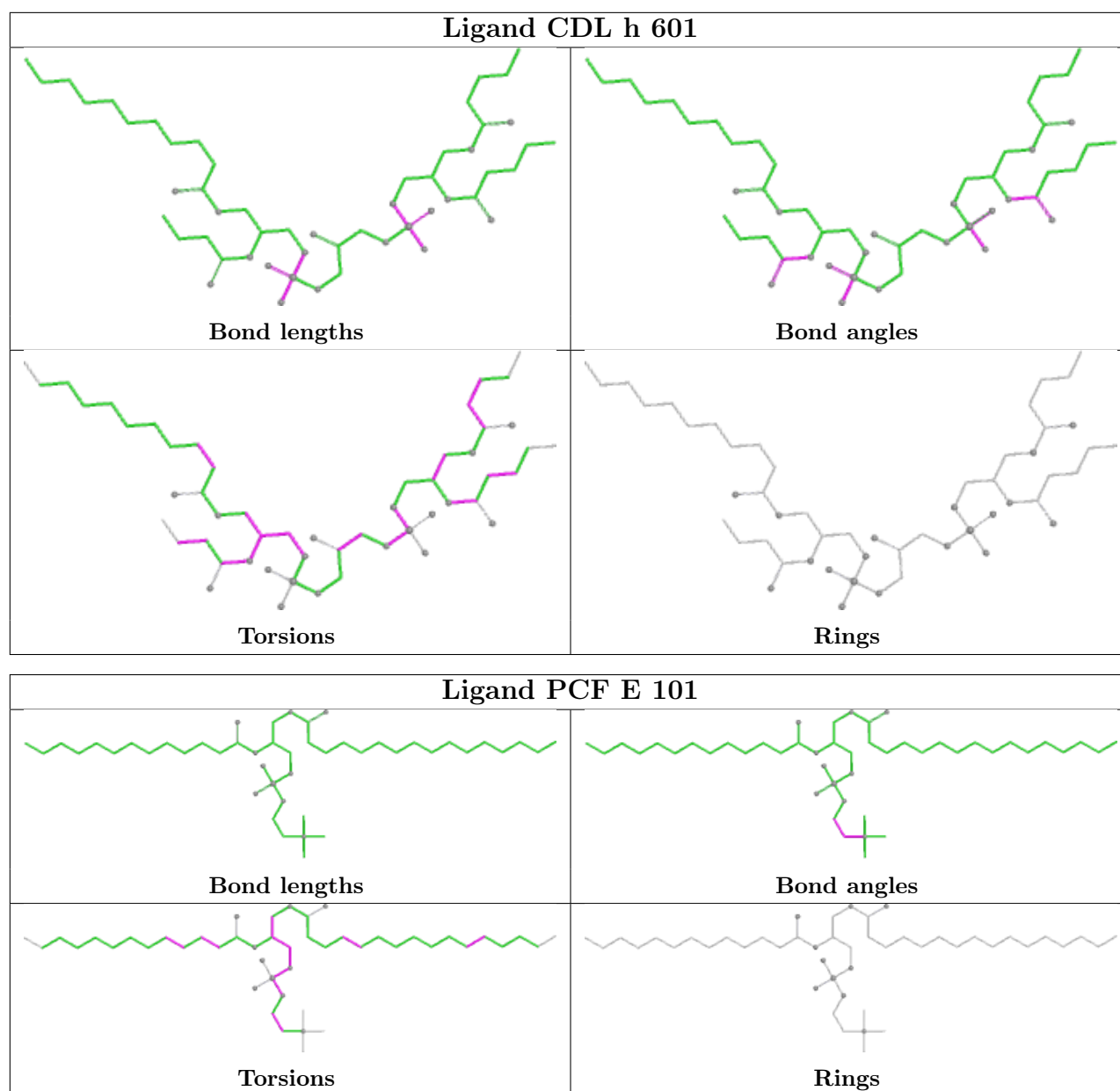


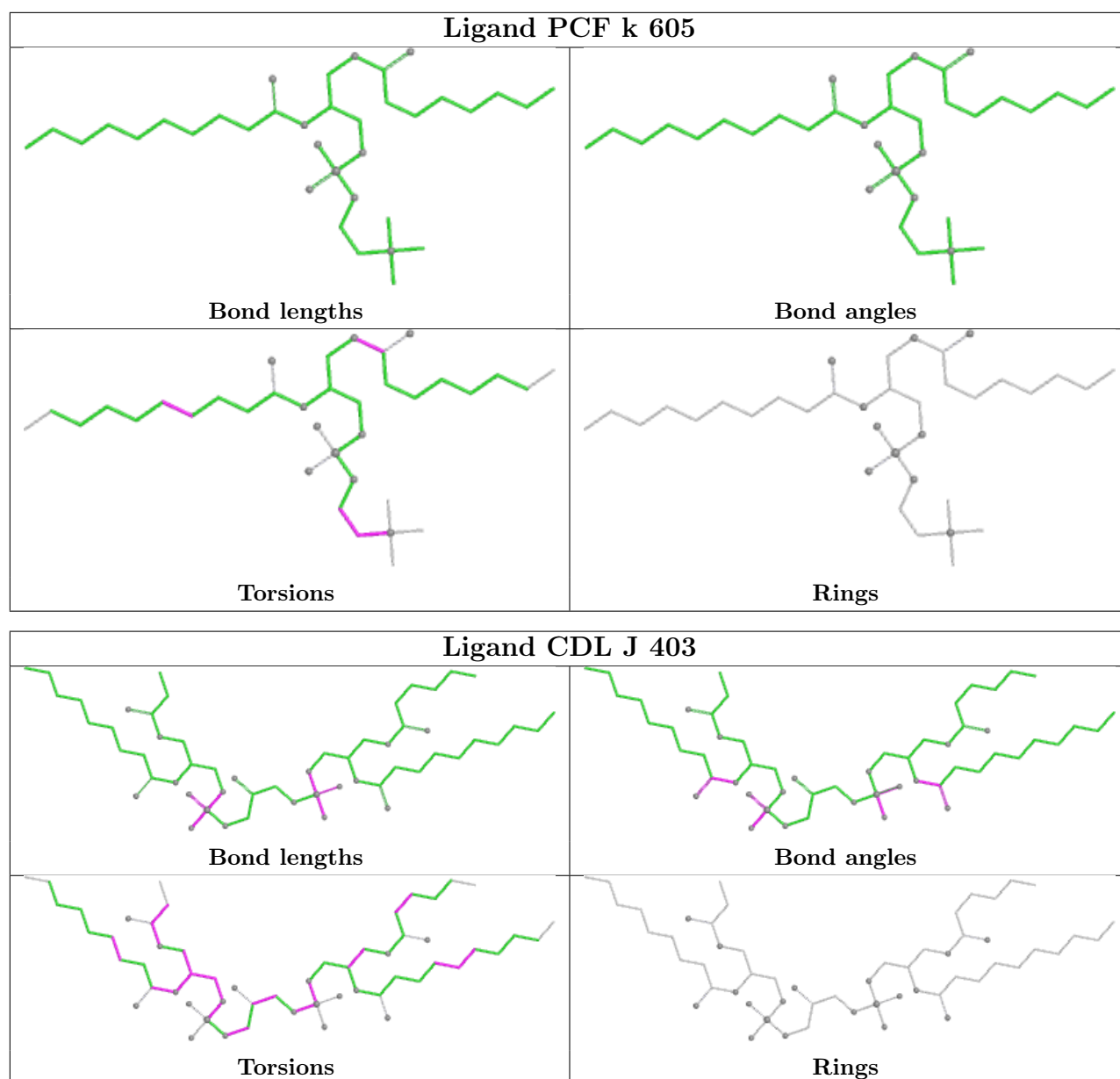


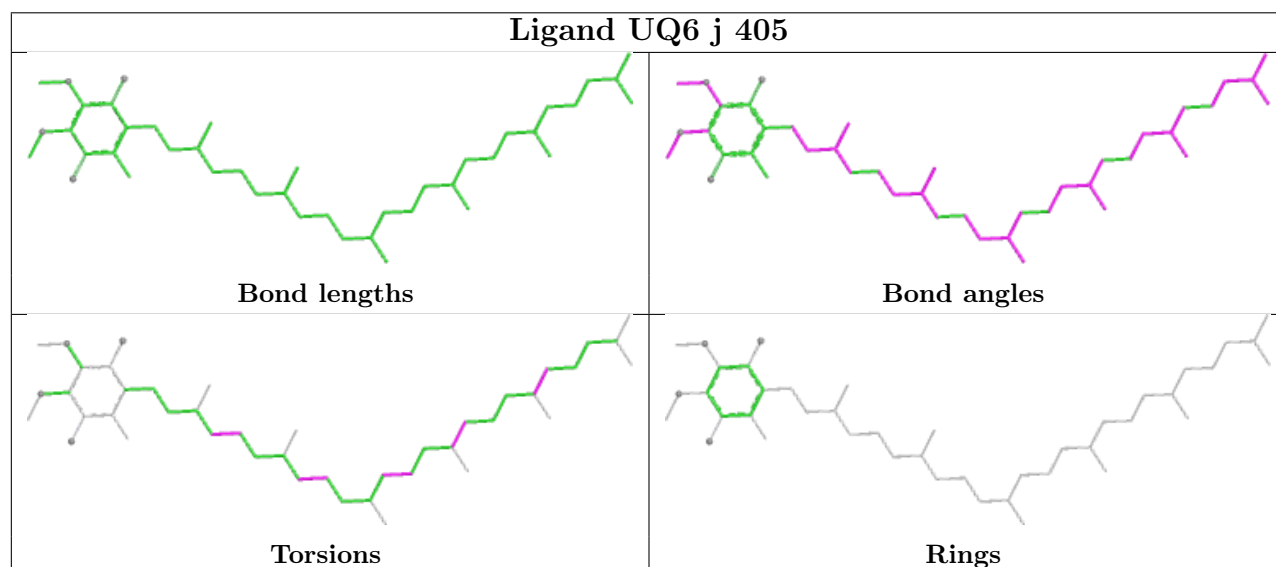
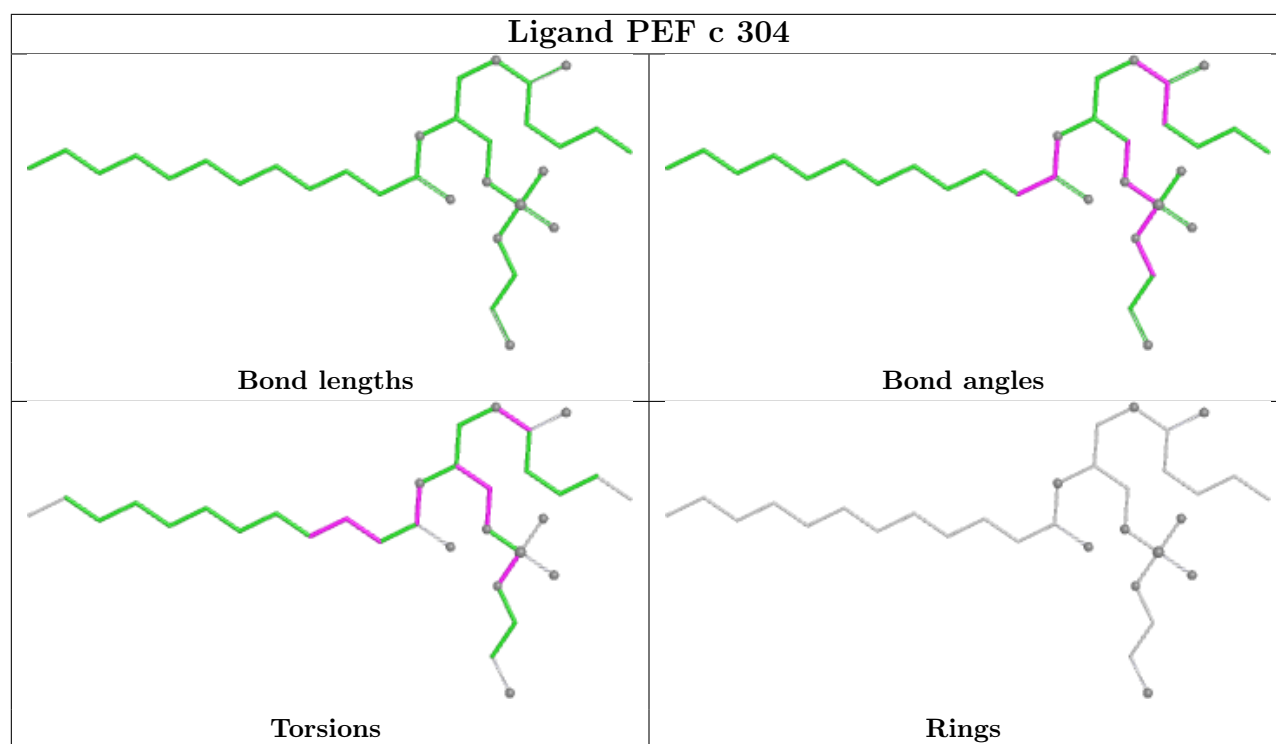


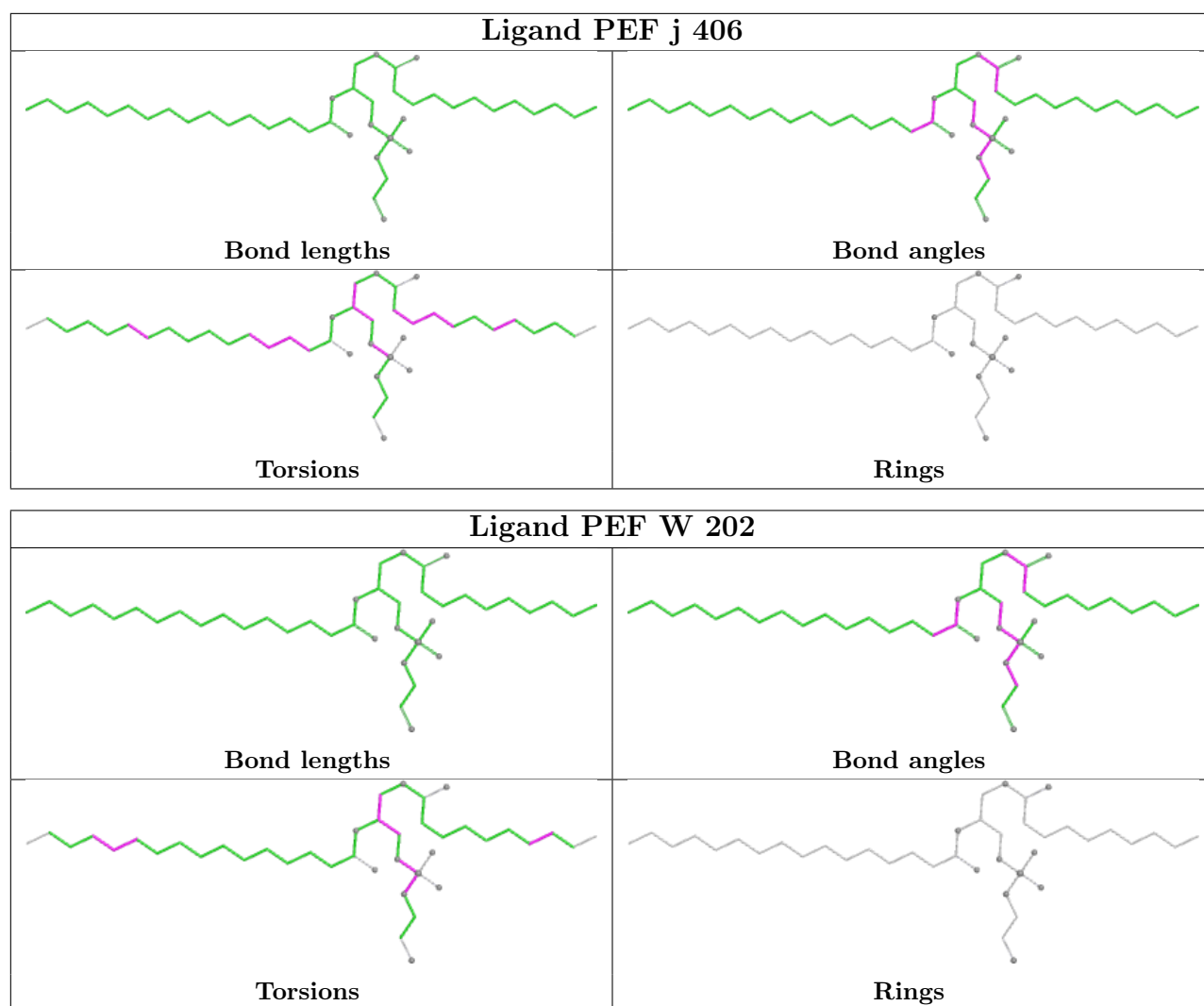


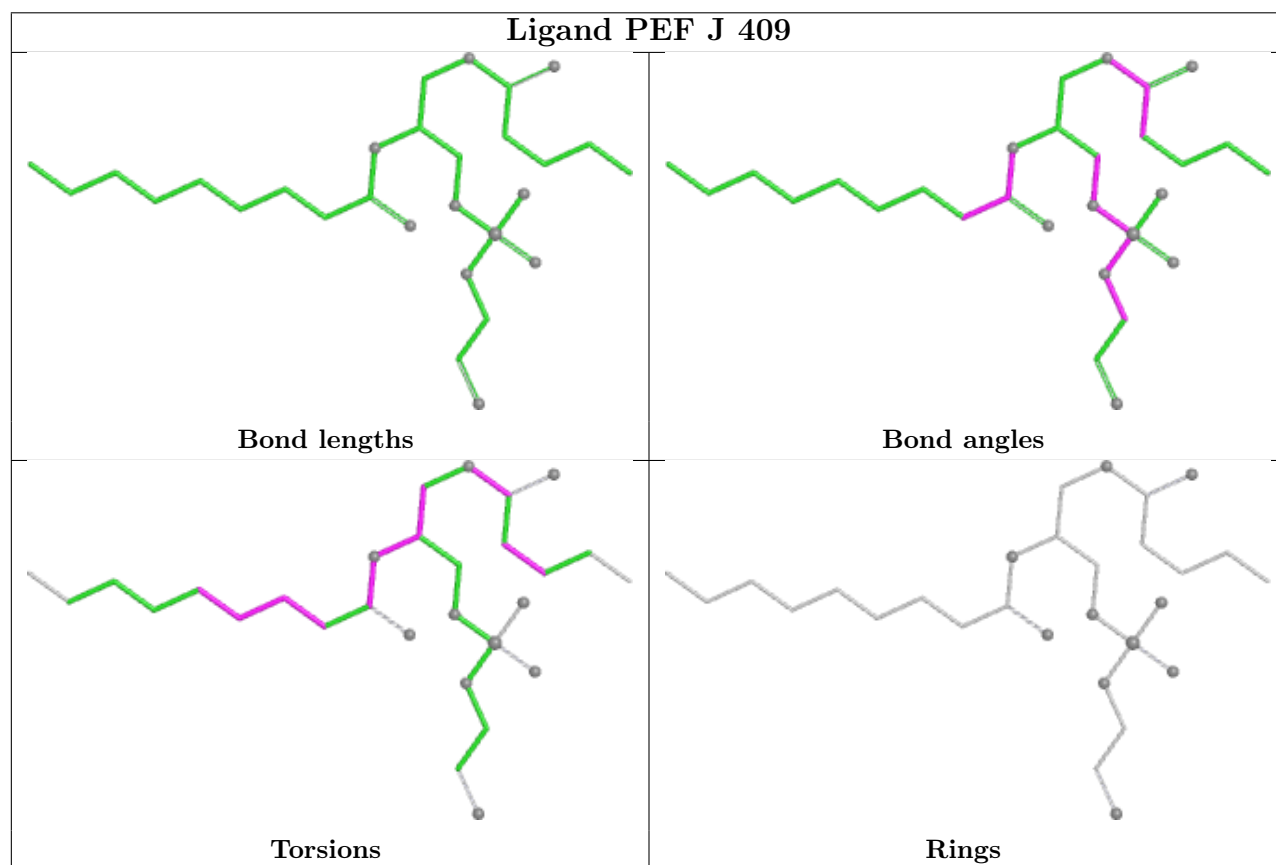
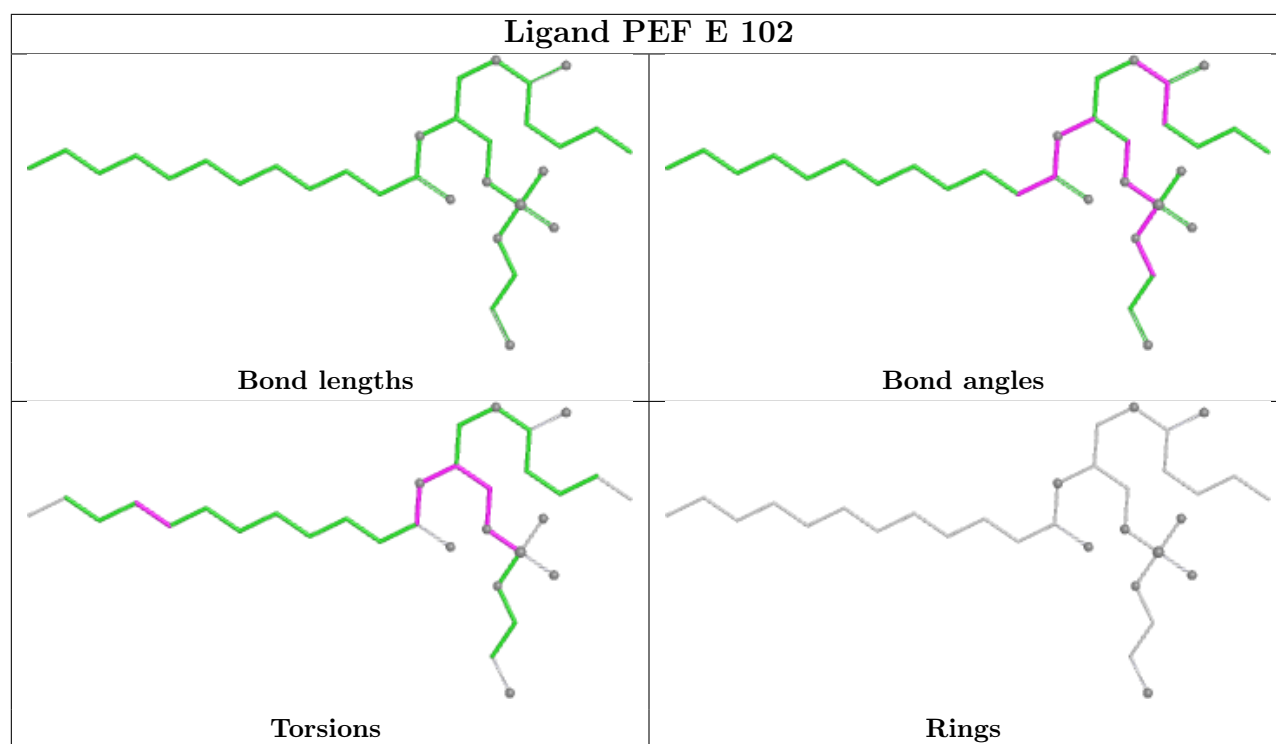


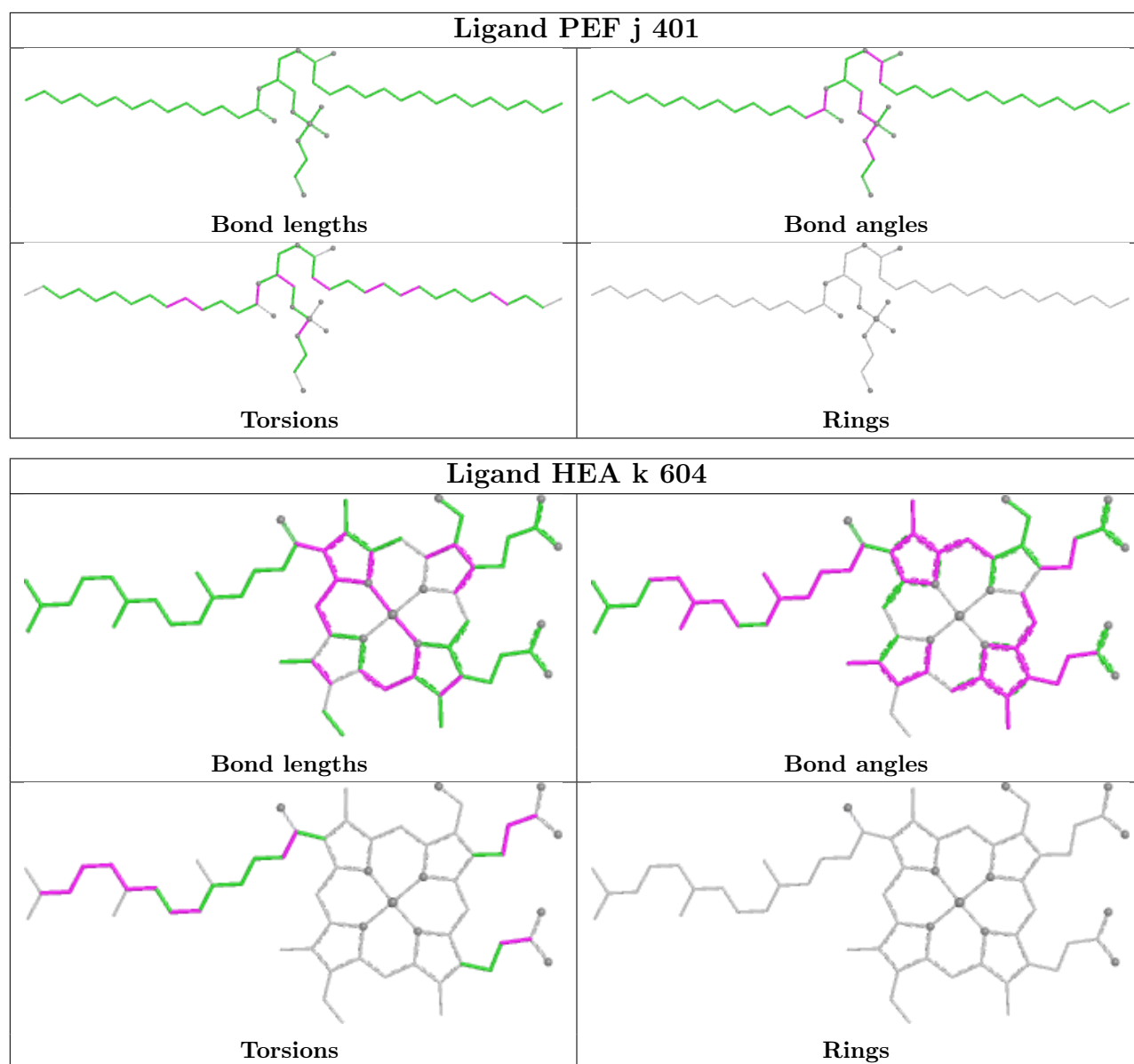




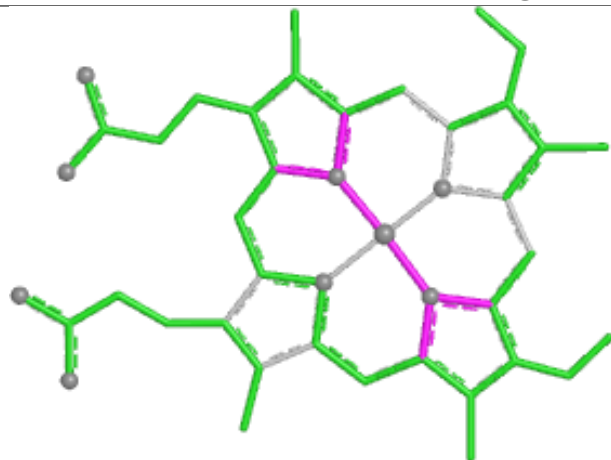




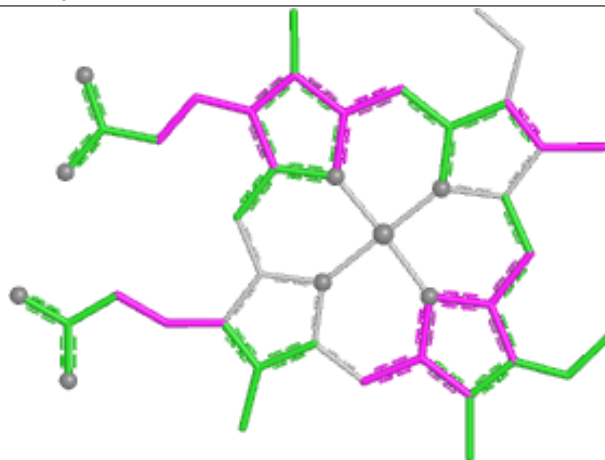




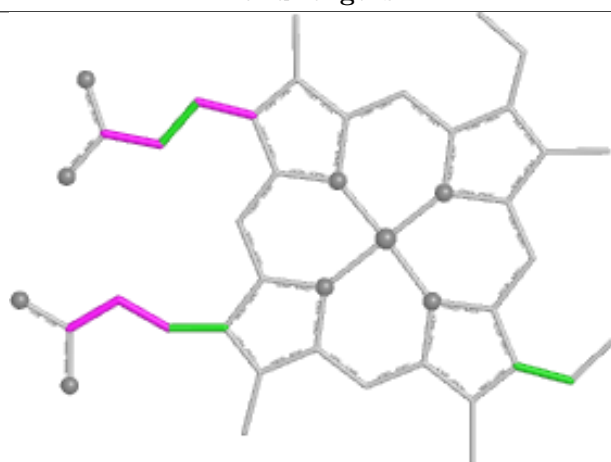
Ligand HEM j 404



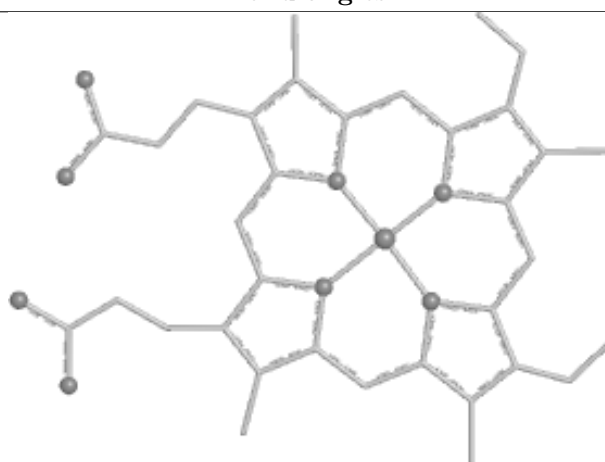
Bond lengths



Bond angles

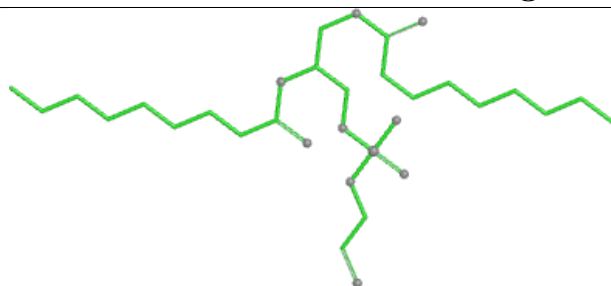


Torsions

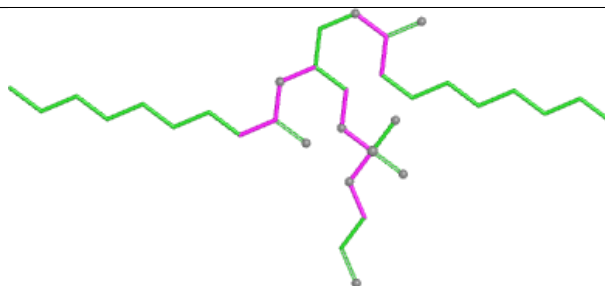


Rings

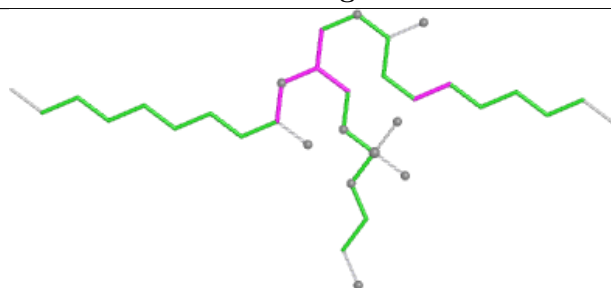
Ligand PEF v 101



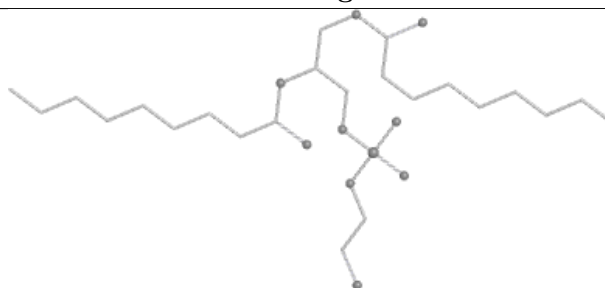
Bond lengths



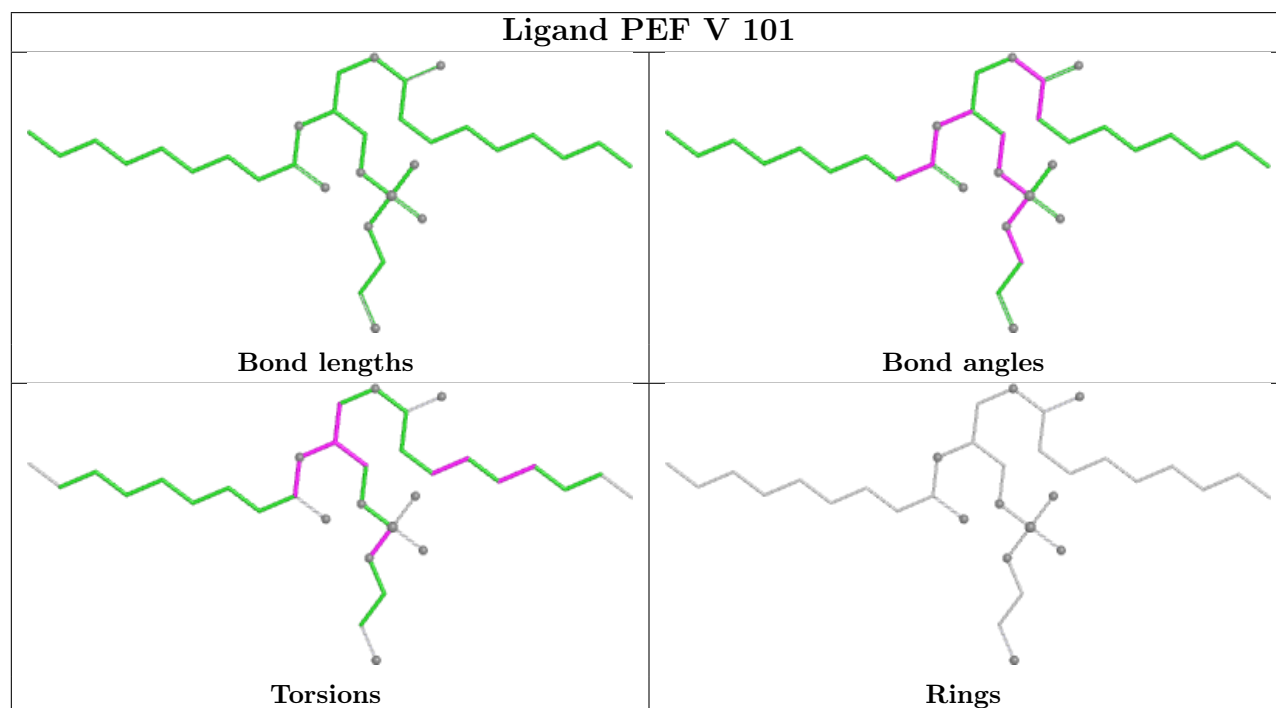
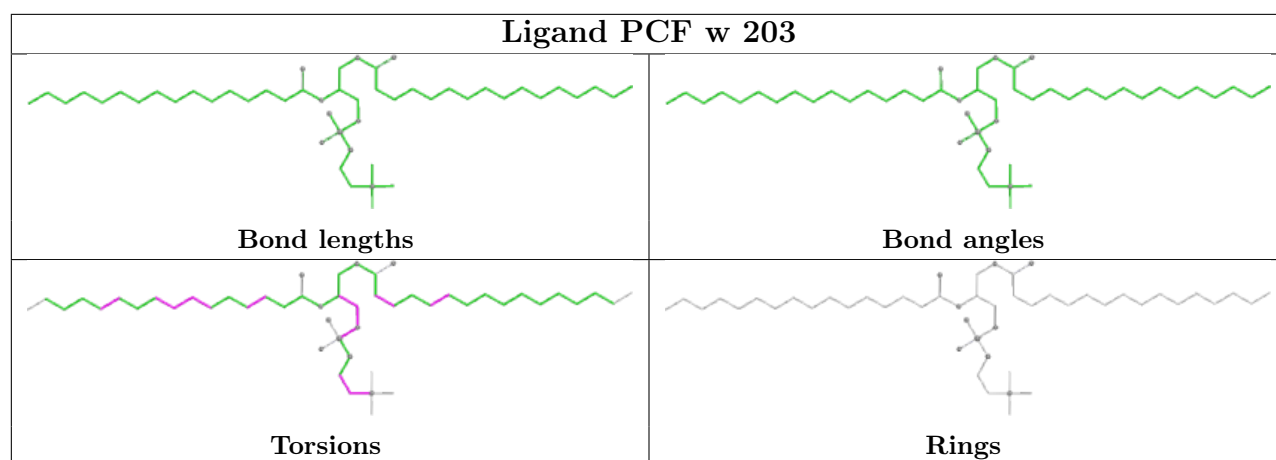
Bond angles

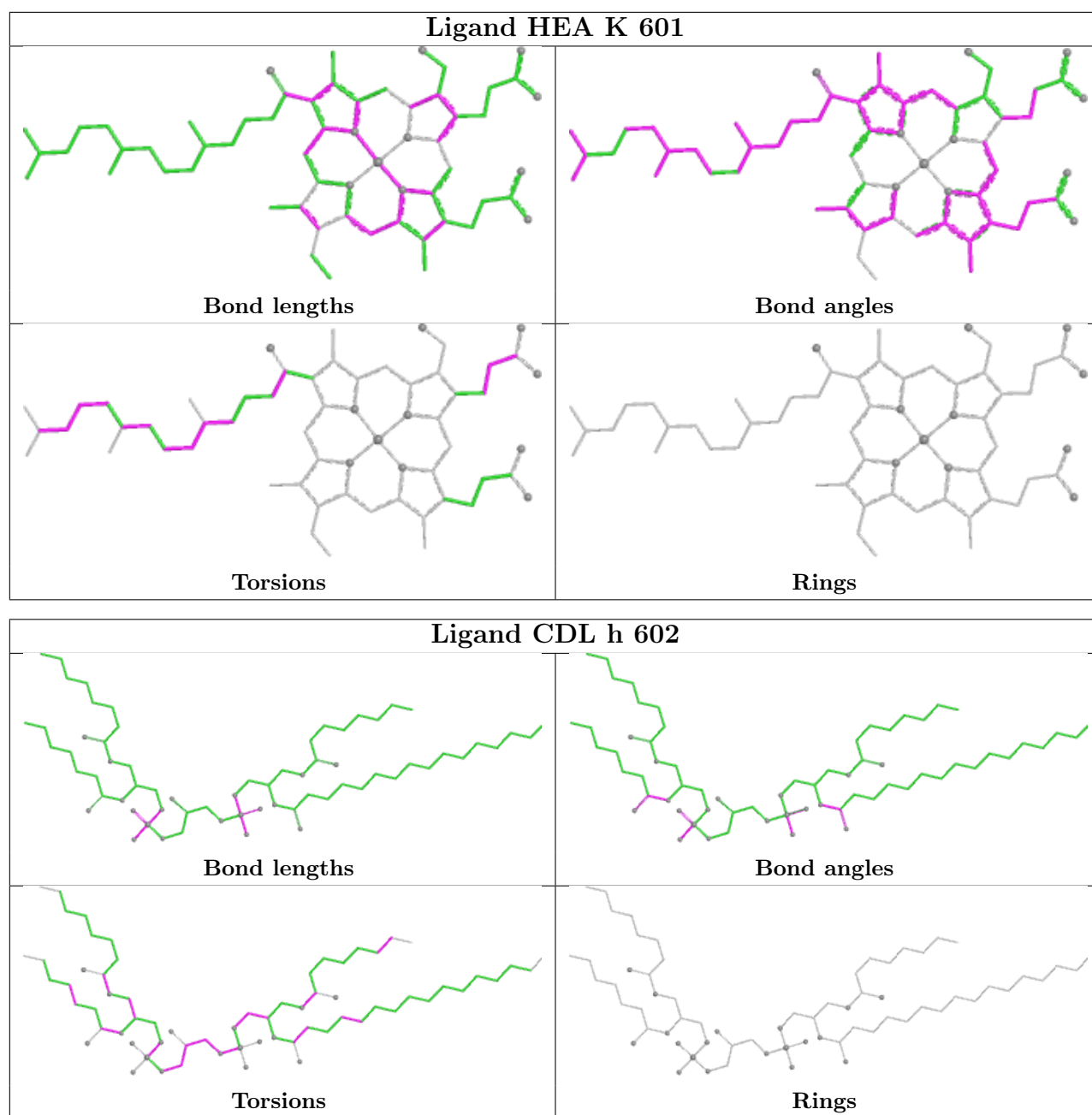


Torsions

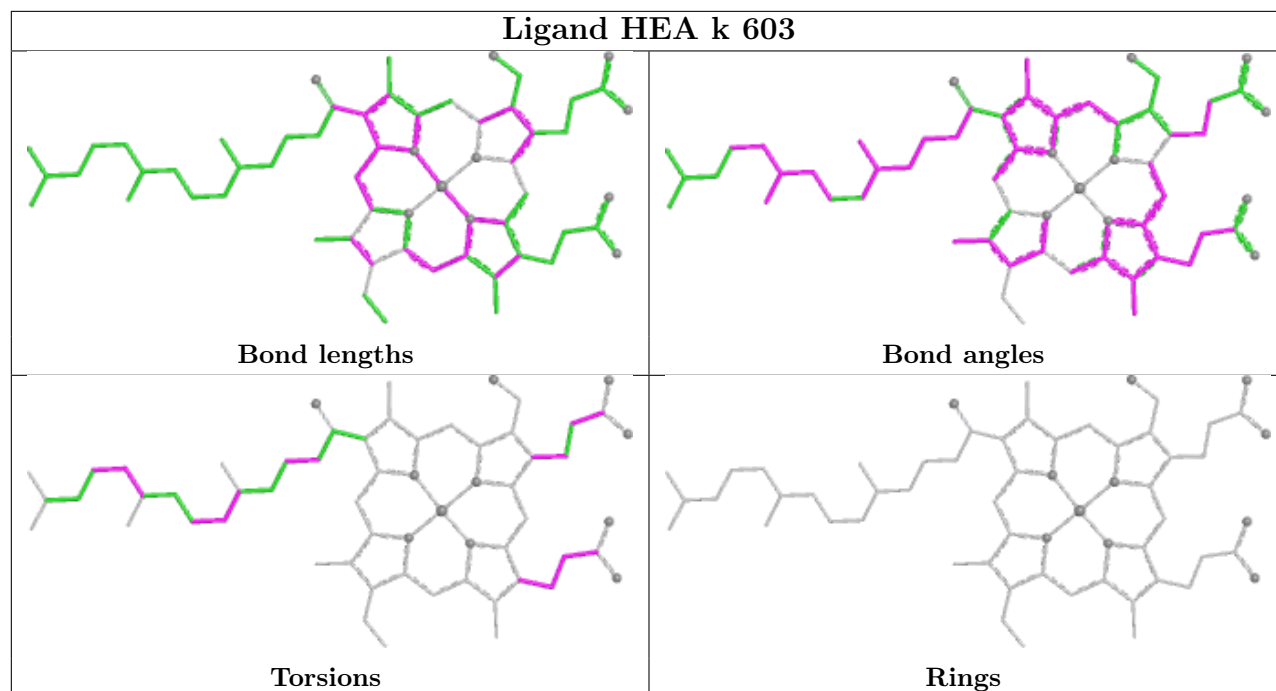


Rings

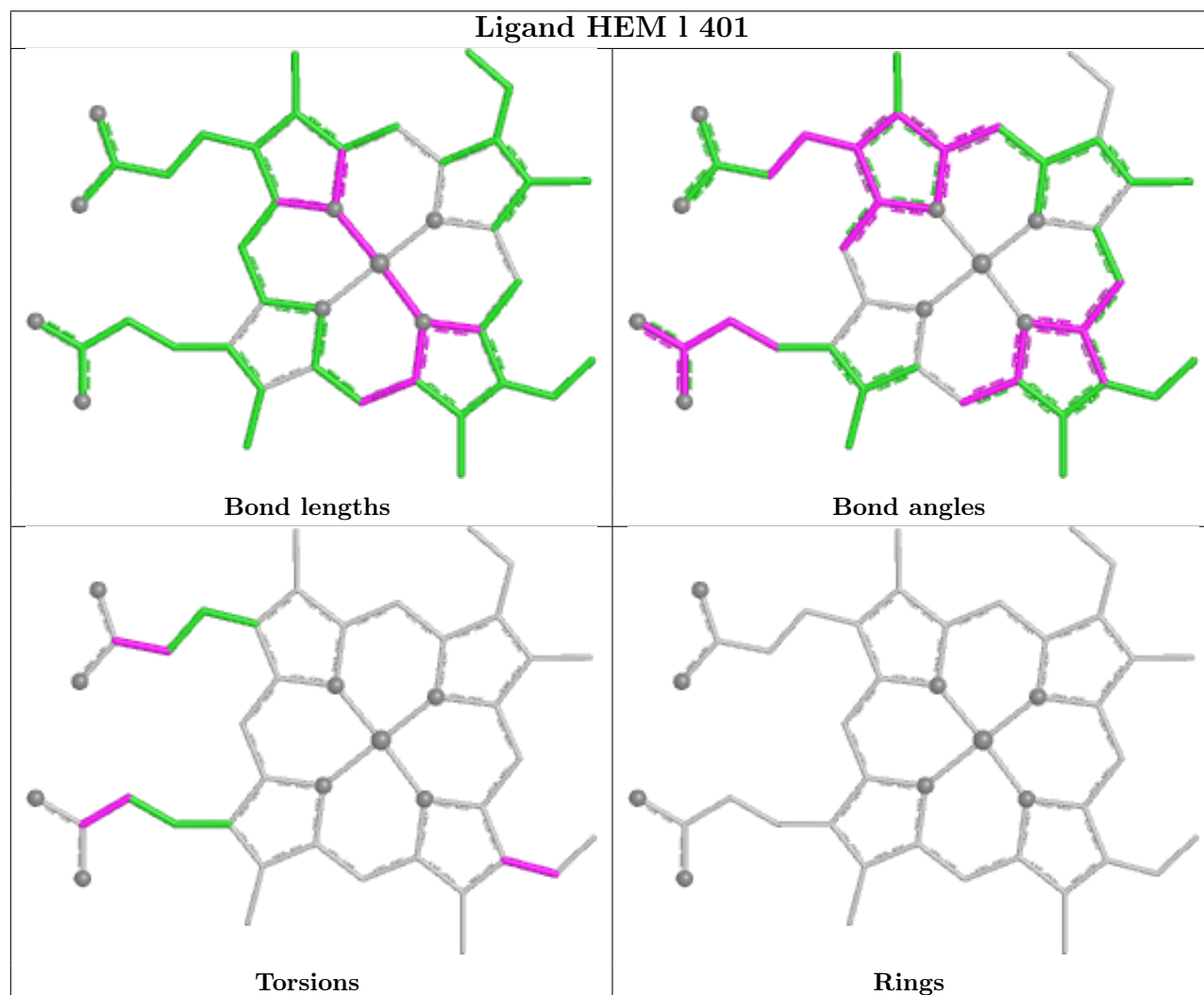


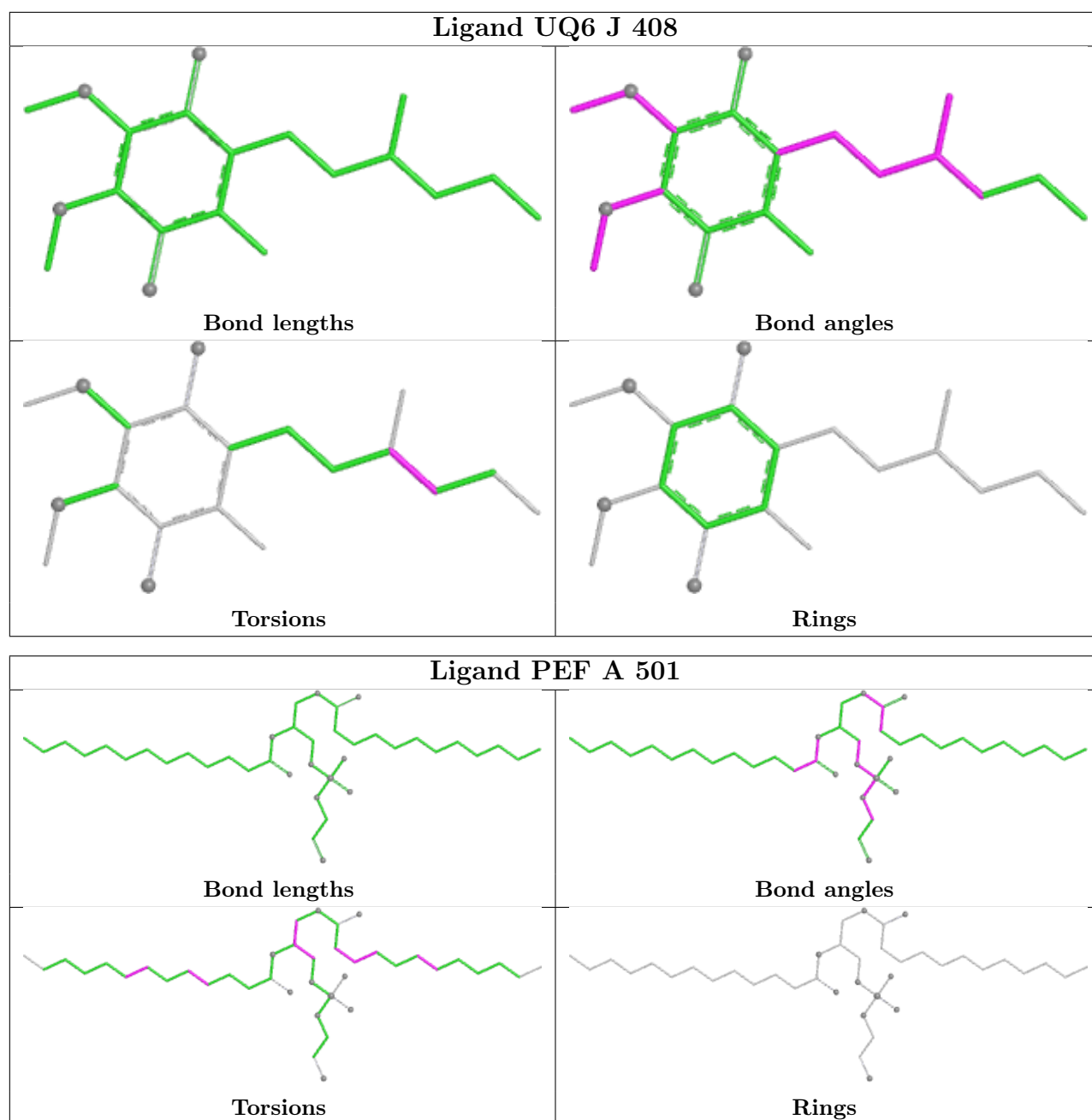


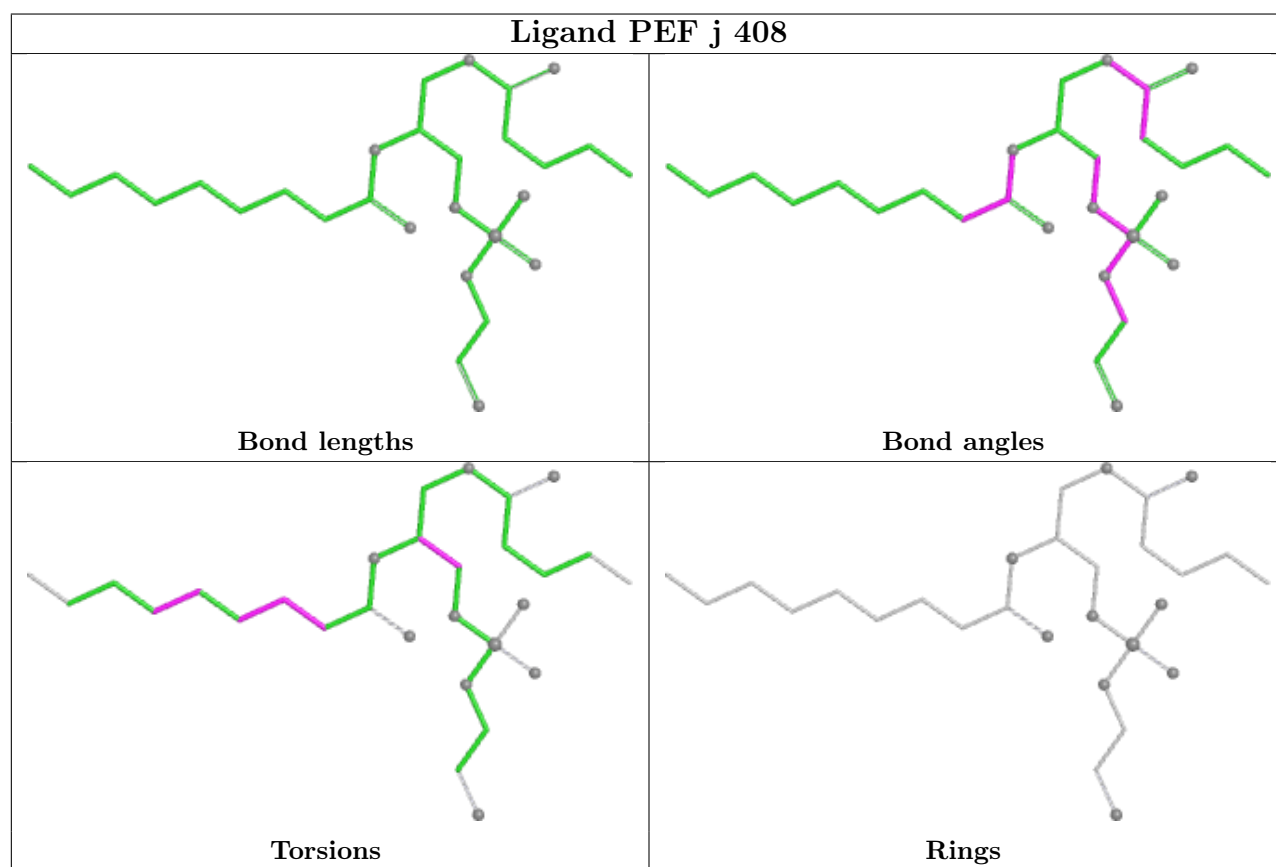
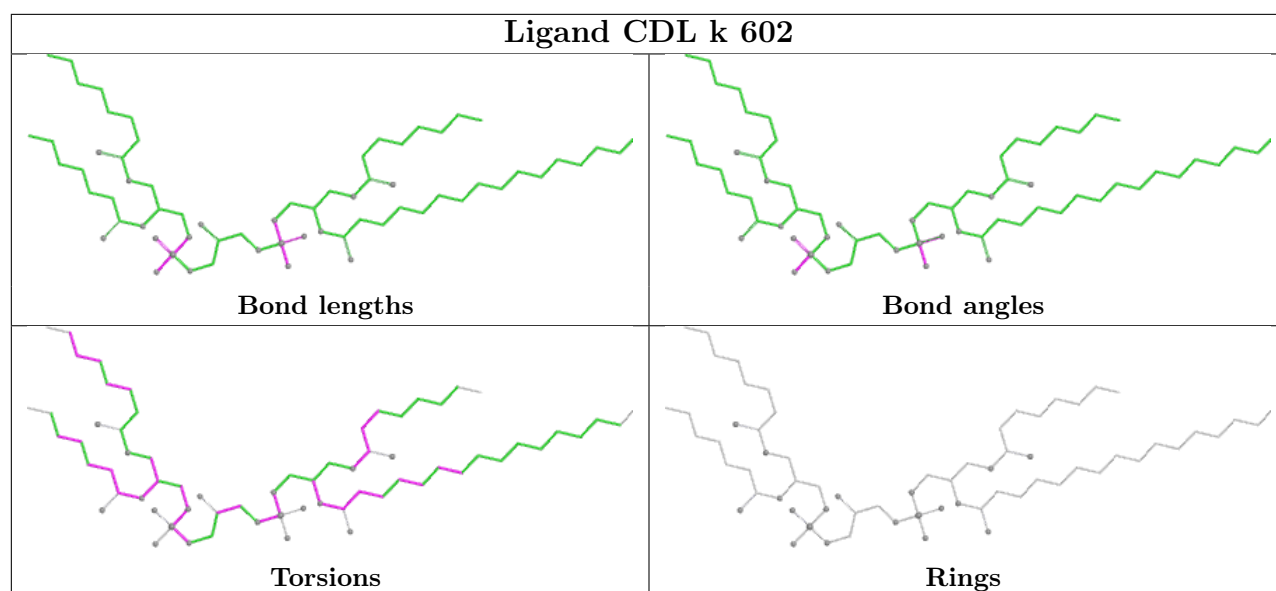
Ligand HEA k 603

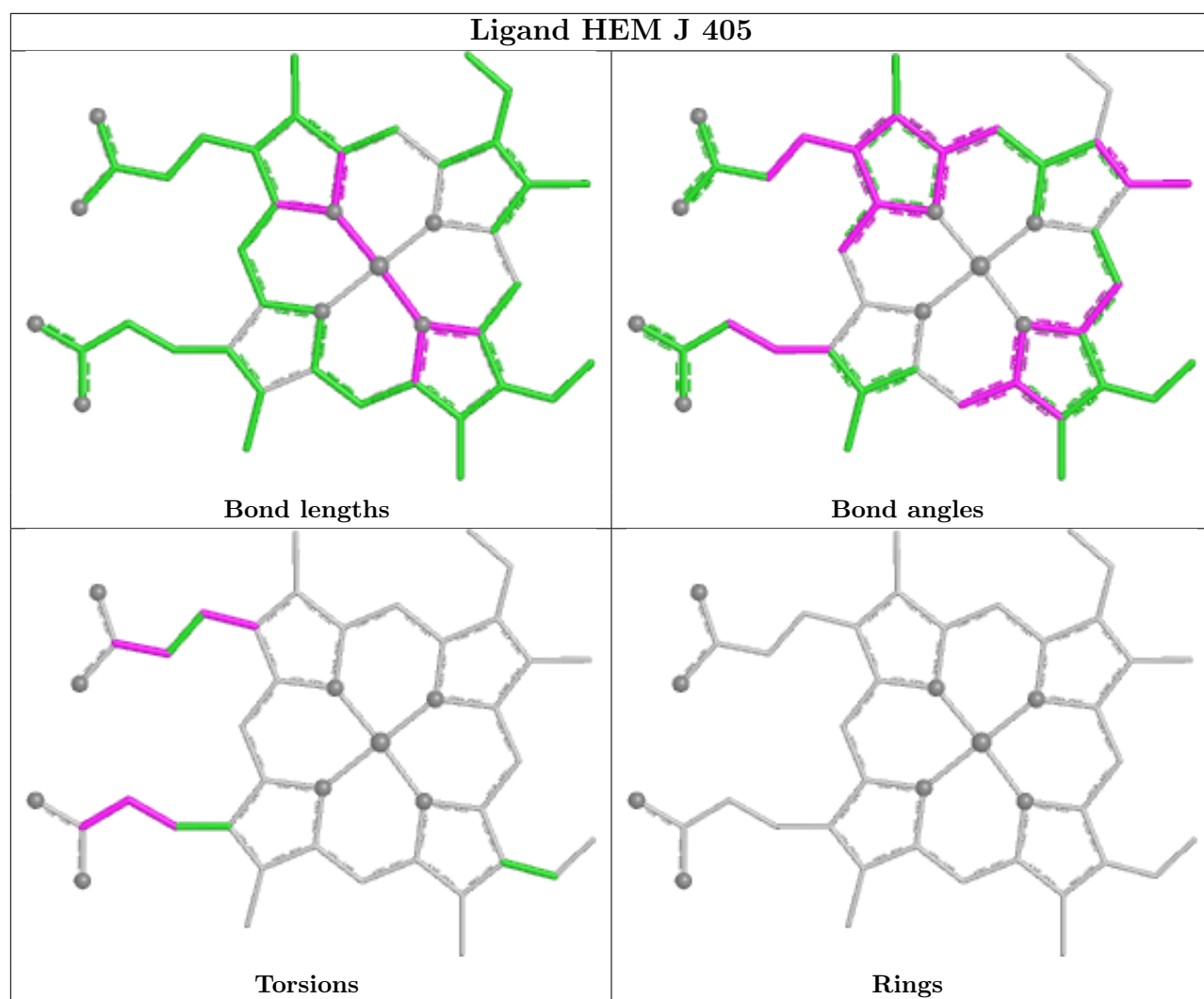


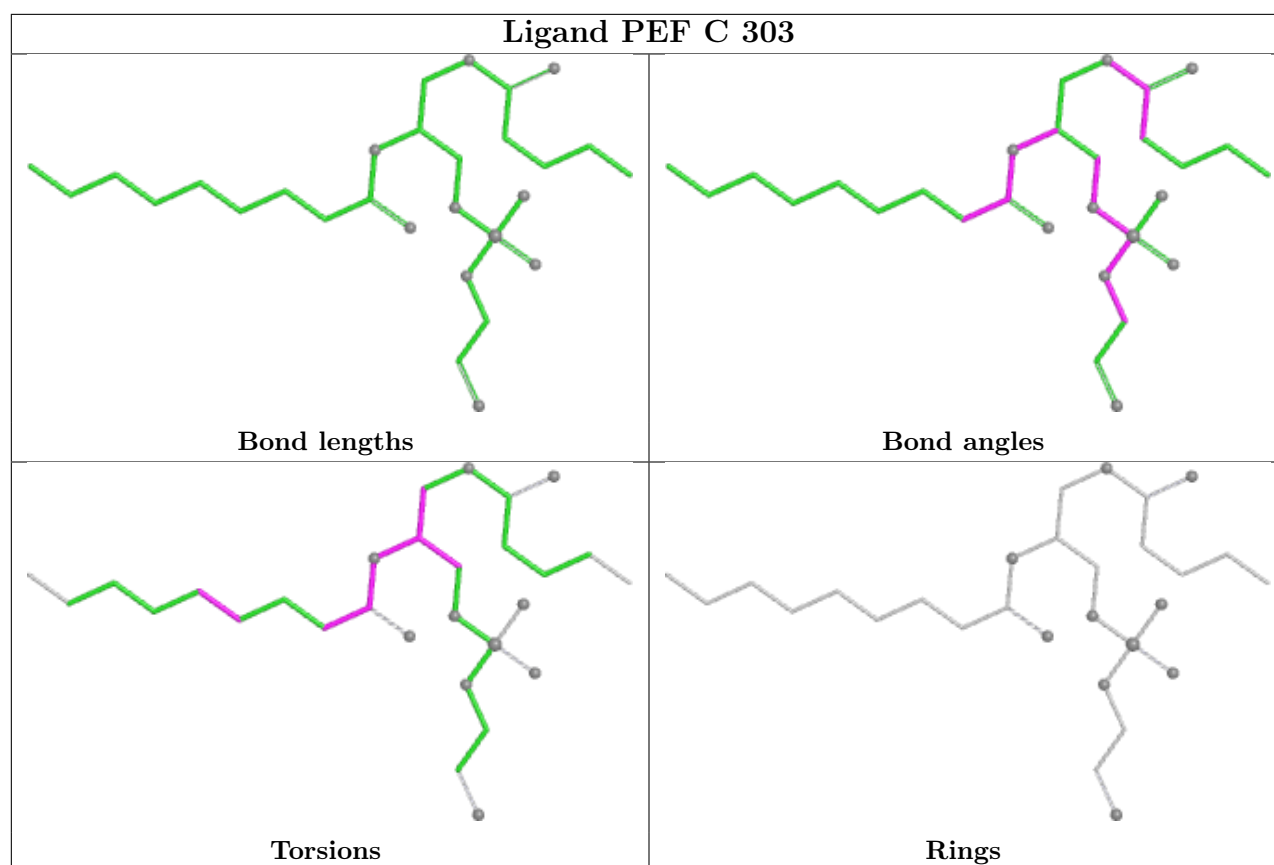
Ligand HEM l 401











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.

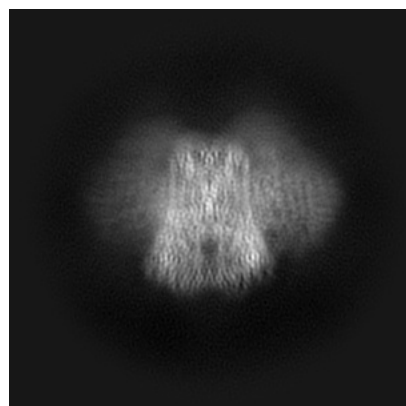
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27940. These allow visual inspection of the internal detail of the map and identification of artifacts.

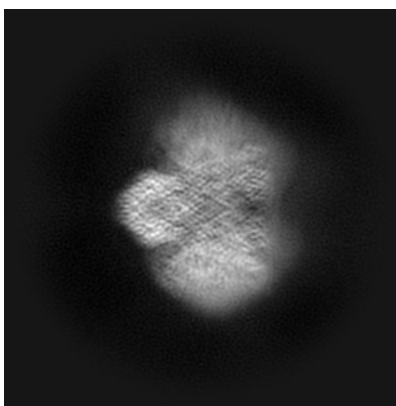
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

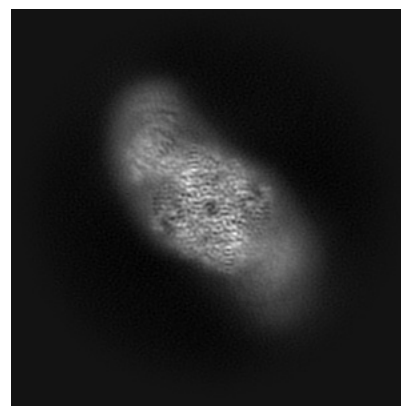
6.1.1 Primary map



X

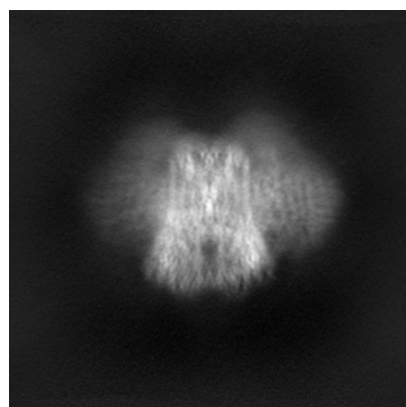


Y

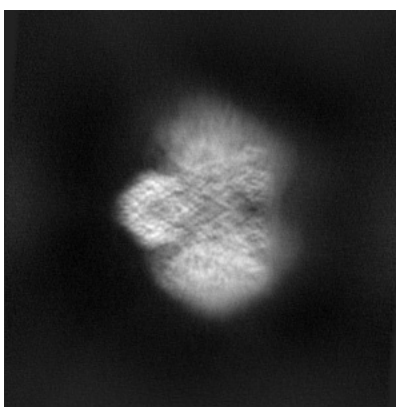


Z

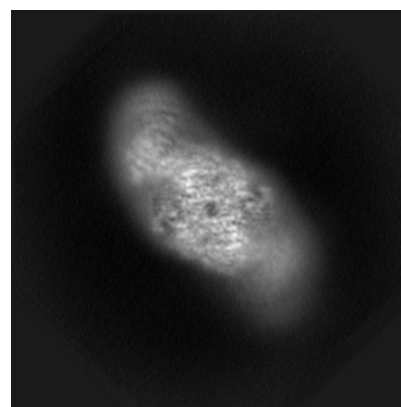
6.1.2 Raw map



X



Y

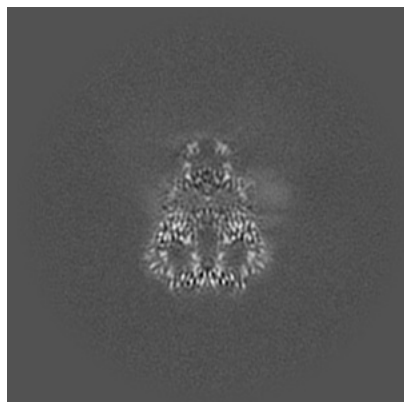


Z

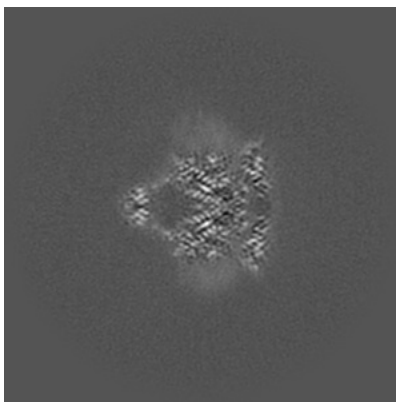
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

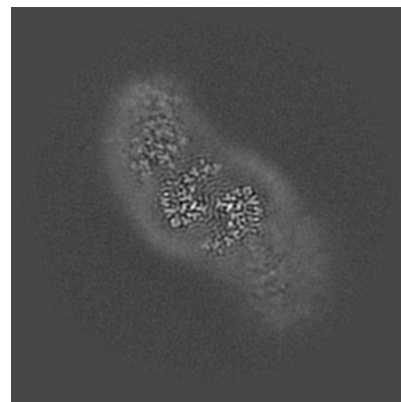
6.2.1 Primary map



X Index: 180

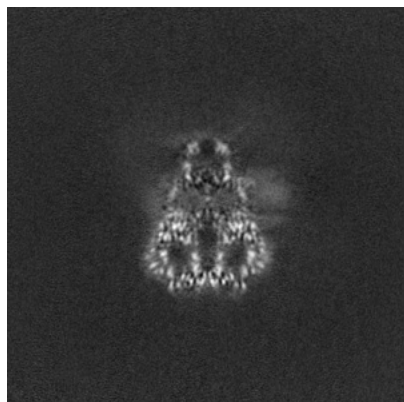


Y Index: 180

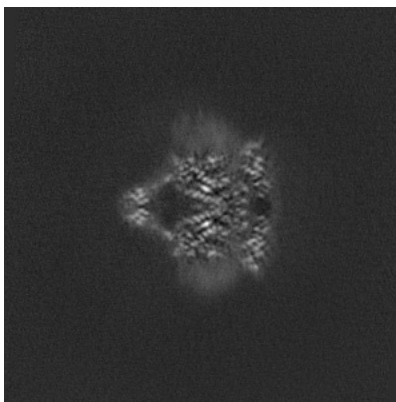


Z Index: 180

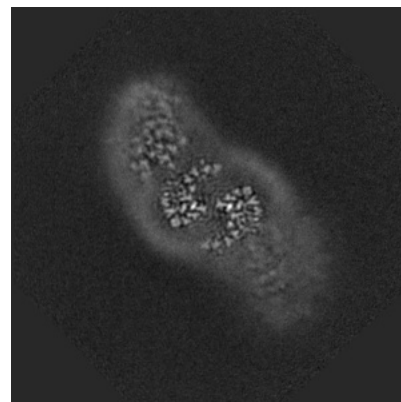
6.2.2 Raw map



X Index: 180



Y Index: 180

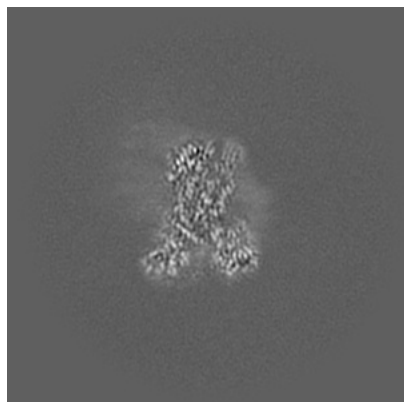


Z Index: 180

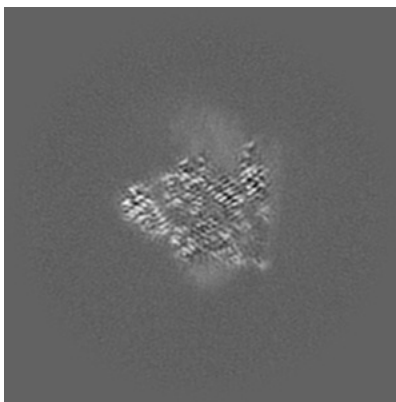
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

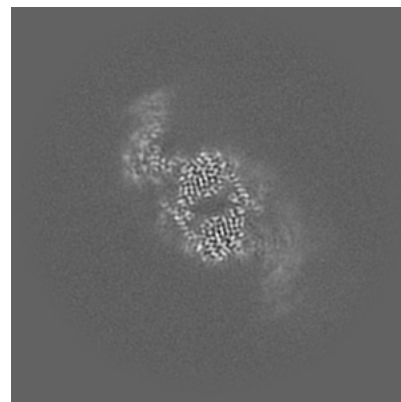
6.3.1 Primary map



X Index: 202

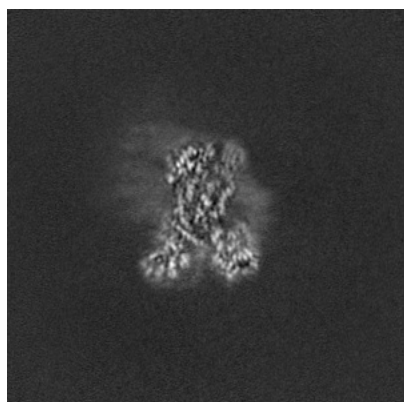


Y Index: 170

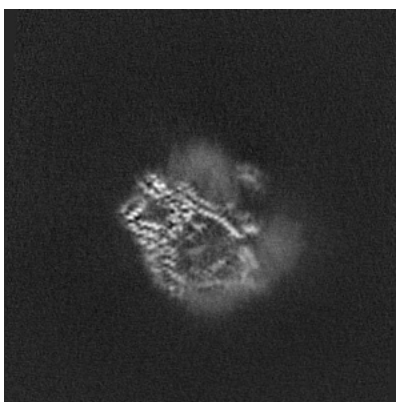


Z Index: 153

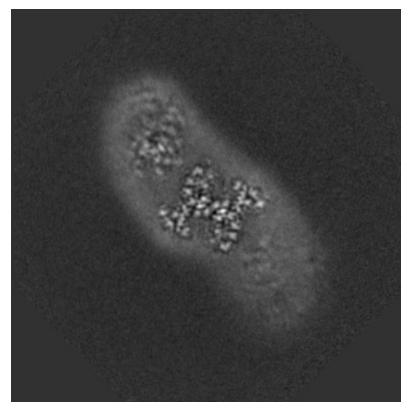
6.3.2 Raw map



X Index: 202



Y Index: 214

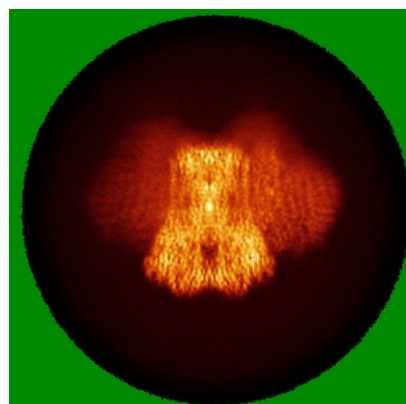


Z Index: 197

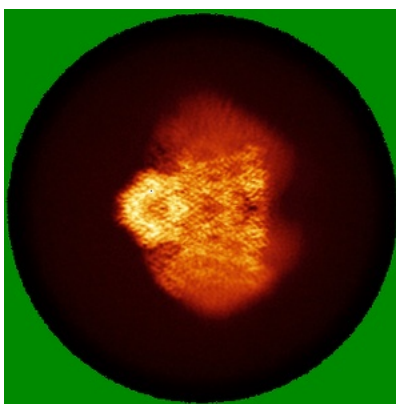
The images above show the largest variance slices of the map in three orthogonal directions.

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

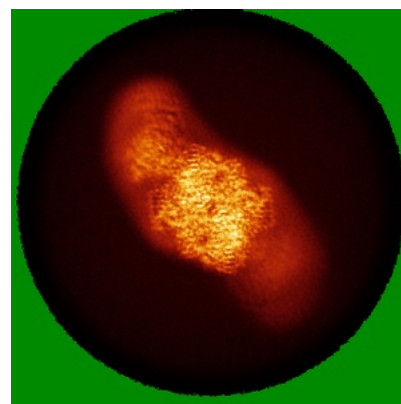
6.4.1 Primary map



X

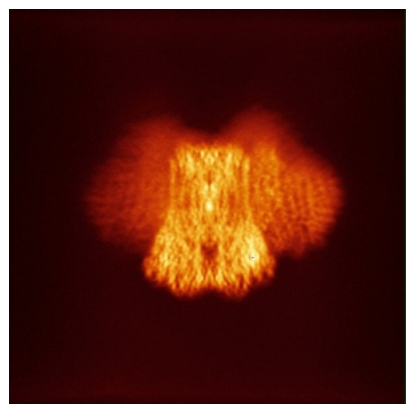


Y

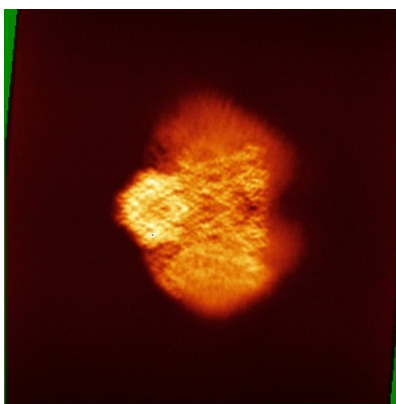


Z

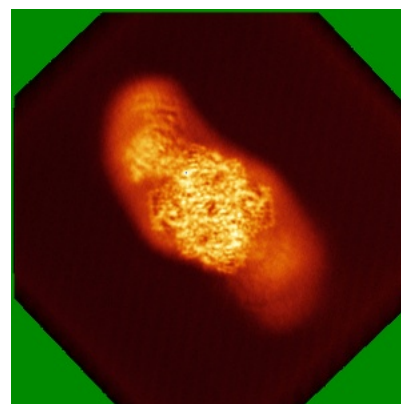
6.4.2 Raw map



X



Y

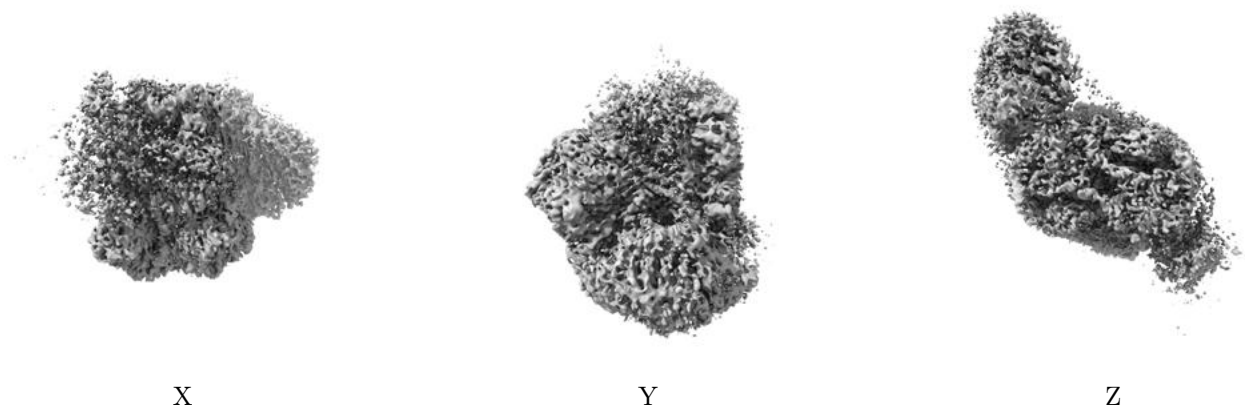


Z

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.

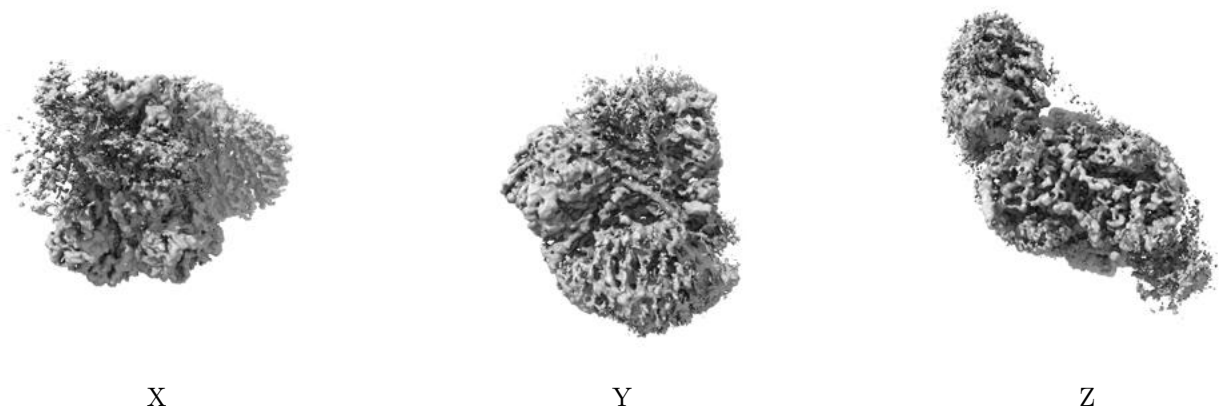
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.245. 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.

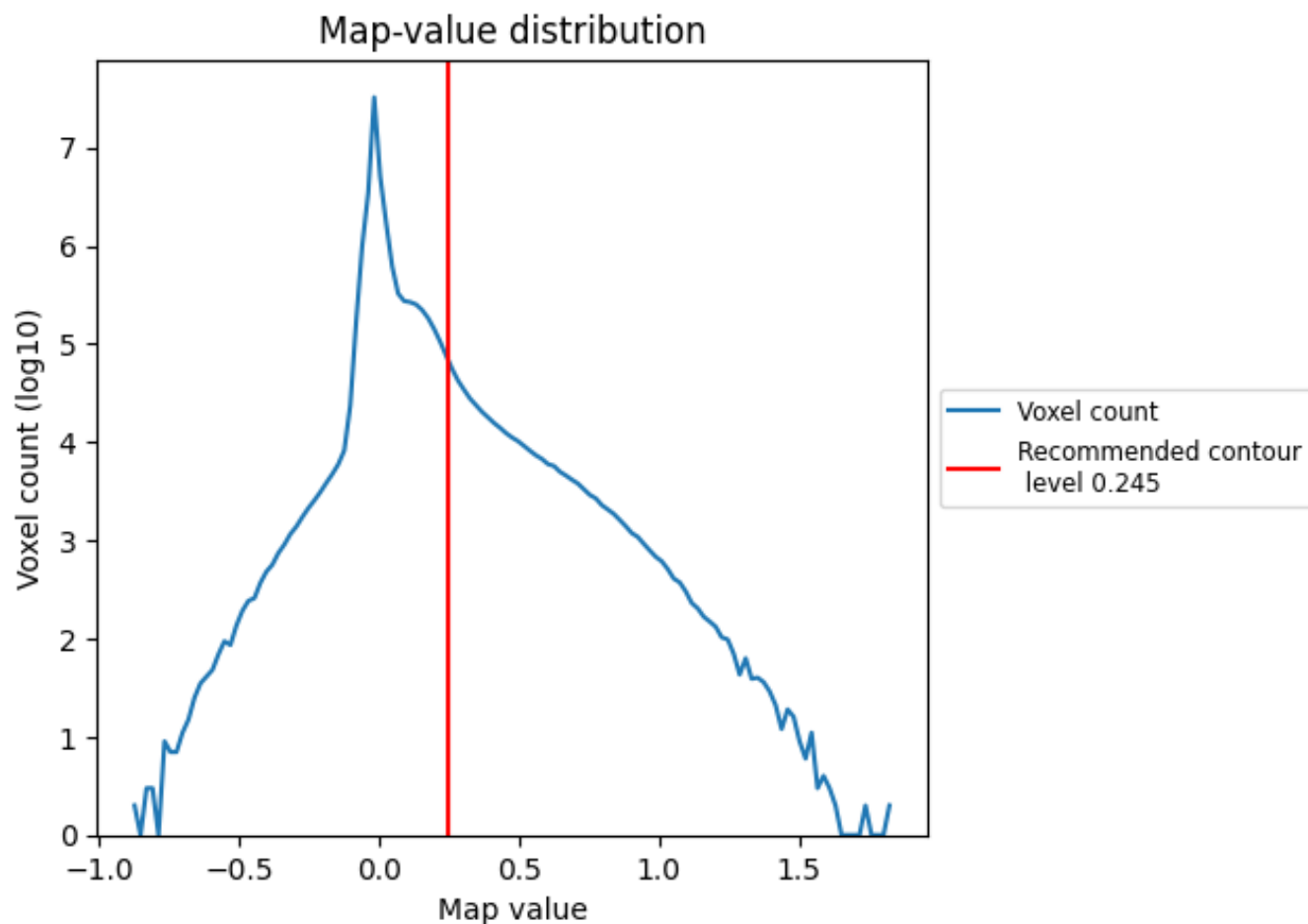
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

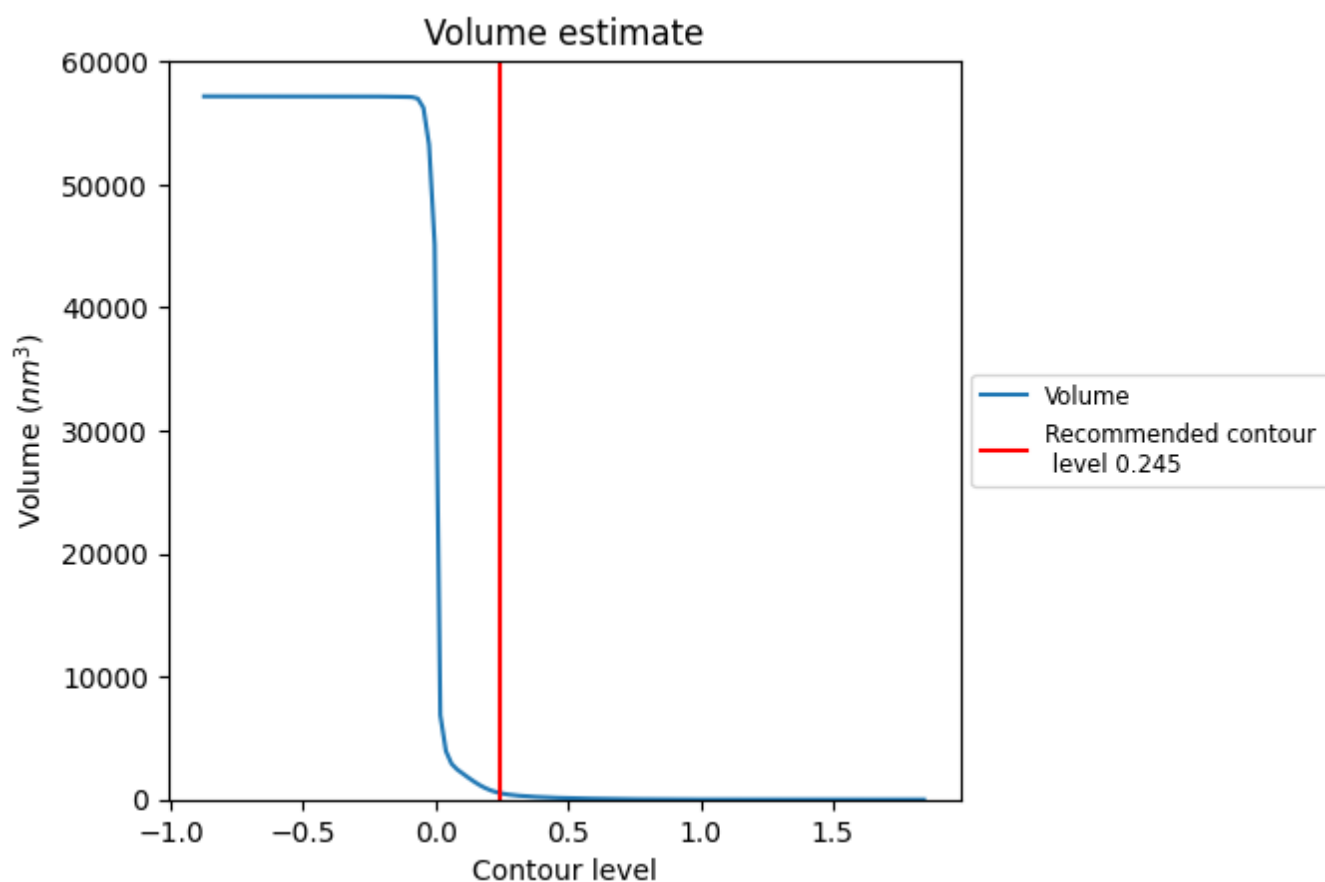
This section contains the results of statistical analysis of the map.

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.

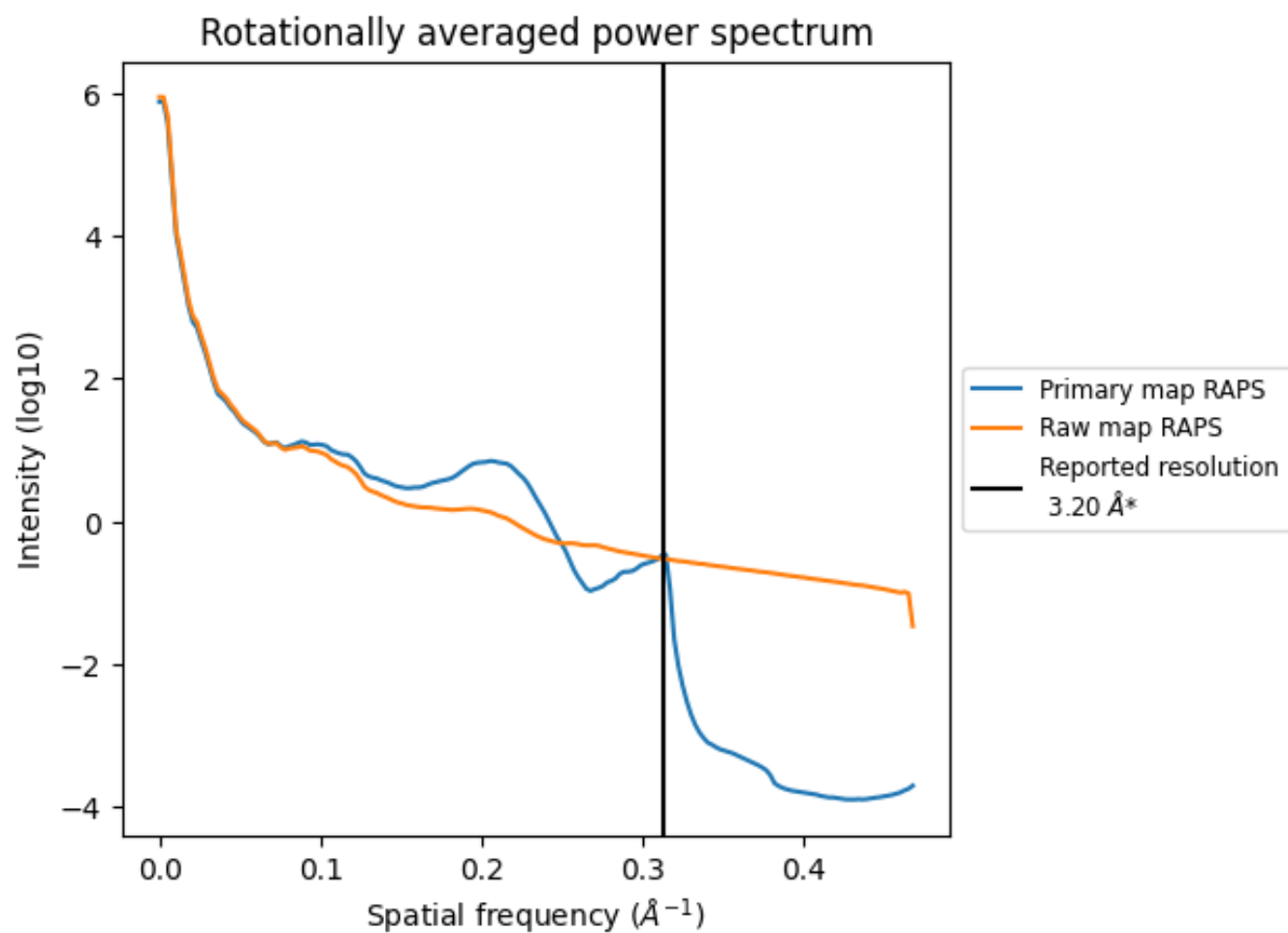
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 525 nm³; this corresponds to an approximate mass of 474 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 ⓘ

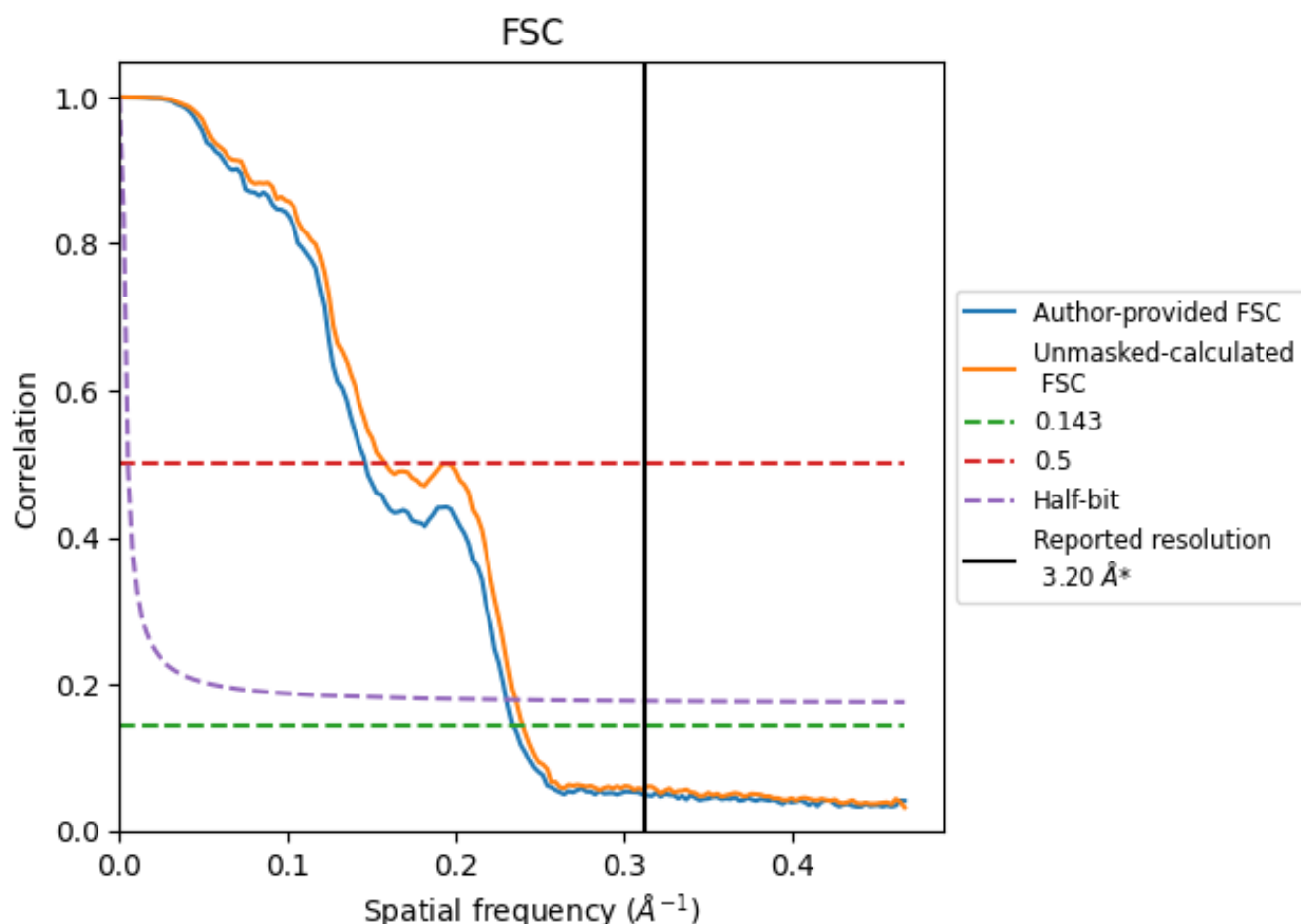


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	4.27	6.84	4.34
Unmasked-calculated*	4.17	6.32	4.24

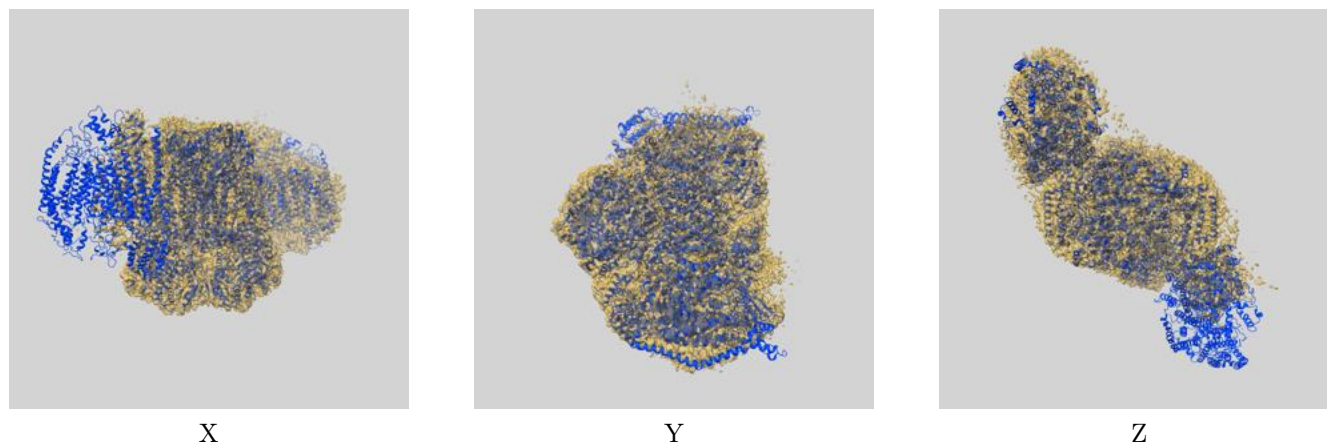
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

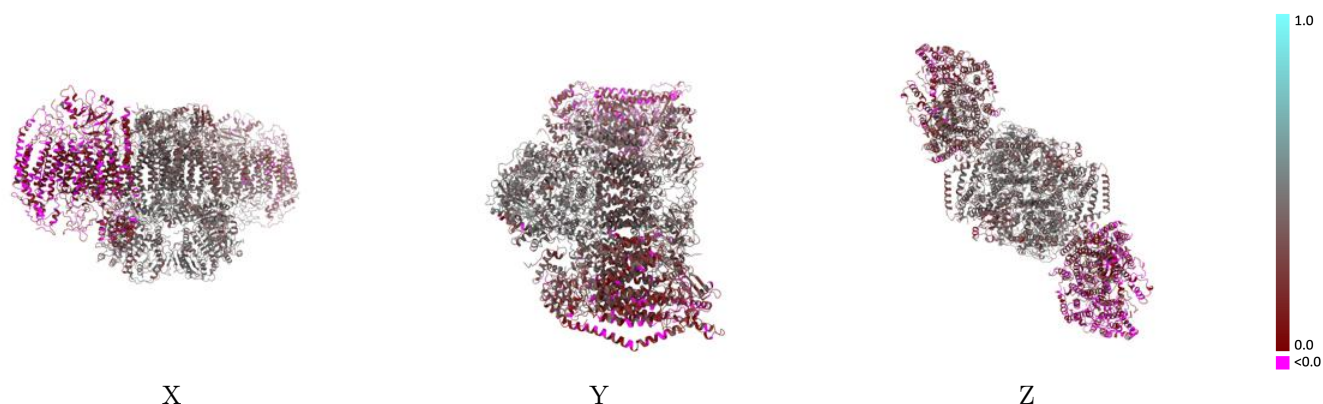
This section contains information regarding the fit between EMDB map EMD-27940 and PDB model 8E7S. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



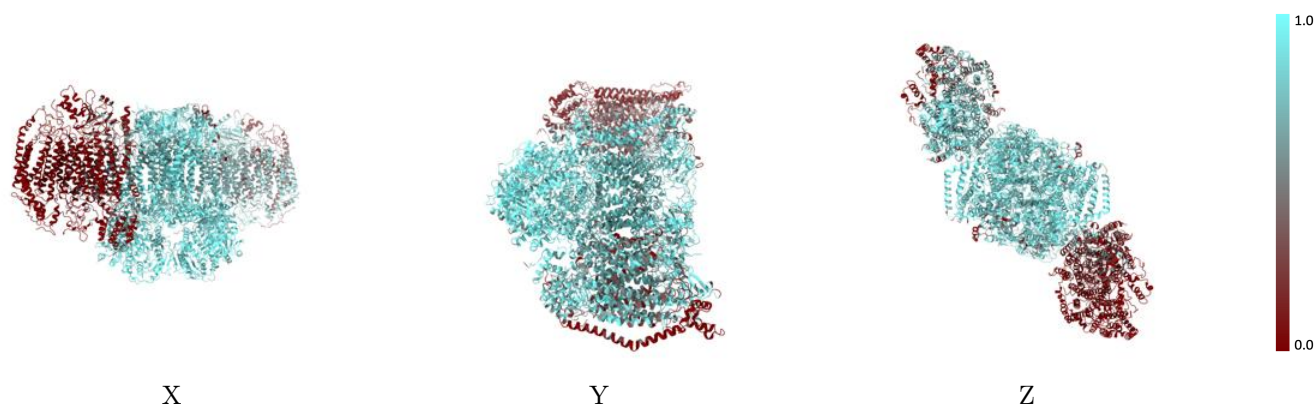
The images above show the 3D surface view of the map at the recommended contour level 0.245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



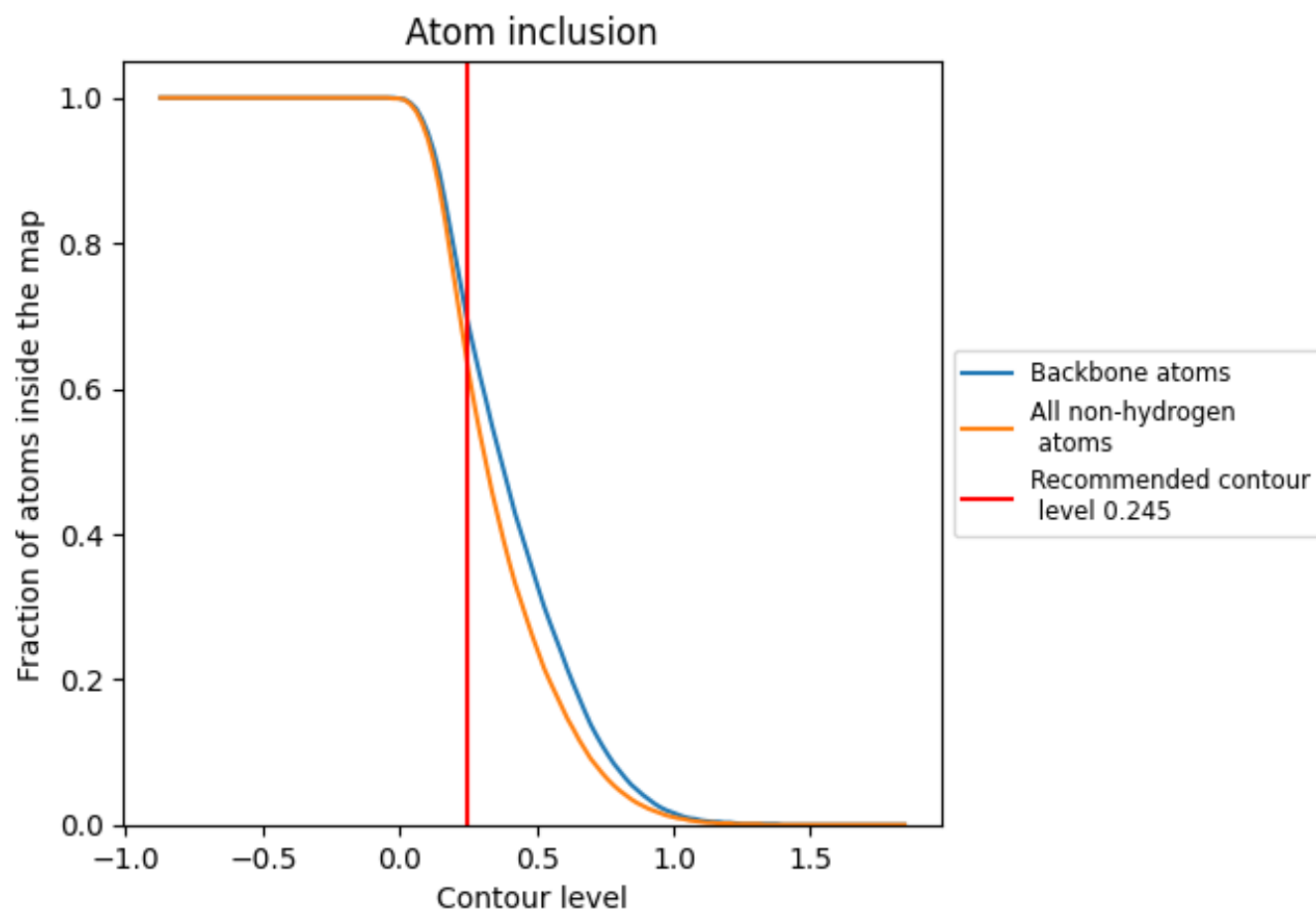
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.245).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 64% 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 (0.245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6380	 0.3120
A	 0.9260	 0.4260
B	 0.9380	 0.4330
C	 0.7330	 0.3570
D	 0.7440	 0.3710
E	 0.7950	 0.4000
F	 0.9010	 0.4340
G	 0.8490	 0.3690
H	 0.8320	 0.4310
J	 0.8400	 0.4220
K	 0.7100	 0.3240
L	 0.9050	 0.4290
M	 0.4320	 0.2750
N	 0.5230	 0.2610
O	 0.6000	 0.1920
P	 0.8130	 0.2850
Q	 0.7890	 0.2870
R	 0.7200	 0.2440
S	 0.0580	 0.1440
T	 0.7080	 0.2960
U	 0.1840	 0.1570
V	 0.5940	 0.2850
W	 0.7810	 0.3480
a	 0.9270	 0.4310
b	 0.9430	 0.4290
c	 0.6810	 0.3420
d	 0.5920	 0.3560
e	 0.7970	 0.3840
f	 0.9050	 0.4280
g	 0.8450	 0.3860
h	 0.8990	 0.4320
j	 0.8680	 0.4220
k	 0.1350	 0.1560
l	 0.9090	 0.4210
m	 0.0000	 0.1350



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Chain	Atom inclusion	Q-score
n	 0.0000	 0.0710
o	 0.0010	 0.0460
p	 0.1510	 0.1210
q	 0.0530	 0.1440
r	 0.1020	 0.0670
s	 0.0000	 0.0210
t	 0.0280	 0.0850
u	 0.0000	 0.0380
v	 0.2750	 0.1630
w	 0.3370	 0.2200