



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 02:43 PM UTC

PDB ID : 6T0B / pdb_00006t0b
EMDB ID : EMD-10340
Title : The III2-IV(5B)2 respiratory supercomplex from *S. cerevisiae*
Authors : Marechal, A.; Pinotsis, N.; Hartley, A.
Deposited on : 2019-10-02
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

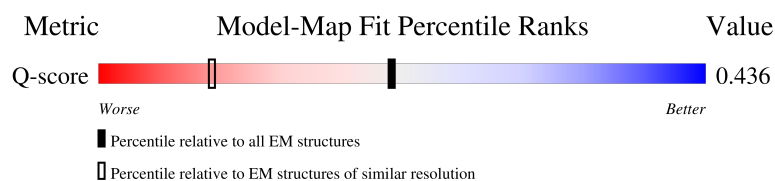
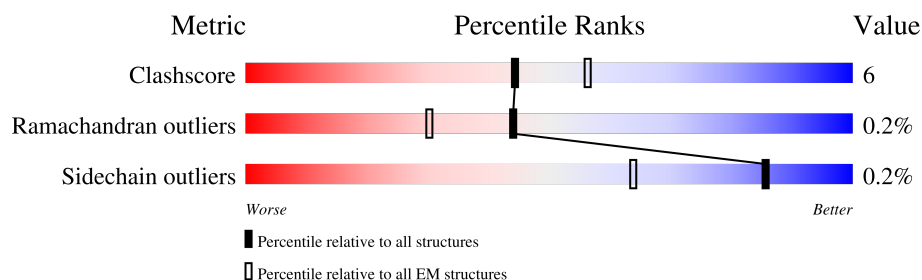
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	431	 88% 12%
1	L	431	 86% 14%
2	B	352	 89% 11%
2	M	352	 86% 14%

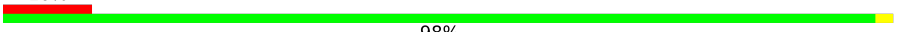
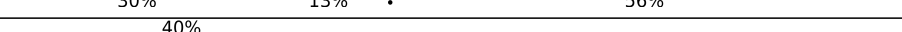
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Mol	Chain	Length	Quality of chain
3	C	385	
3	N	385	
4	D	248	
4	O	248	
5	E	185	
5	P	185	
6	F	147	
6	Q	147	
7	G	127	
7	R	127	
8	H	94	
8	S	94	
9	I	66	
9	T	66	
10	J	77	
10	U	77	
11	a	534	
11	n	534	
12	b	236	
12	o	236	
13	c	269	
13	p	269	
14	d	130	
14	q	130	
15	e	134	

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Mol	Chain	Length	Quality of chain
15	r	134	
16	f	108	
16	s	108	
17	g	59	
17	t	59	
18	h	51	
18	u	51	
19	i	55	
19	v	55	
20	j	82	
20	w	82	
21	k	131	
21	x	131	
22	l	66	
22	y	66	
23	m	224	
23	z	224	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 64478 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	L	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	M	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	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

- 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	P	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.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	57	Total	C	N	O	0	0
			465	310	77	78		
9	T	57	Total	C	N	O	0	0
			465	310	77	78		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	76	Total	C	N	O	S	0	0
			599	391	98	108	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
			4162	2778	649	713	22		
11	n	534	Total	C	N	O	S	0	0
			4162	2778	649	713	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
			1889	1242	286	351	10		
12	o	236	Total	C	N	O	S	0	0
			1889	1242	286	351	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	p	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	120	Total	C	N	O	S	0	0
			906	571	150	180	5		
14	q	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

- Molecule 15 is a protein called Cytochrome c oxidase polypeptide 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	133	Total	C	N	O	S	0	0
			1075	689	187	197	2		
15	r	133	Total	C	N	O	S	0	0
			1075	689	187	197	2		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	59	Total	C	N	O	0	0
			484	328	83	73		
17	t	59	Total	C	N	O	0	0
			484	328	83	73		

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	51	Total	C	N	O	S	0	0
			409	278	66	64	1		
18	u	51	Total	C	N	O	S	0	0
			409	278	66	64	1		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	55	Total	C	N	O	S	0	0
			456	300	79	74	3		
19	v	55	Total	C	N	O	S	0	0
			456	300	79	74	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	75	Total	C	N	O	S	0	0
			627	403	107	112	5		
20	w	75	Total	C	N	O	S	0	0
			627	403	107	112	5		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	113	Total	C	N	O	S	0	0
			928	605	160	160	3		
21	x	113	Total	C	N	O	S	0	0
			928	605	160	160	3		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	130	GLY	-	expression tag	UNP P32799
k	131	ALA	-	expression tag	UNP P32799
k	132	ARG	-	expression tag	UNP P32799
k	133	GLY	-	expression tag	UNP P32799
k	134	SER	-	expression tag	UNP P32799
k	135	HIS	-	expression tag	UNP P32799
k	136	HIS	-	expression tag	UNP P32799
k	137	HIS	-	expression tag	UNP P32799
k	138	HIS	-	expression tag	UNP P32799
k	139	HIS	-	expression tag	UNP P32799
k	140	HIS	-	expression tag	UNP P32799
x	130	GLY	-	expression tag	UNP P32799
x	131	ALA	-	expression tag	UNP P32799
x	132	ARG	-	expression tag	UNP P32799
x	133	GLY	-	expression tag	UNP P32799
x	134	SER	-	expression tag	UNP P32799
x	135	HIS	-	expression tag	UNP P32799
x	136	HIS	-	expression tag	UNP P32799
x	137	HIS	-	expression tag	UNP P32799
x	138	HIS	-	expression tag	UNP P32799
x	139	HIS	-	expression tag	UNP P32799
x	140	HIS	-	expression tag	UNP P32799

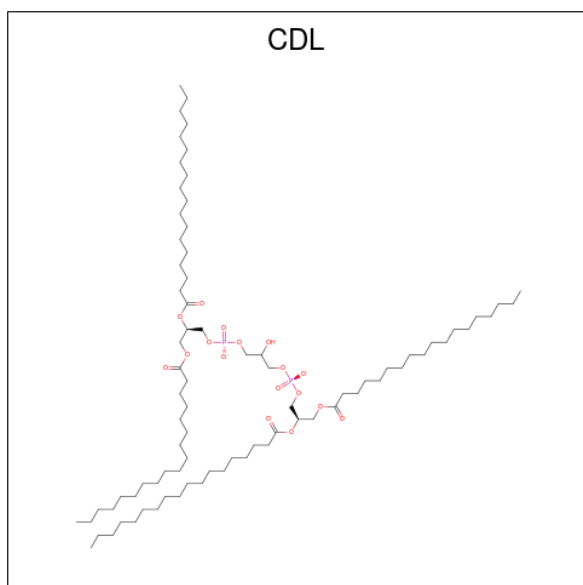
- Molecule 22 is a protein called Cox26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	45	Total	C	N	O	S	0	0
			361	238	63	59	1		
22	y	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 23 is a protein called Respiratory supercomplex factor 2, mitochondrial.

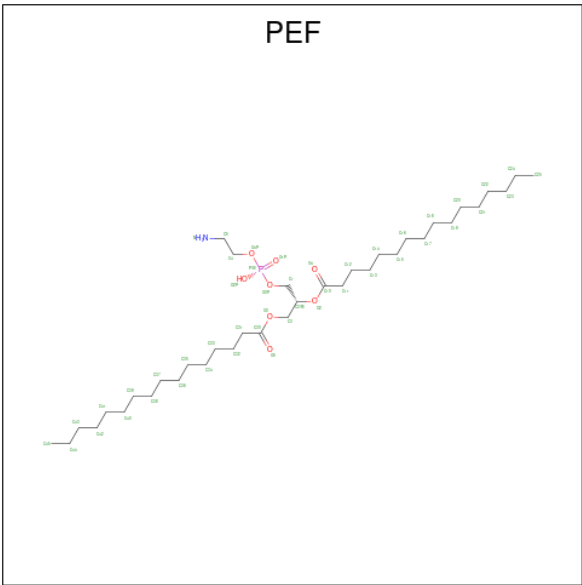
Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	99	Total	C	N	O	S	0	0
			799	511	140	144	4		
23	z	99	Total	C	N	O	S	0	0
			799	511	140	144	4		

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			58	39	17	2	
24	C	1	Total	C	O	P	0
			66	47	17	2	
24	D	1	Total	C	O	P	0
			71	52	17	2	
24	H	1	Total	C	O	P	0
			53	34	17	2	
24	L	1	Total	C	O	P	0
			55	36	17	2	
24	N	1	Total	C	O	P	0
			53	34	17	2	
24	N	1	Total	C	O	P	0
			75	56	17	2	
24	S	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 25 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
25	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
25	E	1	Total	C	N	O	P	0
			42	32	1	8	1	
25	E	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	E	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
25	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	N	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	O	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	S	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	a	1	Total	C	N	O	P	0
			33	23	1	8	1	

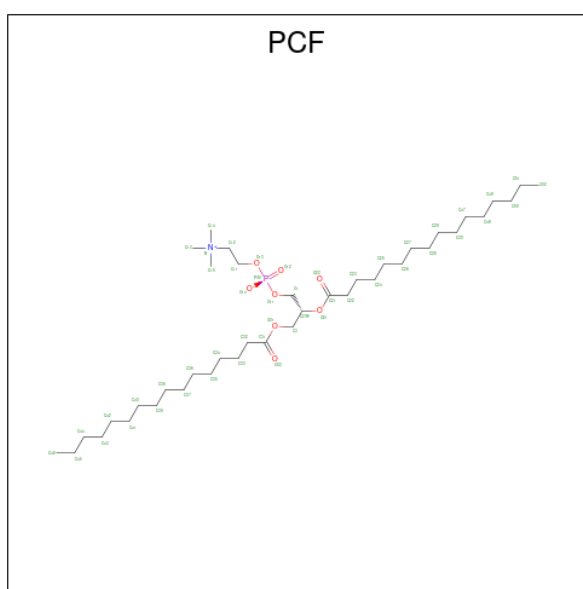
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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 40	C 30	N 1	O 8	P 1	0
25	b	1	Total 40	C 30	N 1	O 8	P 1	0
25	c	1	Total 36	C 26	N 1	O 8	P 1	0
25	c	1	Total 34	C 24	N 1	O 8	P 1	0
25	e	1	Total 41	C 31	N 1	O 8	P 1	0
25	l	1	Total 33	C 23	N 1	O 8	P 1	0
25	n	1	Total 47	C 37	N 1	O 8	P 1	0
25	n	1	Total 33	C 23	N 1	O 8	P 1	0
25	n	1	Total 33	C 23	N 1	O 8	P 1	0
25	o	1	Total 40	C 30	N 1	O 8	P 1	0
25	p	1	Total 36	C 26	N 1	O 8	P 1	0
25	r	1	Total 41	C 31	N 1	O 8	P 1	0

-
- The diagram illustrates the chemical structure of the Heme (HEM) molecule. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and functional groups, such as hydroxyl groups (OH) and carboxylate groups (COO⁻). The atoms are labeled with their respective element symbols and unique identifiers (e.g., O1A, O2A, O1D, O2D for oxygen atoms; CAA, CBA, CAD, CBD for carbon atoms; N1A, N1B, N1C, N1D for nitrogen atoms). The overall structure is highly symmetrical, reflecting the complex nature of the heme molecule.

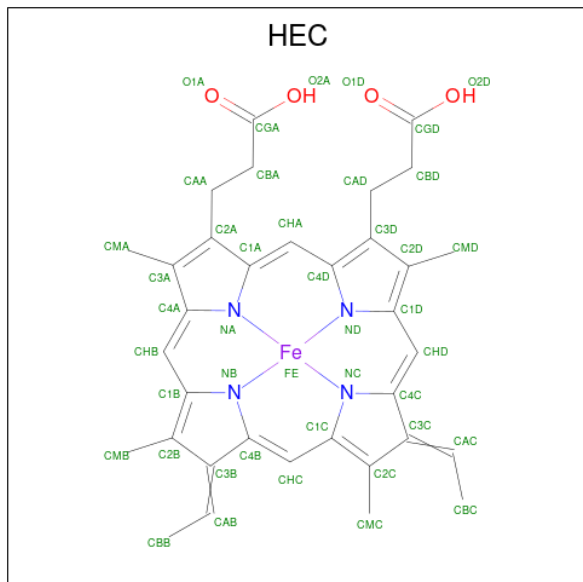
Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$).



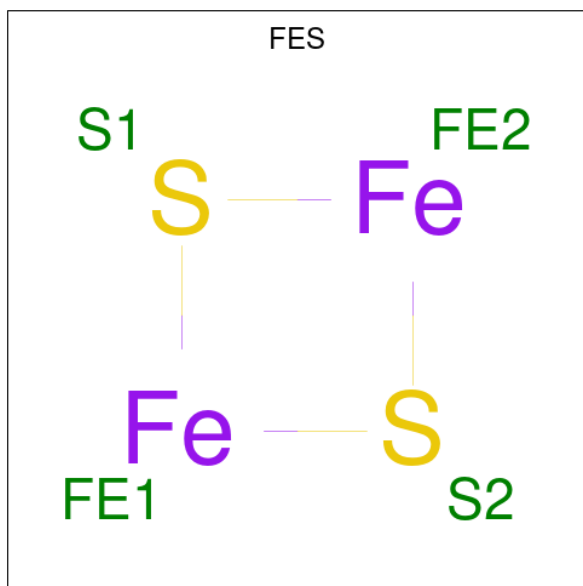
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	I	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	T	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	e	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	r	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 28 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

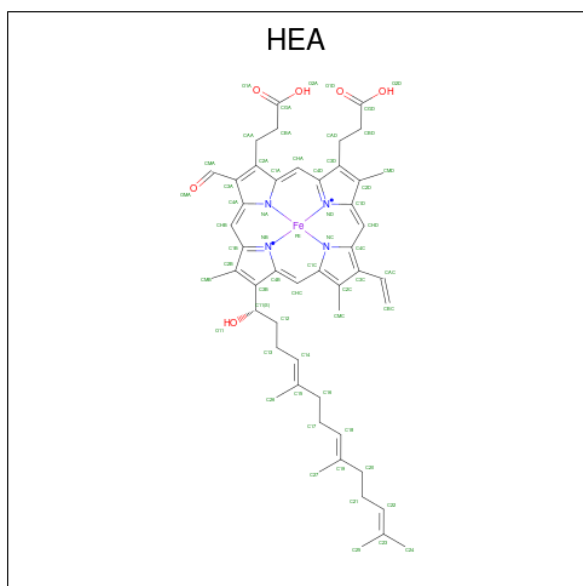


Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Cu	0
			1	1	
30	n	1	Total	Cu	0
			1	1	

- Molecule 31 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

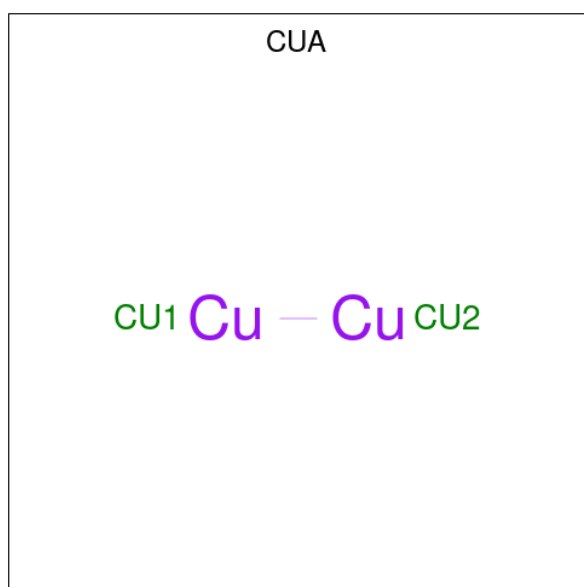
- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total 1	Ca 1	0
32	n	1	Total 1	Ca 1	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
33	a	1	Total 1	Mg 1	0
33	n	1	Total 1	Mg 1	0

- Molecule 34 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
34	b	1	Total 2	Cu 2	0
34	o	1	Total 2	Cu 2	0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

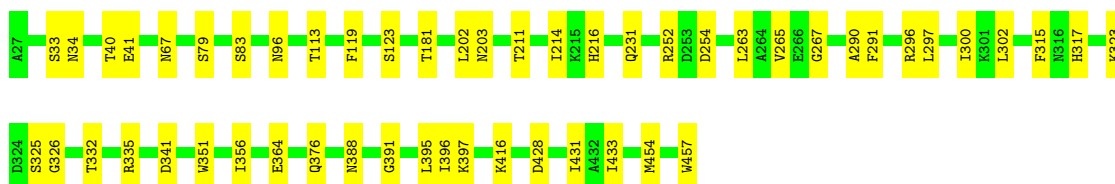
Mol	Chain	Residues	Atoms		AltConf
35	d	1	Total 1	Zn 1	0
35	q	1	Total 1	Zn 1	0

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.

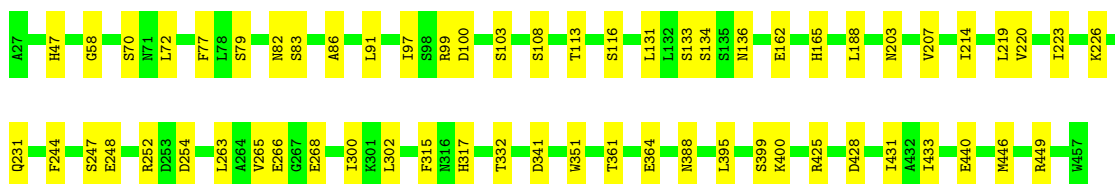
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A: 



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

Chain L: 



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

Chain B: 



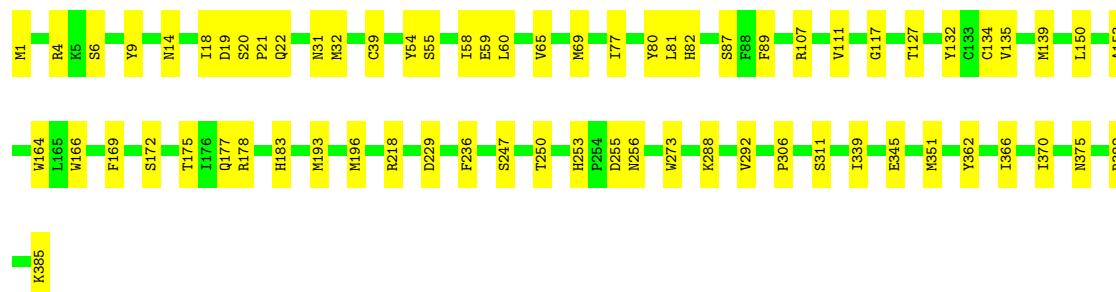
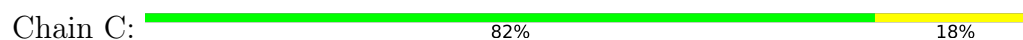
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 

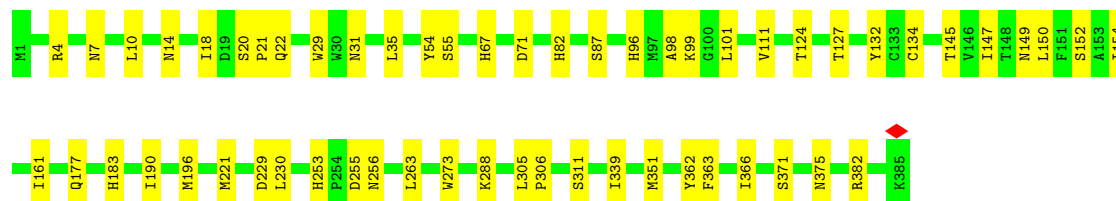
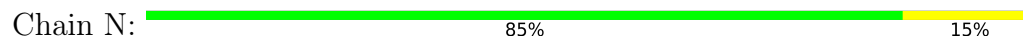




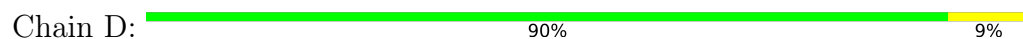
• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b



• Molecule 4: Cytochrome c1, heme protein, mitochondrial



• Molecule 4: Cytochrome c1, heme protein, mitochondrial



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

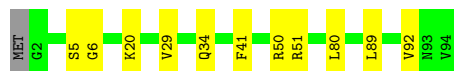






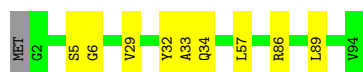
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H: 87% 12%



- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S: 89% 10%



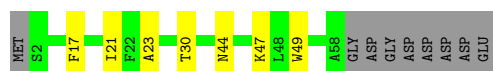
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain I: 76% 11% 14%



- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T: 76% 11% 14%



- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain J: 5% 90% 9%



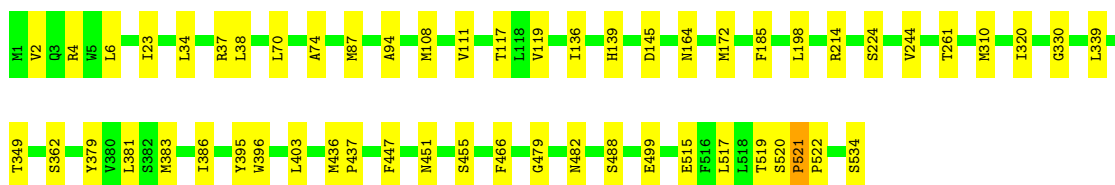
- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain U: 5% 84% 14%

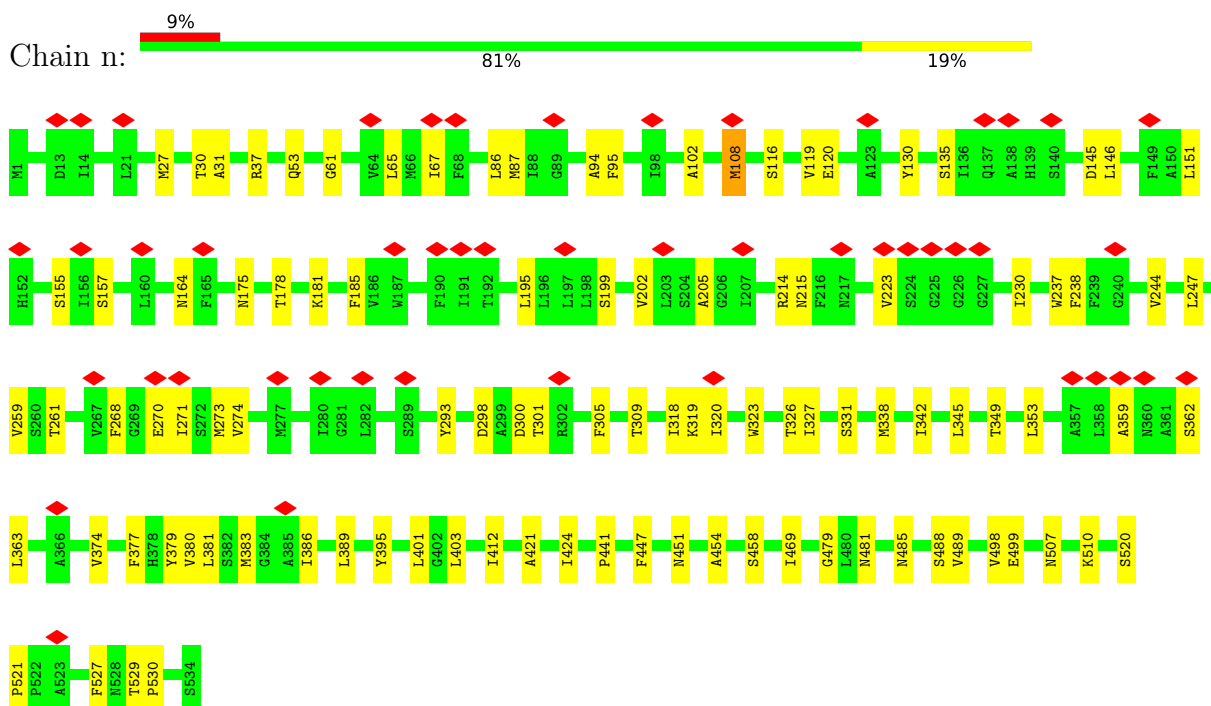


- Molecule 11: Cytochrome c oxidase subunit 1

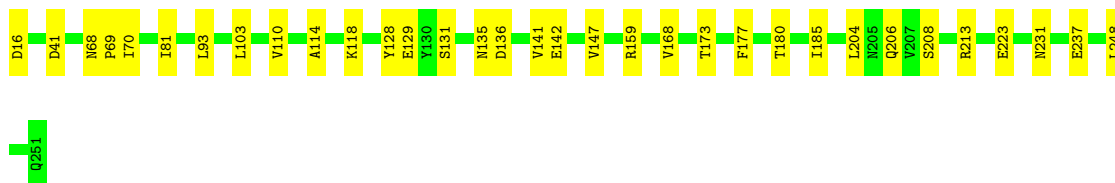
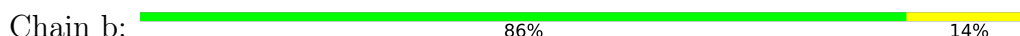
Chain a: 90% 10%



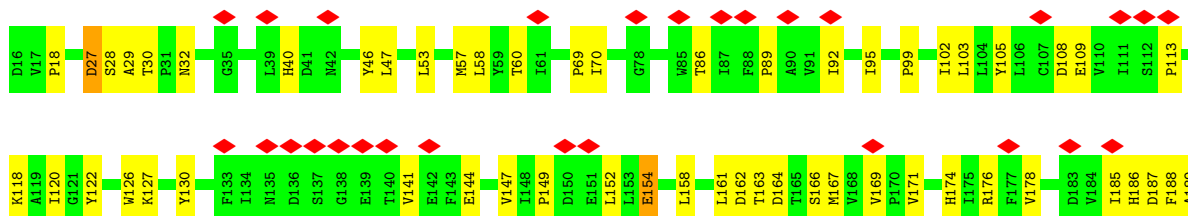
• Molecule 11: Cytochrome c oxidase subunit 1



• Molecule 12: Cytochrome c oxidase subunit 2

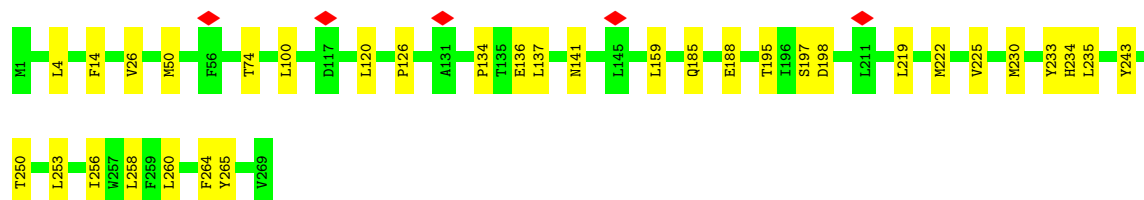
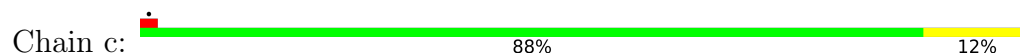


• Molecule 12: Cytochrome c oxidase subunit 2

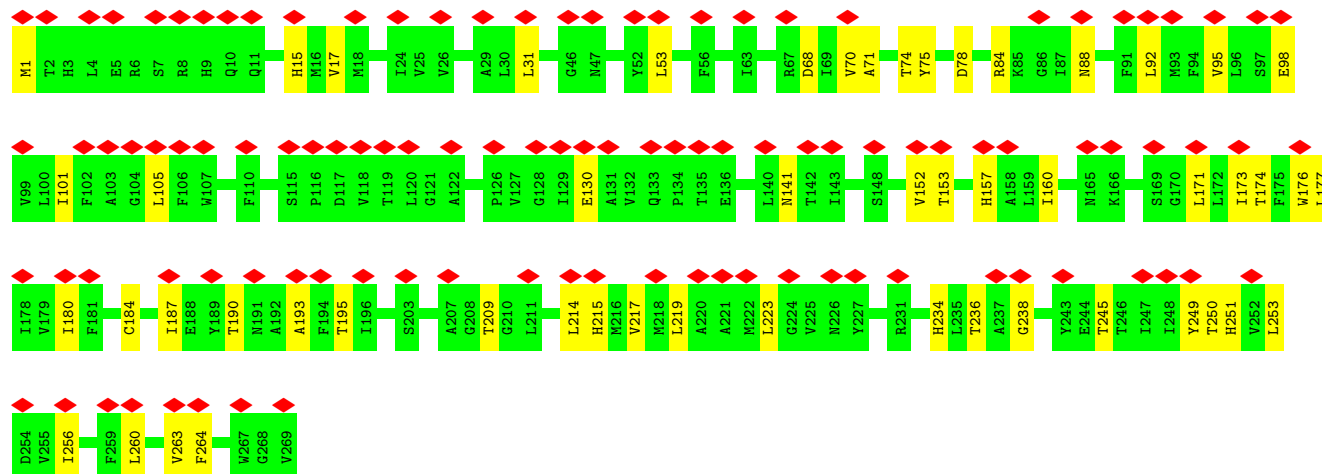
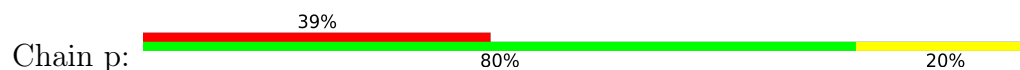




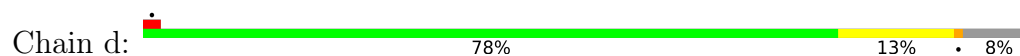
• Molecule 13: Cytochrome c oxidase subunit 3



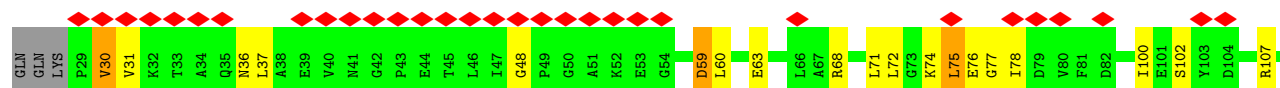
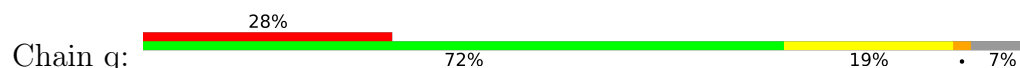
• Molecule 13: Cytochrome c oxidase subunit 3



• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial



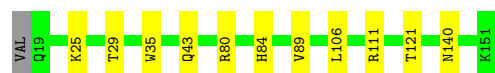
• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial





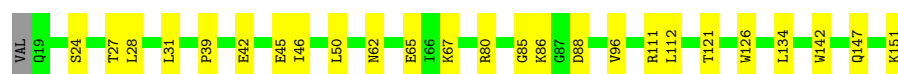
- Molecule 15: Cytochrome c oxidase polypeptide 5B, mitochondrial

Chain e: 91% 8%



- Molecule 15: Cytochrome c oxidase polypeptide 5B, mitochondrial

Chain r: 81% 19%



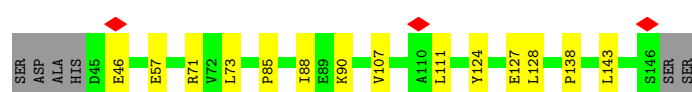
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

Chain f: 85% 9% 6%



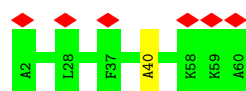
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

Chain s: 81% 13% 6%



- Molecule 17: Cytochrome c oxidase subunit 7

Chain g: 10% 98%



- Molecule 17: Cytochrome c oxidase subunit 7

Chain t: 42% 86% 14%

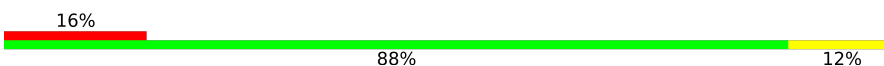


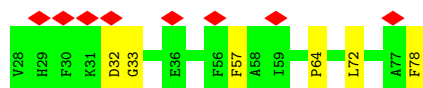
- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h:  88% 12%



- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain u:  16% 88% 12%



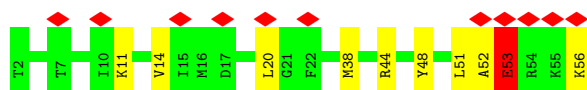
- Molecule 19: Cytochrome c oxidase subunit 7A

Chain i:  84% 16%

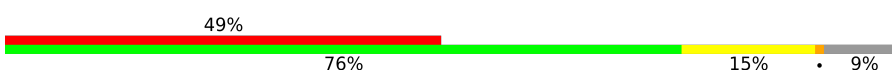


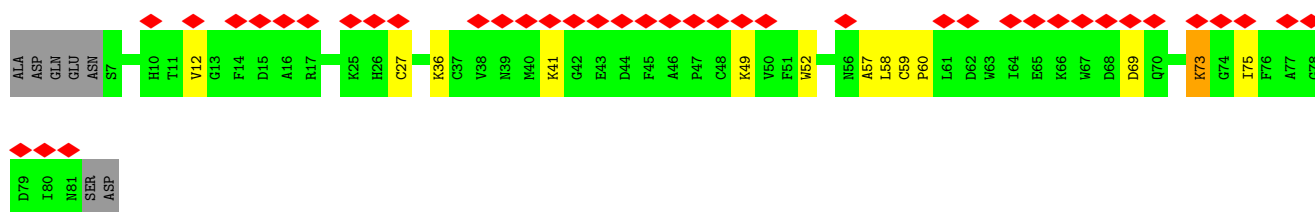
- Molecule 19: Cytochrome c oxidase subunit 7A

Chain v:  20% 82% 16%

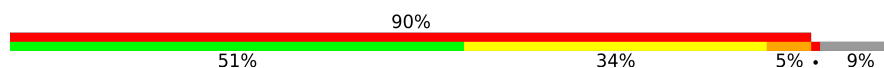


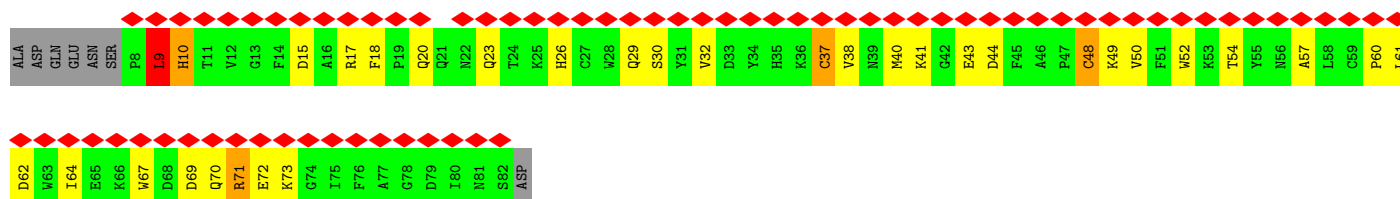
- Molecule 20: Cytochrome c oxidase subunit 6B

Chain j:  49% 76% 15% 9%

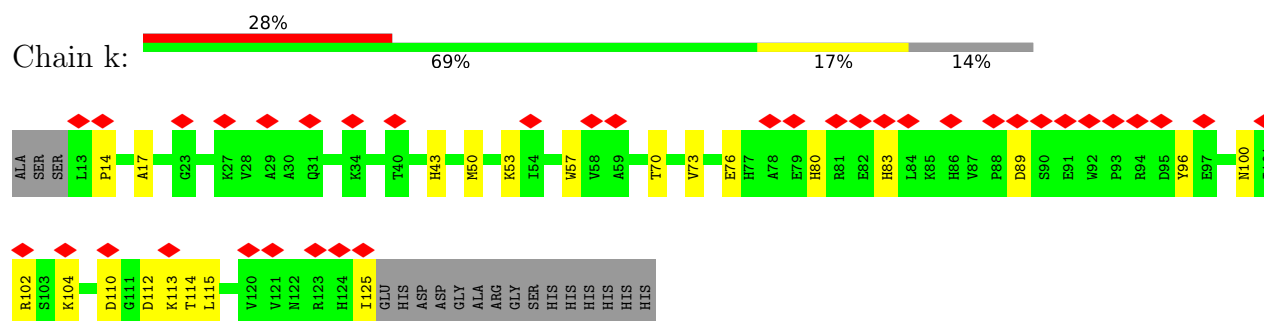


- Molecule 20: Cytochrome c oxidase subunit 6B

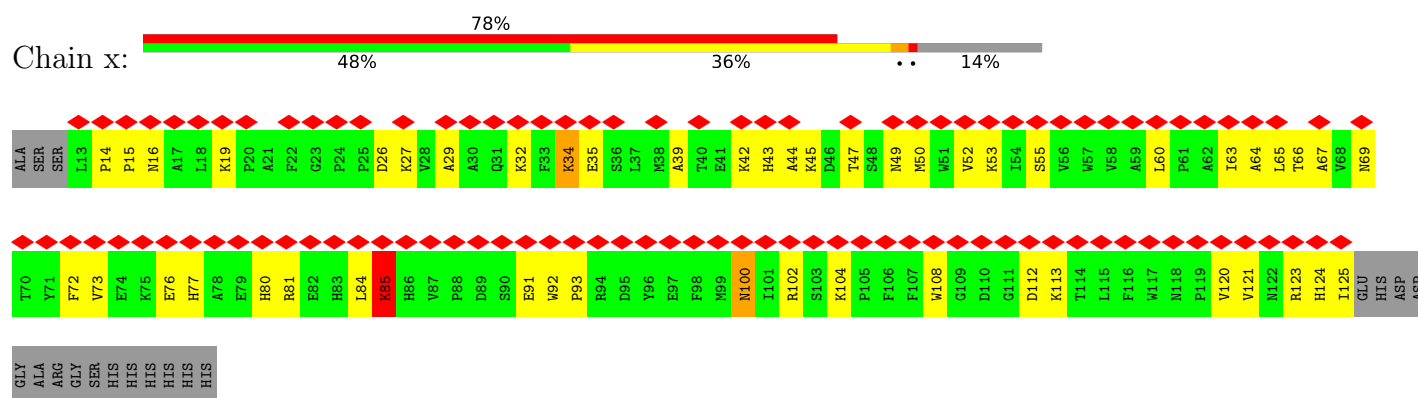
Chain w:  90% 51% 34% 5% 9%



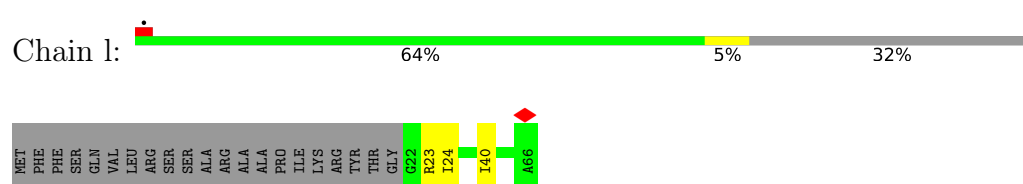
- Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial



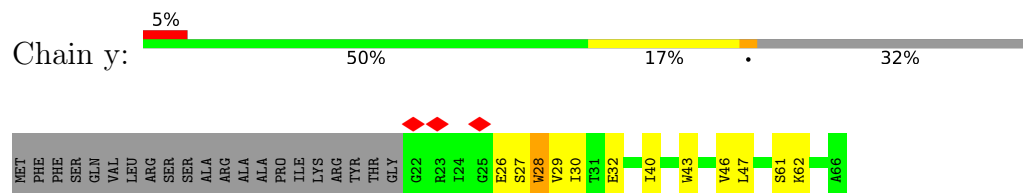
- Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial



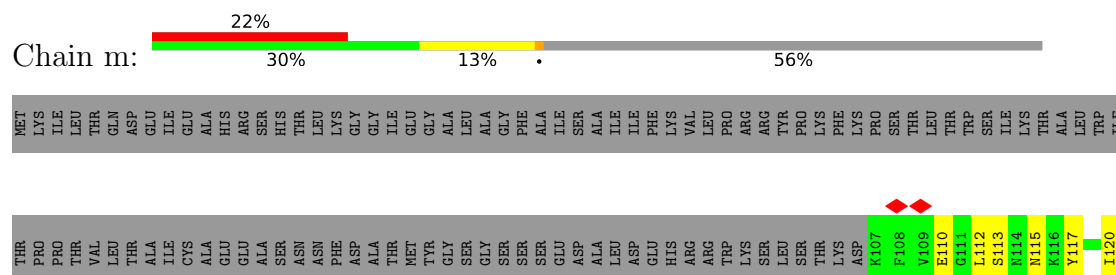
- Molecule 22: Cox26

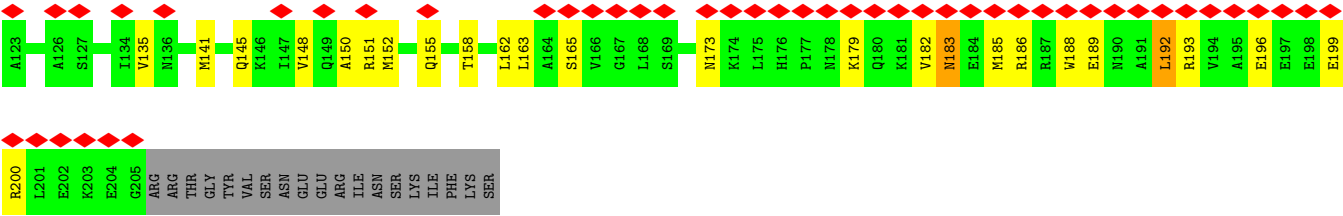


- Molecule 22: Cox26

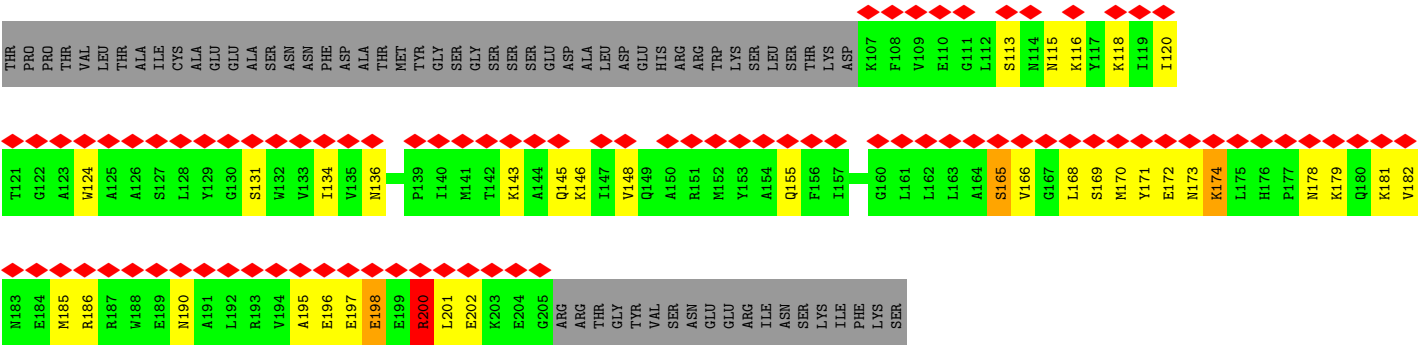


- Molecule 23: Respiratory supercomplex factor 2, mitochondrial





• Molecule 23: Respiratory supercomplex factor 2, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65999	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 ($e^-/\text{\AA}^2$)	56.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.028	Depositor
Minimum map value	-1.743	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	486.08002, 486.08002, 486.08002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	1/3406 (0.0%)	0.59	0/4615
1	L	0.54	0/3406	0.59	0/4615
2	B	0.53	0/2781	0.59	3/3764 (0.1%)
2	M	0.52	0/2781	0.60	0/3764
3	C	0.61	0/3192	0.62	0/4354
3	N	0.57	0/3192	0.62	0/4354
4	D	0.56	0/2012	0.55	0/2740
4	O	0.54	0/2012	0.51	0/2740
5	E	0.49	0/1444	0.93	4/1957 (0.2%)
5	P	0.64	2/1444 (0.1%)	1.10	9/1957 (0.5%)
6	F	0.37	0/647	0.56	0/870
6	Q	0.39	0/647	0.57	0/870
7	G	0.49	0/1040	0.54	0/1408
7	R	0.50	0/1040	0.52	0/1408
8	H	0.50	0/804	0.54	0/1088
8	S	0.50	0/804	0.53	0/1088
9	I	0.47	0/479	0.51	0/646
9	T	0.49	0/479	0.49	0/646
10	J	0.29	0/619	0.53	0/841
10	U	0.26	0/619	0.53	0/841
11	a	0.58	0/4290	0.63	0/5857
11	n	0.49	1/4290 (0.0%)	0.70	0/5857
12	b	0.53	0/1941	0.64	0/2653
12	o	0.51	0/1941	0.85	2/2653 (0.1%)
13	c	0.46	0/2218	0.56	0/3036
13	p	0.35	0/2218	0.71	0/3036
14	d	0.55	0/924	0.69	0/1258
14	q	0.44	0/932	0.86	2/1269 (0.2%)
15	e	0.51	0/1103	0.58	0/1493
15	r	0.44	1/1103 (0.1%)	0.64	0/1493
16	f	0.51	0/868	0.61	0/1174
16	s	0.46	0/868	0.68	0/1174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.51	0/500	0.64	0/681
17	t	0.35	0/500	0.66	0/681
18	h	0.51	0/424	0.59	0/569
18	u	0.36	0/424	0.64	0/569
19	i	0.44	0/468	0.57	0/626
19	v	0.53	1/468 (0.2%)	0.87	1/626 (0.2%)
20	j	0.46	1/649 (0.2%)	0.87	2/880 (0.2%)
20	w	0.52	0/649	1.16	4/879 (0.5%)
21	k	0.29	0/962	0.54	0/1310
21	x	0.46	0/962	1.20	13/1310 (1.0%)
22	l	0.42	0/372	0.62	0/502
22	y	0.39	0/372	0.94	2/502 (0.4%)
23	m	0.49	0/813	1.02	1/1093 (0.1%)
23	z	0.54	0/813	1.24	6/1093 (0.5%)
All	All	0.51	7/63920 (0.0%)	0.69	49/86840 (0.1%)

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
2	B	0	1
2	M	0	1
3	C	0	1
5	E	0	4
5	P	0	12
11	a	0	2
11	n	0	2
12	o	0	3
14	d	0	1
14	q	0	2
16	s	0	1
19	v	0	3
20	w	0	8
21	x	0	3
23	m	0	2
23	z	0	5
All	All	0	51

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	127	GLN	CB-CG	8.38	1.77	1.52
5	P	130	ASN	CG-OD1	6.14	1.35	1.23
11	n	108	MET	SD-CE	-5.92	1.64	1.79
20	j	41	LYS	CD-CE	-5.62	1.35	1.52
15	r	31	LEU	C-N	5.41	1.39	1.34

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	85	LYS	CA-C-N	-8.06	110.47	122.24
21	x	85	LYS	C-N-CA	-8.06	110.47	122.24
21	x	26	ASP	CA-C-N	7.18	133.78	121.29
21	x	26	ASP	C-N-CA	7.18	133.78	121.29
12	o	154	GLU	CA-C-N	-6.94	113.20	122.85

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	201	VAL	Peptide
3	C	107	ARG	Peptide
5	E	127	GLN	Peptide
5	E	135	SER	Peptide
5	E	97	ASN	Peptide

5.2 Too-close contacts [i](#)

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	3345	0	3323	34	0
1	L	3345	0	3323	39	0
2	B	2735	0	2774	23	0
2	M	2735	0	2774	31	0
3	C	3090	0	3129	46	0
3	N	3090	0	3129	40	0
4	D	1951	0	1875	18	0
4	O	1951	0	1875	14	0
5	E	1411	0	1387	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	1411	0	1386	71	0
6	F	633	0	587	3	0
6	Q	633	0	587	1	0
7	G	1019	0	1034	9	0
7	R	1019	0	1034	7	0
8	H	773	0	736	8	0
8	S	773	0	736	7	0
9	I	465	0	459	7	0
9	T	465	0	459	7	0
10	J	599	0	594	7	0
10	U	599	0	594	9	0
11	a	4162	0	4191	41	0
11	n	4162	0	4191	75	0
12	b	1889	0	1866	22	0
12	o	1889	0	1866	64	0
13	c	2146	0	2137	24	0
13	p	2146	0	2137	35	0
14	d	906	0	901	15	0
14	q	913	0	909	20	0
15	e	1075	0	1072	9	0
15	r	1075	0	1072	19	0
16	f	851	0	822	7	0
16	s	851	0	822	10	0
17	g	484	0	517	1	0
17	t	484	0	517	5	0
18	h	409	0	408	5	0
18	u	409	0	408	4	0
19	i	456	0	469	7	0
19	v	456	0	469	5	0
20	j	627	0	577	8	0
20	w	627	0	578	17	0
21	k	928	0	906	19	0
21	x	928	0	906	30	0
22	l	361	0	363	3	0
22	y	361	0	363	10	0
23	m	799	0	819	19	0
23	z	799	0	819	19	0
24	A	58	0	60	3	0
24	C	66	0	76	3	0
24	D	71	0	89	0	0
24	H	53	0	50	2	0
24	L	55	0	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	N	128	0	147	1	0
24	S	48	0	40	2	0
25	A	36	0	45	1	0
25	C	83	0	118	3	0
25	E	116	0	157	7	0
25	H	32	0	37	0	0
25	J	29	0	31	0	0
25	L	31	0	35	0	0
25	N	83	0	115	5	0
25	O	43	0	62	0	0
25	S	36	0	48	1	0
25	a	33	0	39	1	0
25	b	80	0	112	3	0
25	c	70	0	86	3	0
25	e	41	0	58	4	0
25	l	33	0	39	0	0
25	n	113	0	151	5	0
25	o	40	0	56	0	0
25	p	36	0	45	2	0
25	r	41	0	58	3	0
26	C	86	0	60	4	0
26	N	86	0	60	5	0
27	C	39	0	55	0	0
27	H	32	0	38	1	0
27	I	30	0	34	3	0
27	N	50	0	80	2	0
27	T	47	0	71	2	0
27	e	36	0	46	0	0
27	r	36	0	46	1	0
28	D	43	0	31	2	0
28	O	43	0	31	0	0
29	E	4	0	0	0	0
29	P	4	0	0	0	0
30	a	1	0	0	0	0
30	n	1	0	0	0	0
31	a	120	0	108	6	0
31	n	120	0	108	5	0
32	a	1	0	0	0	0
32	n	1	0	0	0	0
33	a	1	0	0	0	0
33	n	1	0	0	0	0
34	b	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	o	2	0	0	0	0
35	d	1	0	0	0	0
35	q	1	0	0	0	0
All	All	64478	0	64476	824	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 6.

The worst 5 of 824 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)
5:P:127:GLN:CB	5:P:127:GLN:CG	1.77	1.61
5:E:111:TRP:O	5:E:114:LYS:HB2	1.56	1.05
5:P:118:ILE:HA	5:P:153:LEU:O	1.55	1.05
5:P:117:PHE:O	5:P:154:ILE:HA	1.64	0.97
5:E:110:LYS:HA	5:E:114:LYS:O	1.69	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	401 (94%)	28 (6%)	0	100	100
1	L	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
2	B	350/352 (99%)	329 (94%)	21 (6%)	0	100	100
2	M	350/352 (99%)	328 (94%)	22 (6%)	0	100	100
3	C	383/385 (100%)	370 (97%)	13 (3%)	0	100	100
3	N	383/385 (100%)	373 (97%)	10 (3%)	0	100	100
4	D	245/248 (99%)	238 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	245/248 (99%)	240 (98%)	5 (2%)	0	100	100
5	E	183/185 (99%)	157 (86%)	26 (14%)	0	100	100
5	P	183/185 (99%)	149 (81%)	33 (18%)	1 (0%)	24	55
6	F	73/147 (50%)	67 (92%)	6 (8%)	0	100	100
6	Q	73/147 (50%)	71 (97%)	2 (3%)	0	100	100
7	G	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
7	R	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
8	H	91/94 (97%)	84 (92%)	7 (8%)	0	100	100
8	S	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
9	I	55/66 (83%)	55 (100%)	0	0	100	100
9	T	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
10	J	74/77 (96%)	70 (95%)	4 (5%)	0	100	100
10	U	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
11	a	532/534 (100%)	504 (95%)	27 (5%)	1 (0%)	43	72
11	n	532/534 (100%)	502 (94%)	28 (5%)	2 (0%)	30	60
12	b	234/236 (99%)	215 (92%)	19 (8%)	0	100	100
12	o	234/236 (99%)	206 (88%)	28 (12%)	0	100	100
13	c	267/269 (99%)	260 (97%)	7 (3%)	0	100	100
13	p	267/269 (99%)	263 (98%)	4 (2%)	0	100	100
14	d	118/130 (91%)	98 (83%)	20 (17%)	0	100	100
14	q	119/130 (92%)	101 (85%)	16 (13%)	2 (2%)	7	25
15	e	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
15	r	131/134 (98%)	115 (88%)	15 (12%)	1 (1%)	16	44
16	f	100/108 (93%)	94 (94%)	6 (6%)	0	100	100
16	s	100/108 (93%)	94 (94%)	6 (6%)	0	100	100
17	g	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
17	t	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
18	h	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
18	u	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
19	v	53/55 (96%)	47 (89%)	6 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	j	73/82 (89%)	68 (93%)	5 (7%)	0	100	100
20	w	73/82 (89%)	62 (85%)	9 (12%)	2 (3%)	4	15
21	k	111/131 (85%)	104 (94%)	7 (6%)	0	100	100
21	x	111/131 (85%)	95 (86%)	16 (14%)	0	100	100
22	l	43/66 (65%)	41 (95%)	2 (5%)	0	100	100
22	y	43/66 (65%)	38 (88%)	5 (12%)	0	100	100
23	m	97/224 (43%)	90 (93%)	7 (7%)	0	100	100
23	z	97/224 (43%)	87 (90%)	7 (7%)	3 (3%)	3	12
All	All	7745/8382 (92%)	7252 (94%)	481 (6%)	12 (0%)	44	72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	P	187	ILE
11	n	120	GLU
11	n	521	PRO
20	w	10	HIS
23	z	173	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	370 (100%)	0	100	100
1	L	370/370 (100%)	370 (100%)	0	100	100
2	B	301/301 (100%)	301 (100%)	0	100	100
2	M	301/301 (100%)	301 (100%)	0	100	100
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	338/338 (100%)	338 (100%)	0	100	100
4	D	205/206 (100%)	205 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	151/151 (100%)	148 (98%)	3 (2%)	48	80
5	P	151/151 (100%)	149 (99%)	2 (1%)	61	86
6	F	68/131 (52%)	68 (100%)	0	100	100
6	Q	68/131 (52%)	67 (98%)	1 (2%)	57	84
7	G	110/111 (99%)	110 (100%)	0	100	100
7	R	110/111 (99%)	110 (100%)	0	100	100
8	H	77/78 (99%)	77 (100%)	0	100	100
8	S	77/78 (99%)	77 (100%)	0	100	100
9	I	47/54 (87%)	47 (100%)	0	100	100
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	65 (100%)	0	100	100
10	U	65/66 (98%)	65 (100%)	0	100	100
11	a	447/447 (100%)	447 (100%)	0	100	100
11	n	447/447 (100%)	447 (100%)	0	100	100
12	b	209/209 (100%)	209 (100%)	0	100	100
12	o	209/209 (100%)	209 (100%)	0	100	100
13	c	228/228 (100%)	228 (100%)	0	100	100
13	p	228/228 (100%)	226 (99%)	2 (1%)	70	89
14	d	101/111 (91%)	101 (100%)	0	100	100
14	q	102/111 (92%)	102 (100%)	0	100	100
15	e	114/115 (99%)	114 (100%)	0	100	100
15	r	114/115 (99%)	114 (100%)	0	100	100
16	f	91/96 (95%)	91 (100%)	0	100	100
16	s	91/96 (95%)	91 (100%)	0	100	100
17	g	50/50 (100%)	50 (100%)	0	100	100
17	t	50/50 (100%)	50 (100%)	0	100	100
18	h	41/41 (100%)	41 (100%)	0	100	100
18	u	41/41 (100%)	41 (100%)	0	100	100
19	i	46/46 (100%)	46 (100%)	0	100	100
19	v	46/46 (100%)	46 (100%)	0	100	100
20	j	67/73 (92%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	w	67/73 (92%)	63 (94%)	4 (6%)	17	47
21	k	99/113 (88%)	99 (100%)	0	100	100
21	x	99/113 (88%)	98 (99%)	1 (1%)	68	88
22	l	36/53 (68%)	36 (100%)	0	100	100
22	y	36/53 (68%)	36 (100%)	0	100	100
23	m	84/191 (44%)	84 (100%)	0	100	100
23	z	84/191 (44%)	83 (99%)	1 (1%)	63	87
All	All	6691/7158 (94%)	6677 (100%)	14 (0%)	85	96

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	p	195	THR
20	w	32	VAL
23	z	113	SER
20	w	48	CYS
21	x	73	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
11	n	399	GLN
12	o	123	GLN
18	u	37	ASN
1	L	156	HIS
1	L	75	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, 8 are monoatomic - leaving 55 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
25	PEF	E	303	-	39,39,46	1.01	2 (5%)	42,44,51	1.25	3 (7%)
25	PEF	r	201	-	40,40,46	0.99	2 (5%)	43,45,51	1.14	3 (6%)
24	CDL	H	101	-	52,52,99	1.22	4 (7%)	58,64,111	1.34	9 (15%)
25	PEF	n	606	-	46,46,46	0.95	2 (4%)	49,51,51	1.16	4 (8%)
25	PEF	S	102	-	35,35,46	1.06	2 (5%)	38,40,51	1.23	3 (7%)
25	PEF	H	102	-	31,31,46	1.11	2 (6%)	34,36,51	1.35	4 (11%)
24	CDL	L	501	-	54,54,99	1.13	4 (7%)	60,66,111	1.29	5 (8%)
25	PEF	N	606	-	42,42,46	0.94	2 (4%)	45,47,51	1.20	4 (8%)
27	PCF	I	101	-	29,29,49	1.28	2 (6%)	35,37,57	1.31	4 (11%)
24	CDL	C	603	-	65,65,99	1.12	4 (6%)	71,77,111	1.39	8 (11%)
31	HEA	n	602	11	67,67,67	2.25	24 (35%)	81,103,103	2.59	39 (48%)
25	PEF	n	607	-	32,32,46	1.14	2 (6%)	35,37,51	1.21	4 (11%)
34	CUA	o	301	12	0,1,1	-	-	-	-	-
27	PCF	H	103	-	31,31,49	1.18	2 (6%)	37,39,57	1.20	4 (10%)
26	HEM	C	602	3	50,50,50	1.80	11 (22%)	67,82,82	1.73	17 (25%)
25	PEF	C	604	-	43,43,46	0.98	2 (4%)	46,48,51	1.11	3 (6%)
27	PCF	T	101	-	46,46,49	1.00	2 (4%)	52,54,57	1.15	4 (7%)
25	PEF	L	502	-	30,30,46	1.16	2 (6%)	33,35,51	1.22	4 (12%)
31	HEA	a	603	11	67,67,67	2.24	23 (34%)	81,103,103	2.53	35 (43%)
25	PEF	C	605	-	38,38,46	1.02	2 (5%)	41,43,51	1.10	2 (4%)
25	PEF	J	101	-	28,28,46	1.23	2 (7%)	31,33,51	1.28	3 (9%)
27	PCF	e	202	-	35,35,49	1.16	2 (5%)	41,43,57	1.18	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEF	l	101	-	32,32,46	1.11	2 (6%)	35,37,51	1.30	5 (14%)
26	HEM	N	601	3	50,50,50	1.75	12 (24%)	67,82,82	1.94	12 (17%)
27	PCF	C	606	-	38,38,49	1.06	2 (5%)	44,46,57	1.32	6 (13%)
25	PEF	O	402	-	42,42,46	1.00	2 (4%)	45,47,51	1.10	3 (6%)
27	PCF	N	607	-	49,49,49	0.93	3 (6%)	55,57,57	1.17	4 (7%)
25	PEF	c	301	-	35,35,46	1.06	2 (5%)	38,40,51	1.14	3 (7%)
25	PEF	o	302	-	39,39,46	1.05	2 (5%)	42,44,51	1.10	4 (9%)
24	CDL	N	604	-	74,74,99	1.05	5 (6%)	80,86,111	1.20	6 (7%)
25	PEF	c	302	-	33,33,46	1.12	2 (6%)	36,38,51	1.07	2 (5%)
28	HEC	O	401	4	46,50,50	2.51	23 (50%)	58,82,82	2.17	19 (32%)
24	CDL	D	402	-	70,70,99	1.03	5 (7%)	76,82,111	1.26	7 (9%)
25	PEF	b	302	-	39,39,46	1.01	2 (5%)	42,44,51	1.13	3 (7%)
25	PEF	a	606	-	32,32,46	1.15	2 (6%)	35,37,51	1.09	3 (8%)
25	PEF	b	303	-	39,39,46	1.04	2 (5%)	42,44,51	1.10	3 (7%)
26	HEM	N	602	3	50,50,50	1.80	12 (24%)	67,82,82	1.73	14 (20%)
29	FES	P	301	5	0,4,4	-	-	-	-	-
25	PEF	E	304	-	33,33,46	1.09	2 (6%)	36,38,51	1.27	5 (13%)
25	PEF	p	301	-	35,35,46	1.10	3 (8%)	38,40,51	1.13	3 (7%)
31	HEA	n	603	11	67,67,67	2.30	24 (35%)	81,103,103	2.57	32 (39%)
28	HEC	D	401	4	46,50,50	2.52	23 (50%)	58,82,82	2.13	18 (31%)
25	PEF	e	201	-	40,40,46	0.97	3 (7%)	43,45,51	1.37	5 (11%)
34	CUA	b	301	12	0,1,1	-	-	-	-	-
26	HEM	C	601	3	50,50,50	1.81	11 (22%)	67,82,82	1.86	15 (22%)
25	PEF	A	502	-	35,35,46	1.07	2 (5%)	38,40,51	1.16	3 (7%)
25	PEF	n	608	-	32,32,46	1.14	2 (6%)	35,37,51	1.13	2 (5%)
31	HEA	a	602	11	67,67,67	2.23	24 (35%)	81,103,103	2.80	40 (49%)
24	CDL	N	603	-	52,52,99	1.23	5 (9%)	58,64,111	1.45	8 (13%)
24	CDL	S	101	-	47,47,99	1.31	4 (8%)	53,59,111	1.44	9 (16%)
25	PEF	E	302	-	41,41,46	1.01	2 (4%)	44,46,51	1.10	3 (6%)
29	FES	E	301	5	0,4,4	-	-	-	-	-
27	PCF	r	202	-	35,35,49	1.15	2 (5%)	41,43,57	1.04	3 (7%)
25	PEF	N	605	-	39,39,46	1.01	2 (5%)	42,44,51	1.17	3 (7%)
24	CDL	A	501	-	57,57,99	1.18	4 (7%)	63,69,111	1.42	8 (12%)

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
25	PEF	E	303	-	-	19/43/43/50	-
25	PEF	r	201	-	-	15/44/44/50	-
24	CDL	H	101	-	-	28/63/63/110	-
25	PEF	n	606	-	-	18/50/50/50	-
25	PEF	S	102	-	-	11/39/39/50	-
25	PEF	H	102	-	-	9/35/35/50	-
24	CDL	L	501	-	-	31/64/64/110	-
25	PEF	N	606	-	-	11/46/46/50	-
27	PCF	I	101	-	-	5/33/33/53	-
24	CDL	C	603	-	-	26/76/76/110	-
31	HEA	n	602	11	-	9/36/76/76	-
25	PEF	n	607	-	-	16/36/36/50	-
27	PCF	H	103	-	-	16/35/35/53	-
26	HEM	C	602	3	-	6/14/54/54	-
25	PEF	C	604	-	-	15/47/47/50	-
27	PCF	T	101	-	-	4/50/50/53	-
25	PEF	L	502	-	-	17/34/34/50	-
31	HEA	a	603	11	-	7/36/76/76	-
25	PEF	C	605	-	-	9/42/42/50	-
25	PEF	J	101	-	-	12/32/32/50	-
27	PCF	e	202	-	-	11/39/39/53	-
25	PEF	l	101	-	-	6/36/36/50	-
26	HEM	N	601	3	-	8/14/54/54	-
27	PCF	C	606	-	-	19/42/42/53	-
25	PEF	O	402	-	-	20/46/46/50	-
27	PCF	N	607	-	-	21/53/53/53	-
25	PEF	c	301	-	-	9/39/39/50	-
25	PEF	o	302	-	-	14/43/43/50	-
24	CDL	N	604	-	-	33/85/85/110	-
25	PEF	c	302	-	-	14/37/37/50	-
28	HEC	O	401	4	-	3/14/54/54	-
24	CDL	D	402	-	-	22/81/81/110	-
25	PEF	b	302	-	-	15/43/43/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEF	a	606	-	-	12/36/36/50	-
25	PEF	b	303	-	-	16/43/43/50	-
26	HEM	N	602	3	-	6/14/54/54	-
29	FES	P	301	5	-	-	0/1/1/1
25	PEF	E	304	-	-	16/37/37/50	-
25	PEF	p	301	-	-	11/39/39/50	-
31	HEA	n	603	11	-	6/36/76/76	-
28	HEC	D	401	4	-	1/14/54/54	-
25	PEF	e	201	-	-	17/44/44/50	-
26	HEM	C	601	3	-	10/14/54/54	-
25	PEF	A	502	-	-	10/39/39/50	-
25	PEF	n	608	-	-	7/36/36/50	-
31	HEA	a	602	11	-	10/36/76/76	-
24	CDL	N	603	-	-	22/63/63/110	-
24	CDL	S	101	-	-	16/58/58/110	-
25	PEF	E	302	-	-	19/45/45/50	-
29	FES	E	301	5	-	-	0/1/1/1
27	PCF	r	202	-	-	11/39/39/53	-
25	PEF	N	605	-	-	19/43/43/50	-
24	CDL	A	501	-	-	25/68/68/110	-

The worst 5 of 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	603	HEA	FE-NB	5.09	2.10	1.94
31	n	602	HEA	FE-NB	5.08	2.10	1.94
31	n	603	HEA	FE-ND	5.06	2.10	1.94
28	O	401	HEC	CHD-C4C	5.06	1.48	1.38
31	a	603	HEA	FE-ND	5.03	2.10	1.94

The worst 5 of 416 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C13-C12-C11	-7.47	102.46	114.39
31	a	603	HEA	C3D-C4D-ND	7.41	117.51	110.35
31	n	603	HEA	C3D-C4D-ND	6.80	116.92	110.35
31	a	602	HEA	C2B-C1B-NB	6.77	117.72	109.90
31	n	602	HEA	C3D-C4D-ND	6.33	116.47	110.35

There are no chirality outliers.

5 of 713 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	501	CDL	CA2-OA2-PA1-OA3
24	A	501	CDL	CA2-OA2-PA1-OA5
24	A	501	CDL	CA3-OA5-PA1-OA2
24	A	501	CDL	CA3-OA5-PA1-OA3
24	A	501	CDL	CB2-OB2-PB2-OB5

There are no ring outliers.

39 monomers are involved in 78 short contacts:

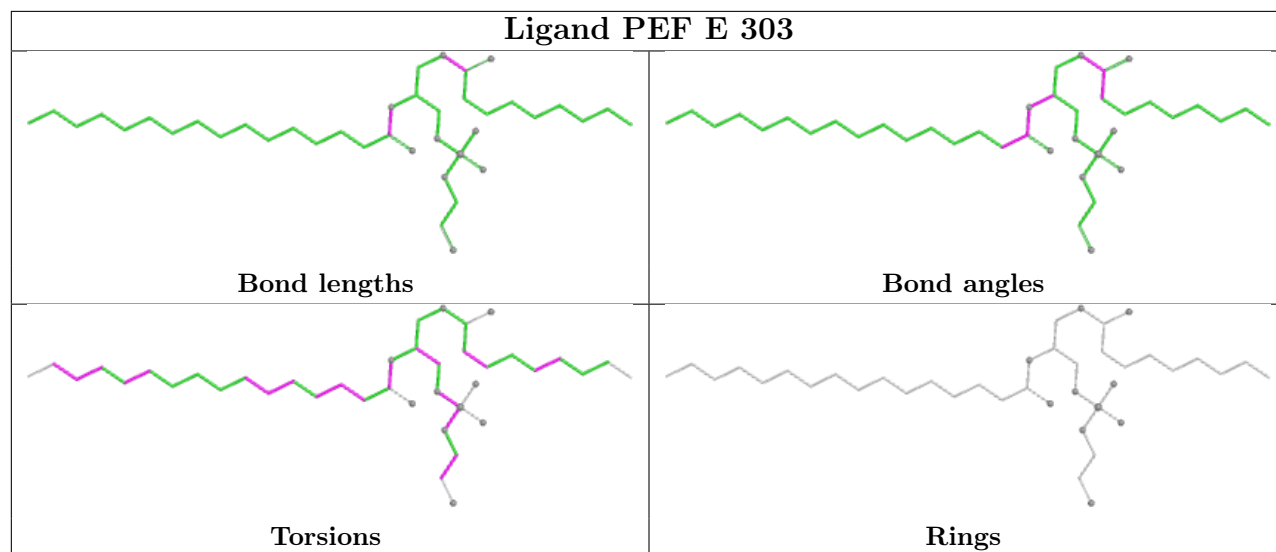
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	E	303	PEF	3	0
25	r	201	PEF	3	0
24	H	101	CDL	2	0
25	n	606	PEF	2	0
25	S	102	PEF	1	0
24	L	501	CDL	1	0
25	N	606	PEF	3	0
27	I	101	PCF	3	0
24	C	603	CDL	3	0
31	n	602	HEA	4	0
25	n	607	PEF	2	0
27	H	103	PCF	1	0
26	C	602	HEM	1	0
25	C	604	PEF	1	0
27	T	101	PCF	2	0
31	a	603	HEA	1	0
25	C	605	PEF	2	0
26	N	601	HEM	4	0
27	N	607	PCF	2	0
24	N	604	CDL	1	0
25	c	302	PEF	3	0
25	b	302	PEF	1	0
25	a	606	PEF	1	0
25	b	303	PEF	2	0
26	N	602	HEM	1	0
25	E	304	PEF	4	0
25	p	301	PEF	2	0
31	n	603	HEA	1	0
28	D	401	HEC	2	0
25	e	201	PEF	4	0

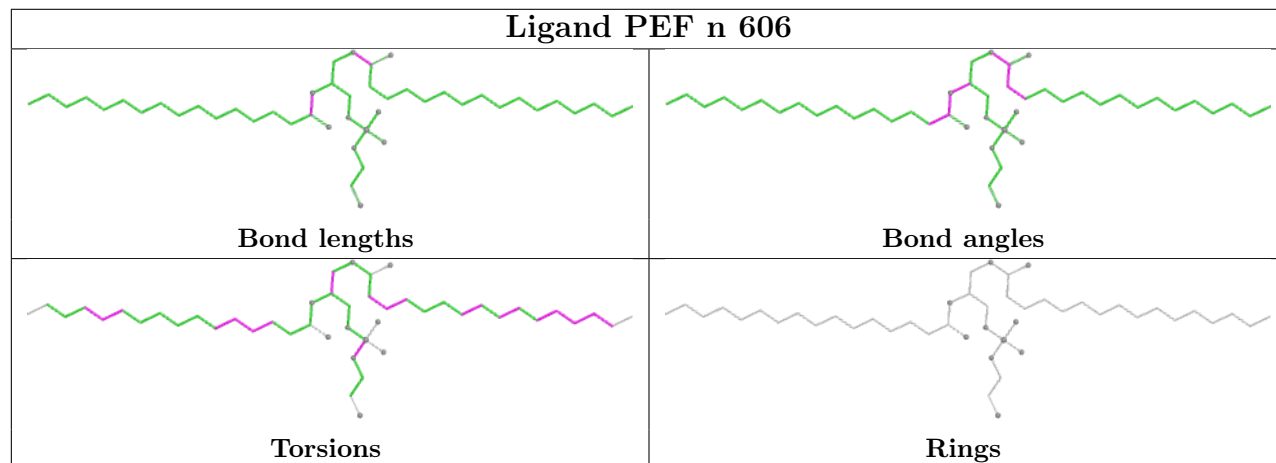
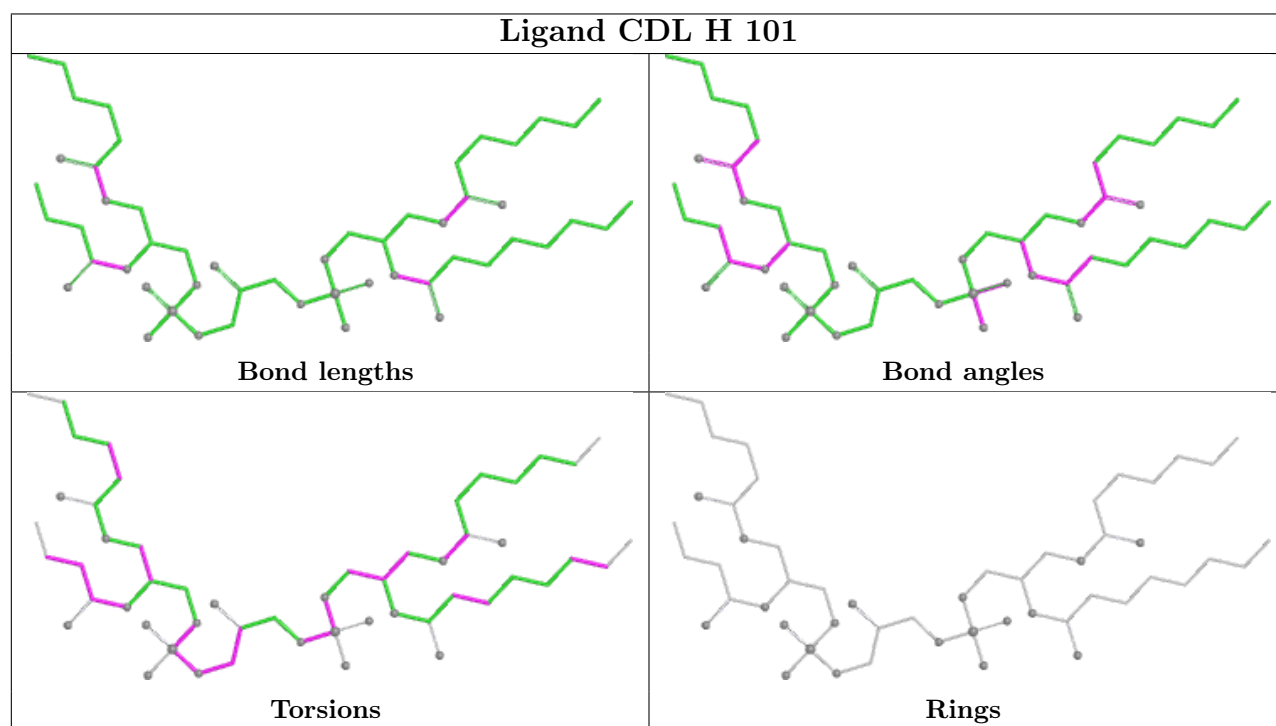
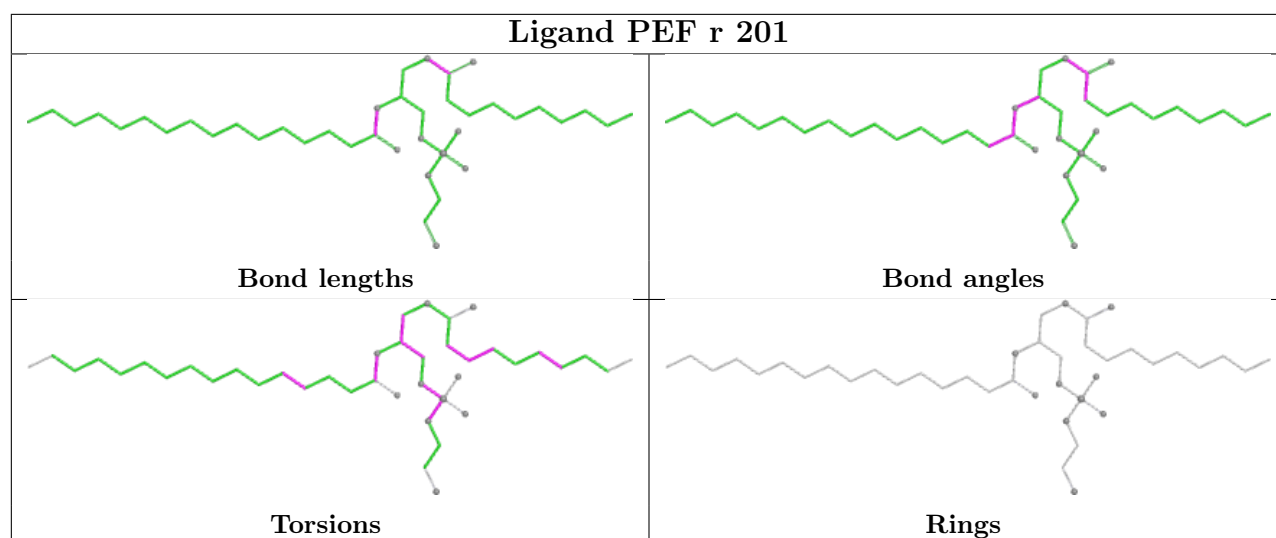
Continued on next page...

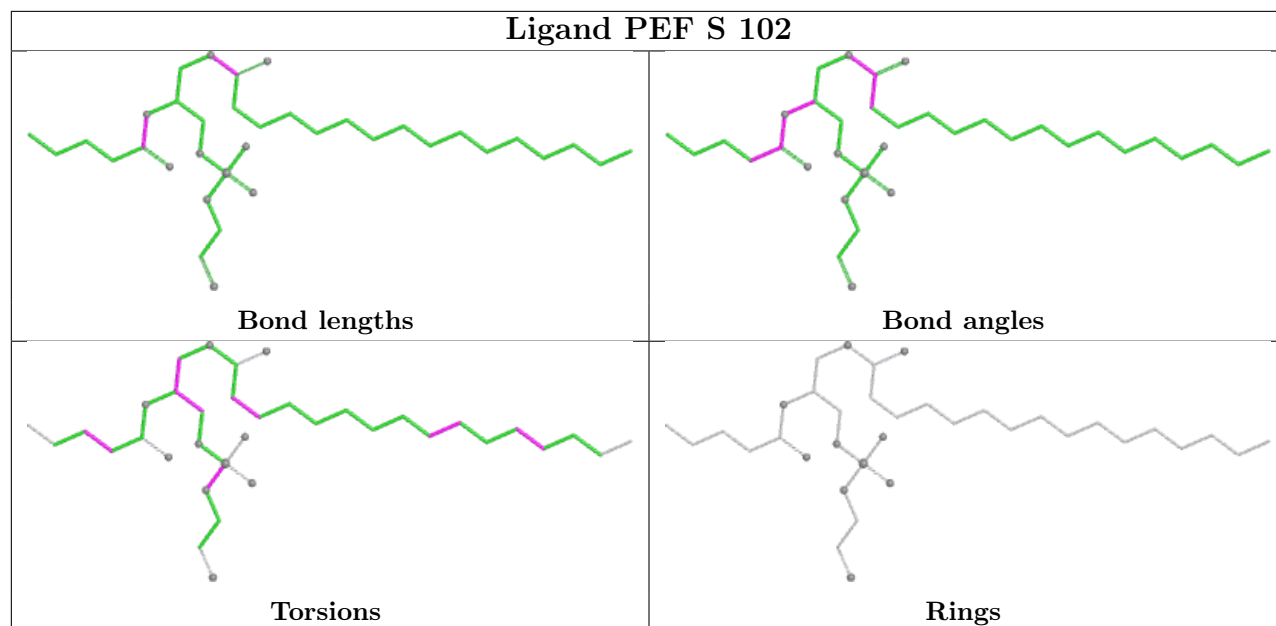
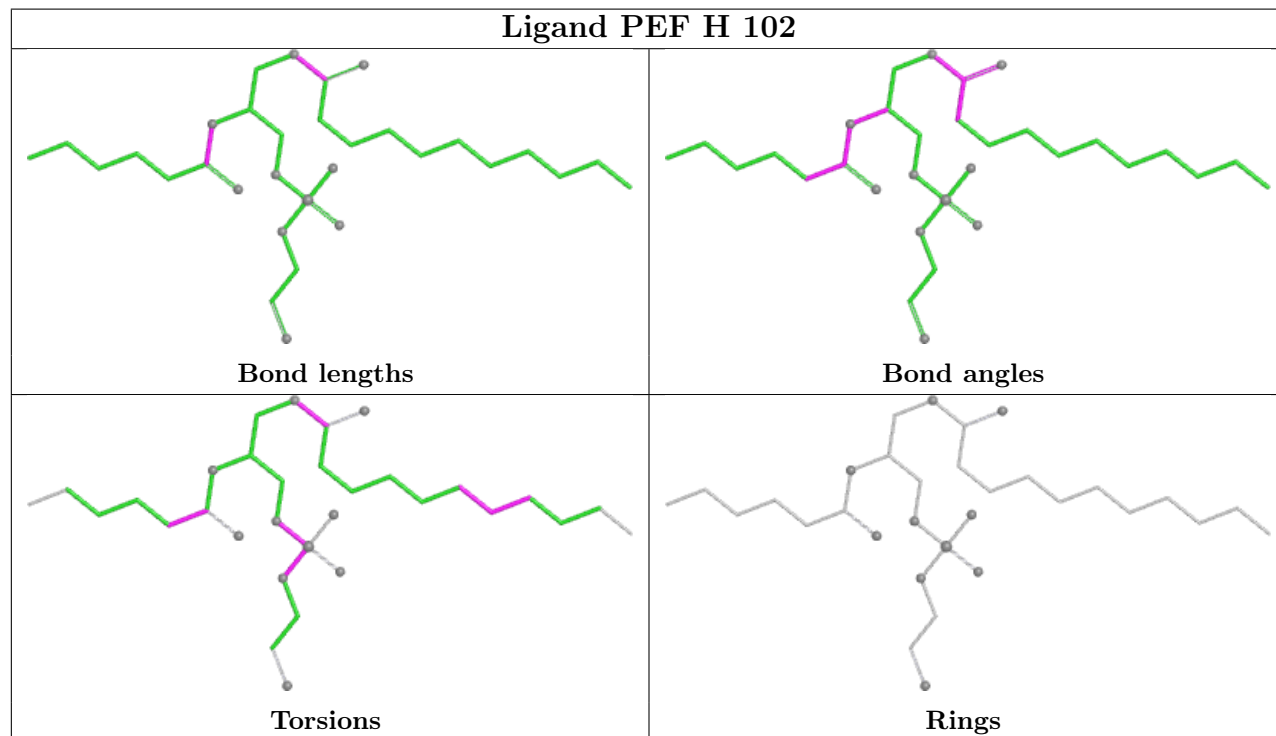
Continued from previous page...

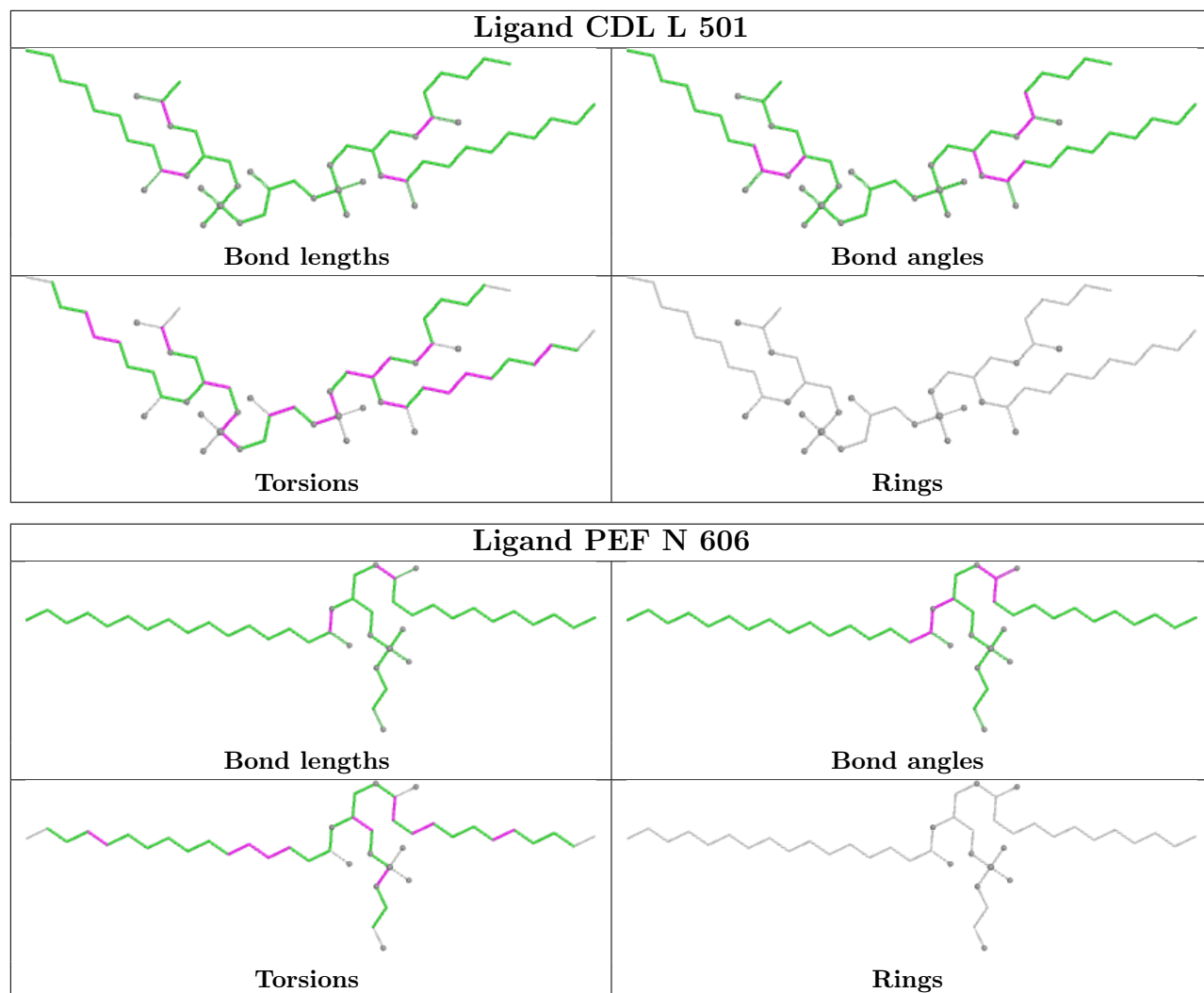
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	601	HEM	3	0
25	A	502	PEF	1	0
25	n	608	PEF	1	0
31	a	602	HEA	5	0
24	S	101	CDL	2	0
25	E	302	PEF	1	0
27	r	202	PCF	1	0
25	N	605	PEF	2	0
24	A	501	CDL	3	0

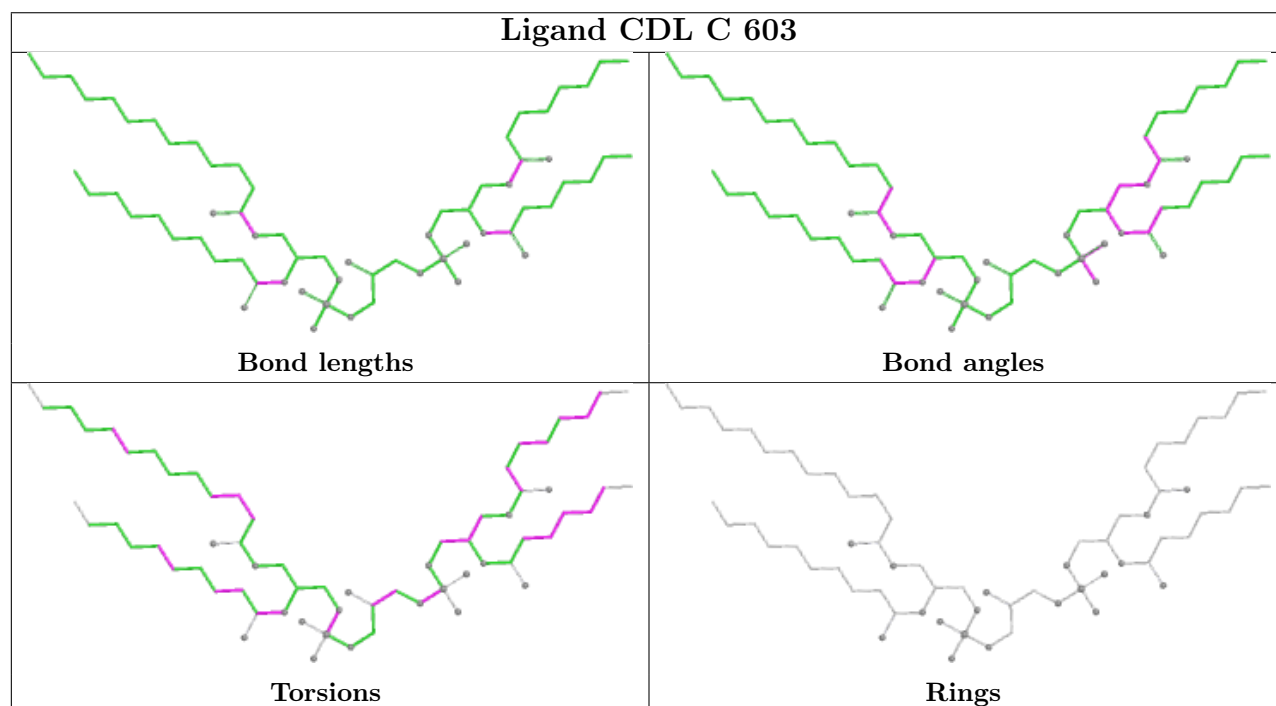
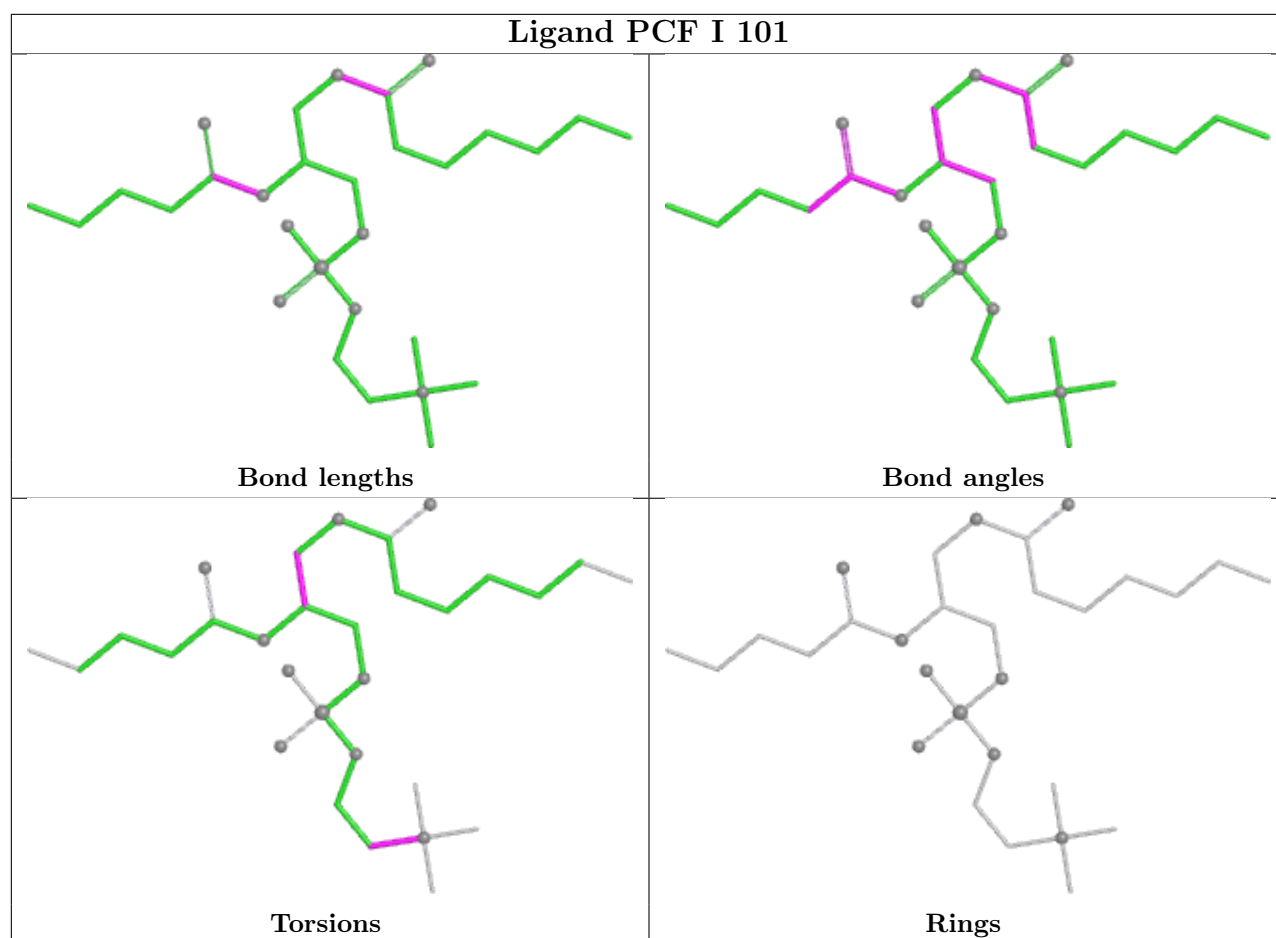
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

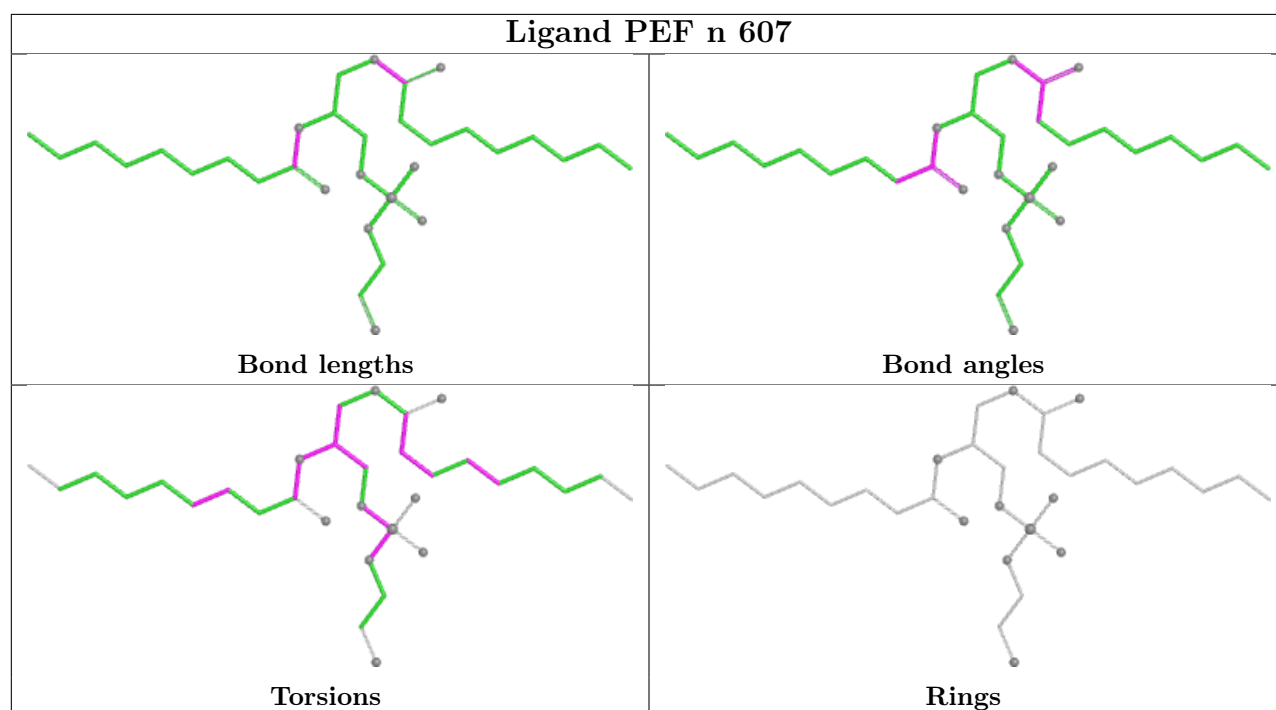
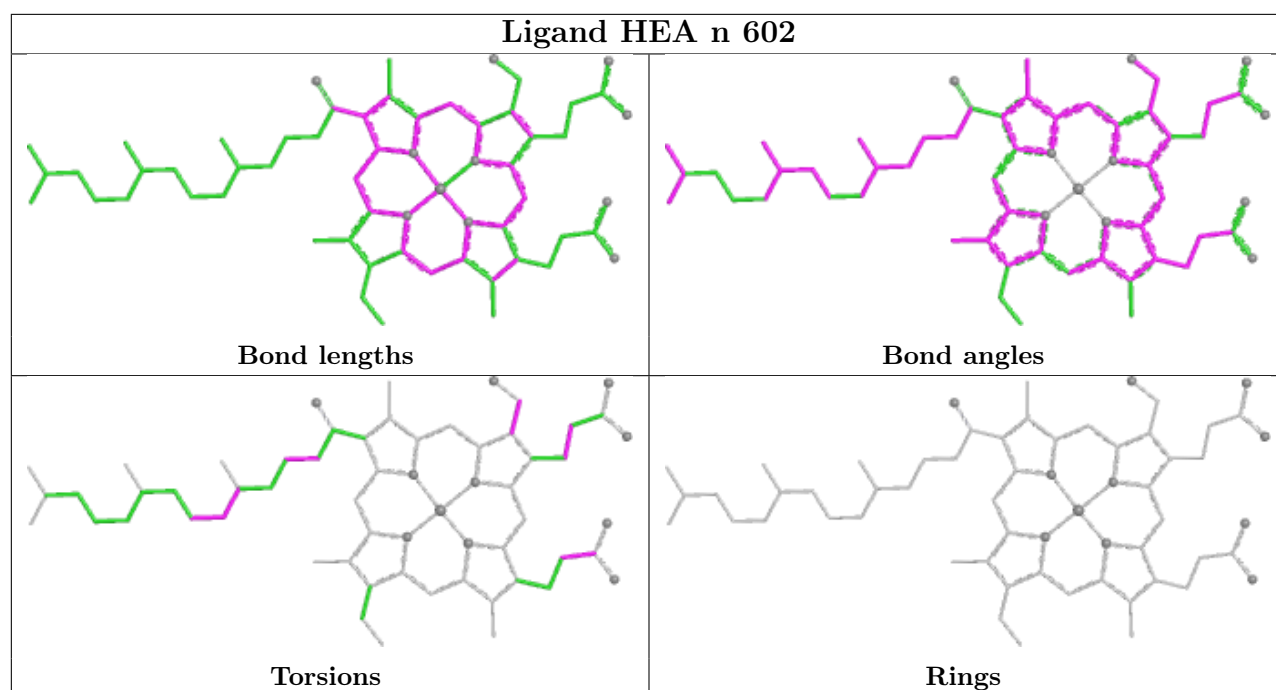


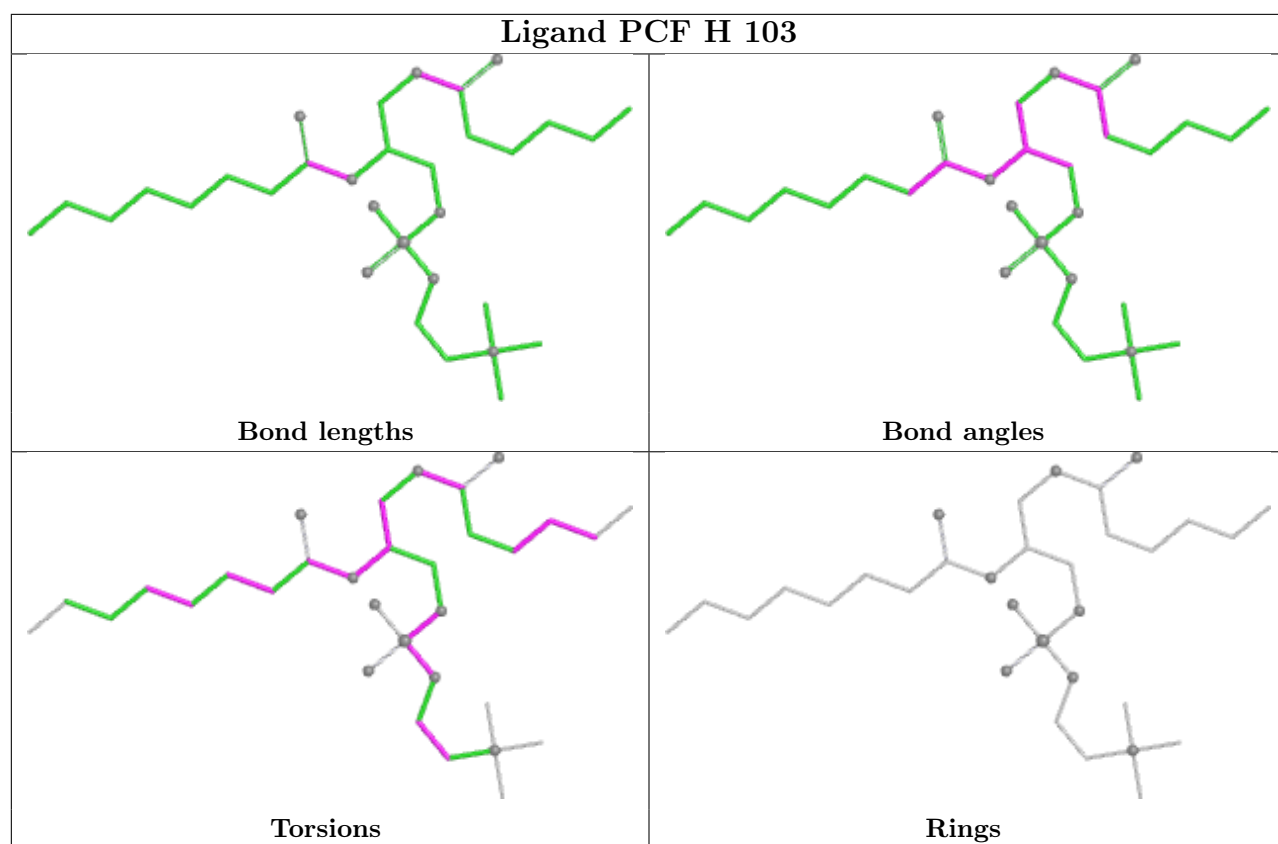


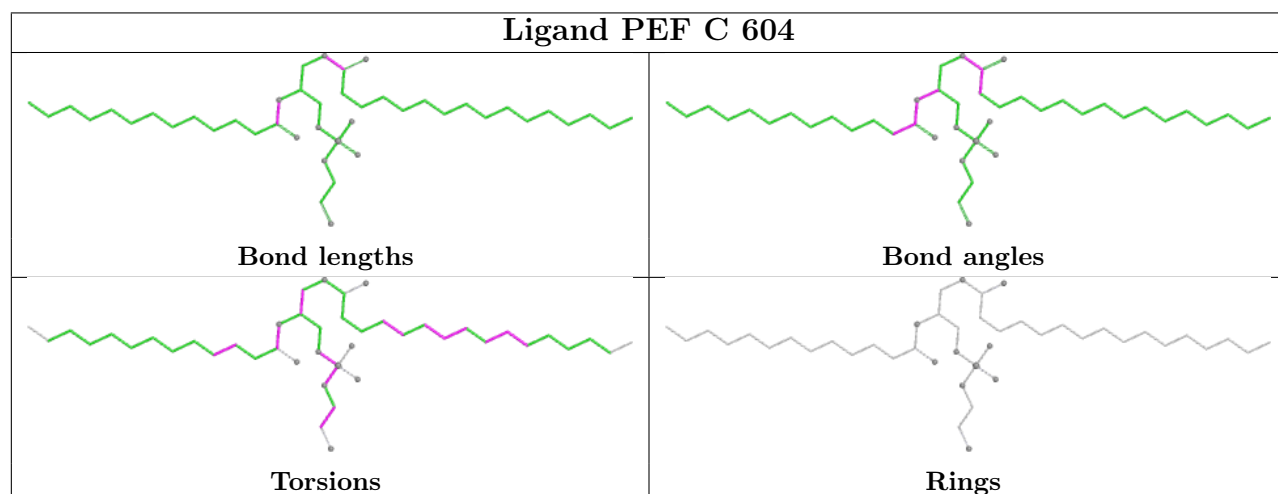
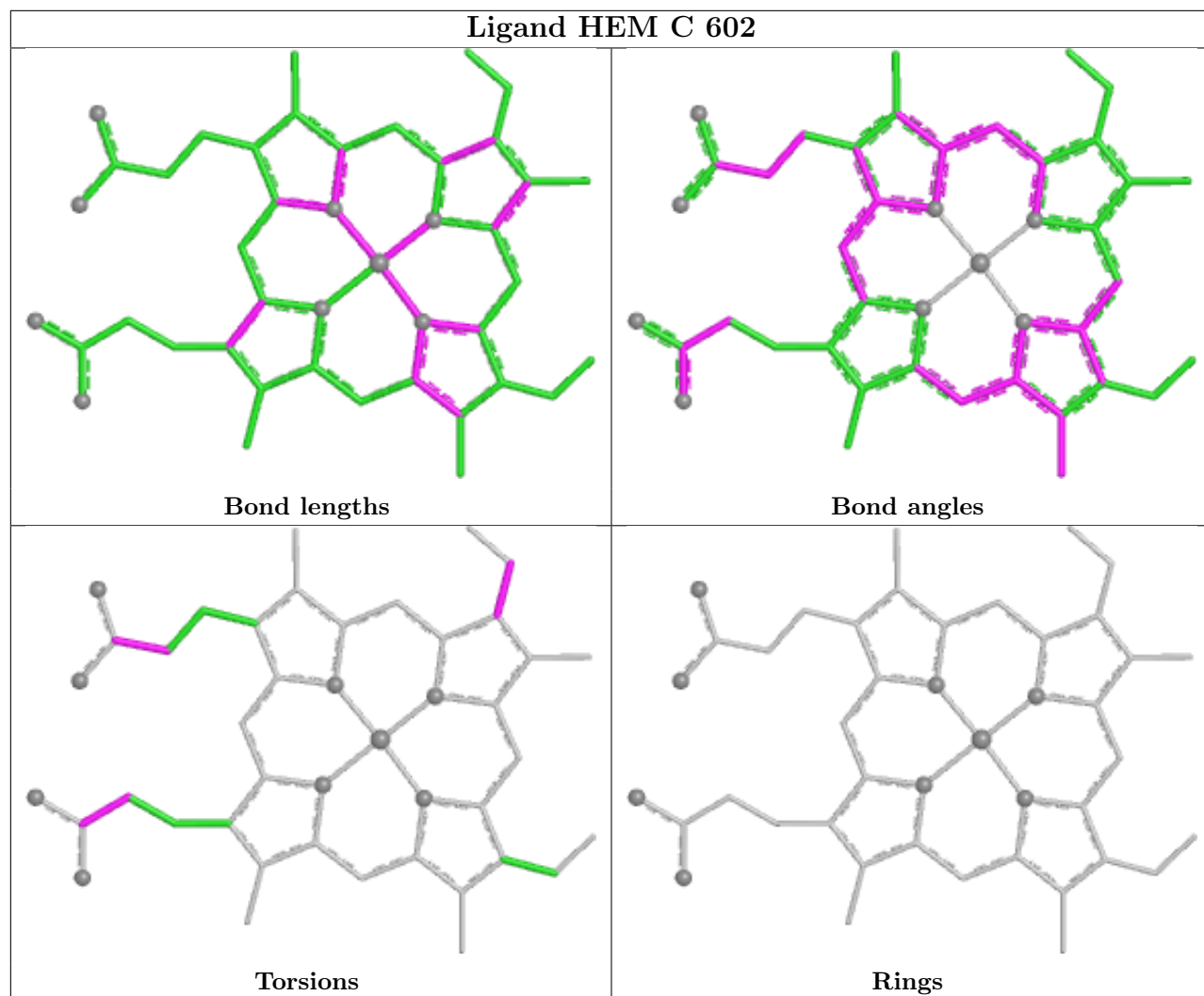
Ligand PEF S 102**Ligand PEF H 102**

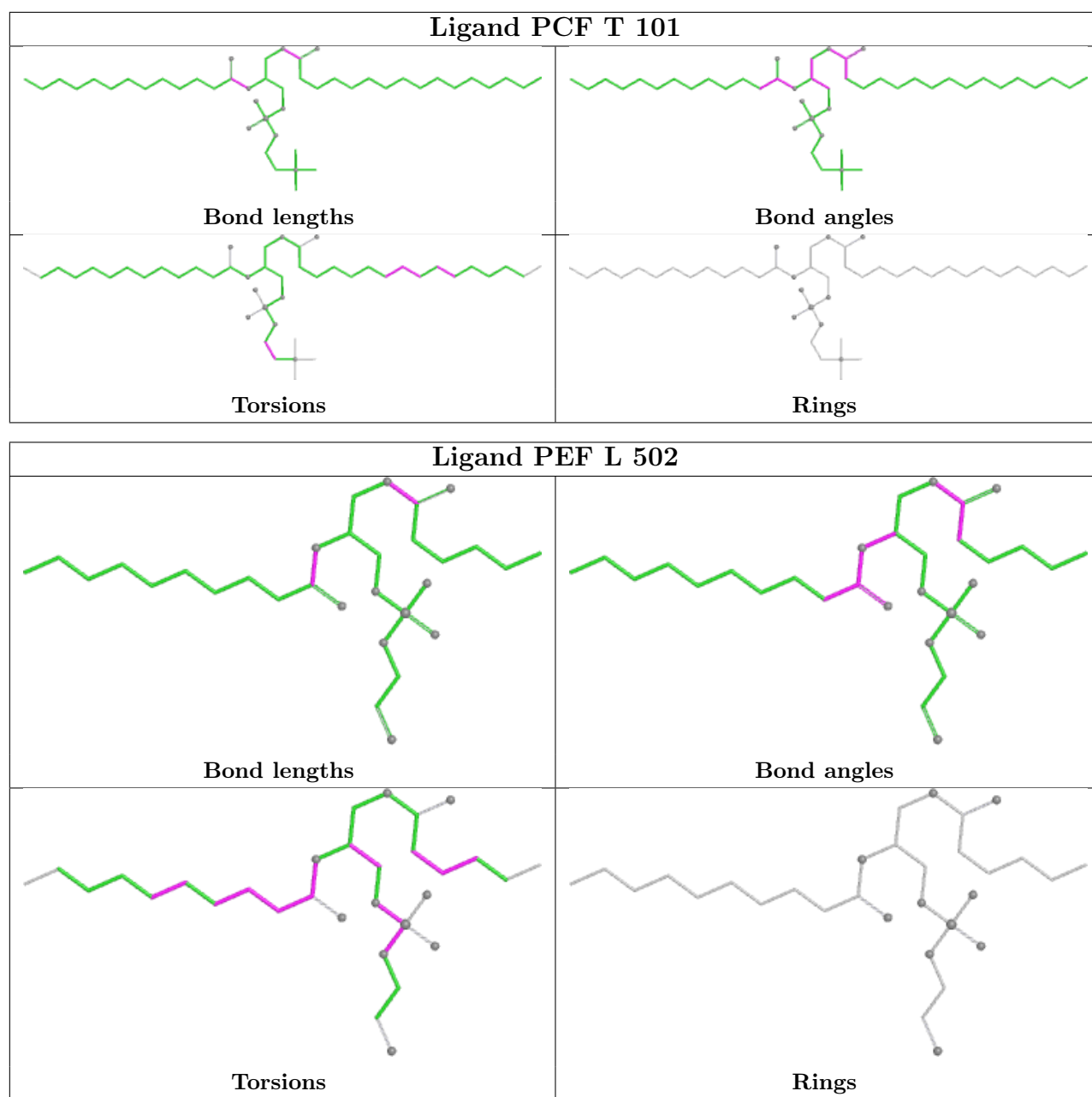


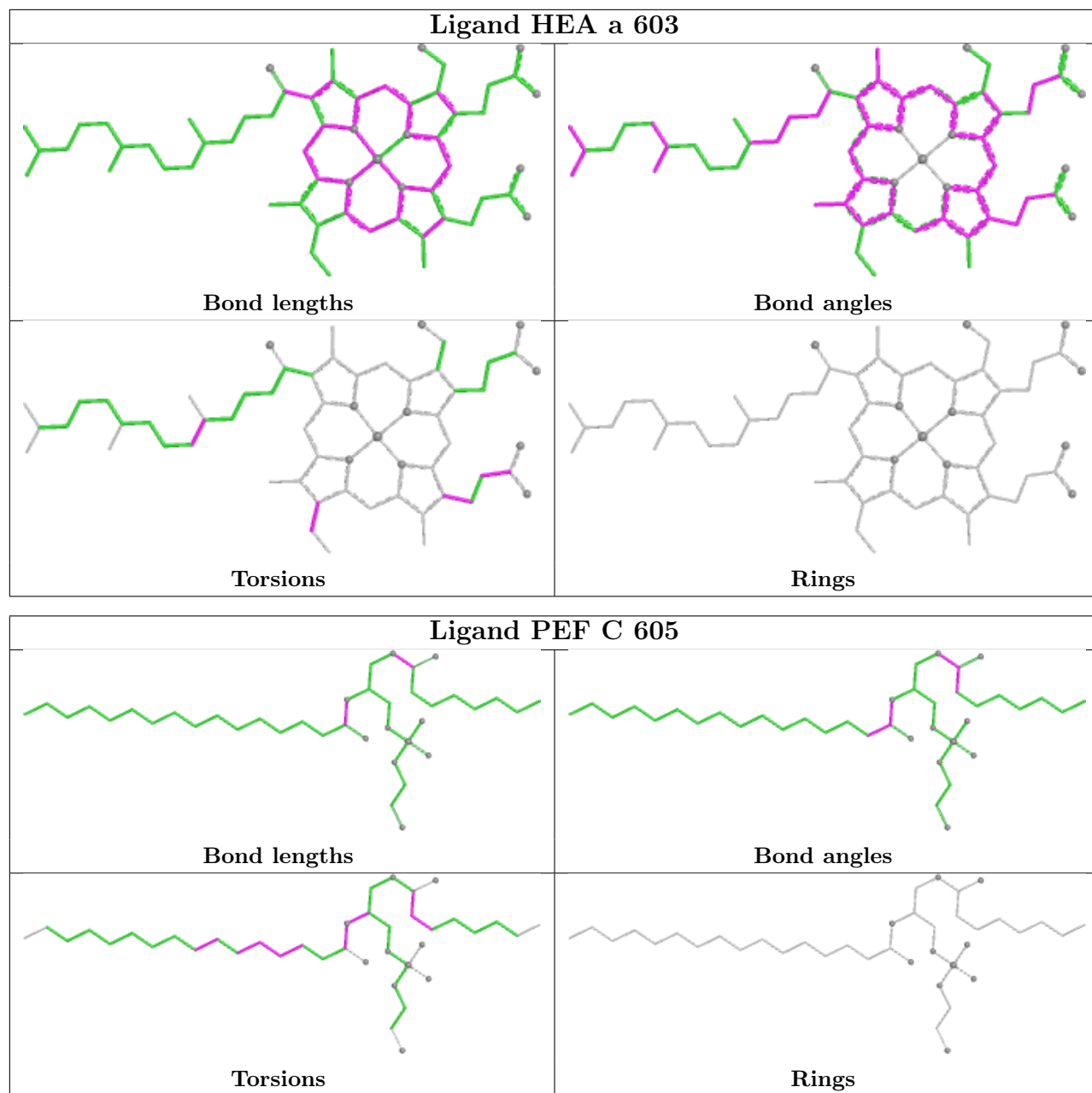


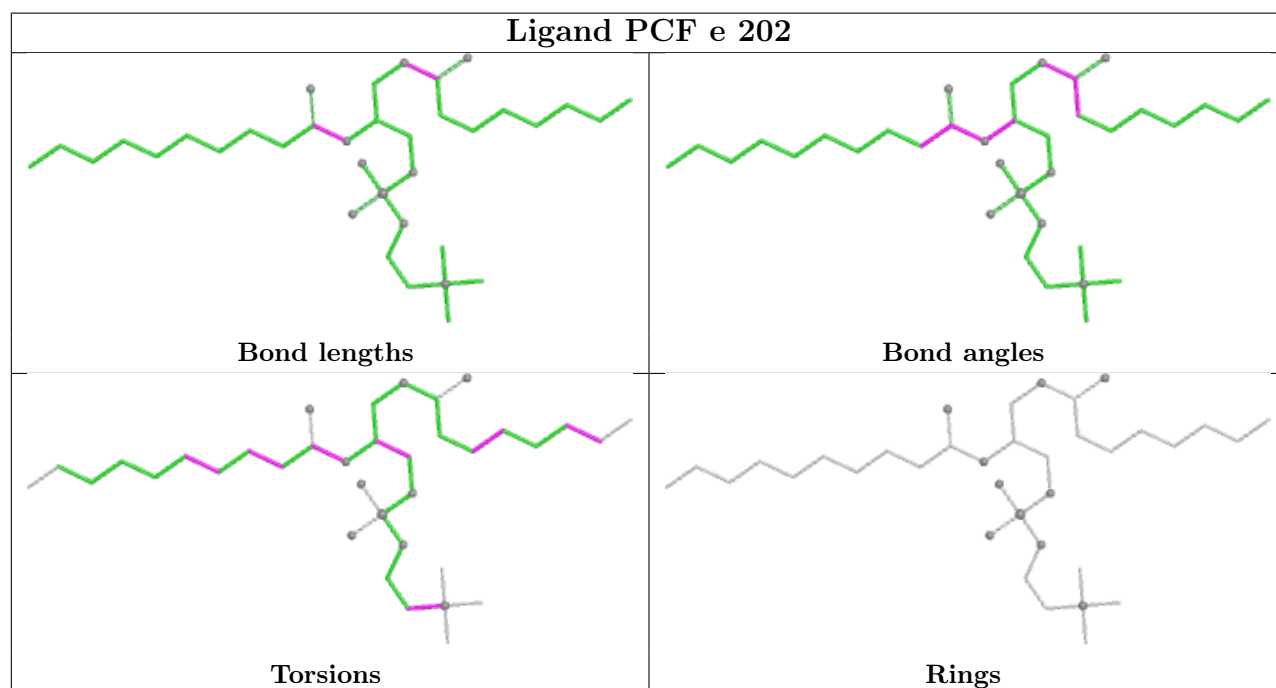
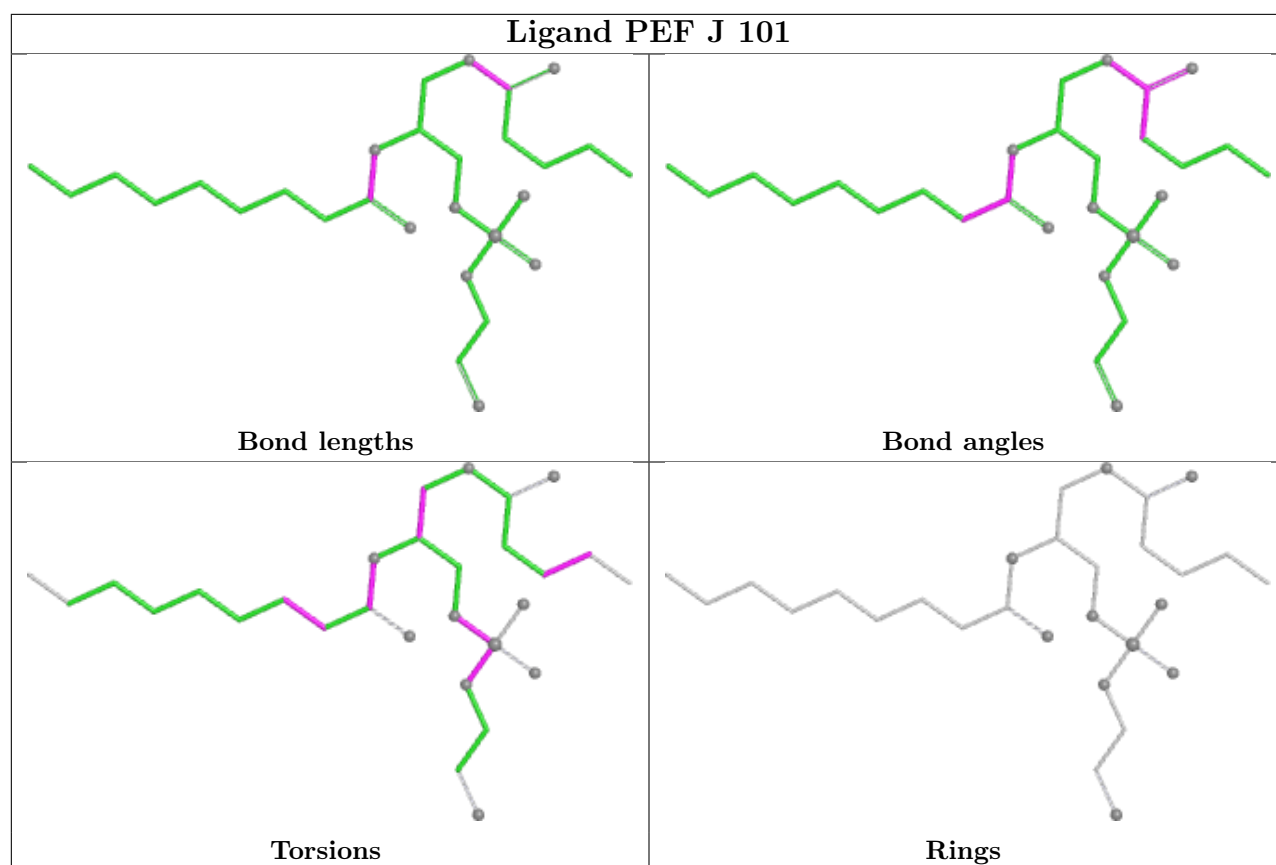




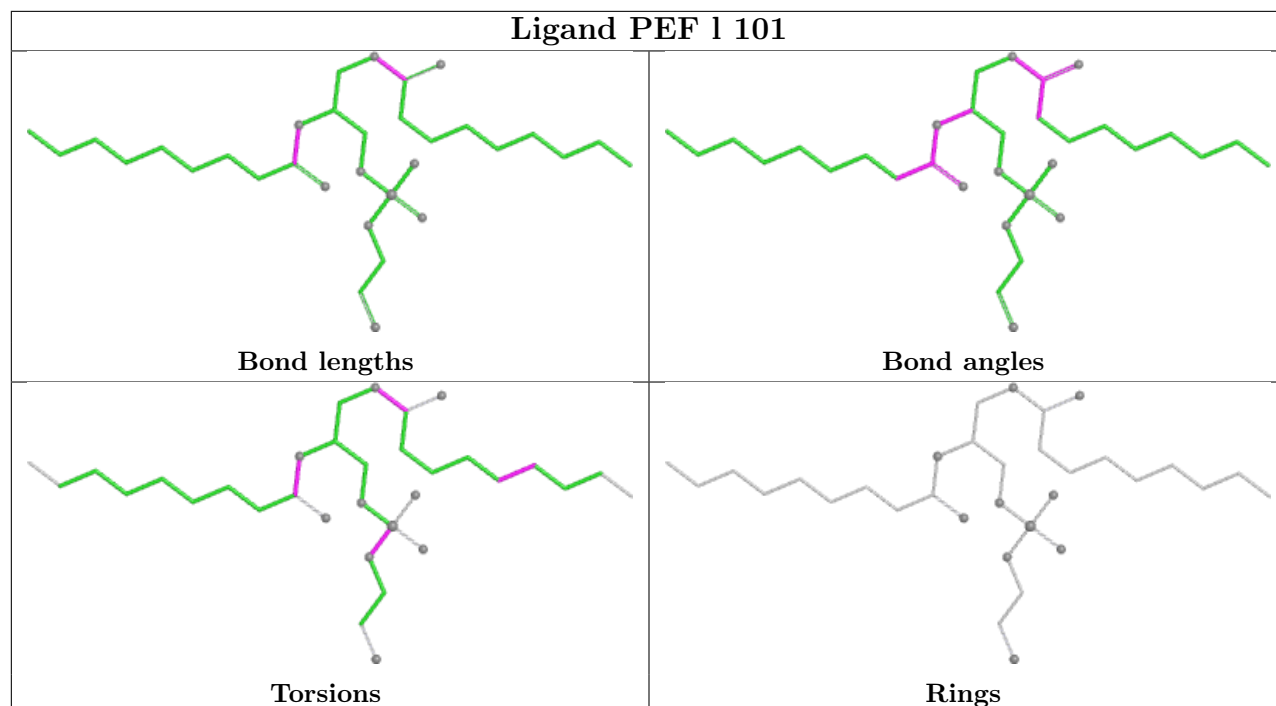




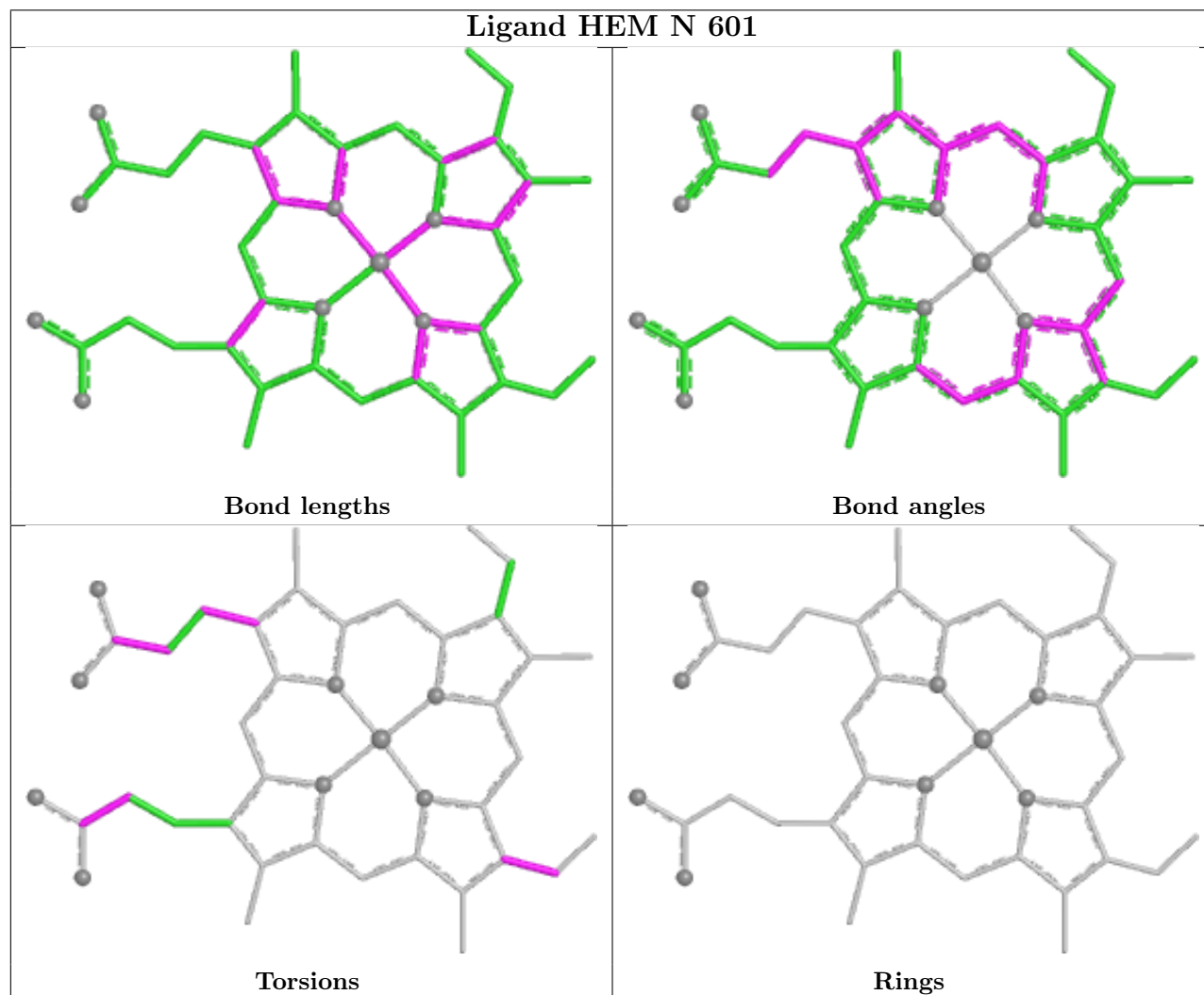


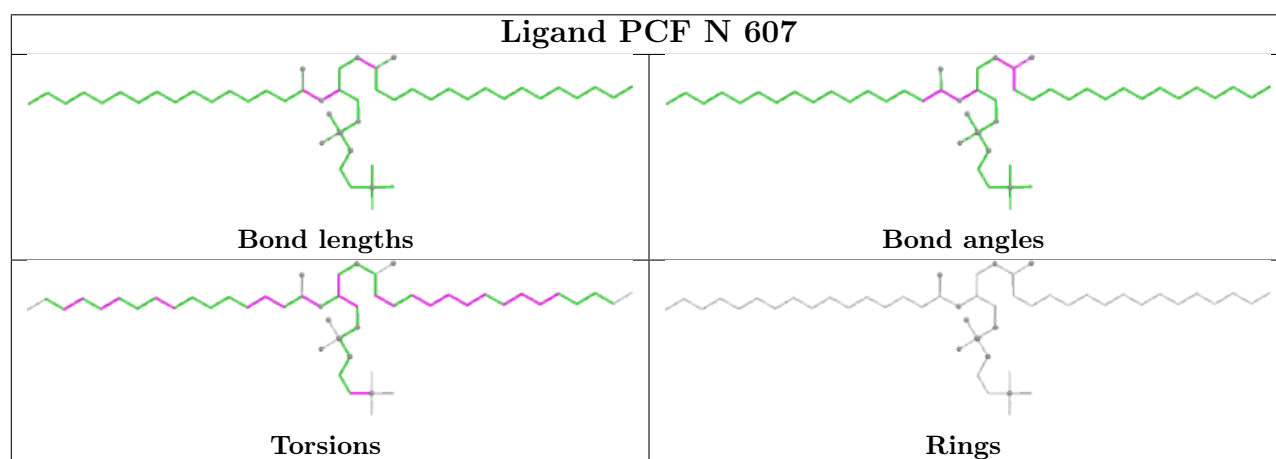
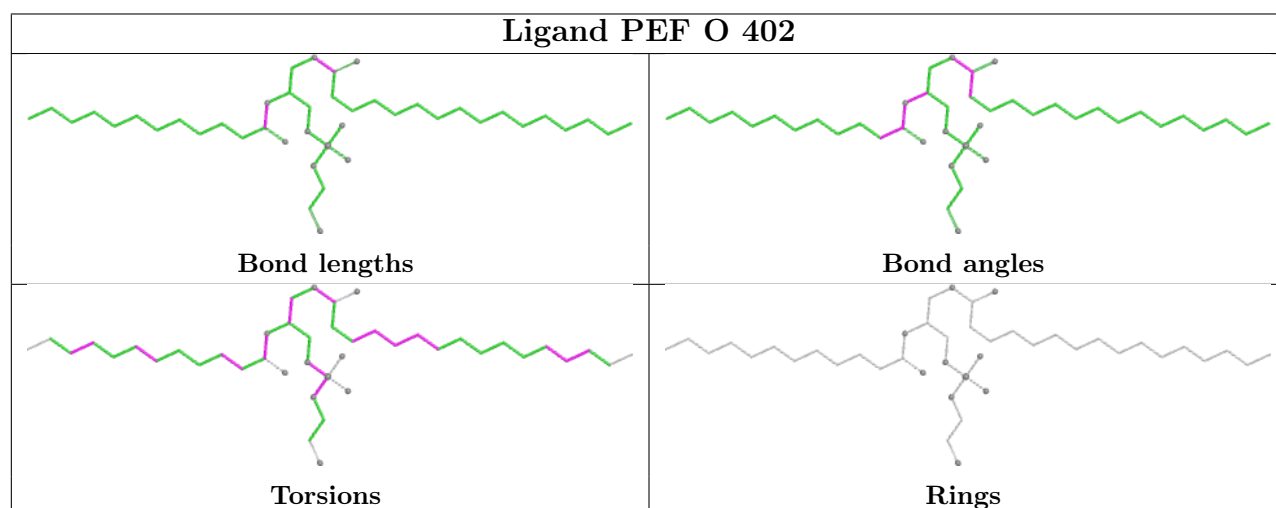
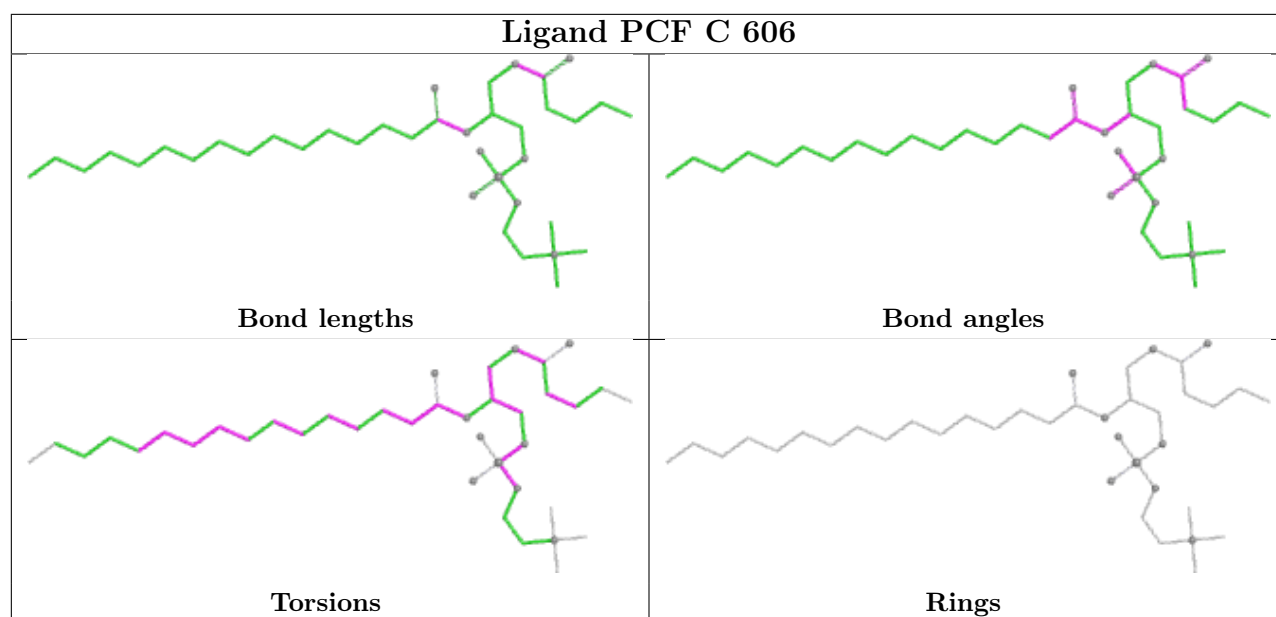


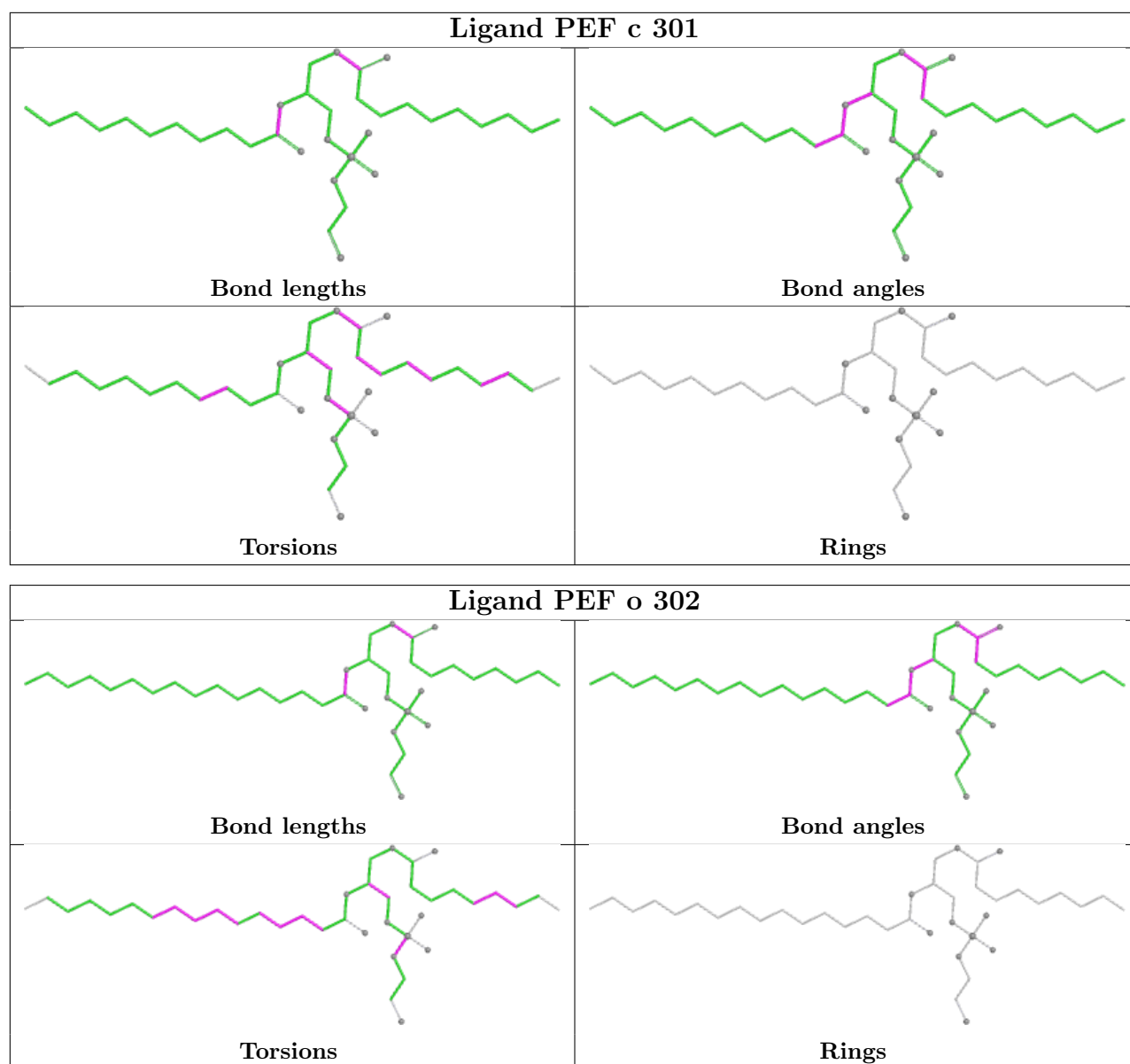
Ligand PEF 1 101

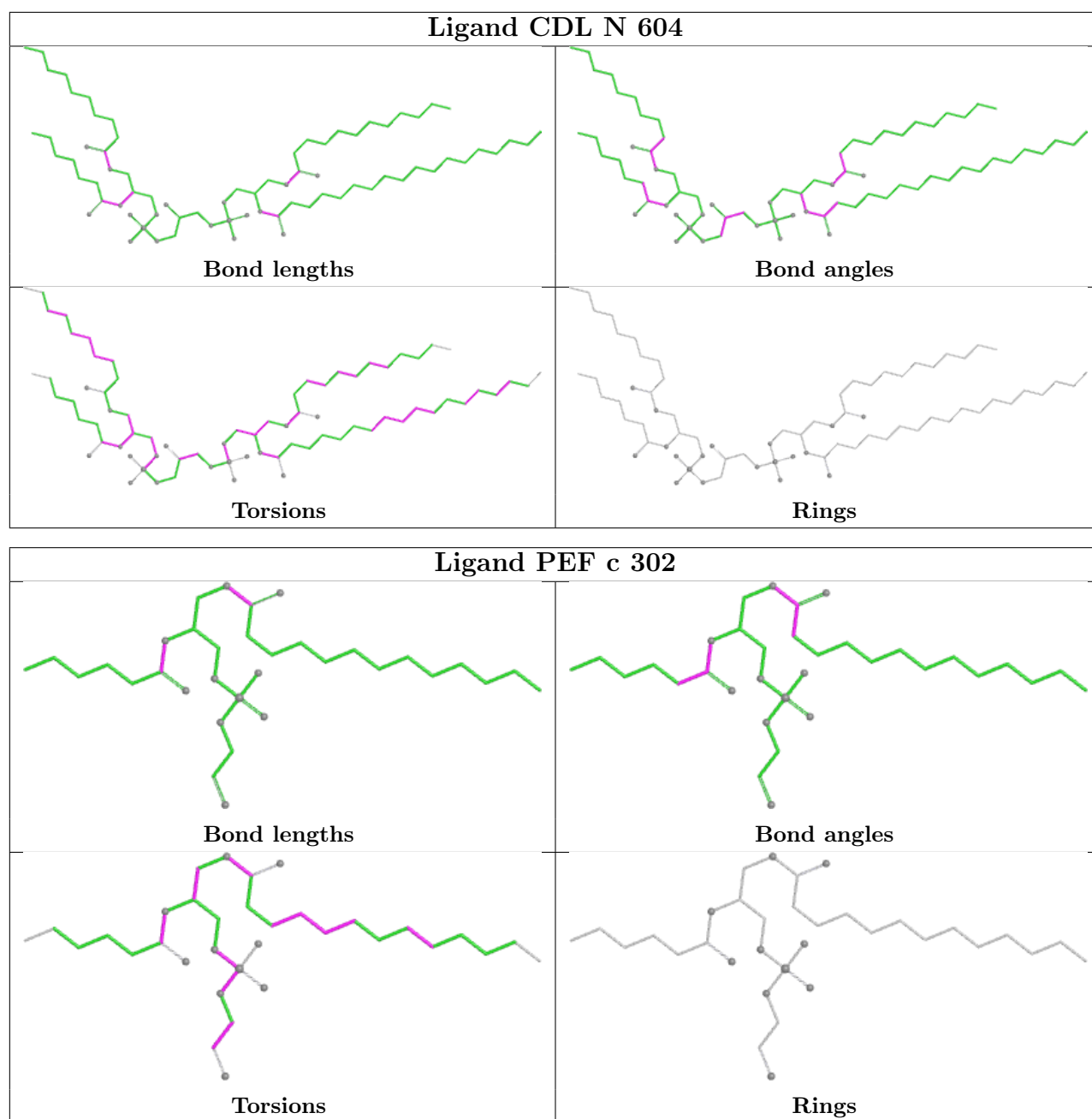


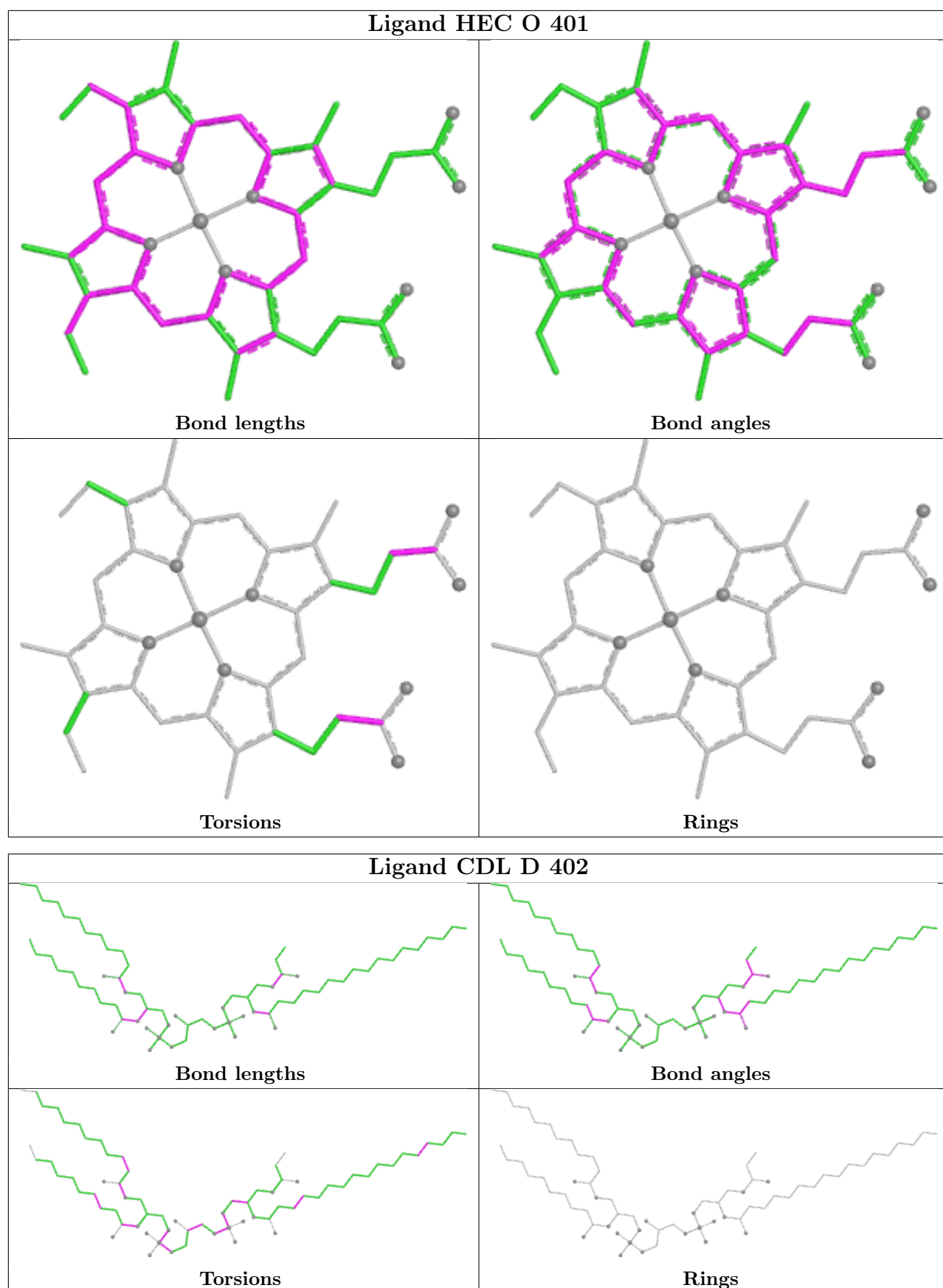
Ligand HEM N 601

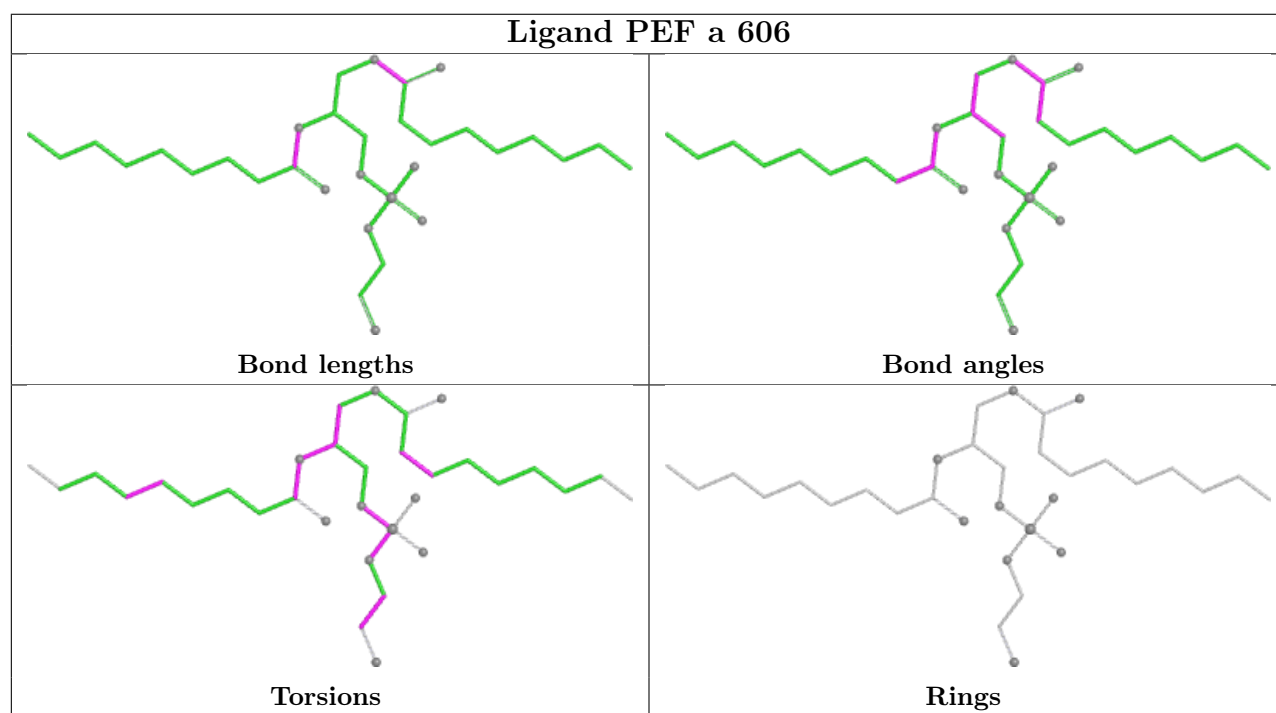
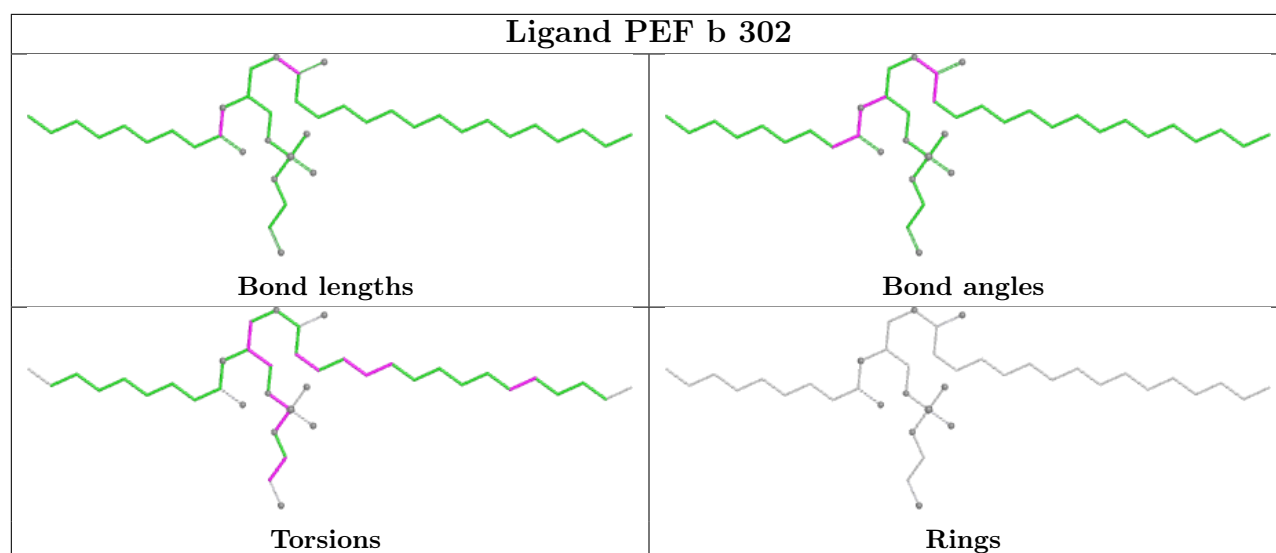


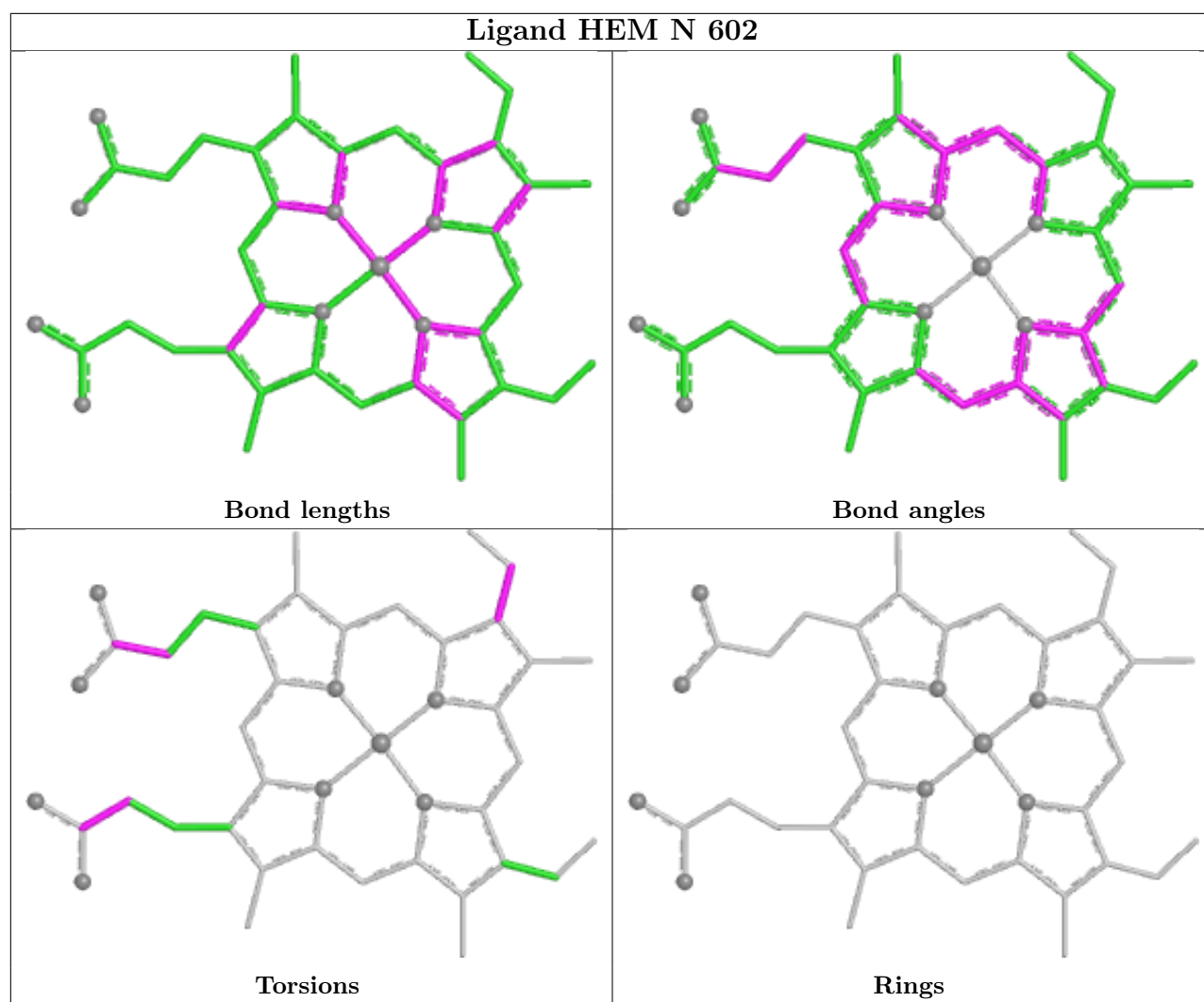
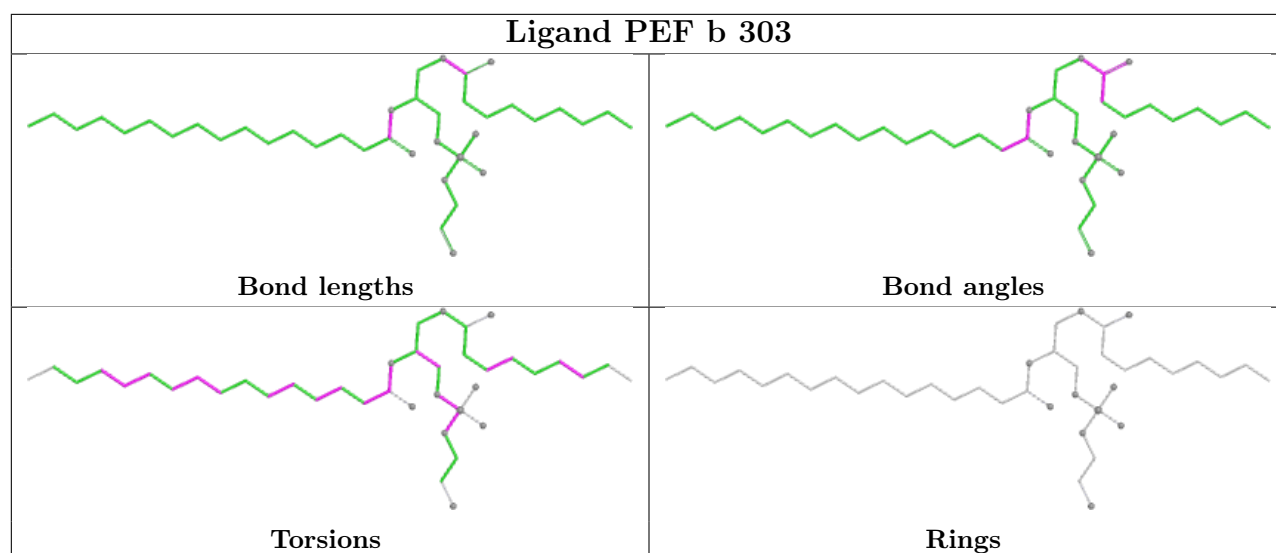


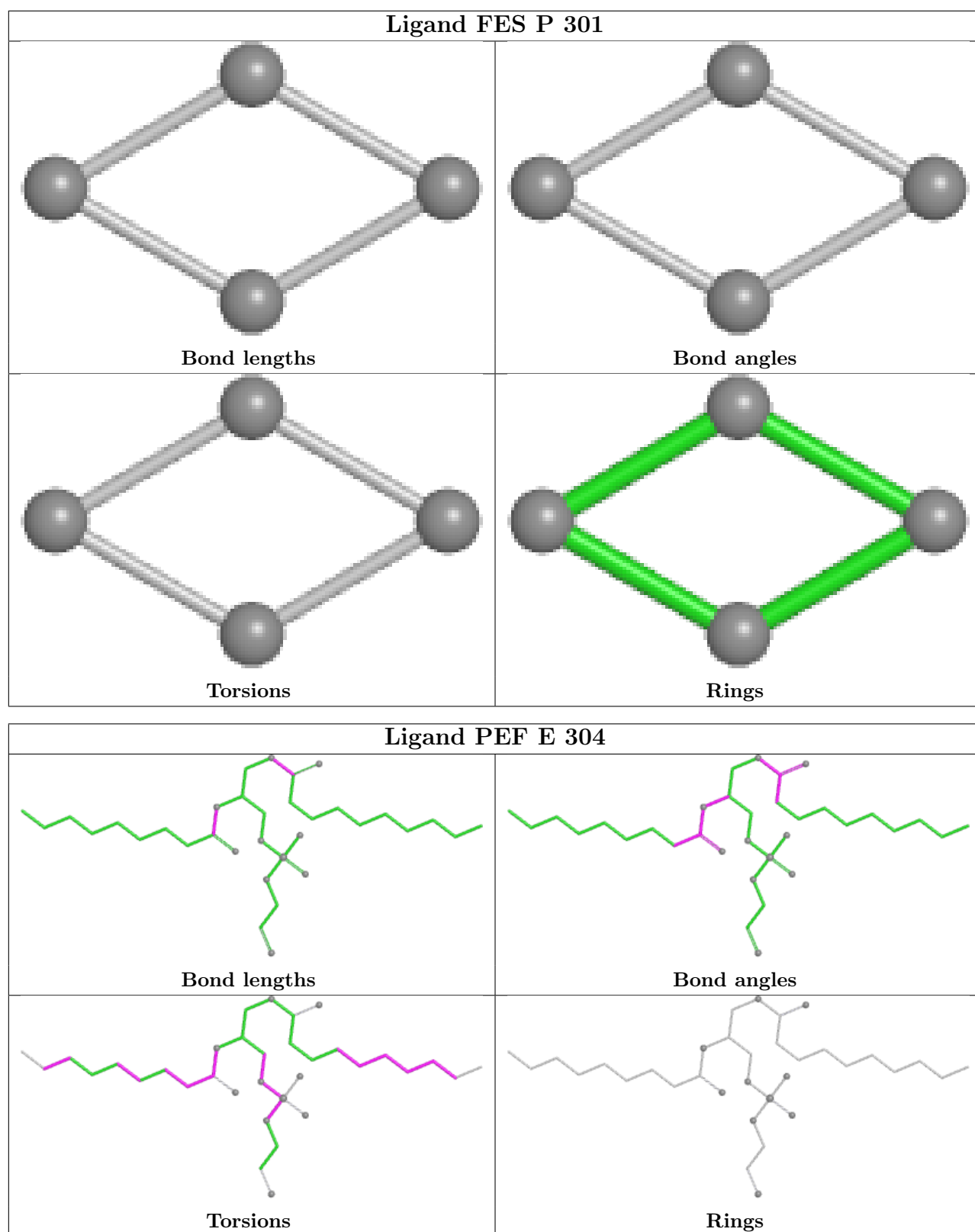


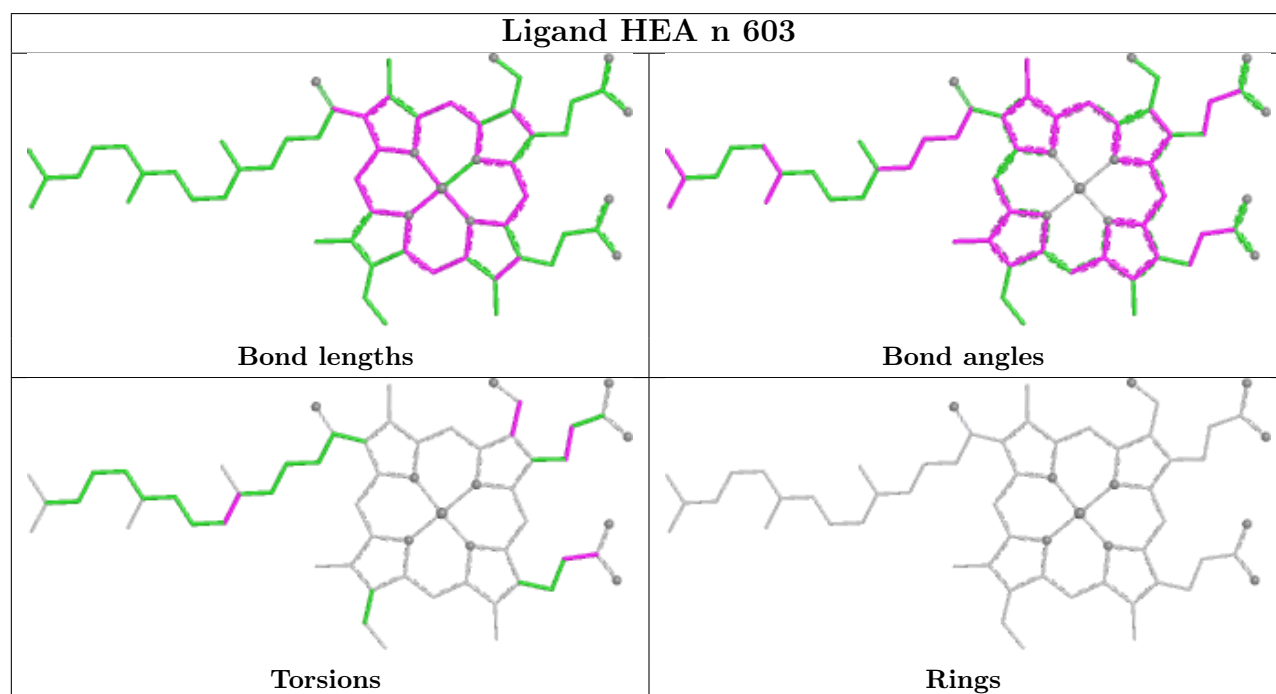
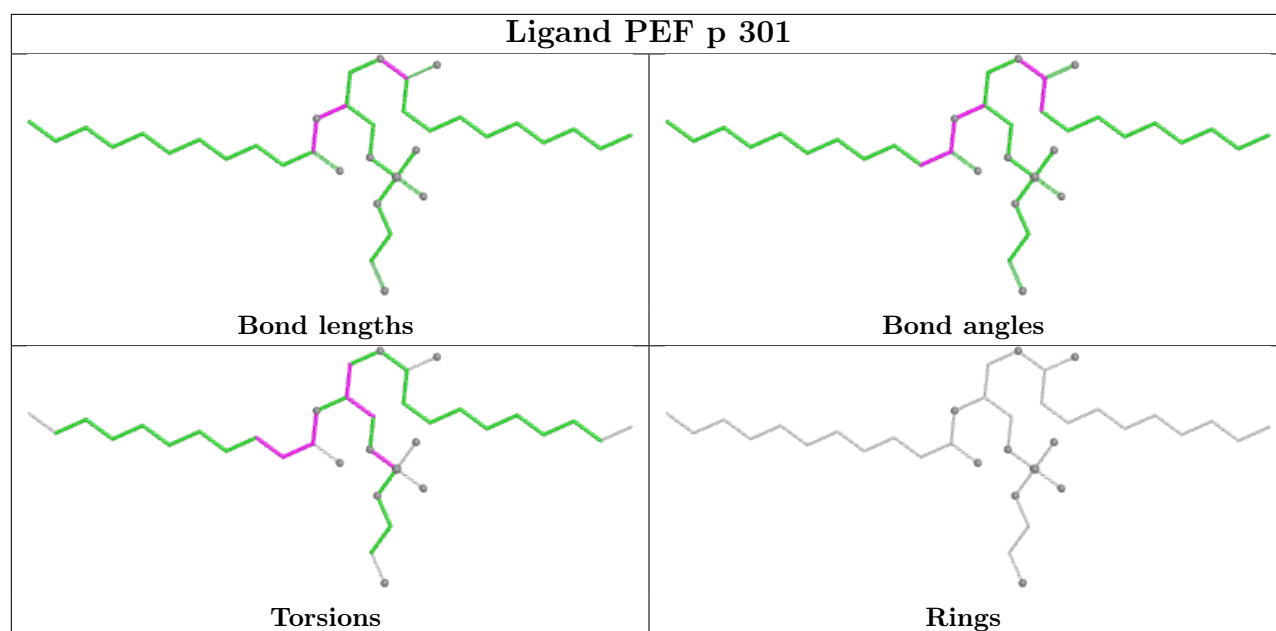


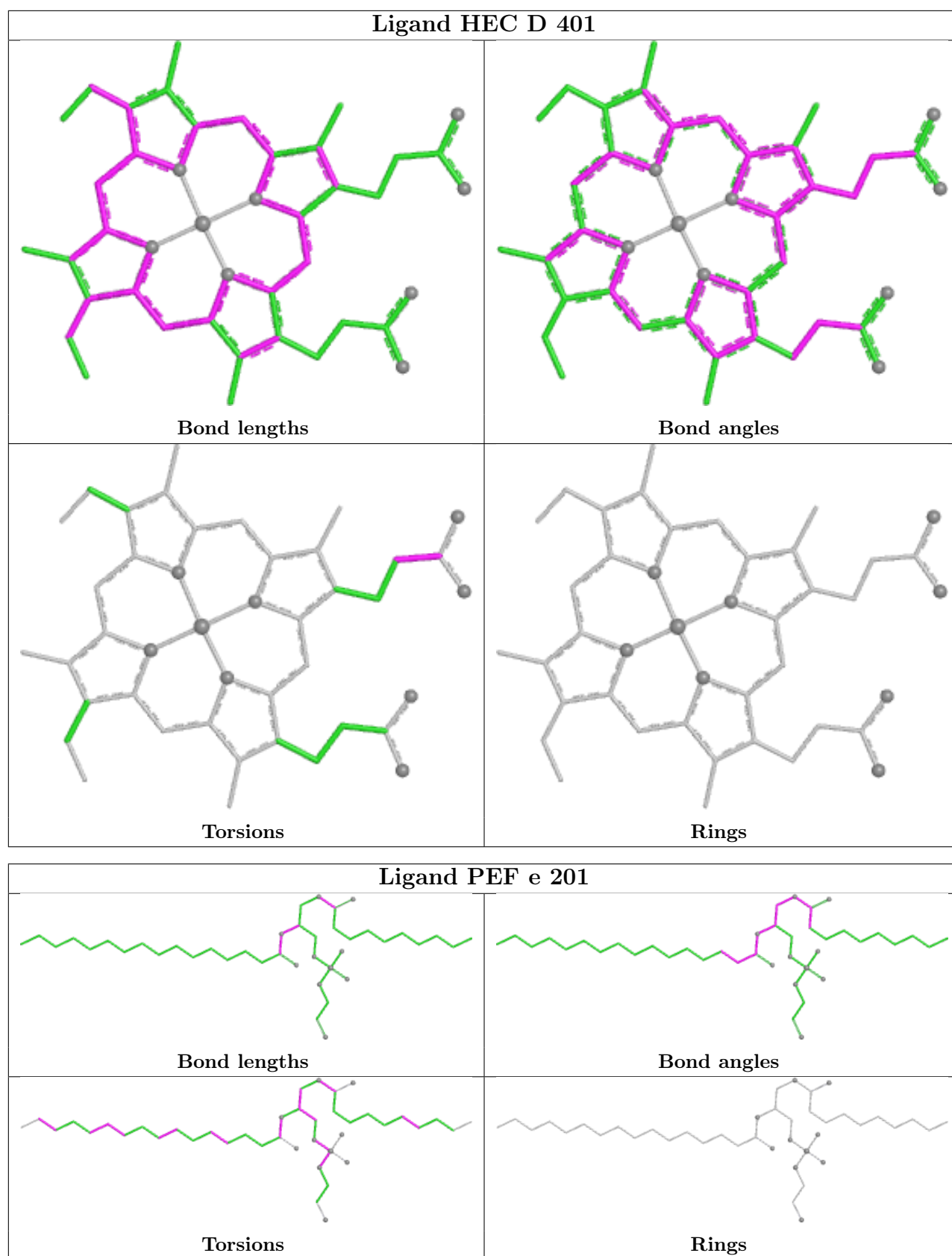


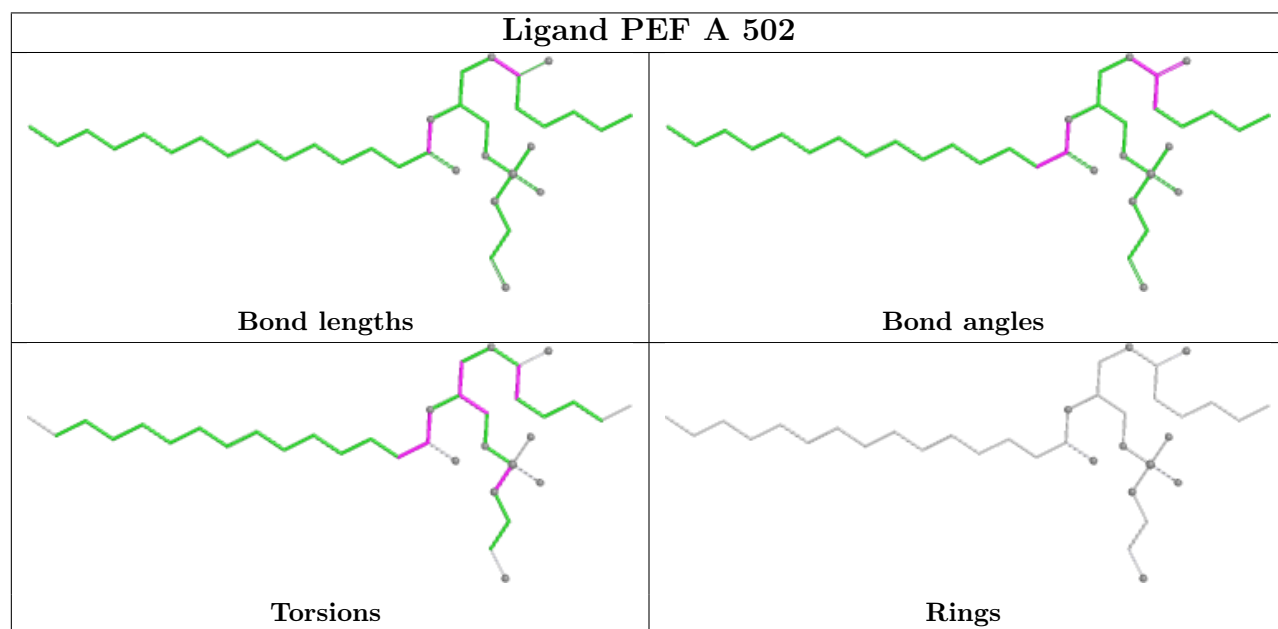
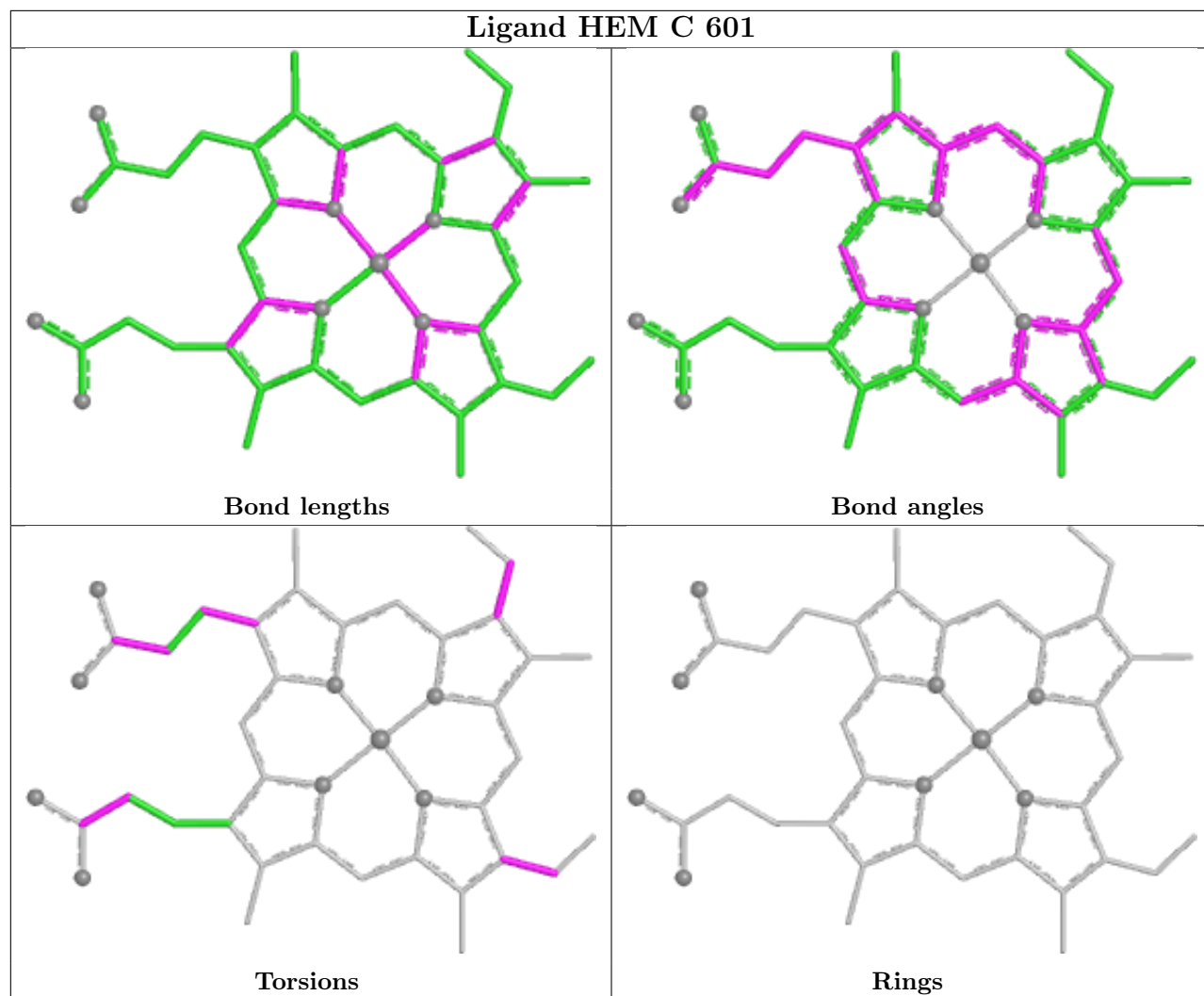


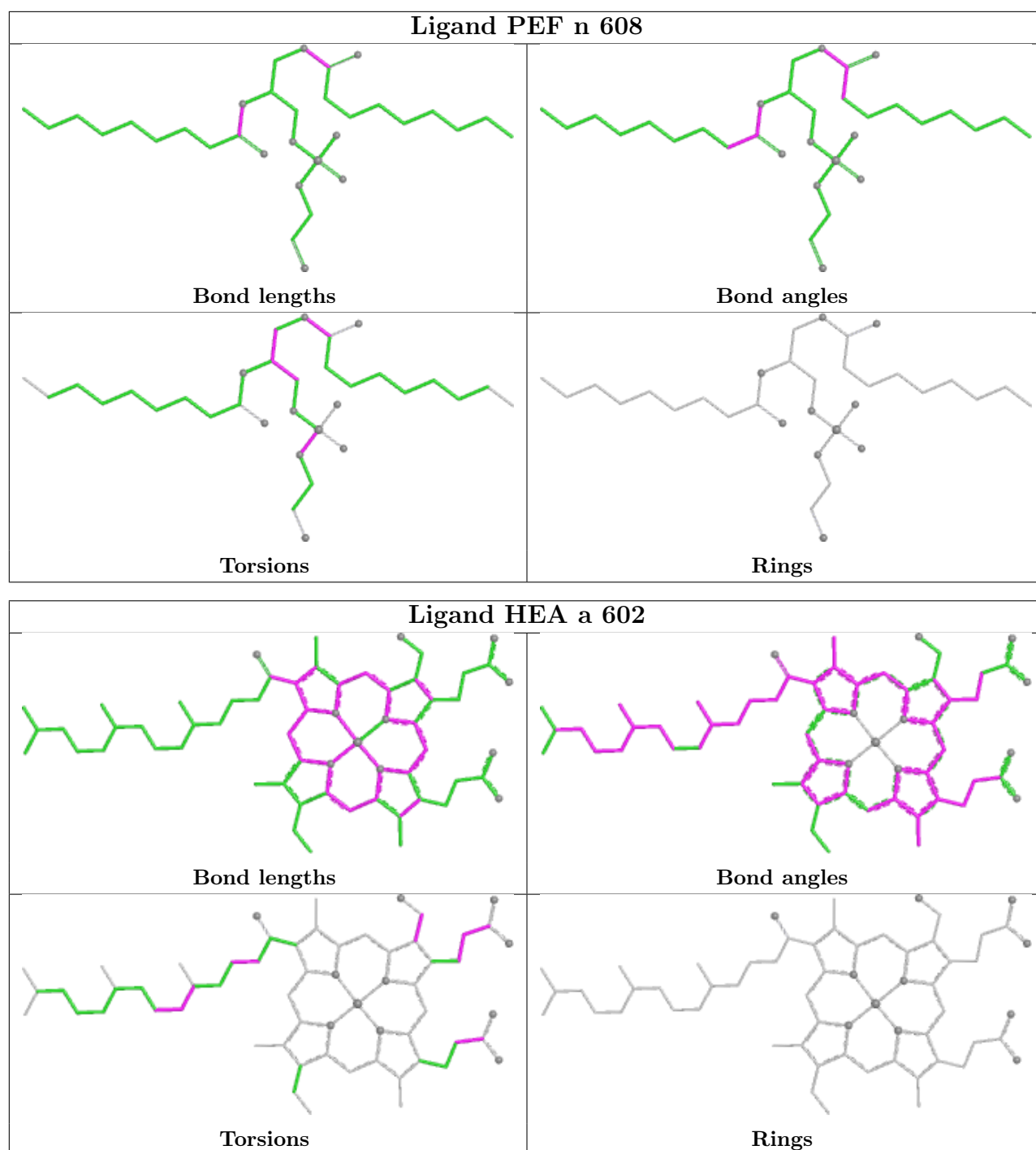


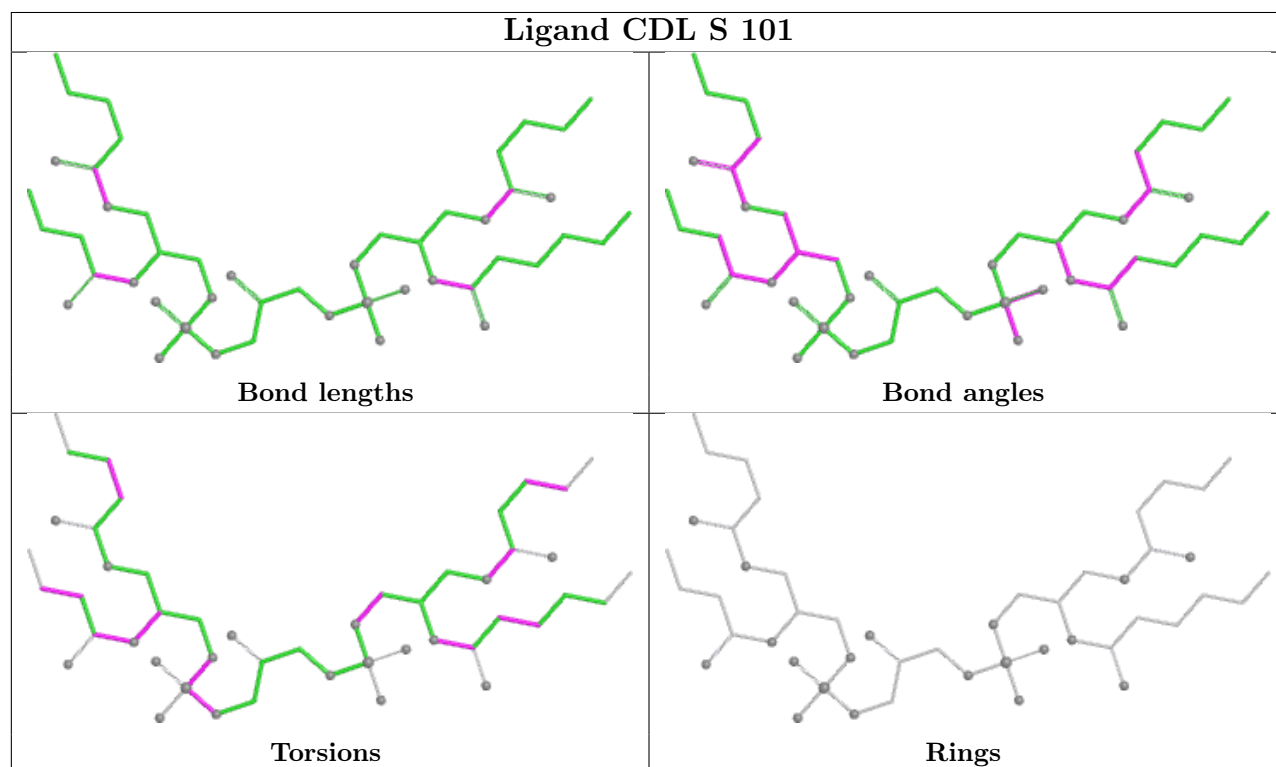
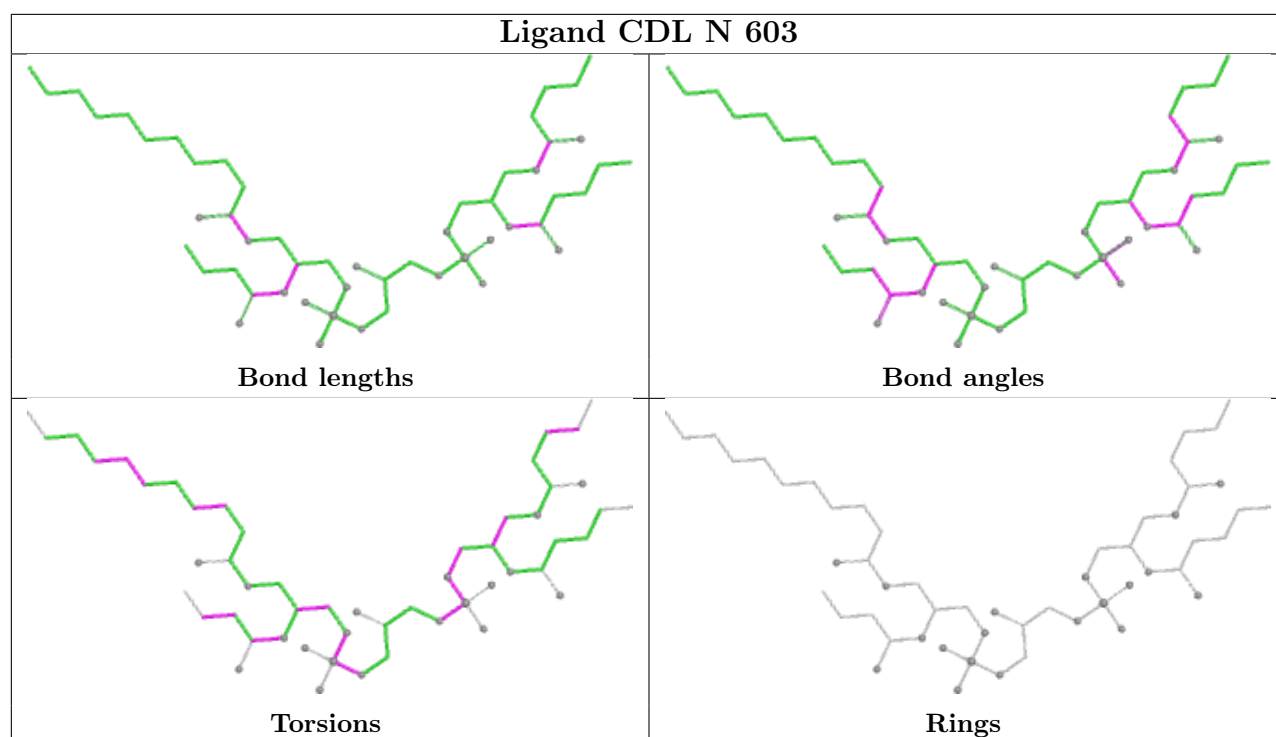


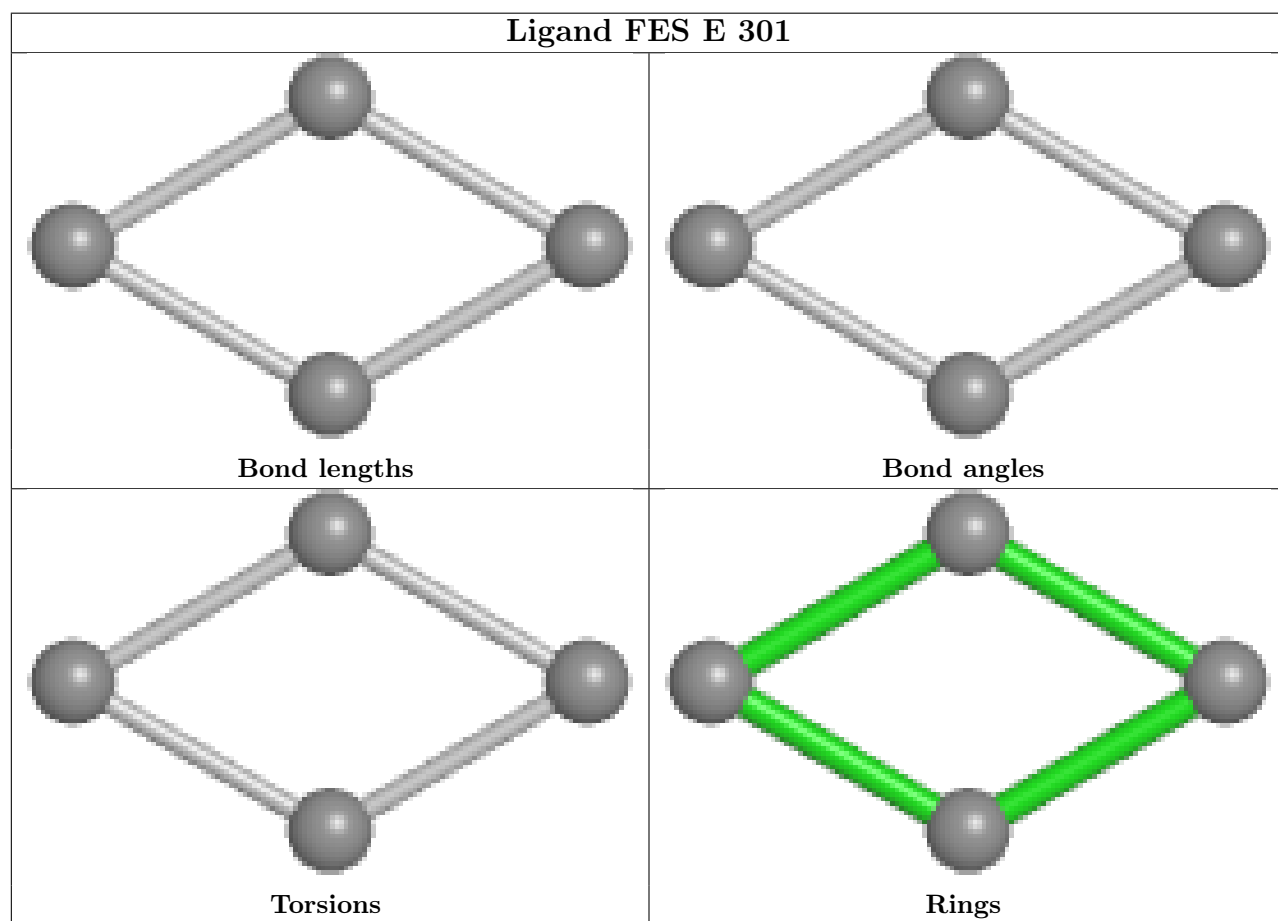
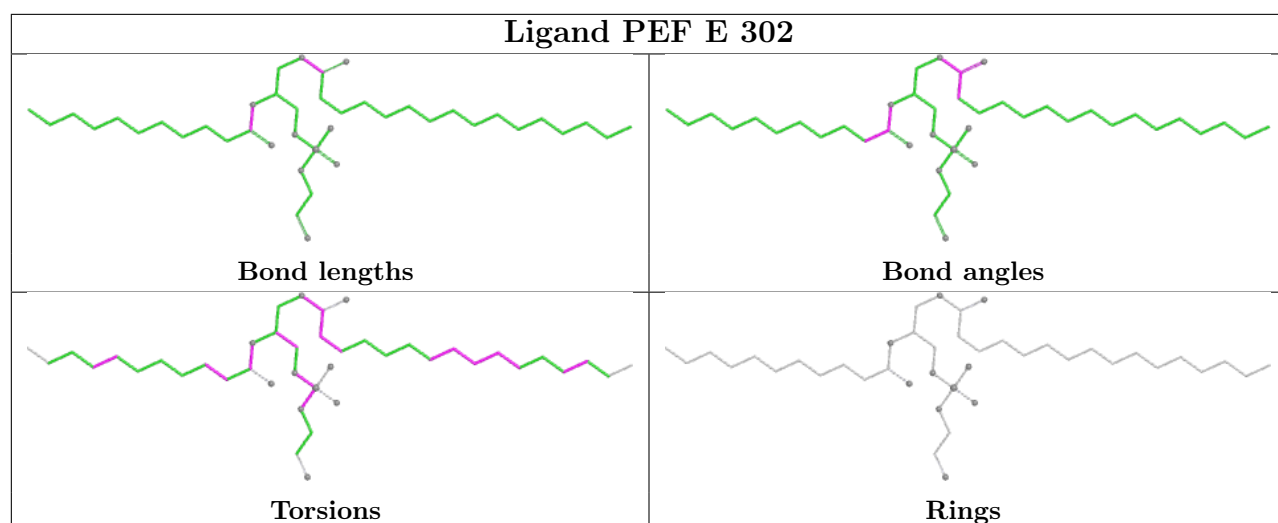


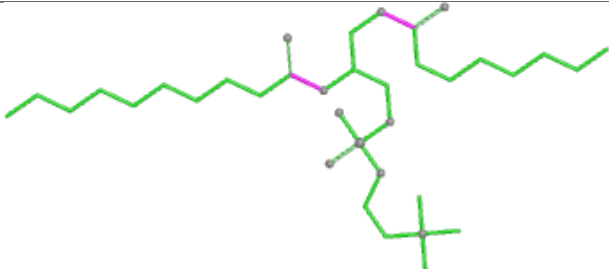
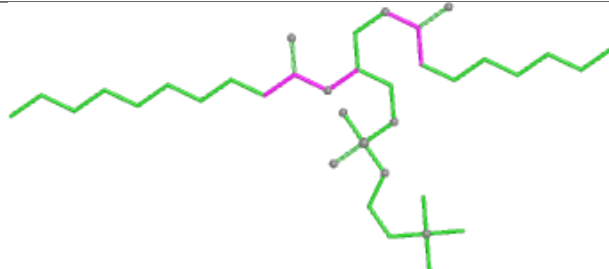
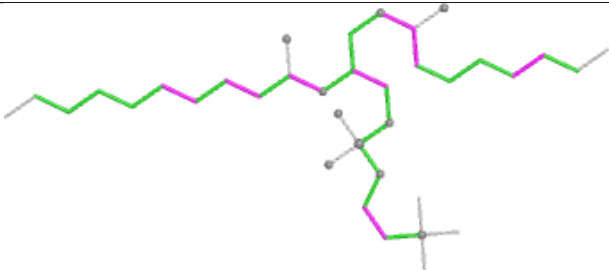
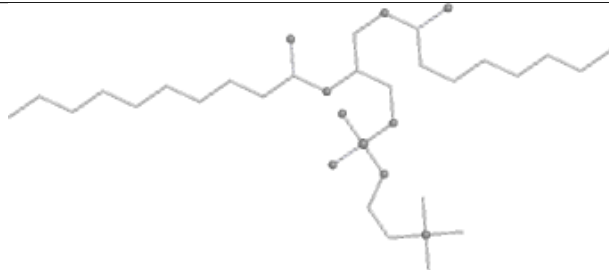
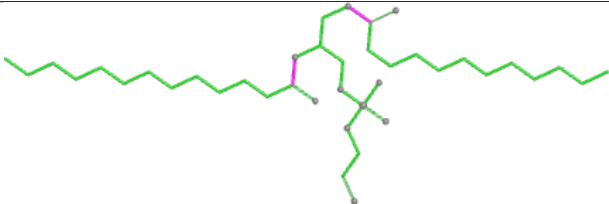
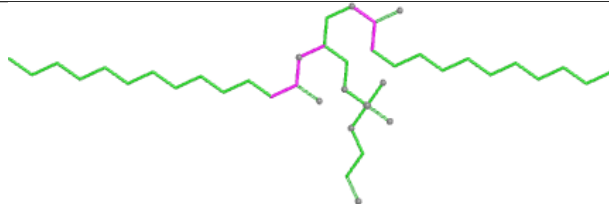
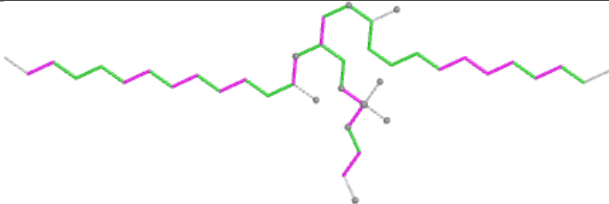
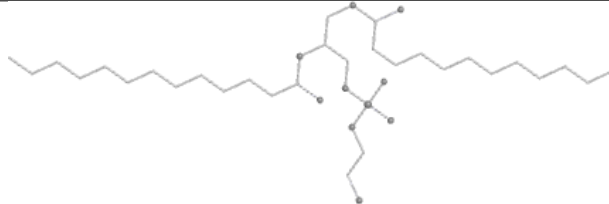


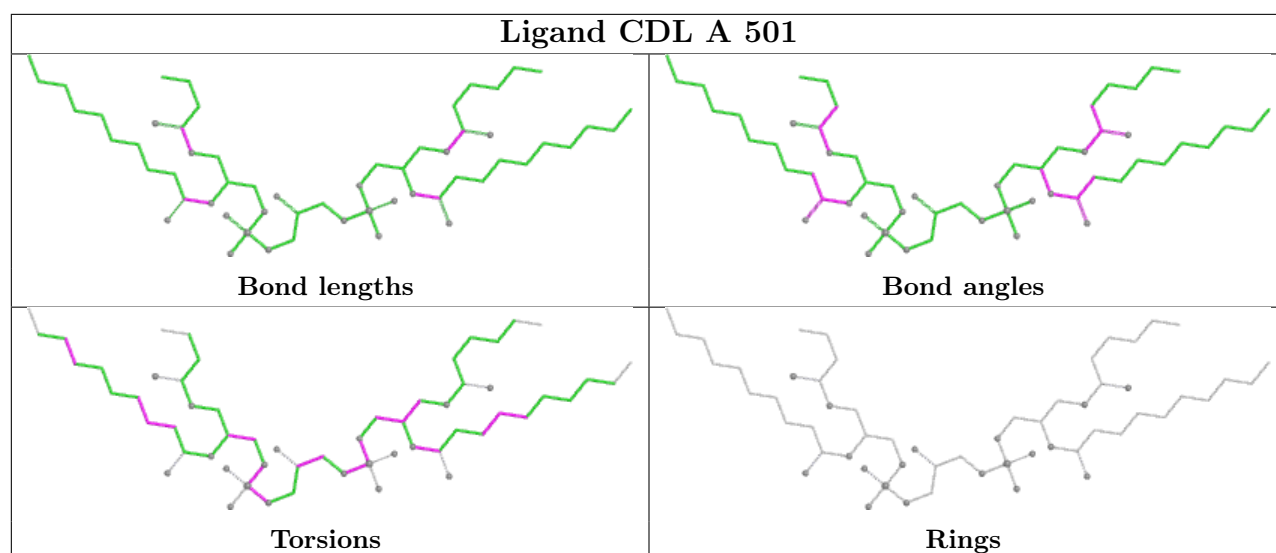








Ligand PCF r 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEF N 605	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

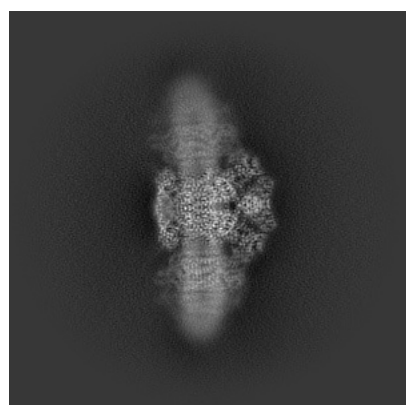
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10340. These allow visual inspection of the internal detail of the map and identification of artifacts.

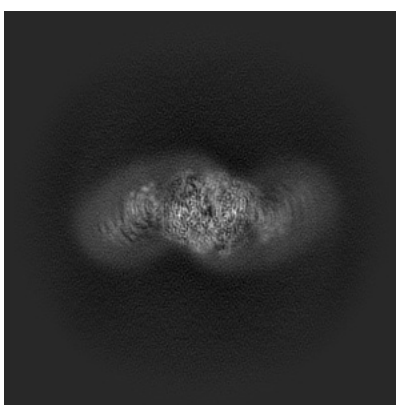
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

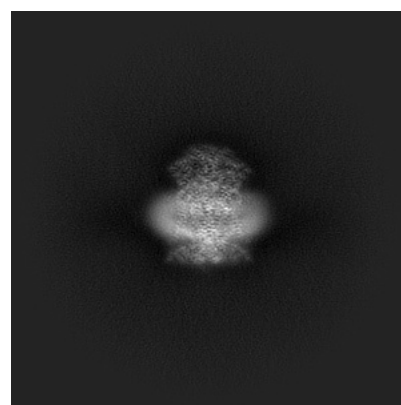
6.1.1 Primary map



X



Y

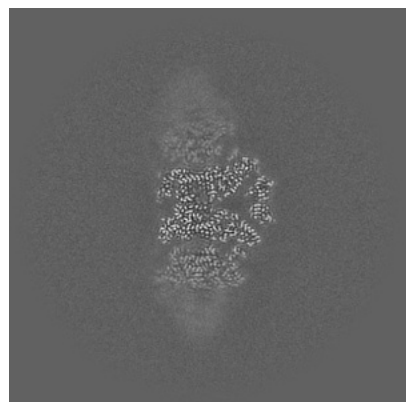


Z

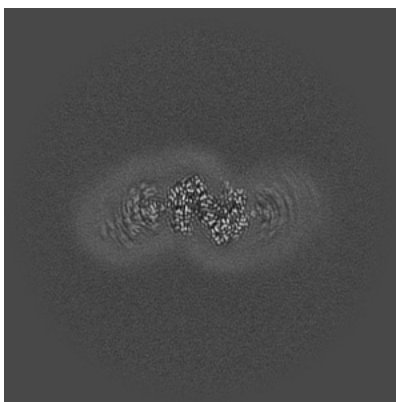
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

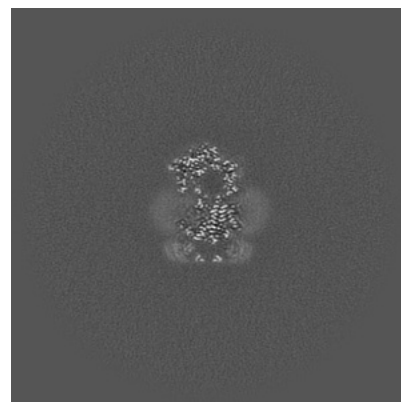
6.2.1 Primary map



X Index: 224



Y Index: 224

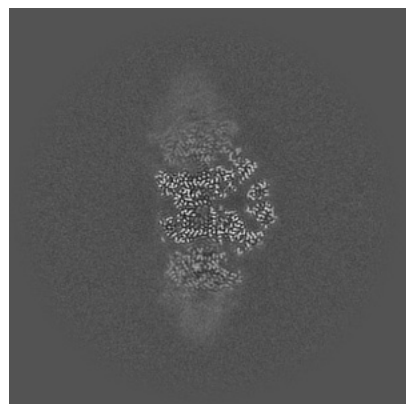


Z Index: 224

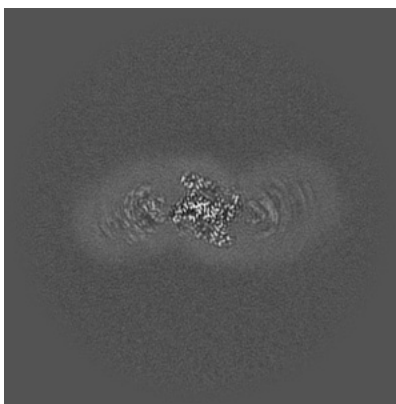
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

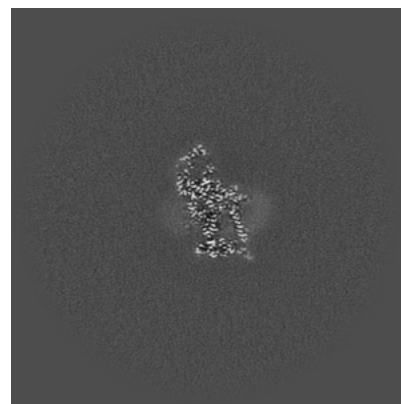
6.3.1 Primary map



X Index: 218



Y Index: 202

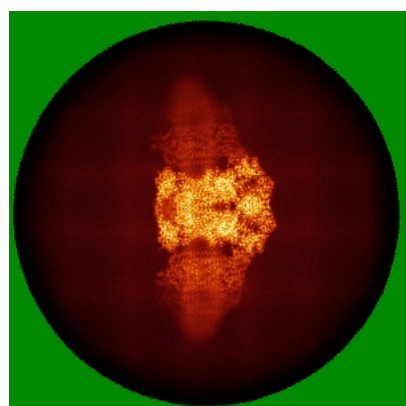


Z Index: 200

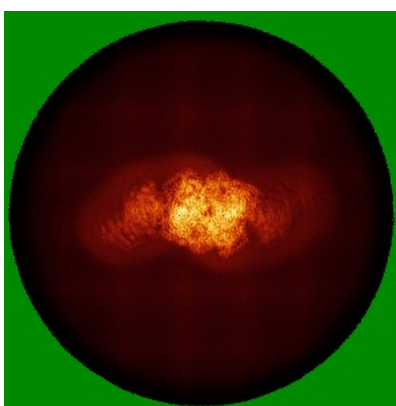
The images above show the largest variance slices of the map in three orthogonal directions.

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

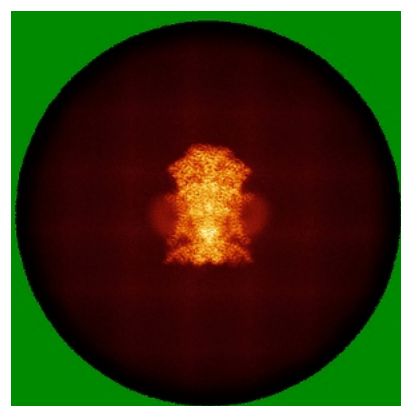
6.4.1 Primary map



X



Y

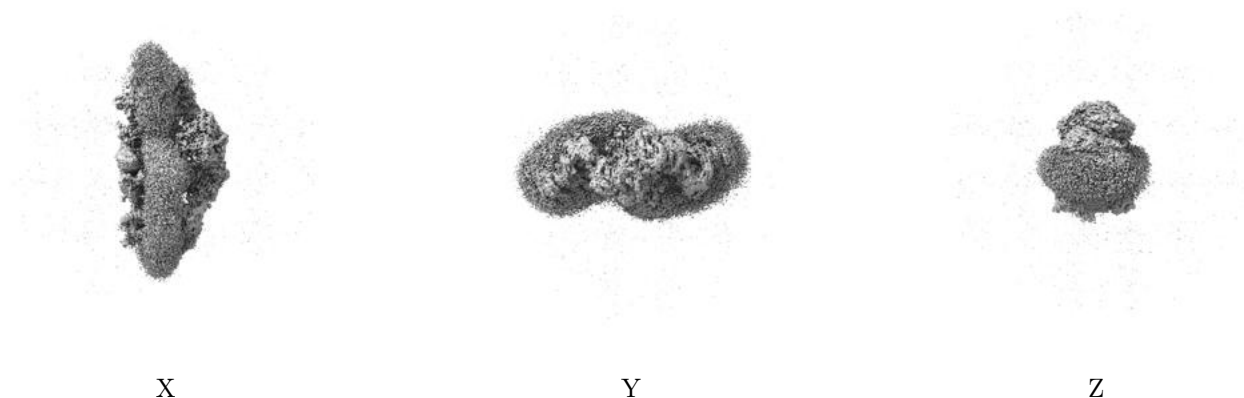


Z

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 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

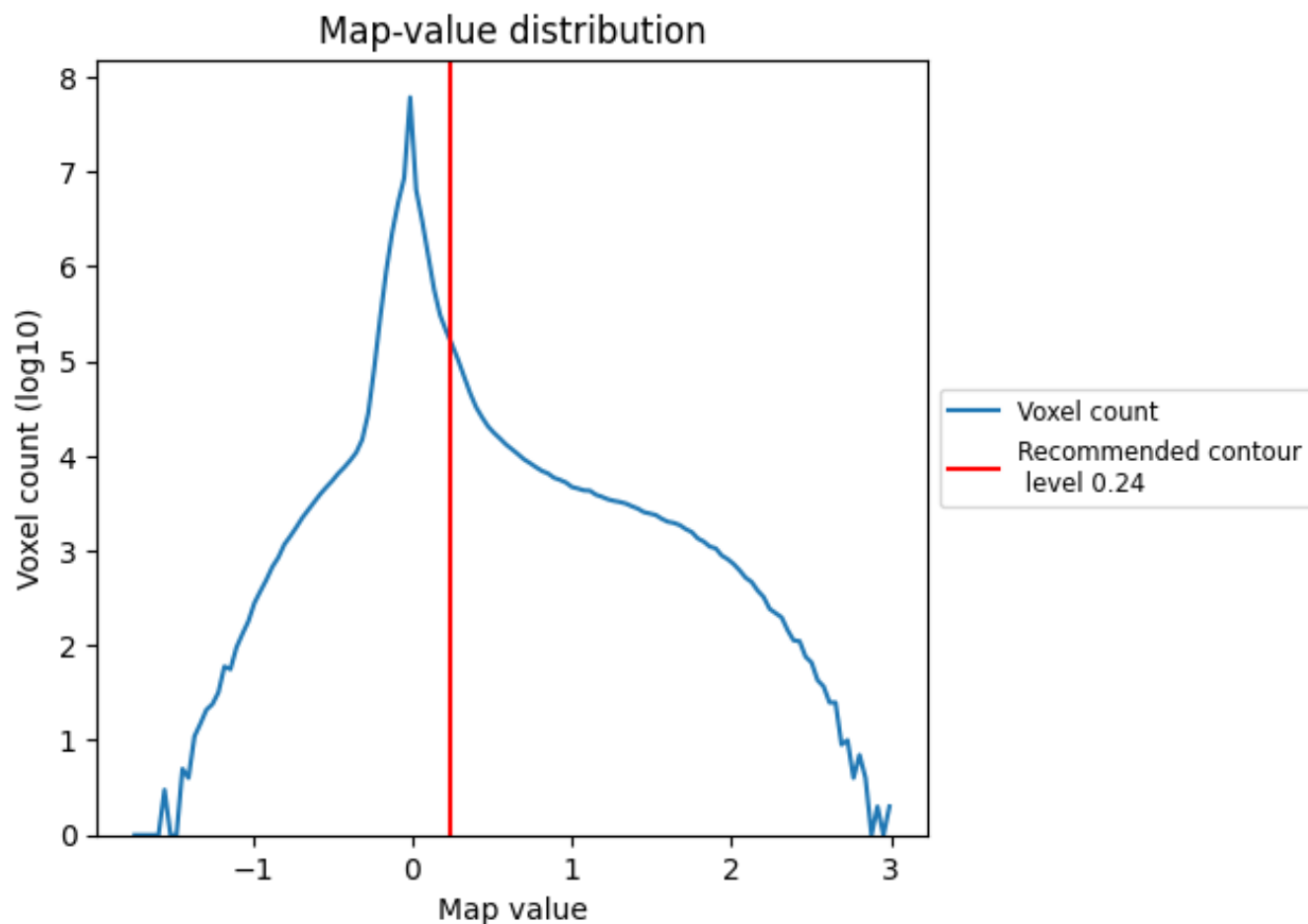
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

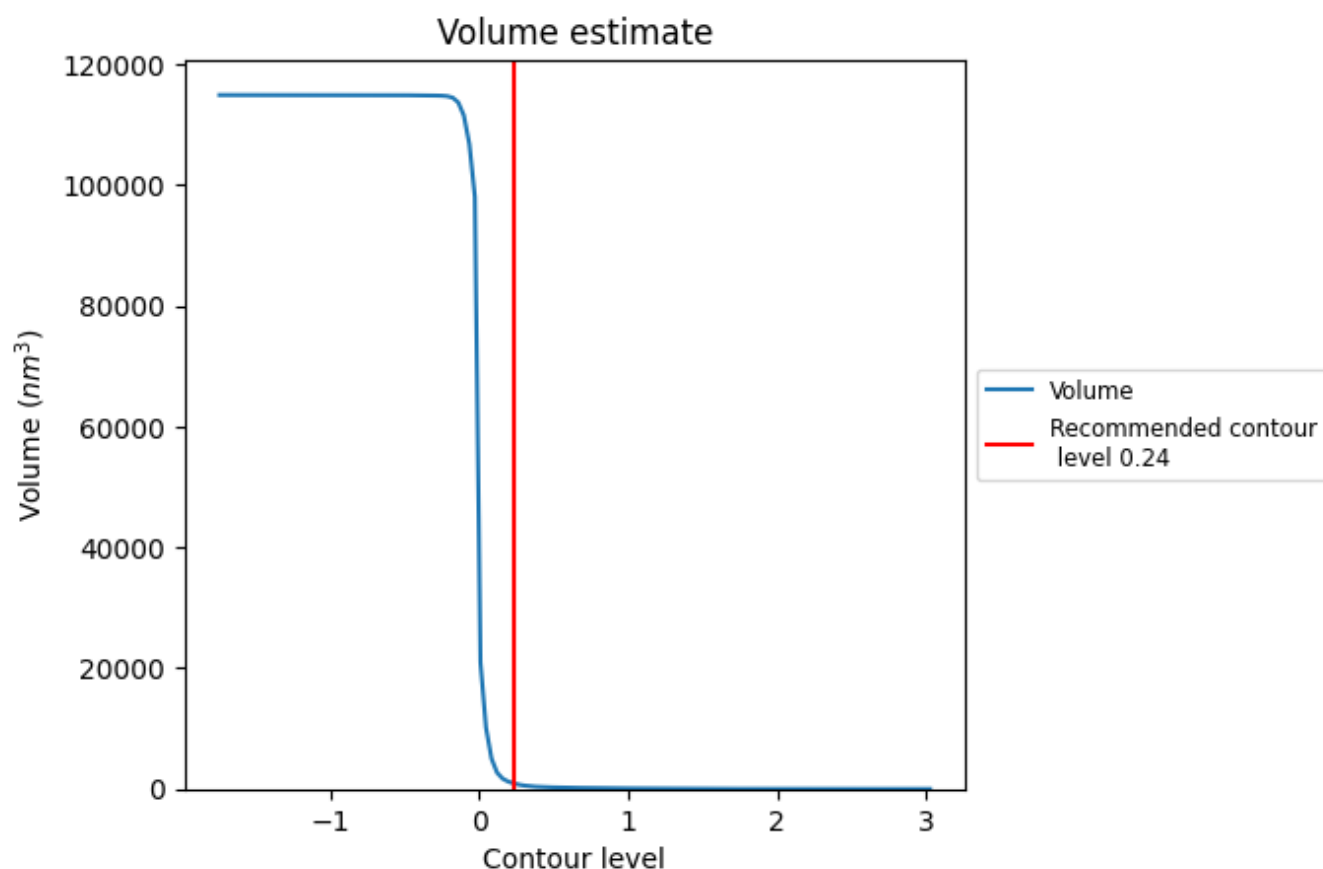
This section contains the results of statistical analysis of the map.

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.

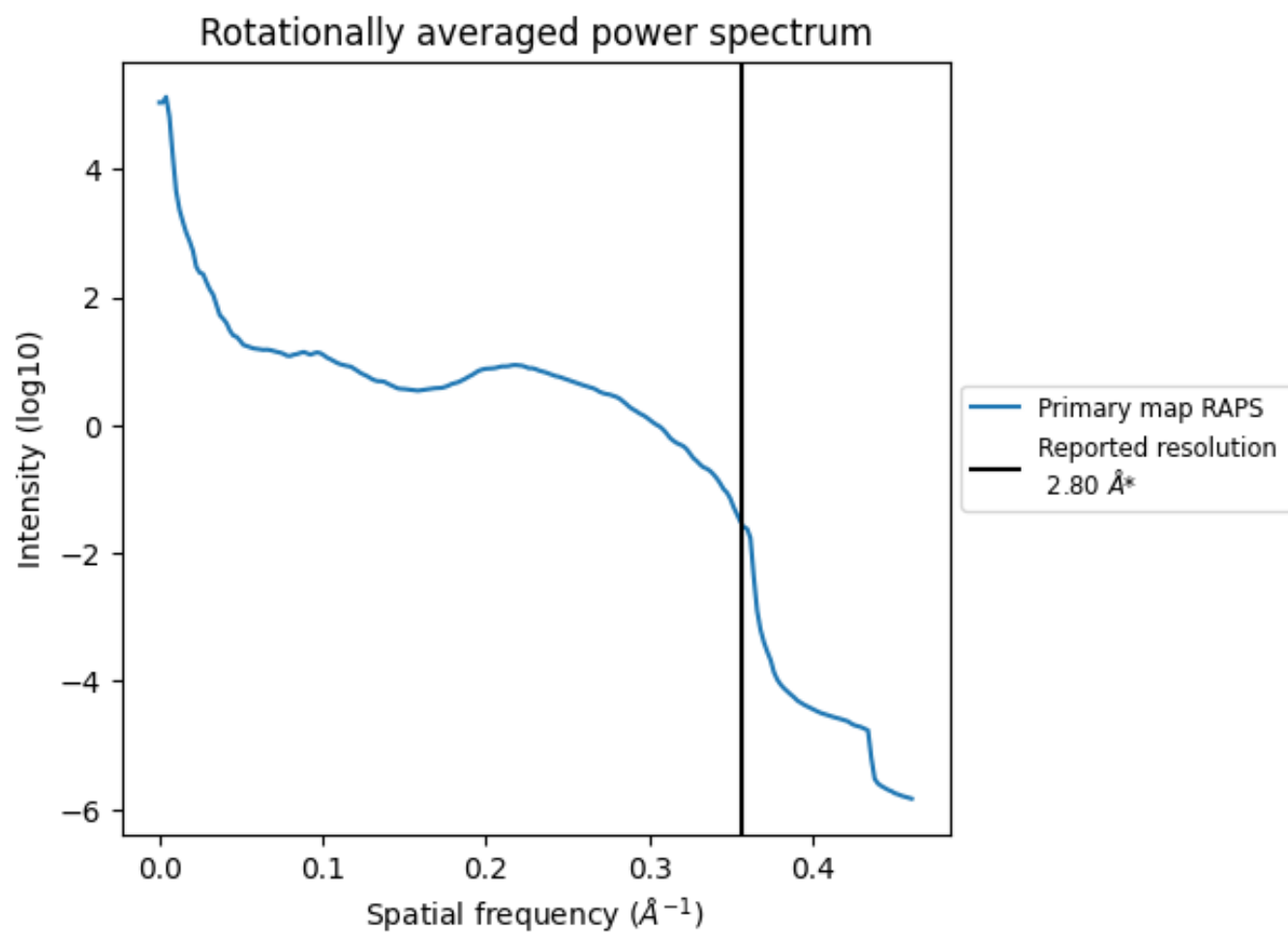
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 878 nm³; this corresponds to an approximate mass of 793 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 ⓘ

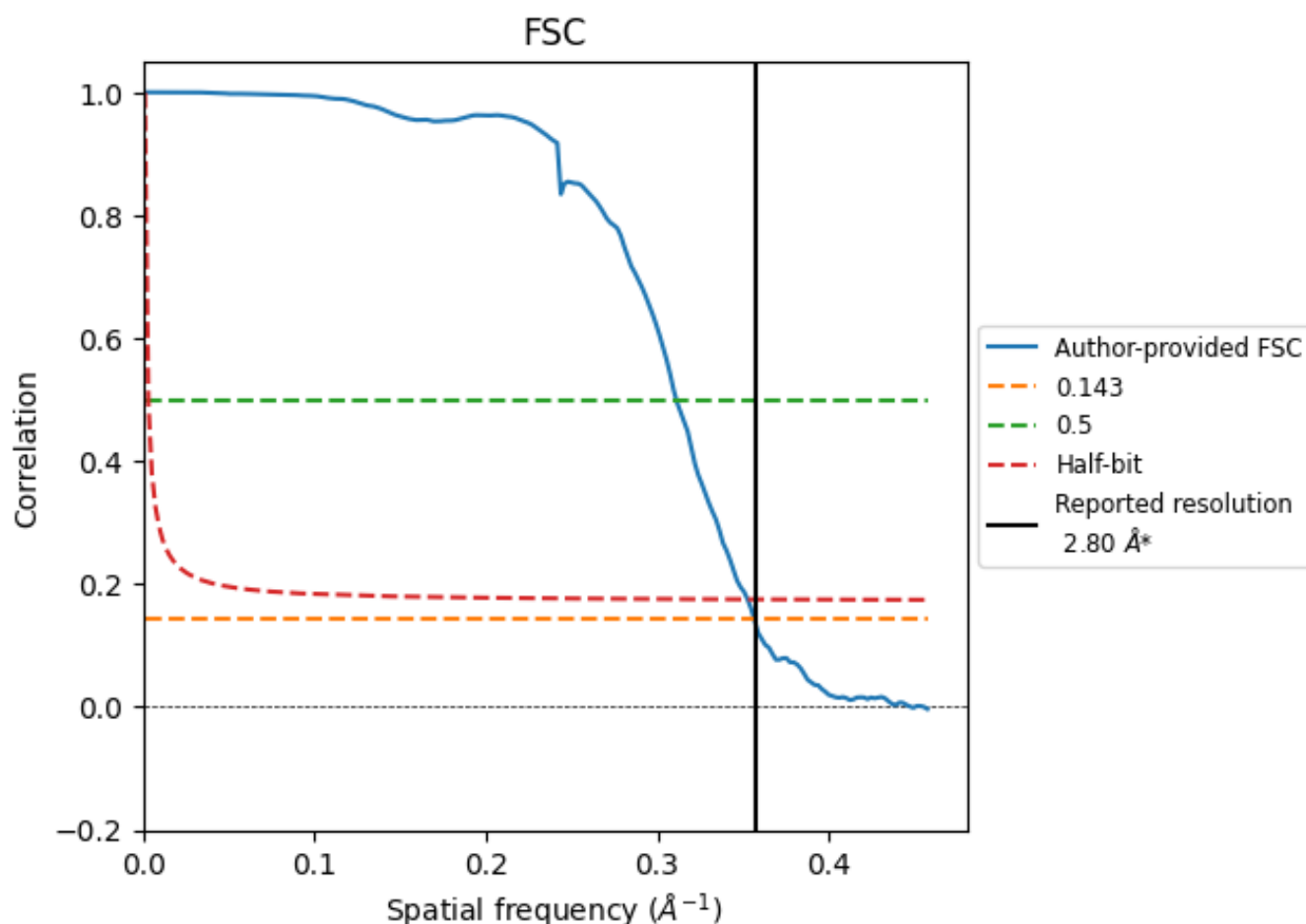


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

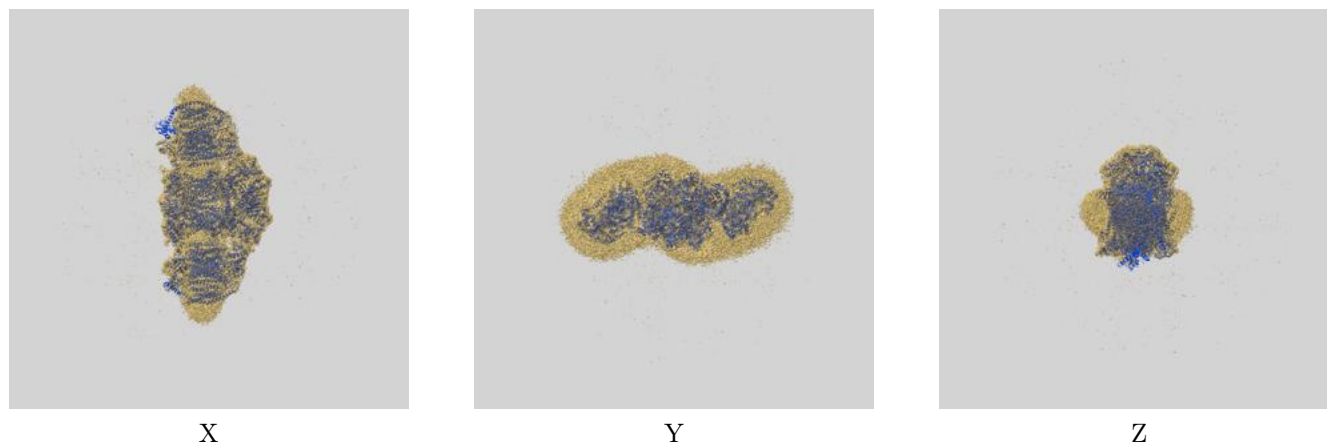
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.21	2.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

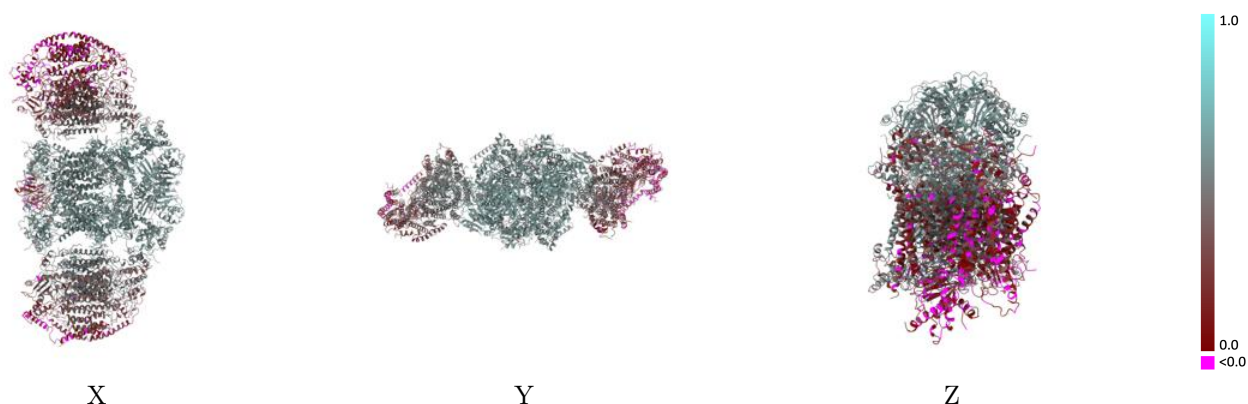
This section contains information regarding the fit between EMDB map EMD-10340 and PDB model 6T0B. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



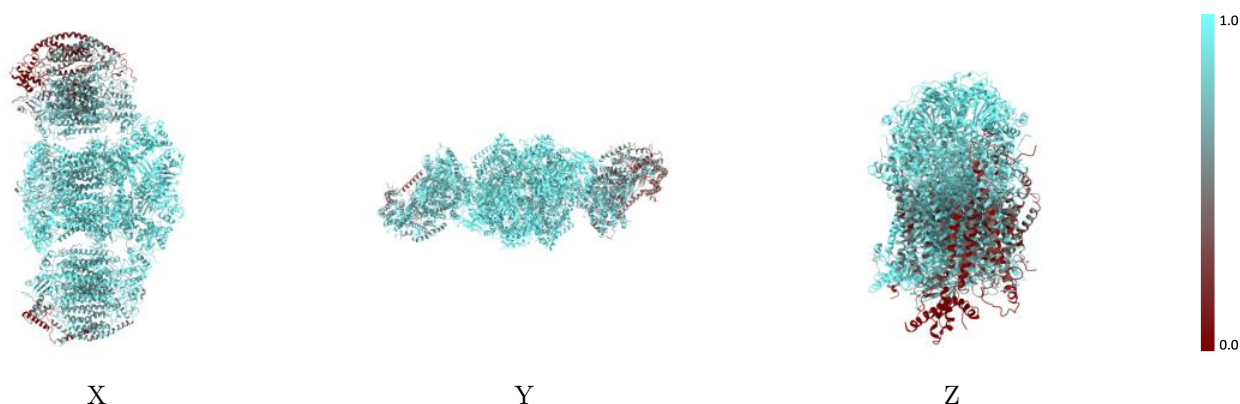
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



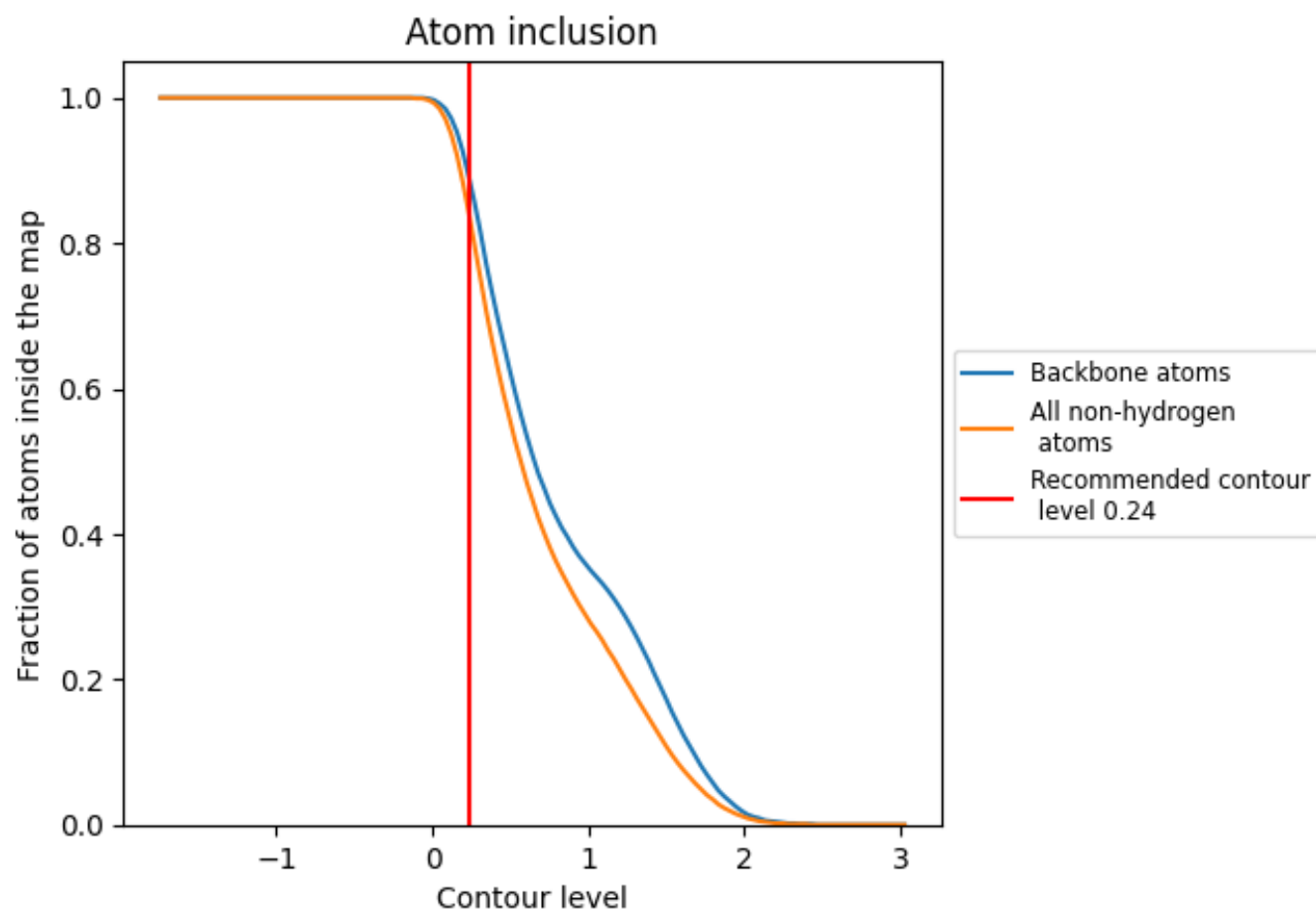
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.4360
A	 0.9740	 0.5720
B	 0.9830	 0.5720
C	 0.9750	 0.5820
D	 0.9800	 0.5780
E	 0.8540	 0.3440
F	 0.9420	 0.5070
G	 0.9690	 0.5670
H	 0.9710	 0.5690
I	 0.9770	 0.5700
J	 0.8420	 0.4960
L	 0.9780	 0.5700
M	 0.9780	 0.5630
N	 0.9800	 0.5850
O	 0.9790	 0.5750
P	 0.8660	 0.3400
Q	 0.9540	 0.5130
R	 0.9660	 0.5680
S	 0.9730	 0.5690
T	 0.9560	 0.5650
U	 0.8290	 0.4880
a	 0.9050	 0.4820
b	 0.8750	 0.4200
c	 0.8110	 0.3190
d	 0.8780	 0.3740
e	 0.9170	 0.5060
f	 0.9180	 0.4260
g	 0.7800	 0.2750
h	 0.8910	 0.4360
i	 0.8780	 0.3990
j	 0.4270	 0.2400
k	 0.5260	 0.1690
l	 0.8820	 0.4460
m	 0.3860	 0.0990
n	 0.7250	 0.3360



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Chain	Atom inclusion	Q-score
o	 0.6550	 0.2310
p	 0.4860	 0.1790
q	 0.5760	 0.2320
r	 0.8550	 0.4200
s	 0.8260	 0.3080
t	 0.4870	 0.1540
u	 0.6780	 0.2870
v	 0.6050	 0.2010
w	 0.0340	 0.0850
x	 0.1430	 0.0690
y	 0.7540	 0.3060
z	 0.1420	 0.0450