



## wwPDB EM Validation Summary Report ⓘ

Dec 26, 2024 – 09:54 AM EST

PDB ID : 6HU9  
EMDB ID : EMD-0262  
Title : III2-IV2 mitochondrial respiratory supercomplex from *S. cerevisiae*  
Authors : Hartley, A.M.; Pinotsis, N.; Marechal, A.  
Deposited on : 2018-10-05  
Resolution : 3.35 Å (reported)  
Based on initial models : 1V54, 1KYO

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

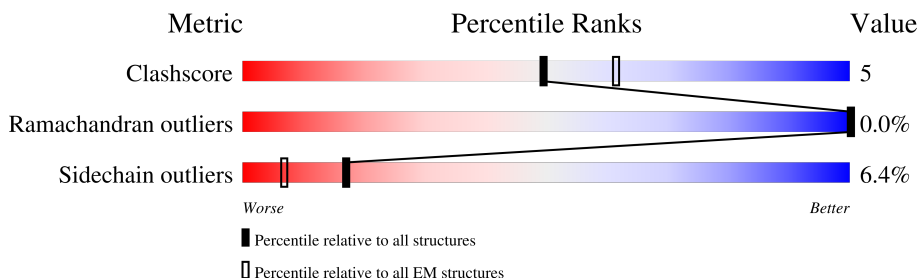
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	83% 16% .
1	L	431	84% 15% .
2	B	352	85% 14%
2	M	352	85% 14% .
3	C	385	79% 19% .
3	N	385	85% 13% .
4	D	248	85% 14% .
4	O	248	87% 12% .

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Mol	Chain	Length	Quality of chain
5	E	185	
5	P	185	
6	F	147	
6	Q	147	
7	G	127	
7	R	127	
8	H	93	
8	S	93	
9	I	66	
9	T	66	
10	J	77	
10	U	77	
11	a	534	
11	m	534	
12	b	236	
12	n	236	
13	c	269	
13	o	269	
14	d	130	
14	p	130	
15	e	133	
15	q	133	
16	f	108	
16	r	108	
17	g	59	

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Mol	Chain	Length	Quality of chain
17	s	59	
18	h	47	
18	t	47	
19	i	55	
19	u	55	
20	j	82	
20	v	82	
21	k	131	
21	w	131	
22	l	66	
22	x	66	

## 2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 63031 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	m	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	n	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	o	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	121	Total	C	N	O	S	0	0
			913	576	151	181	5		
14	p	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		
15	q	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		

- 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	r	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	s	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	47	Total	C	N	O	S	0	0
			383	261	62	59	1		
18	t	47	Total	C	N	O	S	0	0
			383	261	62	59	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	u	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	77	Total	C	N	O	S	0	0
			642	410	109	118	5		
20	v	77	Total	C	N	O	S	0	0
			642	410	109	118	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	w	113	Total	C	N	O	S	0	0
			928	605	160	160	3		

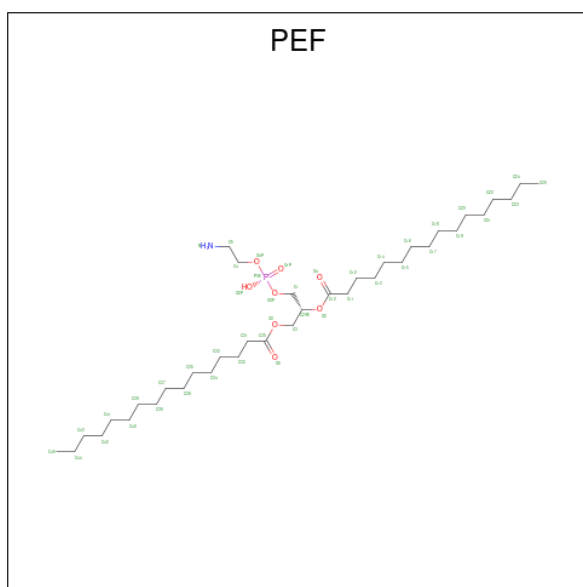
There are 22 discrepancies between the modelled and reference sequences:

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
w	130	GLY	-	expression tag	UNP P32799
w	131	ALA	-	expression tag	UNP P32799
w	132	ARG	-	expression tag	UNP P32799
w	133	GLY	-	expression tag	UNP P32799
w	134	SER	-	expression tag	UNP P32799
w	135	HIS	-	expression tag	UNP P32799
w	136	HIS	-	expression tag	UNP P32799
w	137	HIS	-	expression tag	UNP P32799
w	138	HIS	-	expression tag	UNP P32799
w	139	HIS	-	expression tag	UNP P32799
w	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	x	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 23 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula:  $C_{37}H_{74}NO_8P$ ).



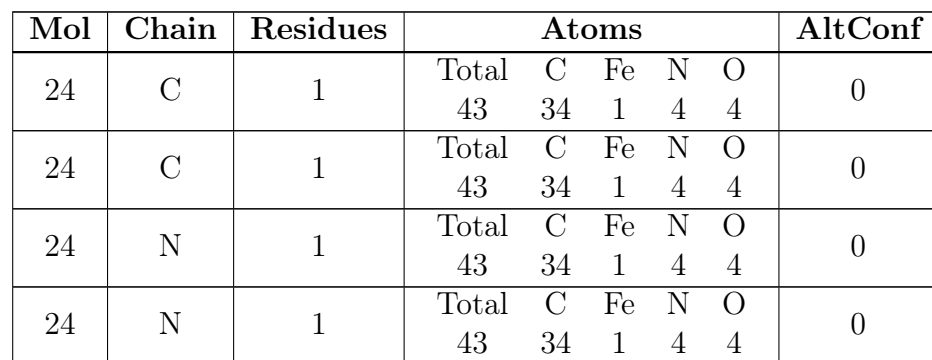
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
23	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
23	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
23	E	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
23	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
23	N	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	N	1	Total	C	N	O	P	0
			31	21	1	8	1	
23	O	1	Total	C	N	O	P	0
			43	33	1	8	1	
23	P	1	Total	C	N	O	P	0
			29	19	1	8	1	
23	S	1	Total	C	N	O	P	0
			36	26	1	8	1	
23	a	1	Total	C	N	O	P	0
			47	37	1	8	1	
23	a	1	Total	C	N	O	P	0
			33	23	1	8	1	

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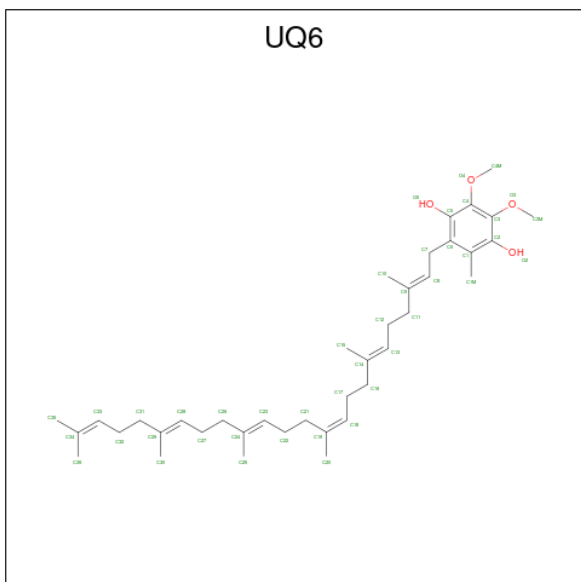
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Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 33	C 23	N 1	O 8	P 1	0
23	b	1	Total 40	C 30	N 1	O 8	P 1	0
23	c	1	Total 36	C 26	N 1	O 8	P 1	0
23	c	1	Total 41	C 31	N 1	O 8	P 1	0
23	e	1	Total 47	C 37	N 1	O 8	P 1	0
23	h	1	Total 47	C 37	N 1	O 8	P 1	0
23	m	1	Total 47	C 37	N 1	O 8	P 1	0
23	m	1	Total 33	C 23	N 1	O 8	P 1	0
23	n	1	Total 40	C 30	N 1	O 8	P 1	0
23	n	1	Total 33	C 23	N 1	O 8	P 1	0
23	o	1	Total 36	C 26	N 1	O 8	P 1	0
23	o	1	Total 41	C 31	N 1	O 8	P 1	0
23	q	1	Total 47	C 37	N 1	O 8	P 1	0
23	t	1	Total 47	C 37	N 1	O 8	P 1	0

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

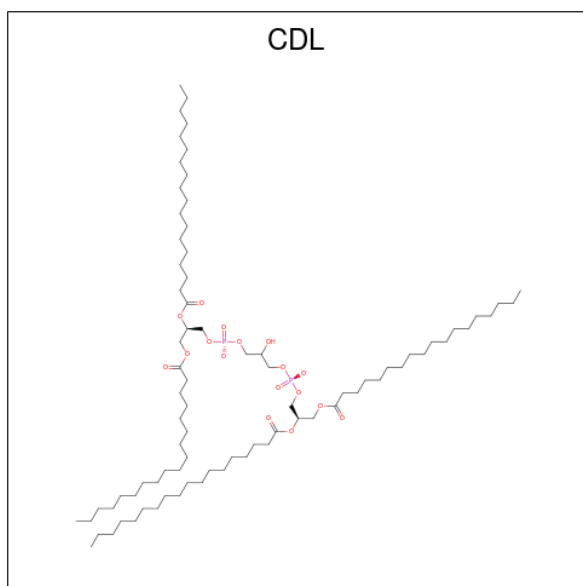


- Molecule 25 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: C<sub>39</sub>H<sub>60</sub>O<sub>4</sub>).



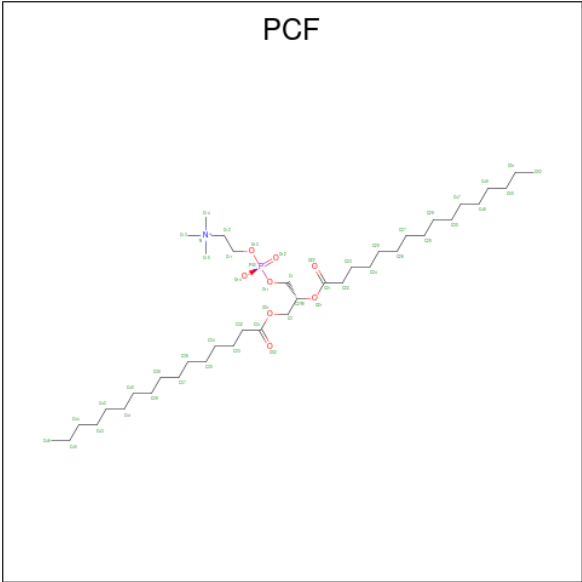
Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total	C	O	1
			86	78	8	

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



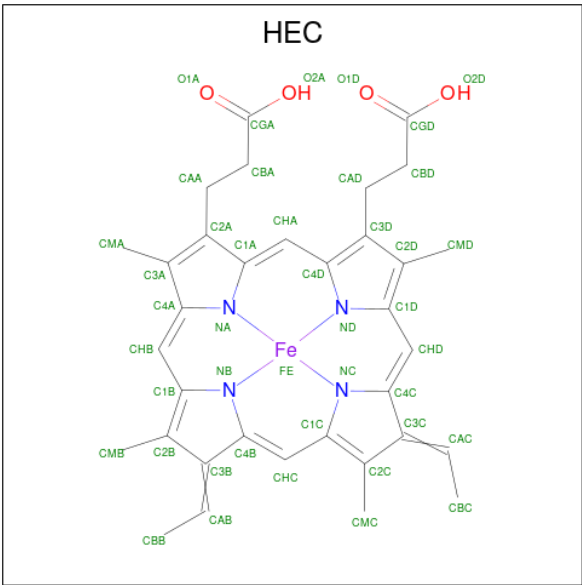
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			58	39	17	2	
26	E	1	Total	C	O	P	0
			53	34	17	2	
26	H	1	Total	C	O	P	0
			66	47	17	2	
26	H	1	Total	C	O	P	0
			71	52	17	2	
26	L	1	Total	C	O	P	0
			55	36	17	2	
26	O	1	Total	C	O	P	0
			67	48	17	2	
26	P	1	Total	C	O	P	0
			48	29	17	2	
26	S	1	Total	C	O	P	0
			53	34	17	2	

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



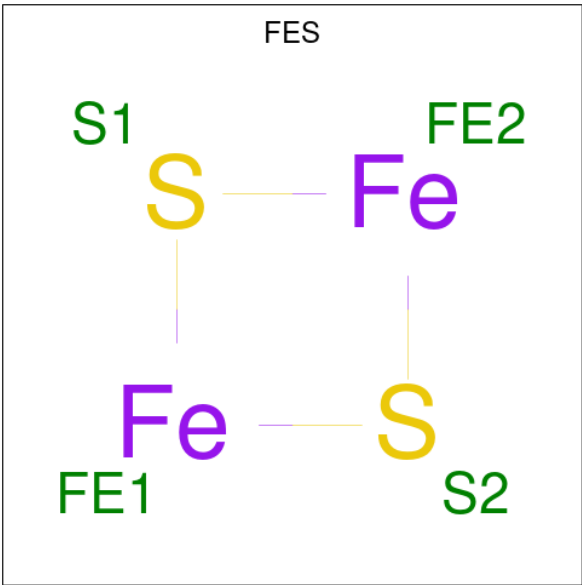
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	I	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	T	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	e	1	Total	C	N	O	P	0
			36	26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

- Molecule 28 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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 (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

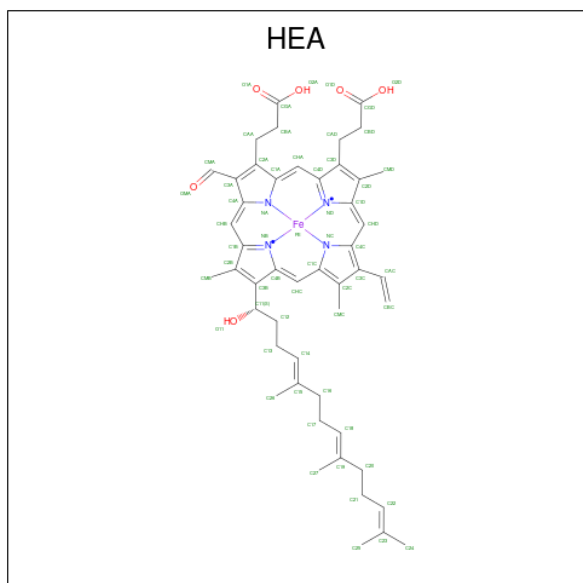


Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 31 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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	m	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	m	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

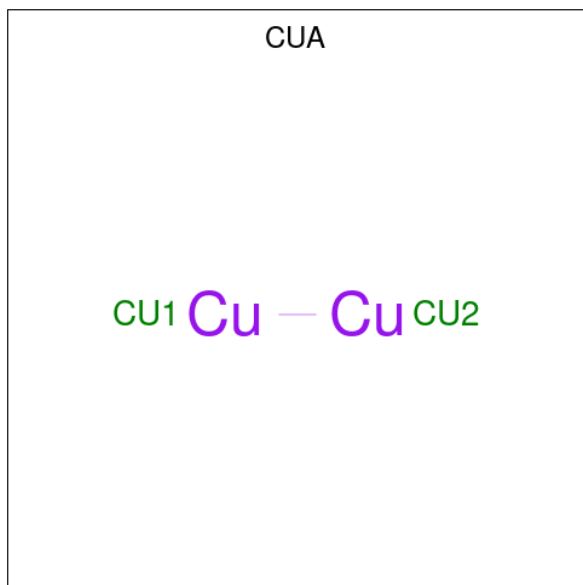
Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Ca	0
			1	1	
32	m	1	Total	Ca	0
			1	1	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



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

- Molecule 34 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		AltConf
34	b	1	Total 1	Cu 1	0
34	b	1	Total 1	Cu 1	0
34	n	1	Total 1	Cu 1	0
34	n	1	Total 1	Cu 1	0

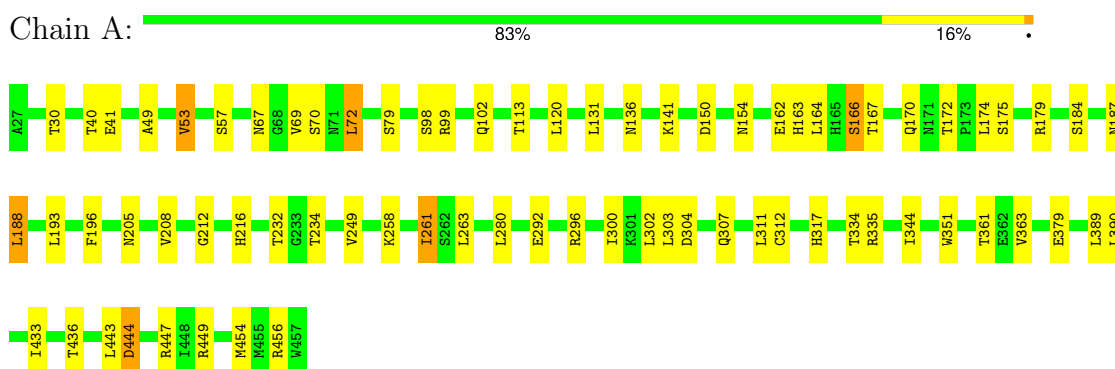
- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

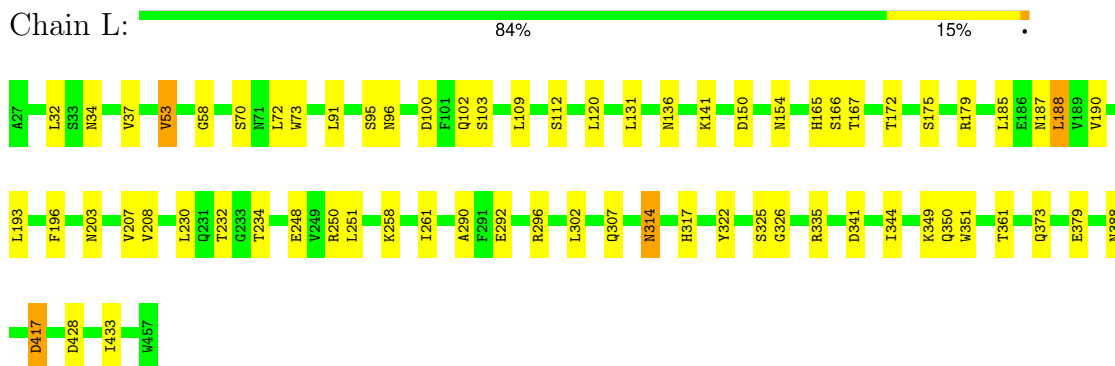
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

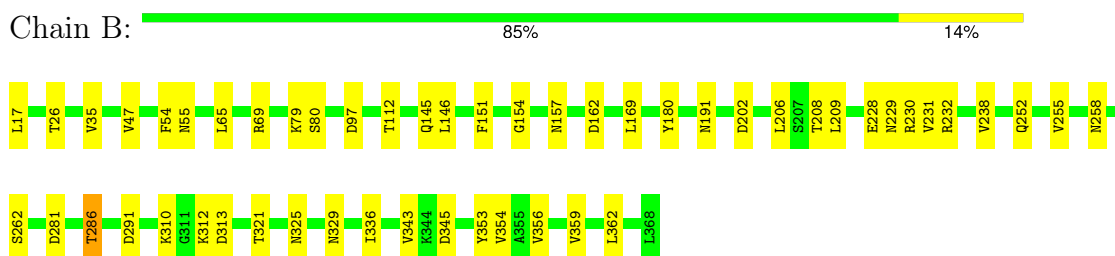
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial




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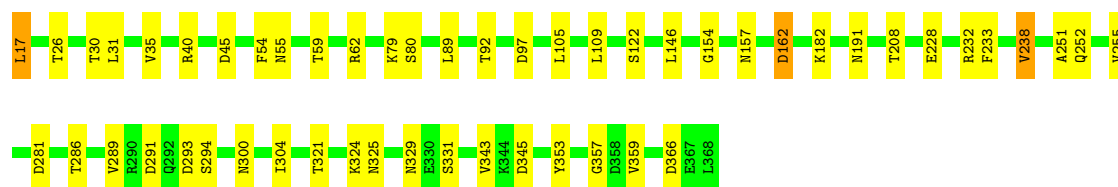


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial




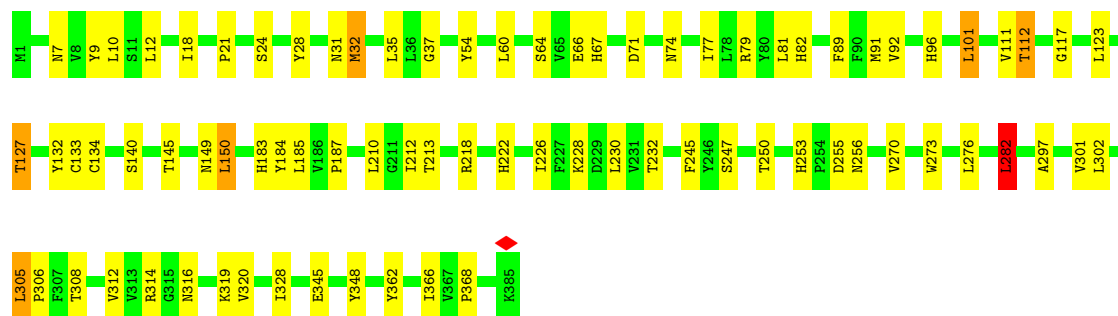
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  85% 14% .




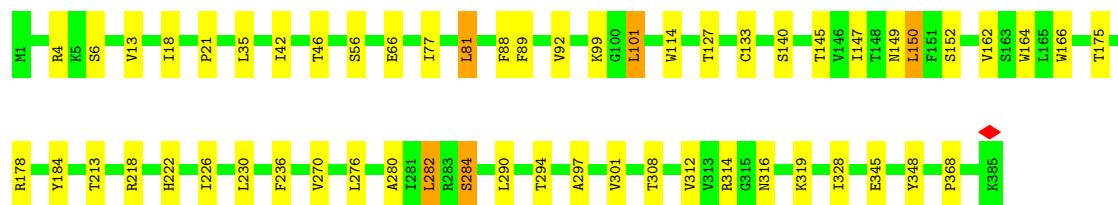
• Molecule 3: Cytochrome b

Chain C:  79% 19% .




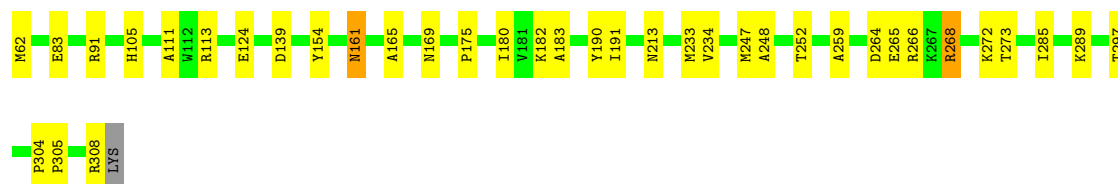
• Molecule 3: Cytochrome b

Chain N:  85% 13% .




• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  85% 14% .

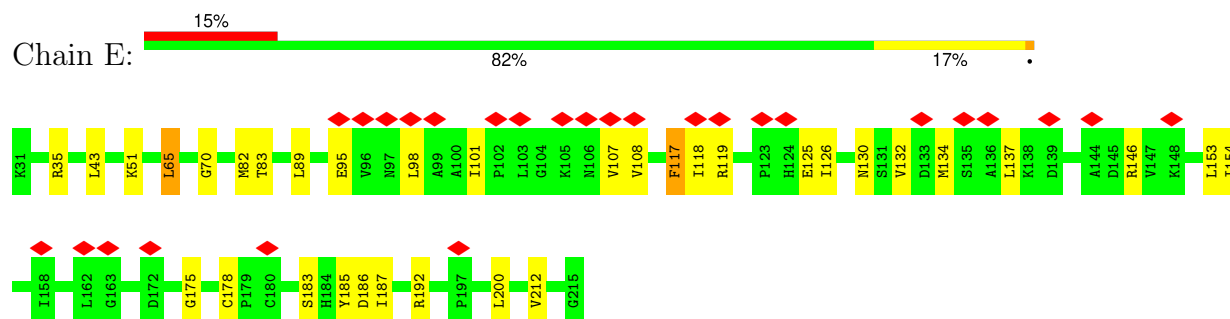


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

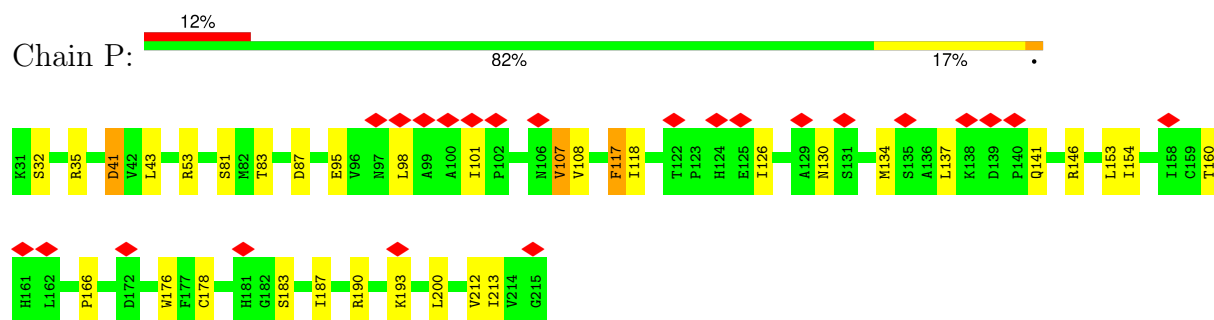
Chain O:  87% 12% .



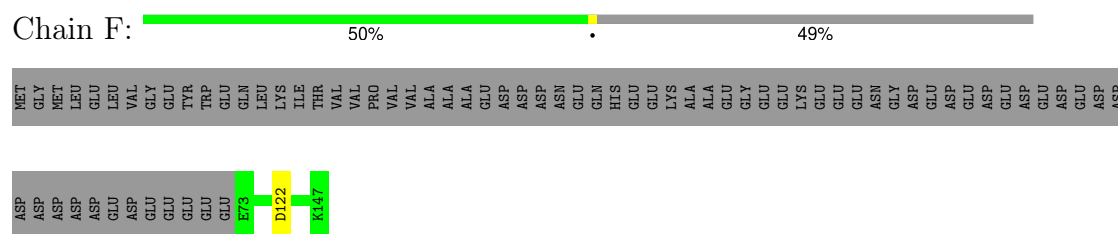
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



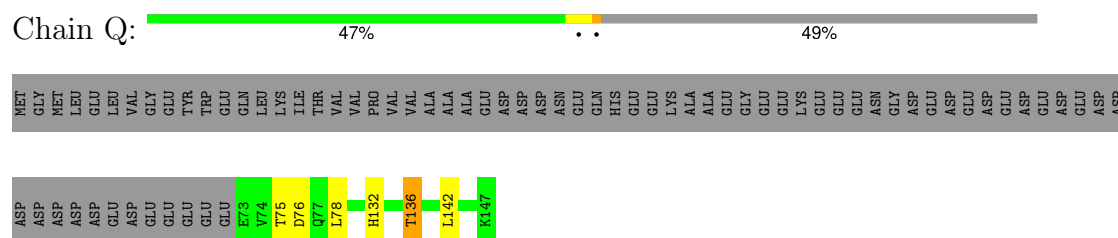
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



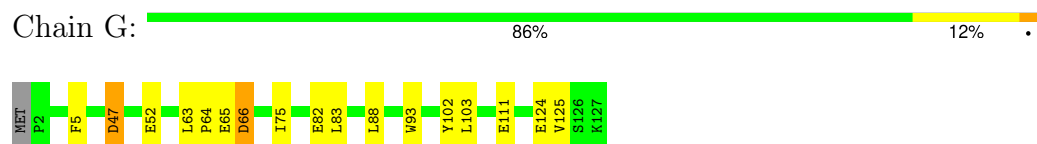
- Molecule 6: Cytochrome b-c1 complex subunit 6




- Molecule 6: Cytochrome b-c1 complex subunit 6



- Molecule 7: Cytochrome b-c1 complex subunit 7




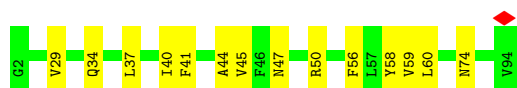
- Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R:  88% 9% ..




- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:  85% 15%



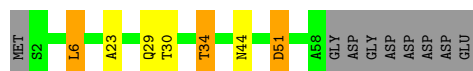
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:  88% 11% .




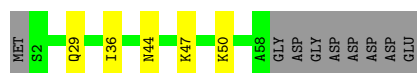
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain I:  76% 6% 5% 14%




- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T:  79% 8% 14%




- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain J:  88% 10% .



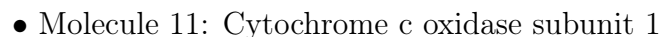
- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain U:  14% 88% 10% .



- Molecule 11: Cytochrome c oxidase subunit 1

Response	Percentage
Yes	93%
No	7%



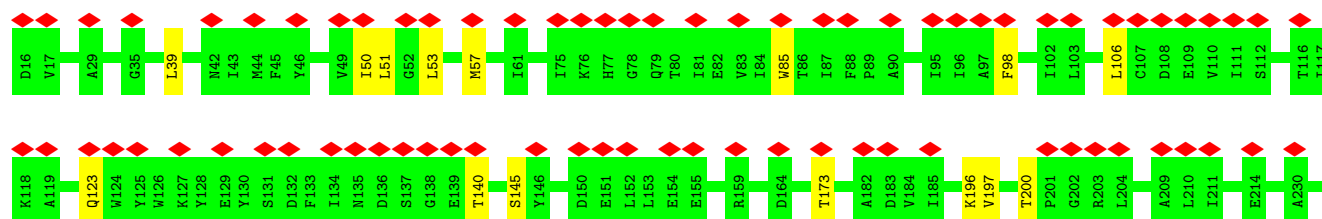
Response	Percentage
Yes	24%
No	93%
Other	7%

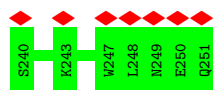


Response	Percentage
Doing a good job	93%
Not doing a good job	7%

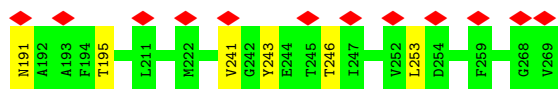


Response	Percentage
Believe the U.S. is a democracy	94%
Believe the U.S. is not a democracy	35%
Unsure	6%

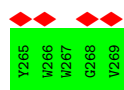
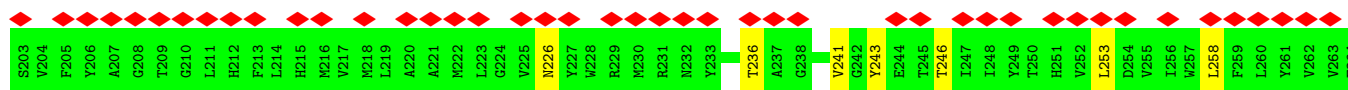
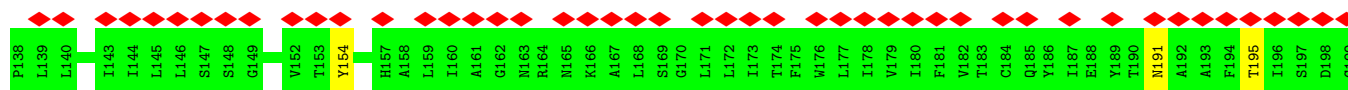
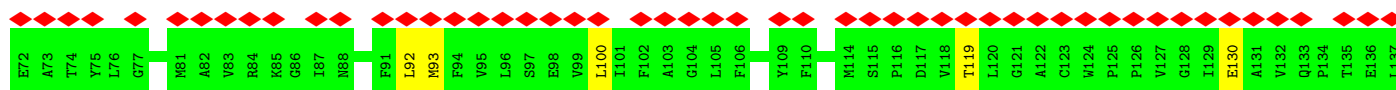
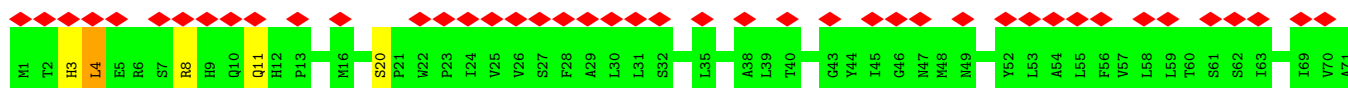
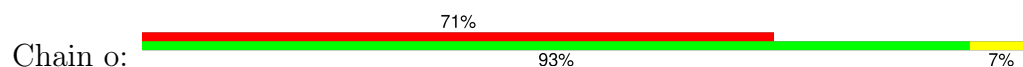




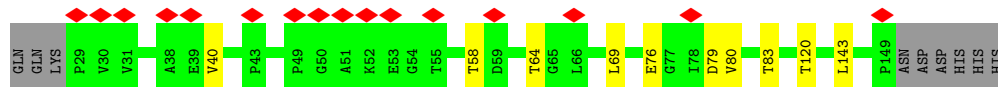
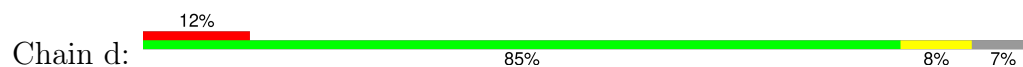
- Molecule 13: Cytochrome c oxidase subunit 3



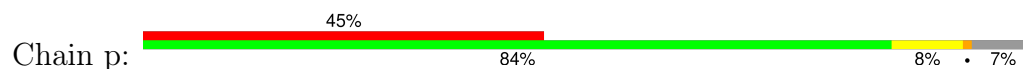
- Molecule 13: Cytochrome c oxidase subunit 3

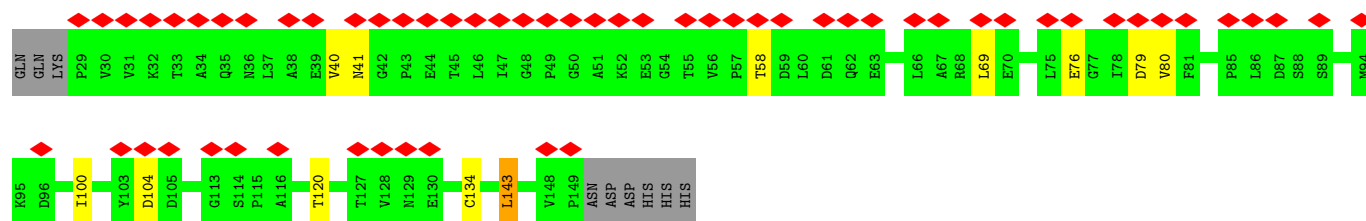


- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial



- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

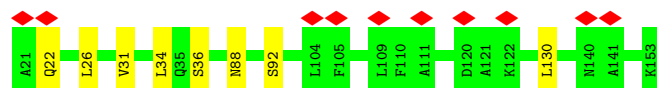
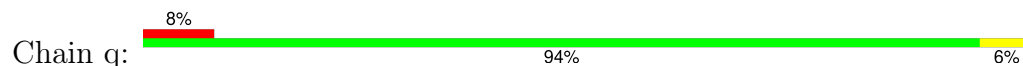




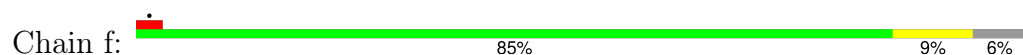
- Molecule 15: Cytochrome c oxidase polypeptide 5A, mitochondrial



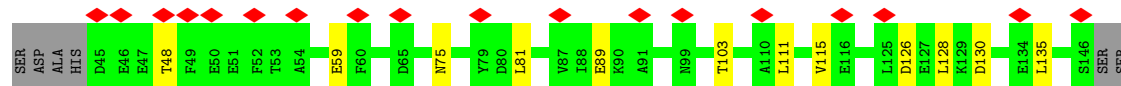
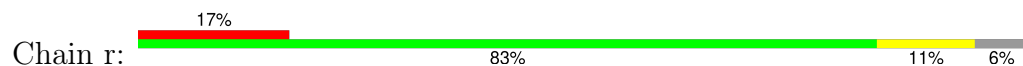
- Molecule 15: Cytochrome c oxidase polypeptide 5A, mitochondrial



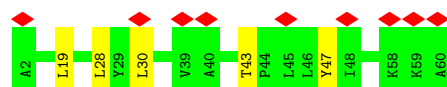
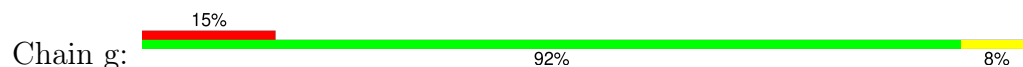
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



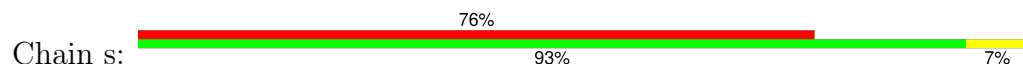
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial



- Molecule 17: Cytochrome c oxidase subunit 7



- Molecule 17: Cytochrome c oxidase subunit 7







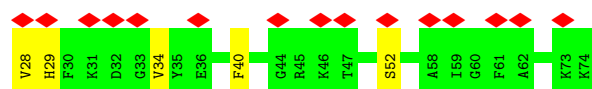
- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h: 100%



- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain t: 32% 89% 11%



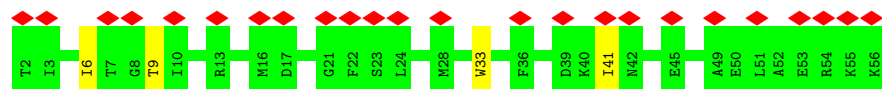
- Molecule 19: Cytochrome c oxidase subunit 7A

Chain i: 7% 93% 7%



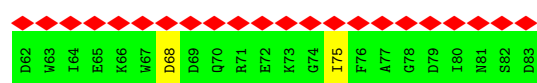
- Molecule 19: Cytochrome c oxidase subunit 7A

Chain u: 44% 93% 7%



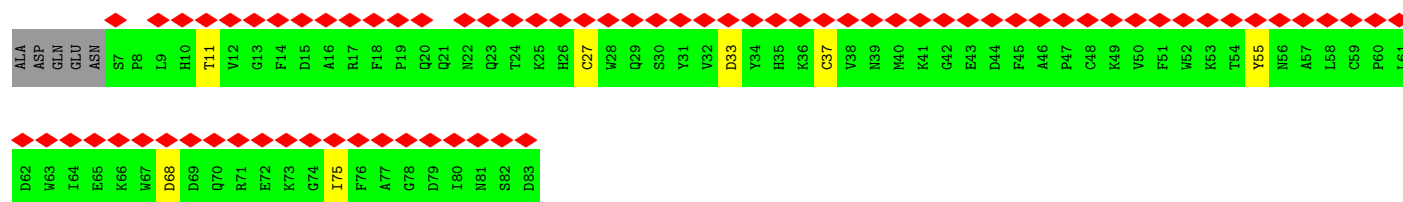
- Molecule 20: Cytochrome c oxidase subunit 6B

Chain j: 87% 84% 10% 6%

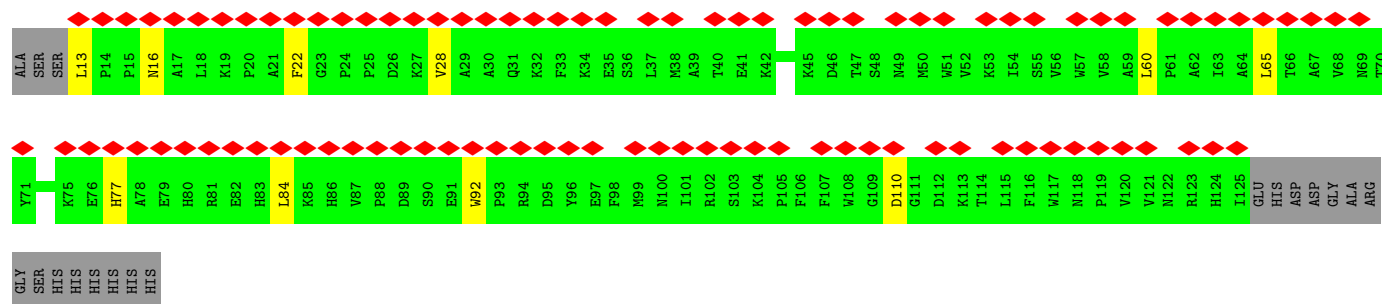
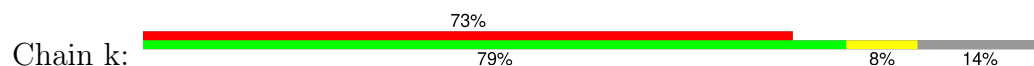


- Molecule 20: Cytochrome c oxidase subunit 6B

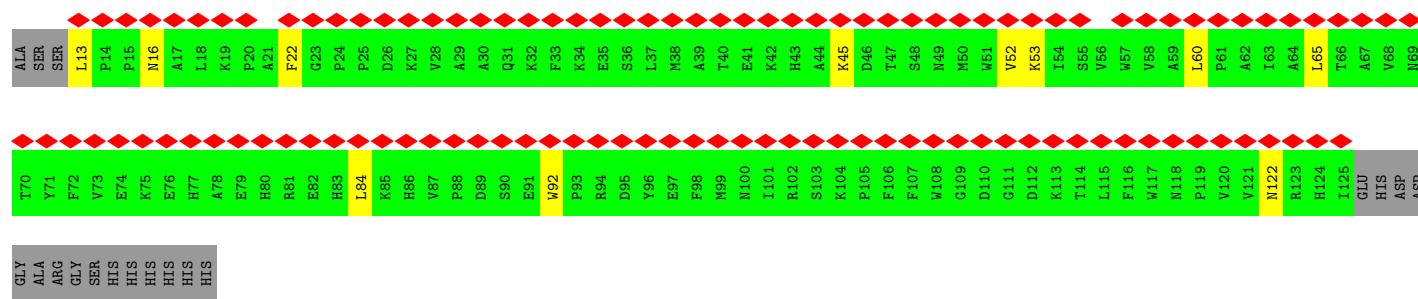
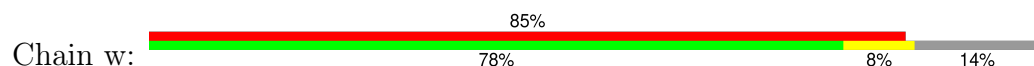
Chain v: 91% 85% 9% 6%



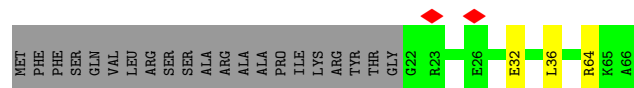
• Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial



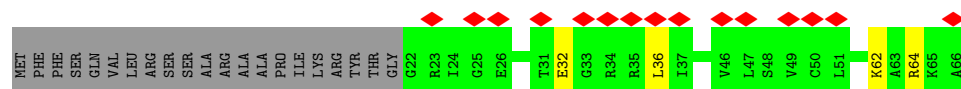
• Molecule 21: Cytochrome c oxidase subunit 6A, mitochondrial



• Molecule 22: Cox26



• Molecule 22: Cox26



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44915	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.645	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.255	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0263	Depositor
Map size ( $\text{\AA}$ )	429.691, 429.691, 429.691	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3861, 1.3861, 1.3861	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/3406	0.55	0/4615
1	L	0.41	0/3406	0.56	1/4615 (0.0%)
2	B	0.39	0/2781	0.53	0/3764
2	M	0.38	0/2781	0.52	0/3764
3	C	0.44	0/3192	0.57	1/4354 (0.0%)
3	N	0.44	0/3192	0.56	1/4354 (0.0%)
4	D	0.44	0/2012	0.49	0/2740
4	O	0.45	0/2012	0.50	0/2740
5	E	0.32	0/1444	0.50	1/1957 (0.1%)
5	P	0.32	0/1444	0.48	0/1957
6	F	0.36	0/647	0.47	0/870
6	Q	0.36	0/647	0.47	0/870
7	G	0.36	0/1040	0.52	0/1408
7	R	0.35	0/1040	0.53	0/1408
8	H	0.40	0/804	0.50	0/1088
8	S	0.42	0/804	0.47	0/1088
9	I	0.41	0/479	0.48	0/646
9	T	0.40	0/479	0.47	0/646
10	J	0.32	0/619	0.46	0/841
10	U	0.31	0/619	0.46	0/841
11	a	0.53	0/4290	0.63	1/5857 (0.0%)
11	m	0.49	0/4290	0.62	1/5857 (0.0%)
12	b	0.48	0/1941	0.62	0/2653
12	n	0.46	0/1941	0.61	0/2653
13	c	0.42	0/2218	0.55	1/3036 (0.0%)
13	o	0.42	0/2218	0.54	1/3036 (0.0%)
14	d	0.44	0/932	0.60	0/1269
14	p	0.46	0/932	0.61	1/1269 (0.1%)
15	e	0.48	0/1074	0.54	0/1451
15	q	0.46	0/1074	0.54	0/1451
16	f	0.46	0/868	0.51	0/1174
16	r	0.47	0/868	0.53	0/1174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	g	0.40	0/500	0.57	0/681
17	s	0.38	0/500	0.58	0/681
18	h	0.53	0/397	0.50	0/533
18	t	0.43	0/397	0.49	0/533
19	i	0.40	0/468	0.49	0/626
19	u	0.39	0/468	0.51	0/626
20	j	0.30	0/664	0.49	0/899
20	v	0.28	0/664	0.47	0/899
21	k	0.29	0/962	0.46	0/1310
21	w	0.29	0/962	0.47	0/1310
22	l	0.39	0/372	0.52	0/502
22	x	0.39	0/372	0.54	0/502
All	All	0.43	0/62220	0.55	9/84548 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	a	0	2
11	m	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	65	LEU	CA-CB-CG	6.29	129.76	115.30
13	c	4	LEU	CA-CB-CG	6.25	129.67	115.30
1	L	251	LEU	CA-CB-CG	5.67	128.35	115.30
13	o	4	LEU	CA-CB-CG	5.60	128.19	115.30
3	N	282	LEU	CA-CB-CG	5.58	128.14	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	a	119	VAL	Peptide
11	a	520	SER	Peptide
11	m	520	SER	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3345	0	3323	33	0
1	L	3345	0	3323	34	0
2	B	2735	0	2774	26	0
2	M	2735	0	2774	29	0
3	C	3090	0	3129	49	0
3	N	3090	0	3129	30	0
4	D	1951	0	1875	25	0
4	O	1951	0	1875	19	0
5	E	1411	0	1386	20	0
5	P	1411	0	1386	17	0
6	F	633	0	587	1	0
6	Q	633	0	587	3	0
7	G	1019	0	1034	13	0
7	R	1019	0	1034	9	0
8	H	773	0	736	10	0
8	S	773	0	736	7	0
9	I	465	0	459	7	0
9	T	465	0	459	5	0
10	J	599	0	594	5	0
10	U	599	0	594	5	0
11	a	4162	0	4191	0	0
11	m	4162	0	4191	0	0
12	b	1889	0	1866	0	0
12	n	1889	0	1866	0	0
13	c	2146	0	2137	0	0
13	o	2146	0	2137	0	0
14	d	913	0	909	0	0
14	p	913	0	910	0	0
15	e	1049	0	1030	0	0
15	q	1049	0	1030	0	0
16	f	851	0	822	0	0
16	r	851	0	822	0	0
17	g	484	0	517	0	0
17	s	484	0	517	0	0
18	h	383	0	386	0	0
18	t	383	0	386	0	0
19	i	456	0	469	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	u	456	0	469	0	0
20	j	642	0	586	0	0
20	v	642	0	586	0	0
21	k	928	0	906	0	0
21	w	928	0	906	0	0
22	l	361	0	363	0	0
22	x	361	0	363	0	0
23	A	44	0	64	2	0
23	C	75	0	99	1	0
23	D	42	0	60	4	0
23	E	29	0	31	1	0
23	H	32	0	37	0	0
23	N	114	0	150	4	0
23	O	43	0	62	2	0
23	P	29	0	31	1	0
23	S	36	0	48	1	0
23	a	113	0	151	0	0
23	b	40	0	56	0	0
23	c	77	0	100	0	0
23	e	47	0	73	0	0
23	h	47	0	73	0	0
23	m	80	0	112	0	0
23	n	73	0	95	0	0
23	o	77	0	100	0	0
23	q	47	0	73	0	0
23	t	47	0	73	0	0
24	C	86	0	60	4	0
24	N	86	0	60	1	0
25	C	86	0	116	7	0
26	C	58	0	60	0	0
26	E	53	0	50	3	0
26	H	137	0	165	5	0
26	L	55	0	54	2	0
26	O	67	0	78	5	0
26	P	48	0	40	0	0
26	S	53	0	50	2	0
27	C	39	0	55	0	0
27	H	32	0	38	1	0
27	I	30	0	34	0	0
27	N	50	0	80	2	0
27	S	32	0	38	0	0
27	T	39	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	e	36	0	46	0	0
27	q	36	0	46	0	0
28	D	43	0	29	1	0
28	O	43	0	29	1	0
29	E	4	0	0	0	0
29	P	4	0	0	0	0
30	a	1	0	0	0	0
30	m	1	0	0	0	0
31	a	120	0	108	0	0
31	m	120	0	108	0	0
32	a	1	0	0	0	0
32	m	1	0	0	0	0
33	a	1	0	0	0	0
33	m	1	0	0	0	0
34	b	2	0	0	0	0
34	n	2	0	0	0	0
35	d	1	0	0	0	0
35	p	1	0	0	0	0
All	All	63031	0	63043	324	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 5.

The worst 5 of 324 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:325:ASN:O	2:M:329:ASN:HB2	1.84	0.77
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.69	0.74
8:S:56:PHE:O	8:S:60:LEU:HB2	1.88	0.73
2:B:258:ASN:O	2:B:262:SER:HB3	1.92	0.69
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.43	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
1	L	429/431 (100%)	411 (96%)	18 (4%)	0	100	100
2	B	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
2	M	350/352 (99%)	333 (95%)	17 (5%)	0	100	100
3	C	383/385 (100%)	371 (97%)	12 (3%)	0	100	100
3	N	383/385 (100%)	371 (97%)	12 (3%)	0	100	100
4	D	245/248 (99%)	239 (98%)	6 (2%)	0	100	100
4	O	245/248 (99%)	240 (98%)	5 (2%)	0	100	100
5	E	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
5	P	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
6	F	73/147 (50%)	72 (99%)	1 (1%)	0	100	100
6	Q	73/147 (50%)	70 (96%)	3 (4%)	0	100	100
7	G	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
7	R	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
8	H	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
8	S	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
9	I	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
9	T	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
10	J	74/77 (96%)	73 (99%)	1 (1%)	0	100	100
10	U	74/77 (96%)	71 (96%)	3 (4%)	0	100	100
11	a	532/534 (100%)	502 (94%)	29 (6%)	1 (0%)	44	71
11	m	532/534 (100%)	506 (95%)	25 (5%)	1 (0%)	44	71
12	b	234/236 (99%)	223 (95%)	11 (5%)	0	100	100
12	n	234/236 (99%)	222 (95%)	12 (5%)	0	100	100
13	c	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
13	o	267/269 (99%)	258 (97%)	9 (3%)	0	100	100
14	d	119/130 (92%)	104 (87%)	15 (13%)	0	100	100
14	p	119/130 (92%)	105 (88%)	14 (12%)	0	100	100
15	e	131/133 (98%)	123 (94%)	7 (5%)	1 (1%)	16	44
15	q	131/133 (98%)	119 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	f	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
16	r	100/108 (93%)	98 (98%)	2 (2%)	0	100	100
17	g	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
17	s	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
18	h	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
18	t	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
19	u	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
20	j	75/82 (92%)	68 (91%)	7 (9%)	0	100	100
20	v	75/82 (92%)	69 (92%)	6 (8%)	0	100	100
21	k	111/131 (85%)	102 (92%)	9 (8%)	0	100	100
21	w	111/131 (85%)	106 (96%)	5 (4%)	0	100	100
22	l	43/66 (65%)	42 (98%)	1 (2%)	0	100	100
22	x	43/66 (65%)	42 (98%)	1 (2%)	0	100	100
All	All	7548/7922 (95%)	7217 (96%)	328 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	e	151	GLN
11	a	521	PRO
11	m	521	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	345 (93%)	25 (7%)	13	39
1	L	370/370 (100%)	350 (95%)	20 (5%)	18	45
2	B	301/301 (100%)	284 (94%)	17 (6%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	301/301 (100%)	289 (96%)	12 (4%)	27	52
3	C	338/338 (100%)	322 (95%)	16 (5%)	22	49
3	N	338/338 (100%)	325 (96%)	13 (4%)	28	54
4	D	205/206 (100%)	200 (98%)	5 (2%)	44	67
4	O	205/206 (100%)	195 (95%)	10 (5%)	21	48
5	E	151/151 (100%)	145 (96%)	6 (4%)	27	52
5	P	151/151 (100%)	140 (93%)	11 (7%)	11	36
6	F	68/131 (52%)	68 (100%)	0	100	100
6	Q	68/131 (52%)	67 (98%)	1 (2%)	60	76
7	G	110/111 (99%)	106 (96%)	4 (4%)	30	56
7	R	110/111 (99%)	105 (96%)	5 (4%)	23	50
8	H	77/77 (100%)	75 (97%)	2 (3%)	41	65
8	S	77/77 (100%)	74 (96%)	3 (4%)	27	54
9	I	47/54 (87%)	44 (94%)	3 (6%)	14	40
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	63 (97%)	2 (3%)	35	61
10	U	65/66 (98%)	64 (98%)	1 (2%)	60	76
11	a	447/447 (100%)	413 (92%)	34 (8%)	11	34
11	m	447/447 (100%)	411 (92%)	36 (8%)	9	32
12	b	209/209 (100%)	192 (92%)	17 (8%)	9	32
12	n	209/209 (100%)	194 (93%)	15 (7%)	12	37
13	c	228/228 (100%)	210 (92%)	18 (8%)	10	33
13	o	228/228 (100%)	208 (91%)	20 (9%)	8	28
14	d	102/111 (92%)	92 (90%)	10 (10%)	6	23
14	p	102/111 (92%)	90 (88%)	12 (12%)	4	16
15	e	110/110 (100%)	104 (94%)	6 (6%)	18	44
15	q	110/110 (100%)	102 (93%)	8 (7%)	11	36
16	f	91/96 (95%)	81 (89%)	10 (11%)	5	19
16	r	91/96 (95%)	79 (87%)	12 (13%)	3	13
17	g	50/50 (100%)	45 (90%)	5 (10%)	6	23
17	s	50/50 (100%)	46 (92%)	4 (8%)	10	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	h	39/39 (100%)	39 (100%)	0	100	100
18	t	39/39 (100%)	34 (87%)	5 (13%)	3	14
19	i	46/46 (100%)	42 (91%)	4 (9%)	8	29
19	u	46/46 (100%)	42 (91%)	4 (9%)	8	29
20	j	69/73 (94%)	61 (88%)	8 (12%)	4	17
20	v	69/73 (94%)	62 (90%)	7 (10%)	6	22
21	k	99/113 (88%)	89 (90%)	10 (10%)	6	22
21	w	99/113 (88%)	88 (89%)	11 (11%)	5	19
22	l	36/53 (68%)	33 (92%)	3 (8%)	9	31
22	x	36/53 (68%)	32 (89%)	4 (11%)	5	19
All	All	6516/6760 (96%)	6097 (94%)	419 (6%)	17	40

5 of 419 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	d	80	VAL
11	m	95	PHE
20	v	33	ASP
15	e	88	ASN
20	j	11	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
11	m	482	ASN
12	n	249	ASN
20	v	29	GLN
1	L	75	ASN
1	L	42	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 70 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 58 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	$\# Z  > 2$
29	FES	E	301	5	0,4,4	-	-	-		
23	PEF	o	301	-	35,35,46	1.08	2 (5%)	38,40,51	1.18	3 (7%)
23	PEF	S	602	-	35,35,46	1.07	2 (5%)	38,40,51	1.12	4 (10%)
27	PCF	T	101	-	38,38,49	1.13	2 (5%)	44,46,57	1.18	2 (4%)
26	CDL	E	302	-	52,52,99	1.22	4 (7%)	58,64,111	1.38	8 (13%)
28	HEC	O	401	4	32,50,50	1.97	10 (31%)	30,82,82	1.77	5 (16%)
31	HEA	m	602	11	58,67,67	2.02	18 (31%)	63,103,103	2.63	31 (49%)
23	PEF	n	304	-	32,32,46	1.11	2 (6%)	35,37,51	1.44	4 (11%)
27	PCF	q	202	-	35,35,49	1.13	2 (5%)	41,43,57	1.18	4 (9%)
23	PEF	E	303	-	28,28,46	1.21	2 (7%)	31,33,51	1.28	2 (6%)
26	CDL	H	602	-	70,70,99	1.05	5 (7%)	76,82,111	1.25	7 (9%)
25	UQ6	C	603[B]	-	43,43,43	2.12	6 (13%)	54,55,55	1.51	12 (22%)
25	UQ6	C	603[A]	-	43,43,43	2.09	6 (13%)	54,55,55	1.40	12 (22%)
24	HEM	C	602	3	42,50,50	1.43	6 (14%)	46,82,82	1.76	11 (23%)
23	PEF	D	402	-	41,41,46	1.03	2 (4%)	44,46,51	1.08	3 (6%)
31	HEA	m	603	11	58,67,67	2.02	16 (27%)	63,103,103	2.37	26 (41%)
23	PEF	b	303	-	39,39,46	1.02	2 (5%)	42,44,51	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	PEF	a	607	-	32,32,46	1.11	2 (6%)	35,37,51	1.37	4 (11%)
27	PCF	H	604	-	31,31,49	1.18	2 (6%)	37,39,57	1.09	2 (5%)
24	HEM	N	601	3	42,50,50	1.37	6 (14%)	46,82,82	1.95	12 (26%)
23	PEF	N	603	-	39,39,46	1.00	2 (5%)	42,44,51	1.22	3 (7%)
27	PCF	C	607	-	38,38,49	1.12	2 (5%)	44,46,57	1.07	2 (4%)
23	PEF	o	302	-	40,40,46	1.04	2 (5%)	43,45,51	1.13	3 (6%)
27	PCF	N	606	-	49,49,49	0.94	3 (6%)	55,57,57	1.04	4 (7%)
27	PCF	I	101	-	29,29,49	1.27	2 (6%)	35,37,57	1.19	3 (8%)
23	PEF	q	201	-	46,46,46	0.95	2 (4%)	49,51,51	1.12	4 (8%)
27	PCF	S	603	-	31,31,49	1.19	2 (6%)	37,39,57	1.25	4 (10%)
23	PEF	c	301	-	35,35,46	1.07	2 (5%)	38,40,51	1.12	2 (5%)
23	PEF	C	605	-	38,38,46	1.04	2 (5%)	41,43,51	1.01	3 (7%)
23	PEF	a	608	-	32,32,46	1.11	2 (6%)	35,37,51	1.27	4 (11%)
26	CDL	L	501	-	54,54,99	1.16	4 (7%)	60,66,111	1.22	5 (8%)
23	PEF	N	604	-	42,42,46	0.95	2 (4%)	45,47,51	0.96	3 (6%)
23	PEF	h	101	-	46,46,46	0.90	2 (4%)	49,51,51	1.05	3 (6%)
23	PEF	A	501	-	43,43,46	0.97	2 (4%)	46,48,51	1.06	3 (6%)
23	PEF	e	201	-	46,46,46	0.93	2 (4%)	49,51,51	1.12	4 (8%)
26	CDL	O	402	-	66,66,99	1.11	4 (6%)	72,78,111	1.21	7 (9%)
28	HEC	D	401	4	32,50,50	2.13	12 (37%)	30,82,82	2.13	8 (26%)
23	PEF	H	603	-	31,31,46	1.17	2 (6%)	34,36,51	1.30	4 (11%)
26	CDL	C	604	-	57,57,99	1.18	4 (7%)	63,69,111	1.39	8 (12%)
23	PEF	n	303	-	39,39,46	1.03	2 (5%)	42,44,51	1.07	3 (7%)
23	PEF	C	606	-	35,35,46	1.08	2 (5%)	38,40,51	1.17	4 (10%)
26	CDL	H	601	-	65,65,99	1.12	4 (6%)	71,77,111	1.23	7 (9%)
23	PEF	m	606	-	46,46,46	0.95	2 (4%)	49,51,51	1.03	2 (4%)
23	PEF	c	302	-	40,40,46	1.02	2 (5%)	43,45,51	1.21	3 (6%)
23	PEF	t	101	-	46,46,46	0.94	2 (4%)	49,51,51	1.16	6 (12%)
26	CDL	S	601	-	52,52,99	1.25	4 (7%)	58,64,111	1.42	8 (13%)
31	HEA	a	603	11	58,67,67	2.02	17 (29%)	63,103,103	2.41	26 (41%)
27	PCF	e	202	-	35,35,49	1.15	2 (5%)	41,43,57	1.15	3 (7%)
23	PEF	P	303	-	28,28,46	1.20	2 (7%)	31,33,51	1.30	4 (12%)
23	PEF	O	403	-	42,42,46	0.98	2 (4%)	45,47,51	1.10	4 (8%)
23	PEF	N	605	-	30,30,46	1.18	2 (6%)	33,35,51	1.25	4 (12%)
24	HEM	C	601	3	42,50,50	1.38	5 (11%)	46,82,82	2.07	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	FES	P	301	5	0,4,4	-	-	-		
26	CDL	P	302	-	47,47,99	1.29	4 (8%)	53,59,111	1.53	10 (18%)
24	HEM	N	602	3	42,50,50	1.39	6 (14%)	46,82,82	1.87	12 (26%)
23	PEF	a	606	-	46,46,46	0.94	2 (4%)	49,51,51	1.09	3 (6%)
23	PEF	m	607	-	32,32,46	1.09	2 (6%)	35,37,51	1.26	4 (11%)
31	HEA	a	602	11	58,67,67	2.04	15 (25%)	63,103,103	2.69	31 (49%)

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
29	FES	E	301	5	-	-	0/1/1/1
23	PEF	o	301	-	-	9/39/39/50	-
23	PEF	S	602	-	-	11/39/39/50	-
27	PCF	T	101	-	-	15/42/42/53	-
26	CDL	E	302	-	-	22/63/63/110	-
28	HEC	O	401	4	-	0/10/54/54	-
31	HEA	m	602	11	-	10/32/76/76	-
23	PEF	n	304	-	-	16/36/36/50	-
27	PCF	q	202	-	-	10/39/39/53	-
23	PEF	E	303	-	-	14/32/32/50	-
26	CDL	H	602	-	-	25/81/81/110	-
25	UQ6	C	603[B]	-	-	13/39/39/39	0/1/1/1
25	UQ6	C	603[A]	-	-	9/39/39/39	0/1/1/1
24	HEM	C	602	3	-	4/12/54/54	-
23	PEF	D	402	-	-	15/45/45/50	-
31	HEA	m	603	11	-	1/32/76/76	-
23	PEF	b	303	-	-	15/43/43/50	-
23	PEF	a	607	-	-	12/36/36/50	-
27	PCF	H	604	-	-	14/35/35/53	-
24	HEM	N	601	3	-	8/12/54/54	-
23	PEF	N	603	-	-	14/43/43/50	-
27	PCF	C	607	-	-	8/42/42/53	-
23	PEF	o	302	-	-	9/44/44/50	-
27	PCF	N	606	-	-	19/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PCF	I	101	-	-	14/33/33/53	-
23	PEF	q	201	-	-	20/50/50/50	-
27	PCF	S	603	-	-	12/35/35/53	-
23	PEF	c	301	-	-	7/39/39/50	-
23	PEF	C	605	-	-	9/42/42/50	-
23	PEF	a	608	-	-	8/36/36/50	-
26	CDL	L	501	-	-	24/64/64/110	-
23	PEF	N	604	-	-	21/46/46/50	-
23	PEF	h	101	-	-	18/50/50/50	-
23	PEF	A	501	-	-	13/47/47/50	-
23	PEF	e	201	-	-	16/50/50/50	-
26	CDL	O	402	-	-	23/77/77/110	-
28	HEC	D	401	4	-	2/10/54/54	-
23	PEF	H	603	-	-	6/35/35/50	-
26	CDL	C	604	-	-	17/68/68/110	-
23	PEF	n	303	-	-	18/43/43/50	-
23	PEF	C	606	-	-	11/39/39/50	-
26	CDL	H	601	-	-	19/76/76/110	-
23	PEF	m	606	-	-	10/50/50/50	-
23	PEF	c	302	-	-	9/44/44/50	-
23	PEF	t	101	-	-	16/50/50/50	-
26	CDL	S	601	-	-	11/63/63/110	-
31	HEA	a	603	11	-	7/32/76/76	-
27	PCF	e	202	-	-	12/39/39/53	-
23	PEF	P	303	-	-	10/32/32/50	-
23	PEF	O	403	-	-	13/46/46/50	-
23	PEF	N	605	-	-	17/34/34/50	-
24	HEM	C	601	3	-	8/12/54/54	-
29	FES	P	301	5	-	-	0/1/1/1
26	CDL	P	302	-	-	19/58/58/110	-
24	HEM	N	602	3	-	4/12/54/54	-
23	PEF	a	606	-	-	9/50/50/50	-
23	PEF	m	607	-	-	6/36/36/50	-
31	HEA	a	602	11	-	7/32/76/76	-



The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	401	HEC	C2B-C3B	6.31	1.47	1.40
25	C	603[B]	UQ6	C5-C4	6.26	1.49	1.39
25	C	603[A]	UQ6	C5-C6	6.16	1.49	1.40
25	C	603[B]	UQ6	C5-C6	6.16	1.49	1.40
25	C	603[A]	UQ6	C2-C3	6.04	1.49	1.39

The worst 5 of 377 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C3D-C4D-ND	7.19	117.30	110.35
31	a	603	HEA	C3D-C4D-ND	7.19	117.30	110.35
28	D	401	HEC	CMB-C2B-C3B	7.12	134.19	125.82
31	m	602	HEA	C3D-C4D-ND	6.95	117.07	110.35
31	m	603	HEA	C3D-C4D-ND	6.81	116.93	110.35

There are no chirality outliers.

5 of 689 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	501	PEF	O4P-C4-C5-N
23	A	501	PEF	C11-C10-O2-C2
23	A	501	PEF	C1-O3P-P-O2P
23	A	501	PEF	C1-O3P-P-O4P
23	A	501	PEF	C4-O4P-P-O1P

There are no ring outliers.

26 monomers are involved in 49 short contacts:

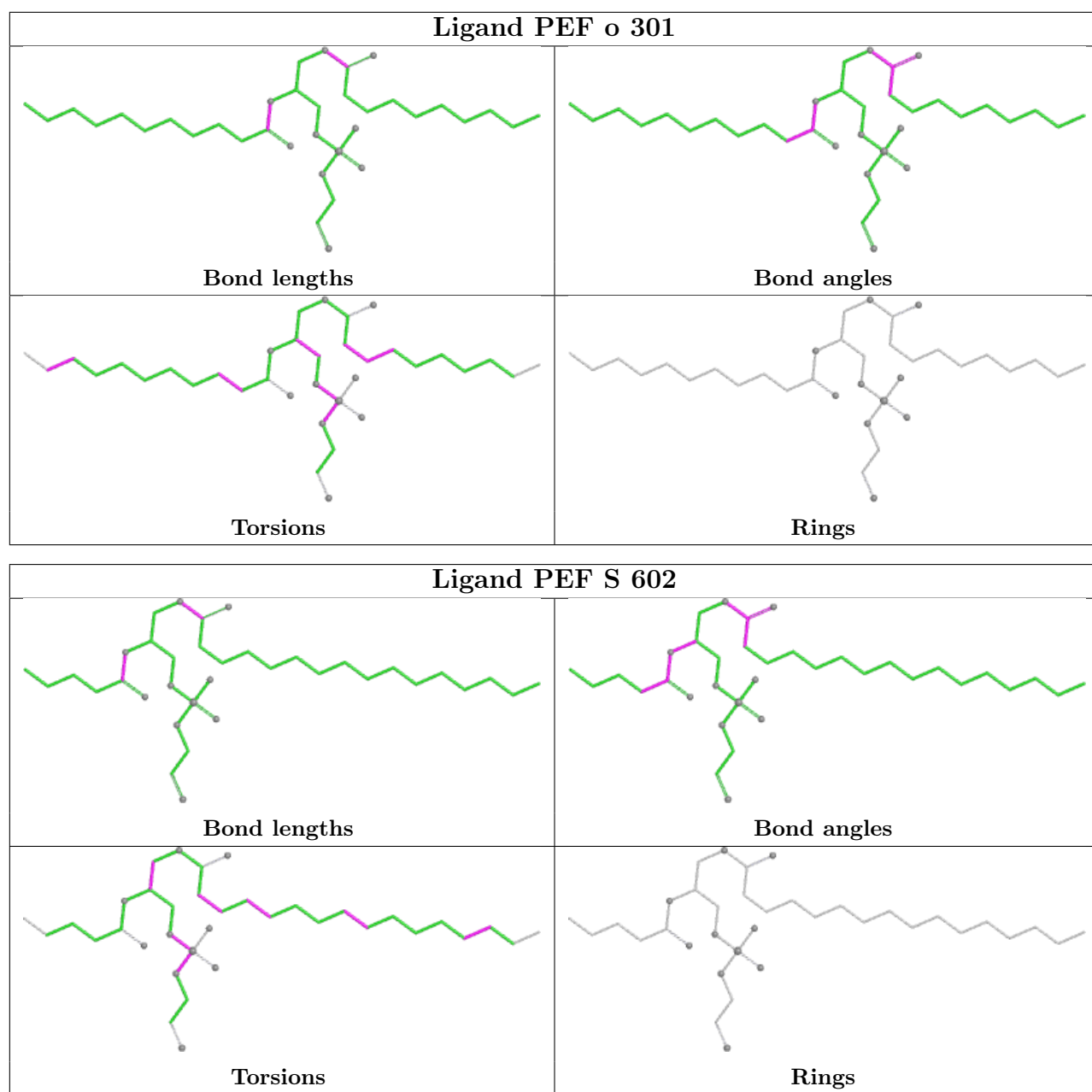
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	S	602	PEF	1	0
27	T	101	PCF	1	0
26	E	302	CDL	3	0
28	O	401	HEC	1	0
23	E	303	PEF	1	0
26	H	602	CDL	3	0
25	C	603[B]	UQ6	5	0
25	C	603[A]	UQ6	2	0
24	C	602	HEM	2	0
23	D	402	PEF	4	0
27	H	604	PCF	1	0

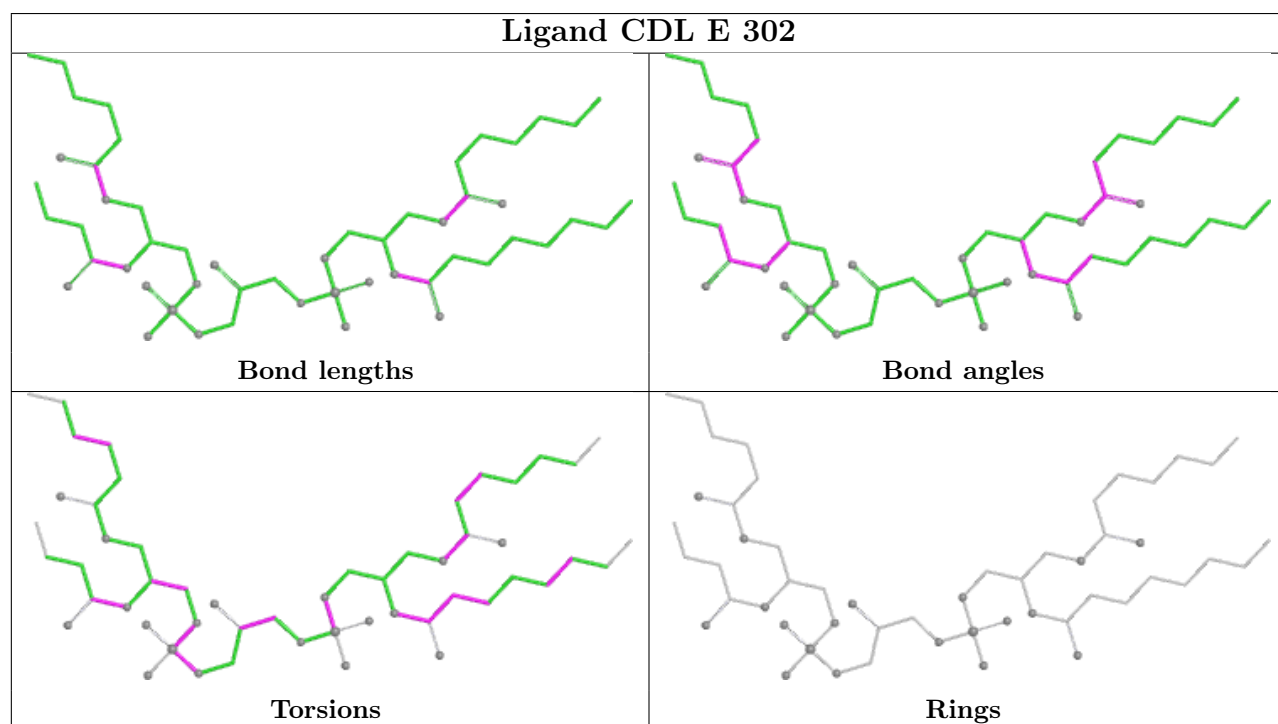
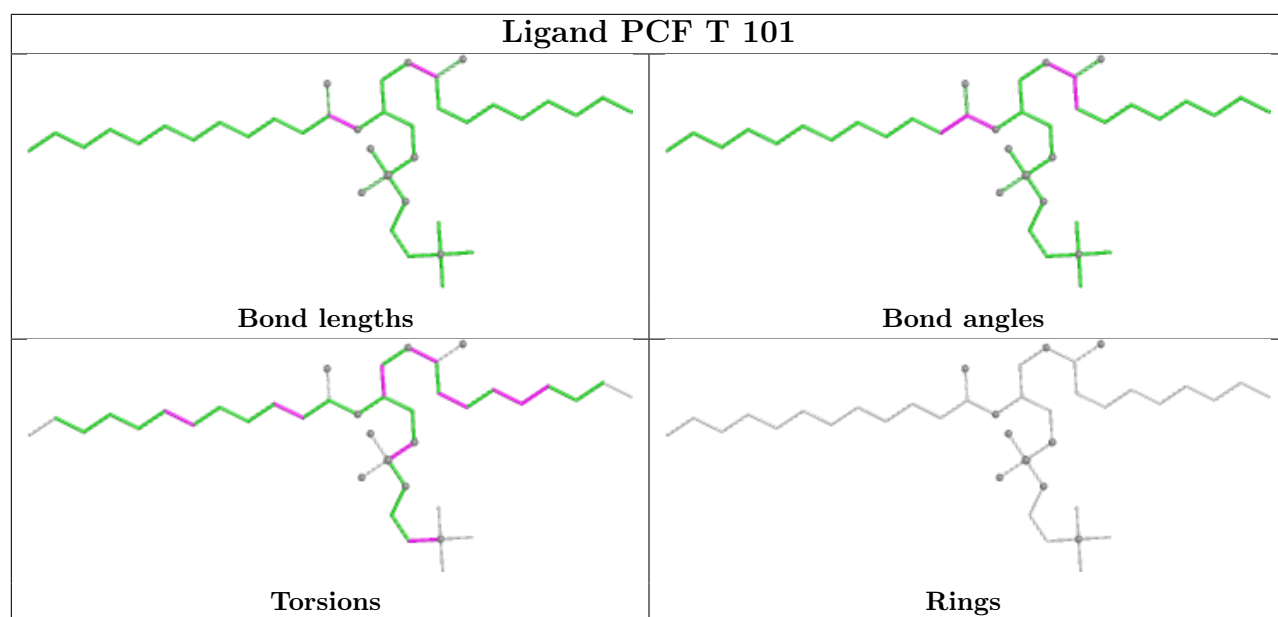
*Continued on next page...*

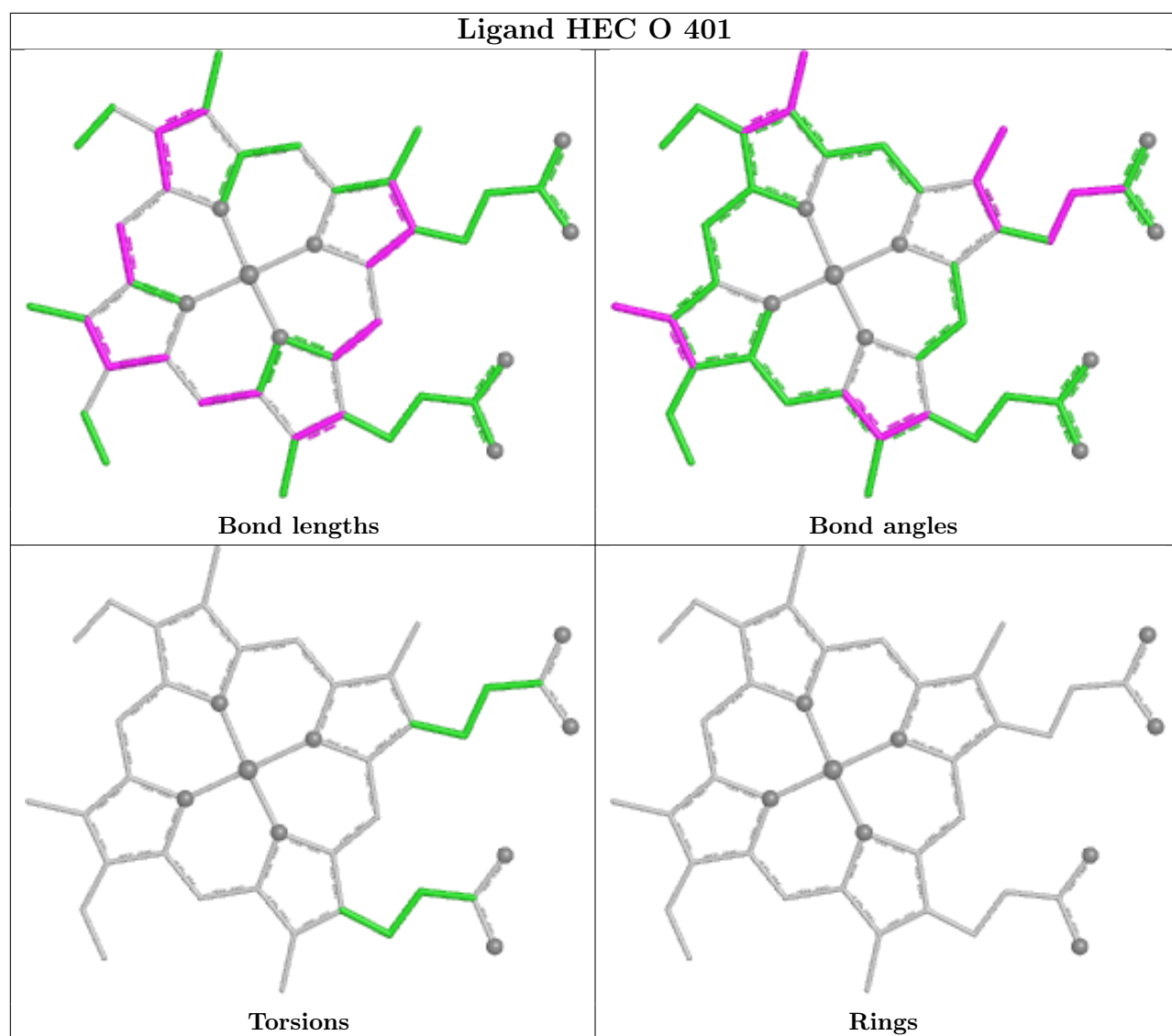
*Continued from previous page...*

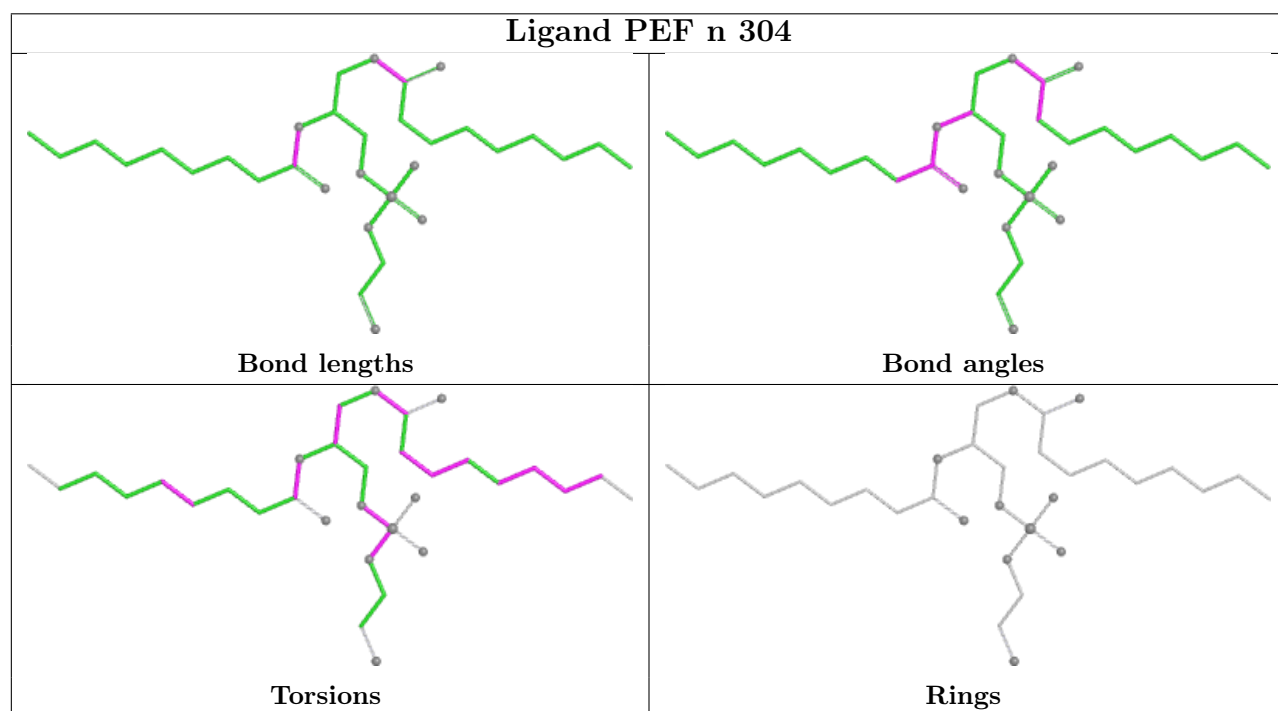
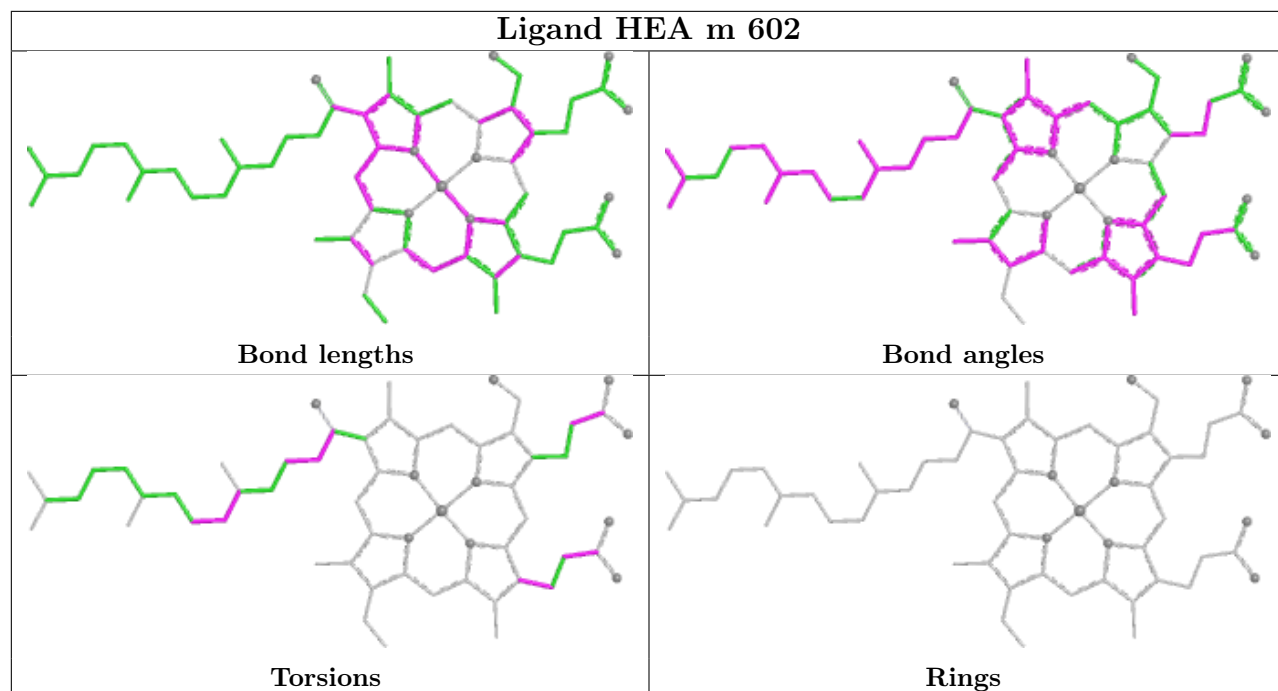
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	N	601	HEM	1	0
23	N	603	PEF	2	0
27	N	606	PCF	2	0
23	C	605	PEF	1	0
26	L	501	CDL	2	0
23	N	604	PEF	1	0
23	A	501	PEF	2	0
26	O	402	CDL	5	0
28	D	401	HEC	1	0
26	H	601	CDL	2	0
26	S	601	CDL	2	0
23	P	303	PEF	1	0
23	O	403	PEF	2	0
23	N	605	PEF	1	0
24	C	601	HEM	2	0

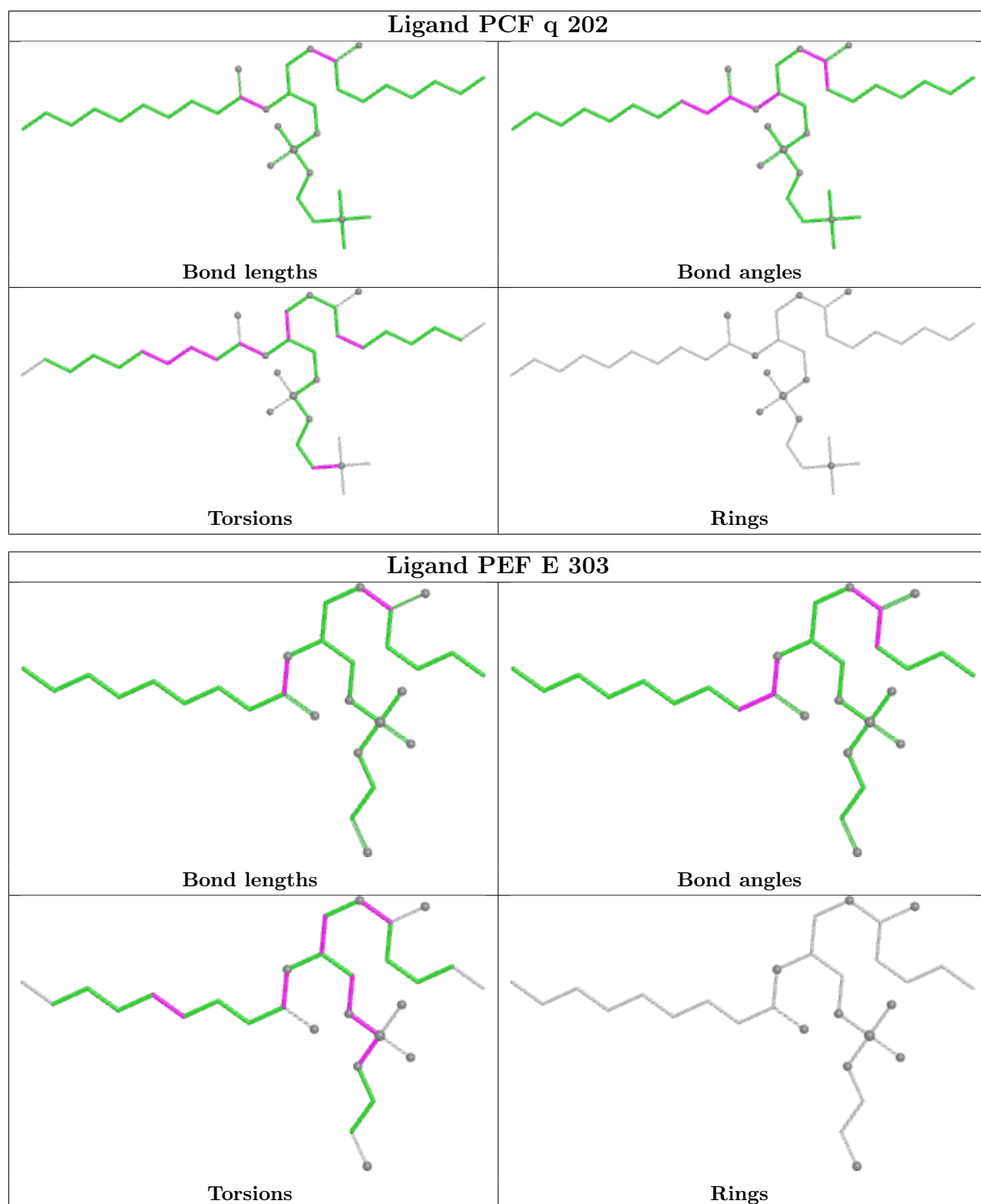
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

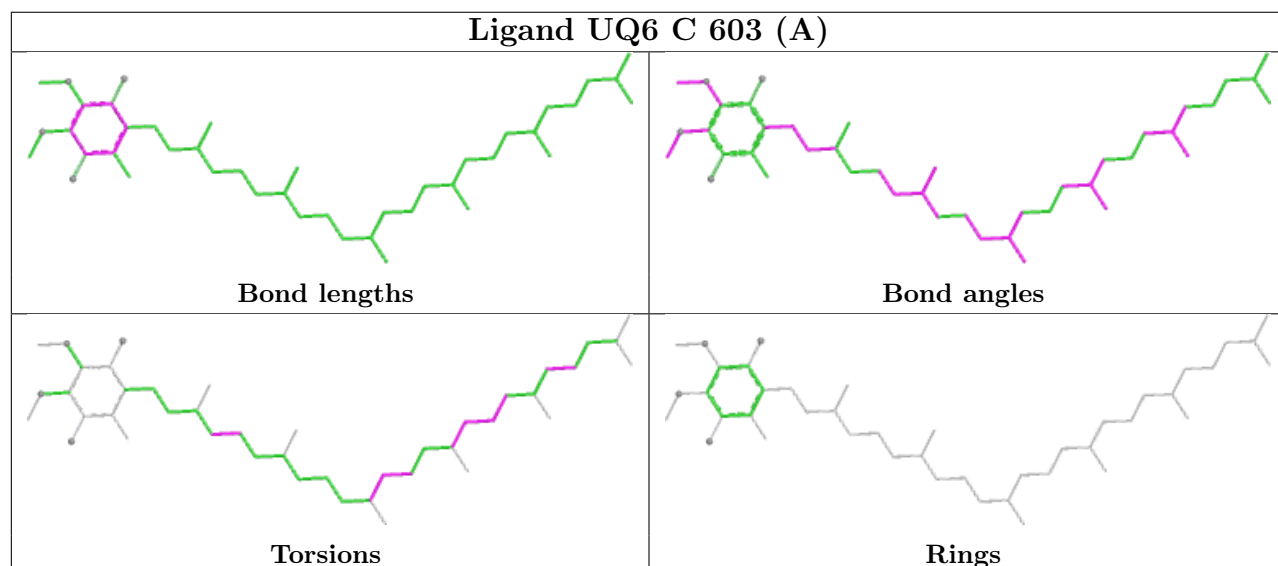
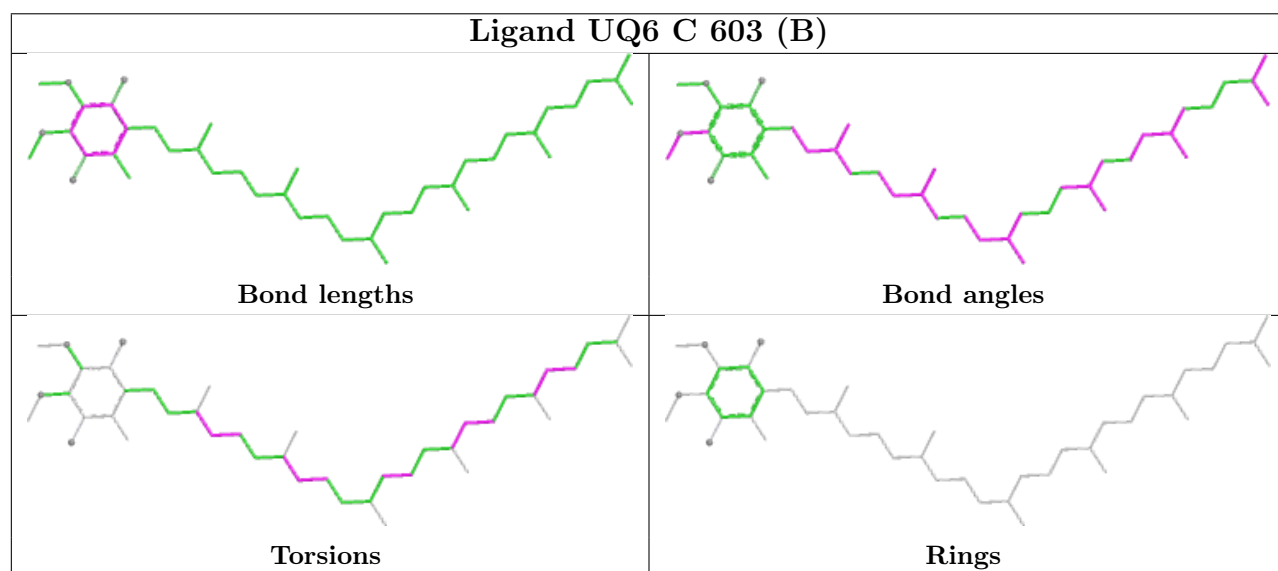
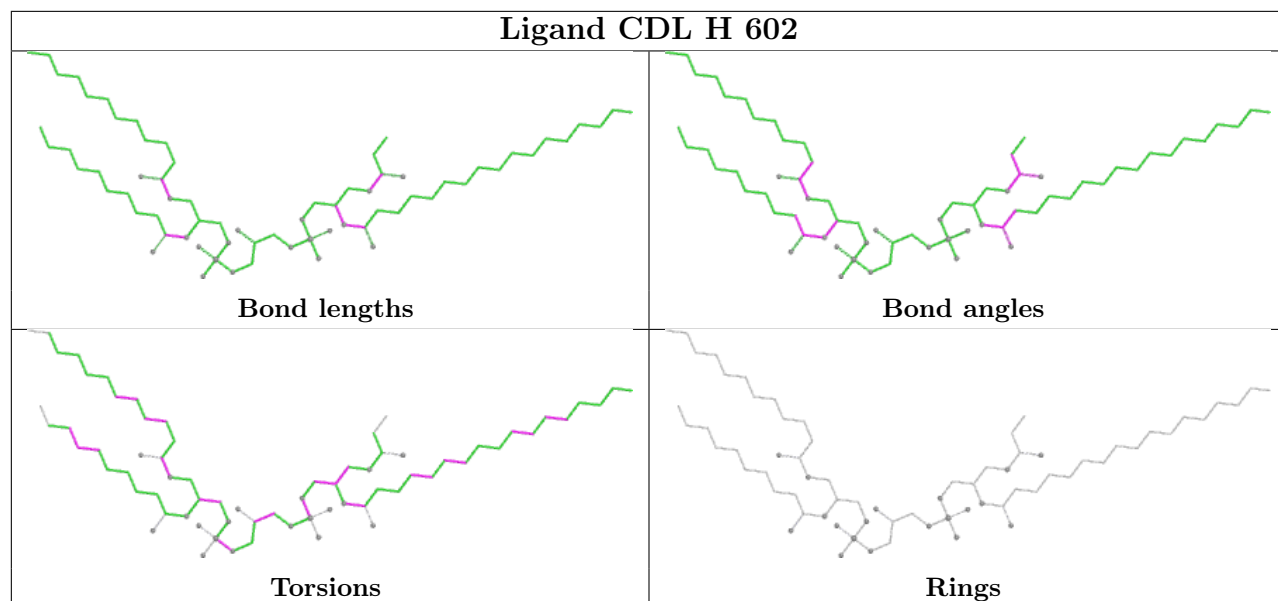




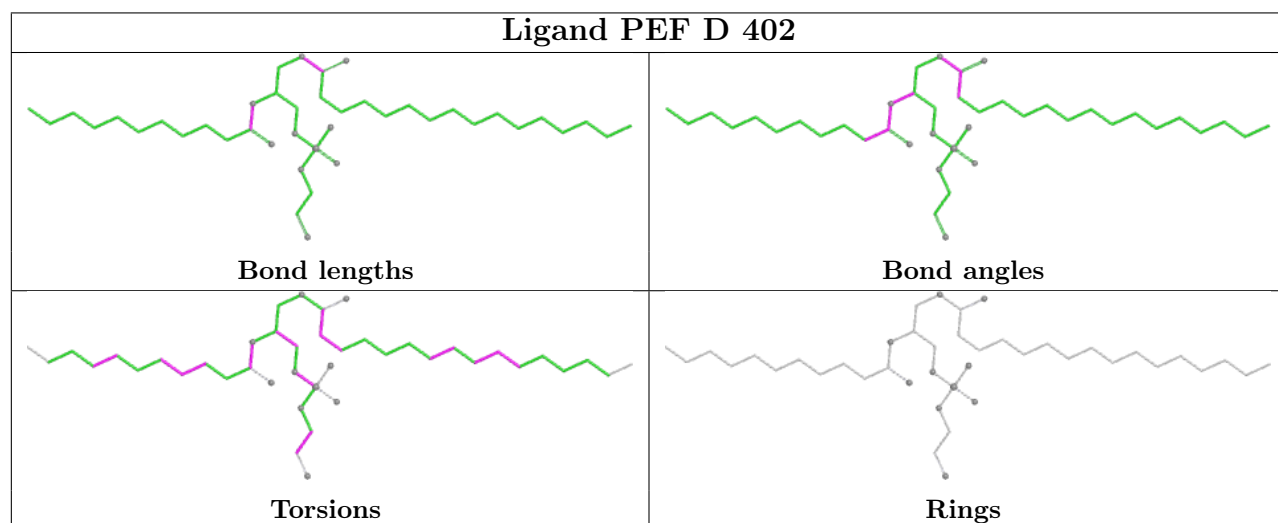
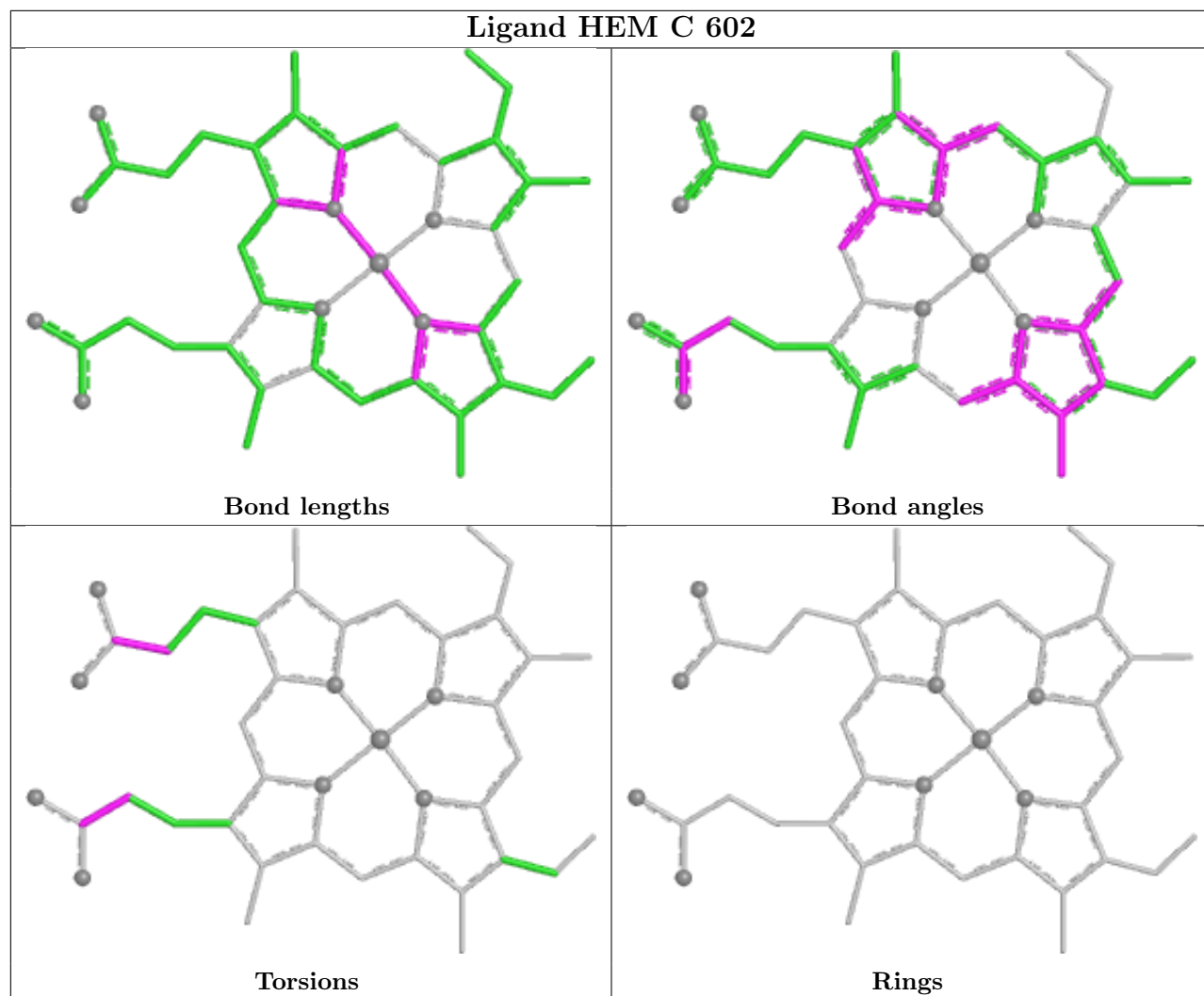


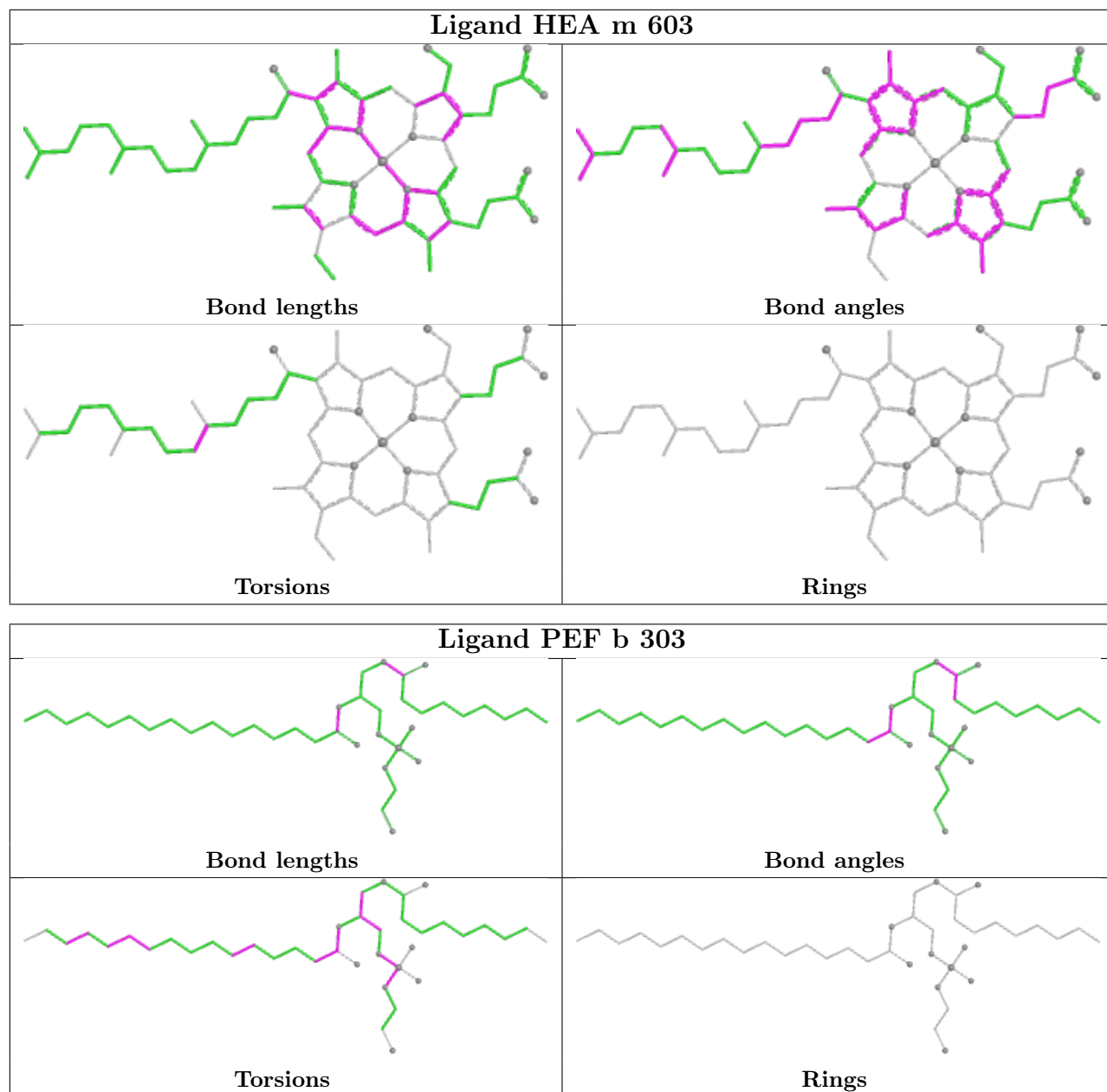


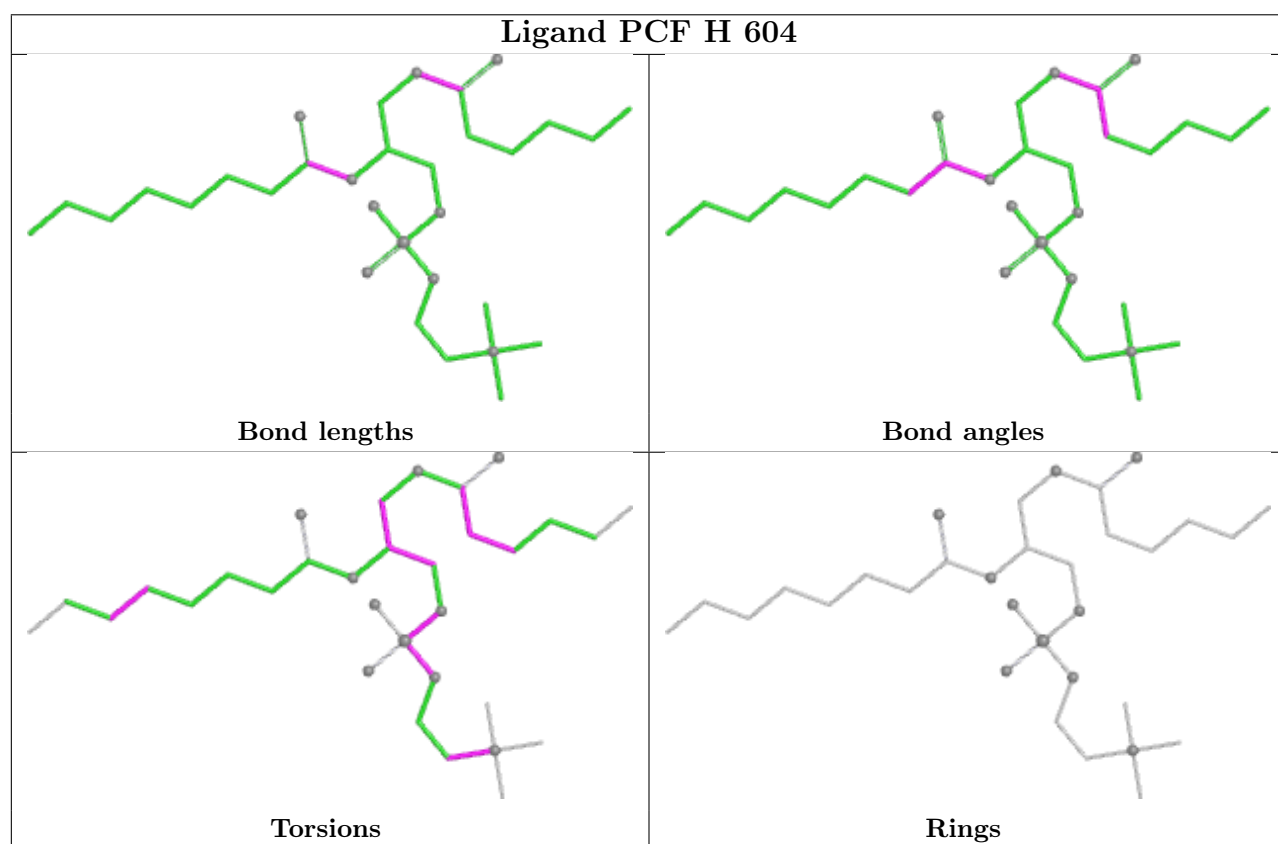
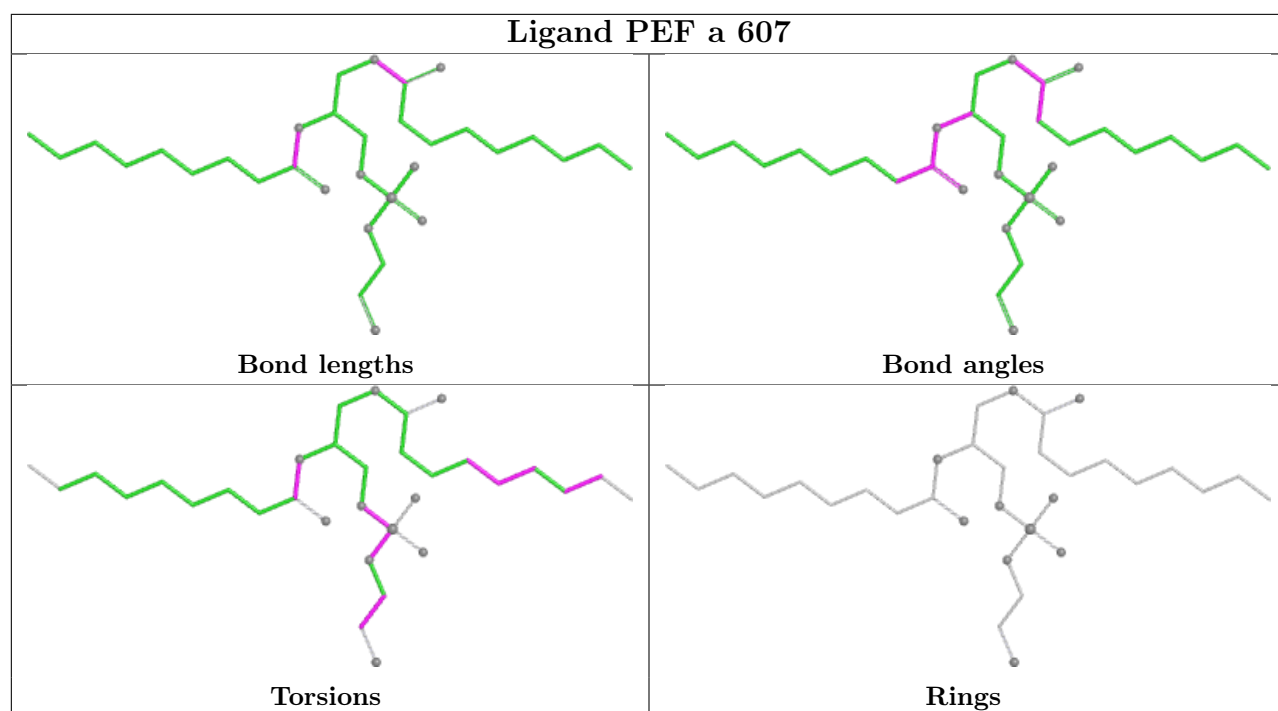


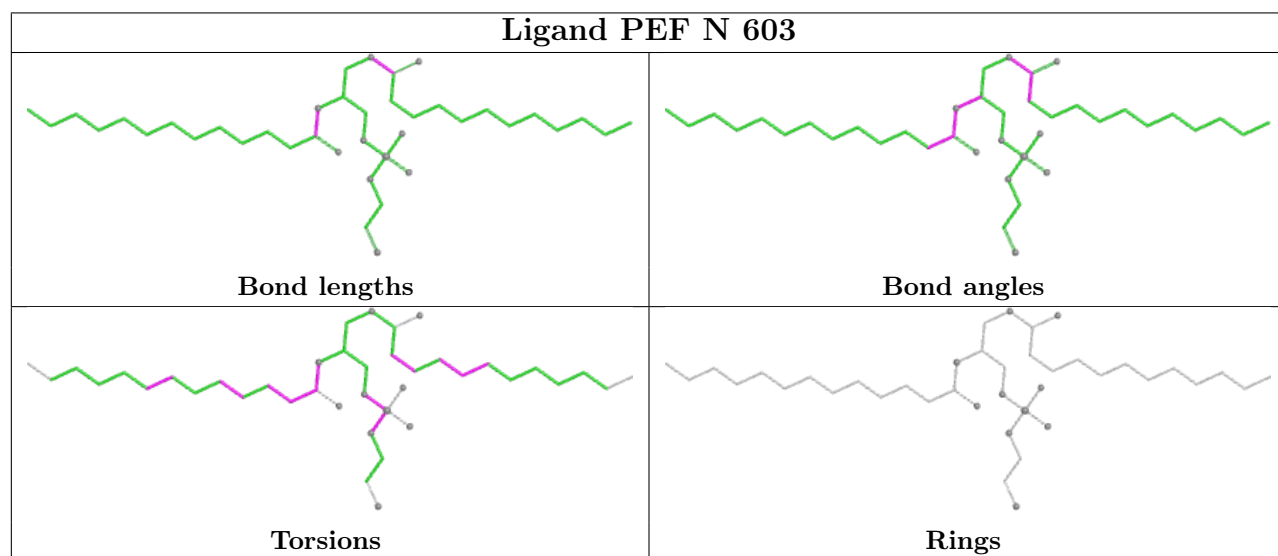
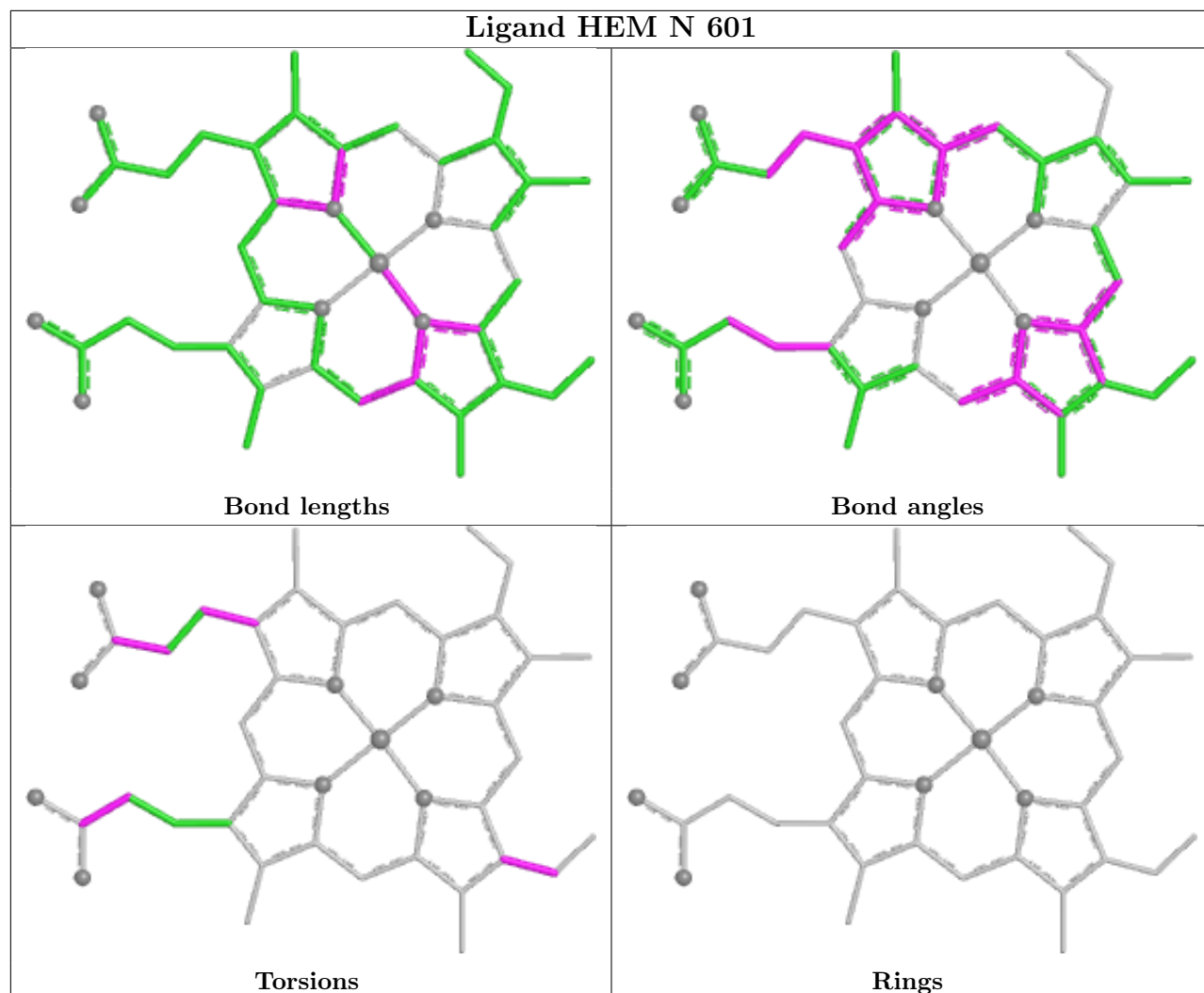


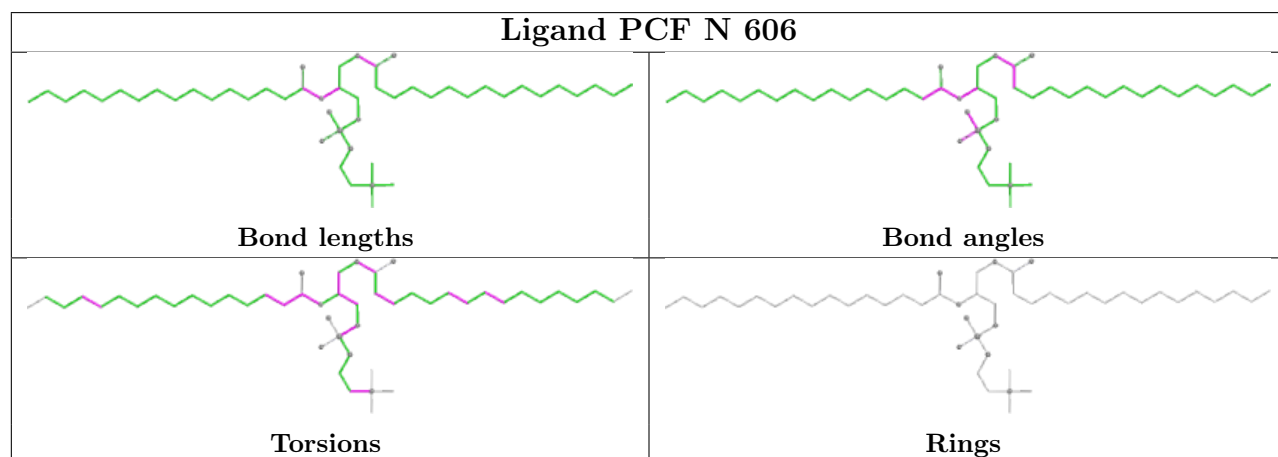
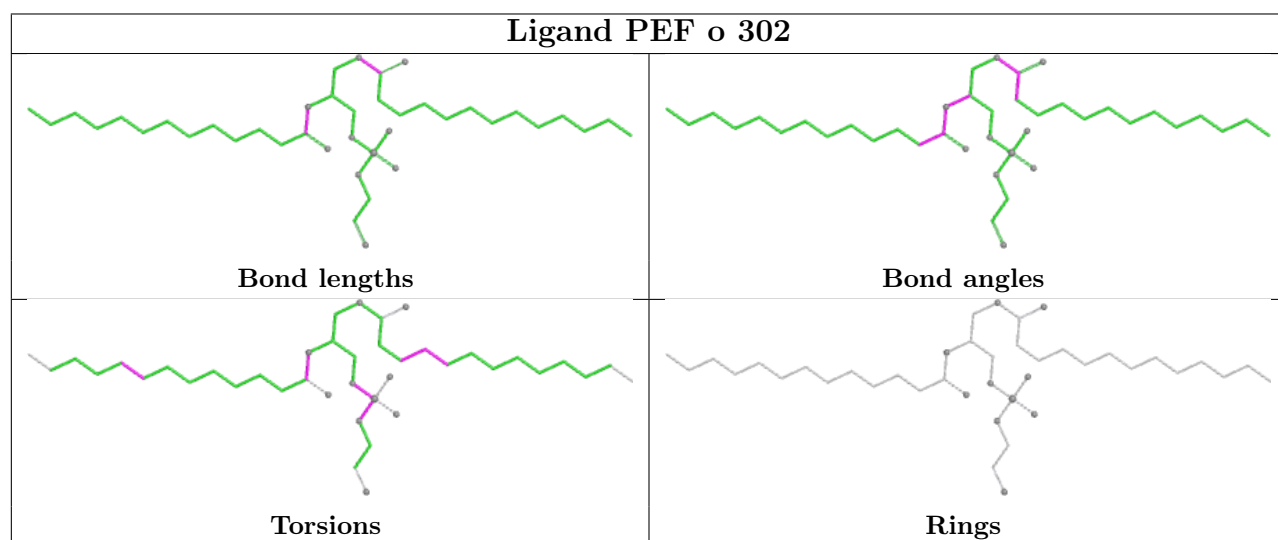
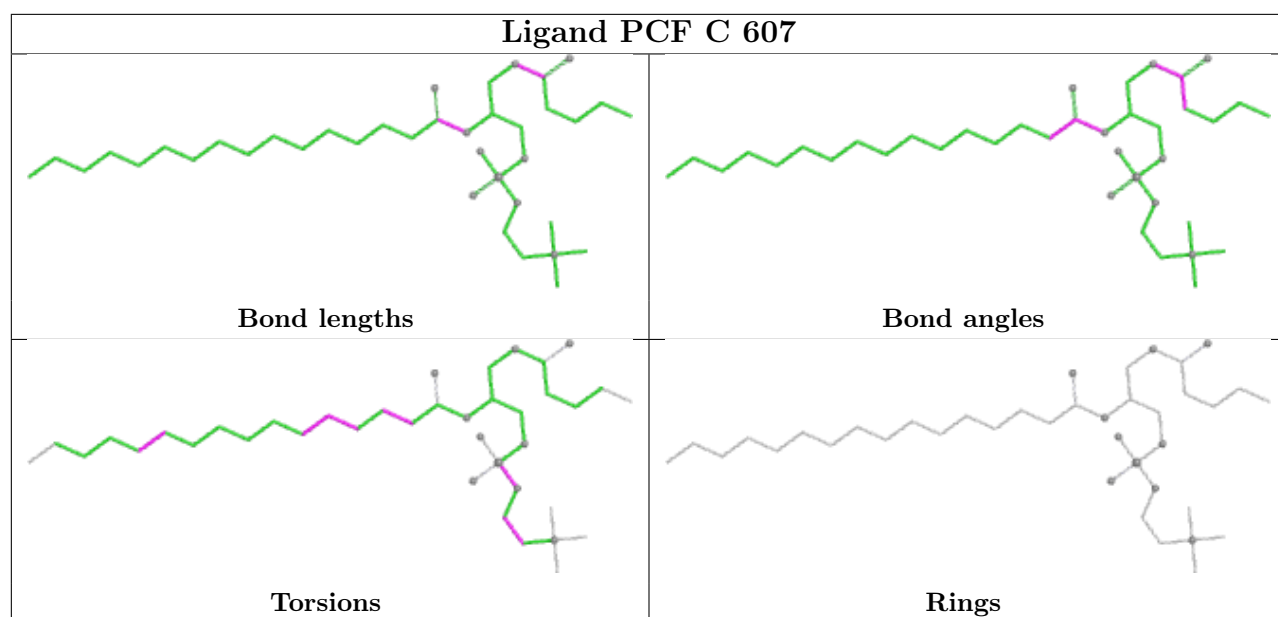


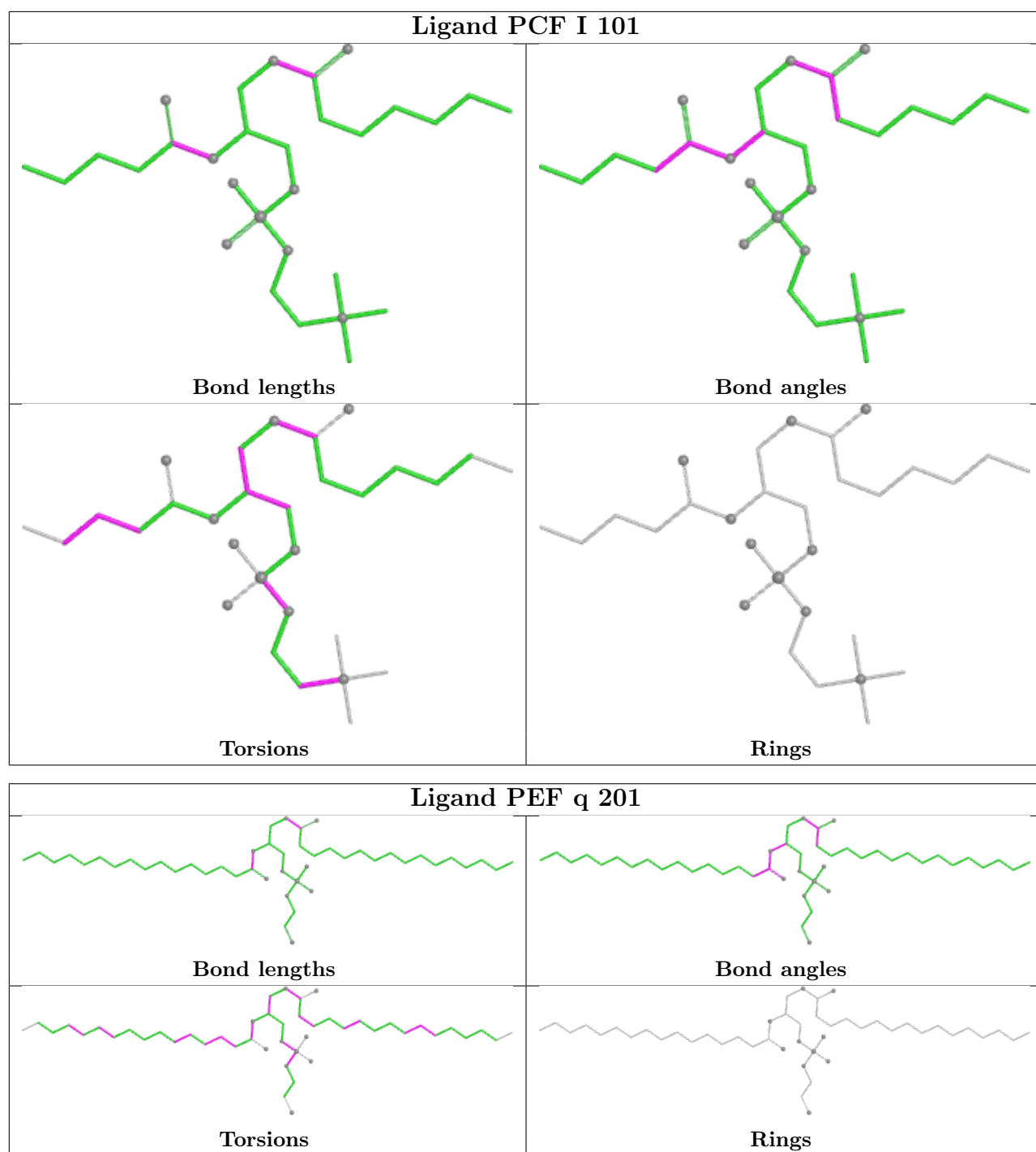


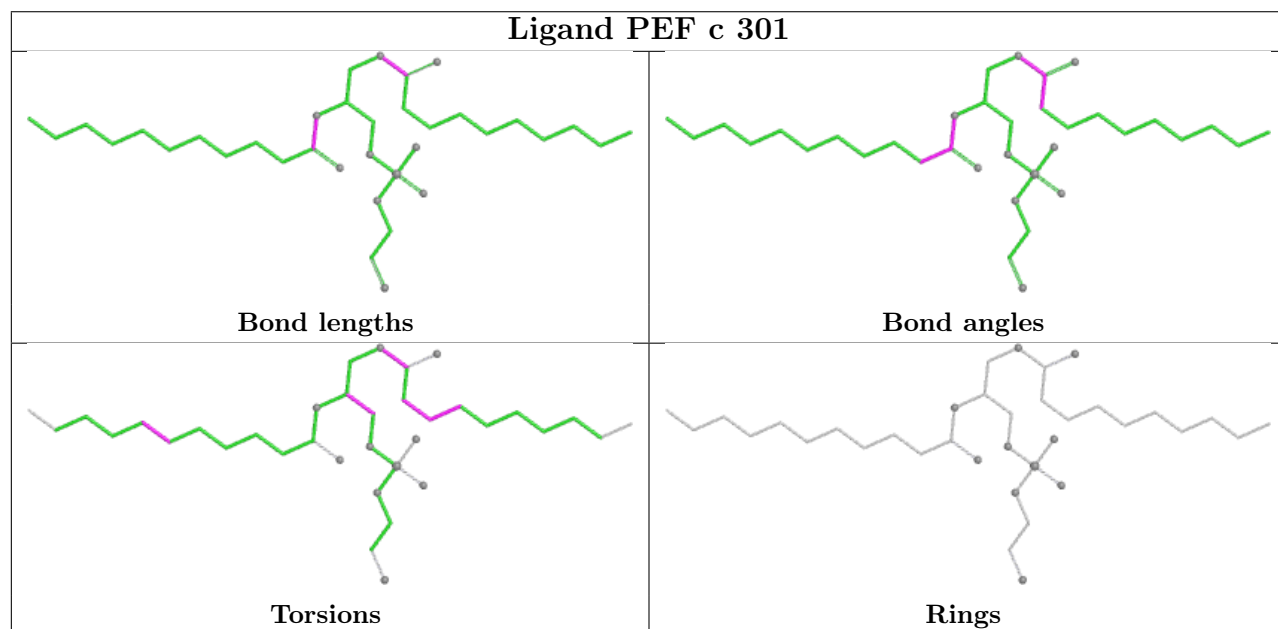
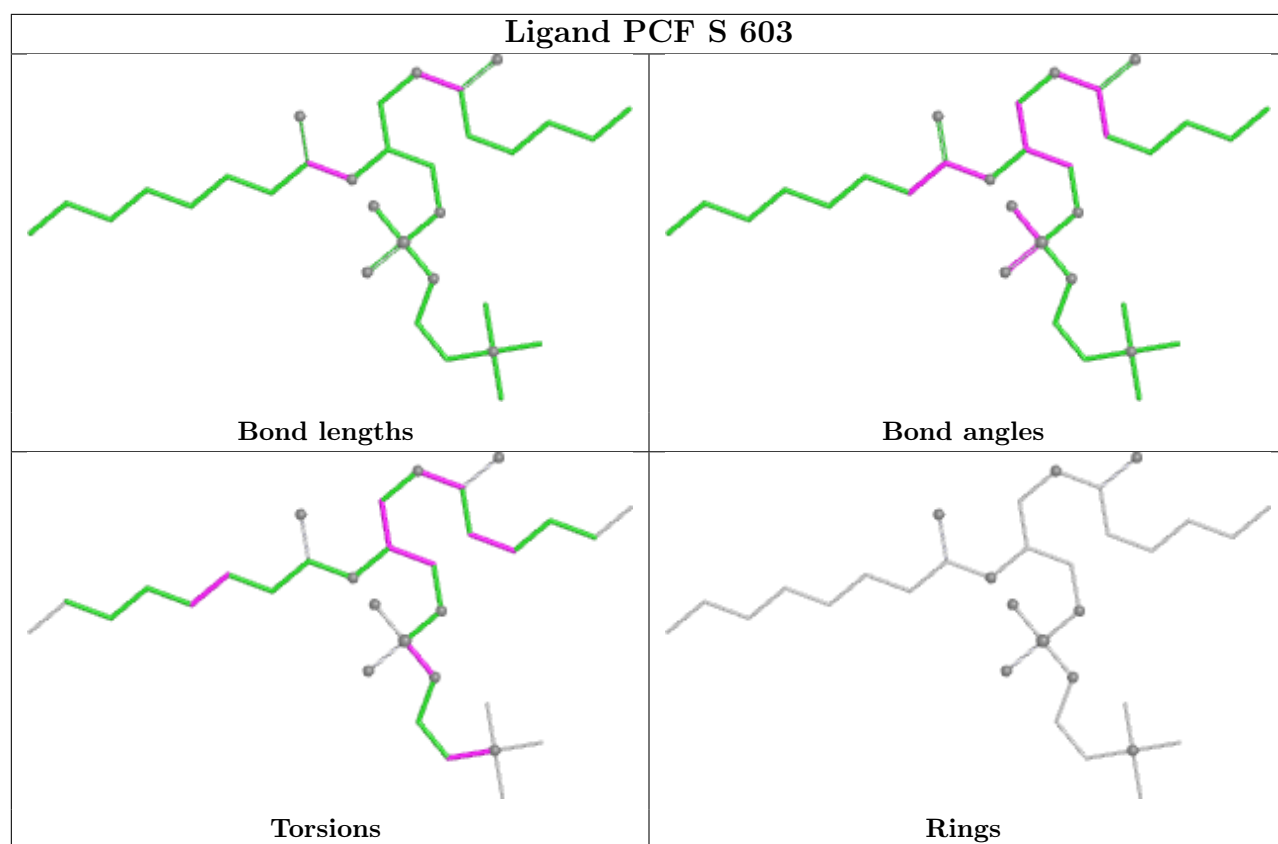


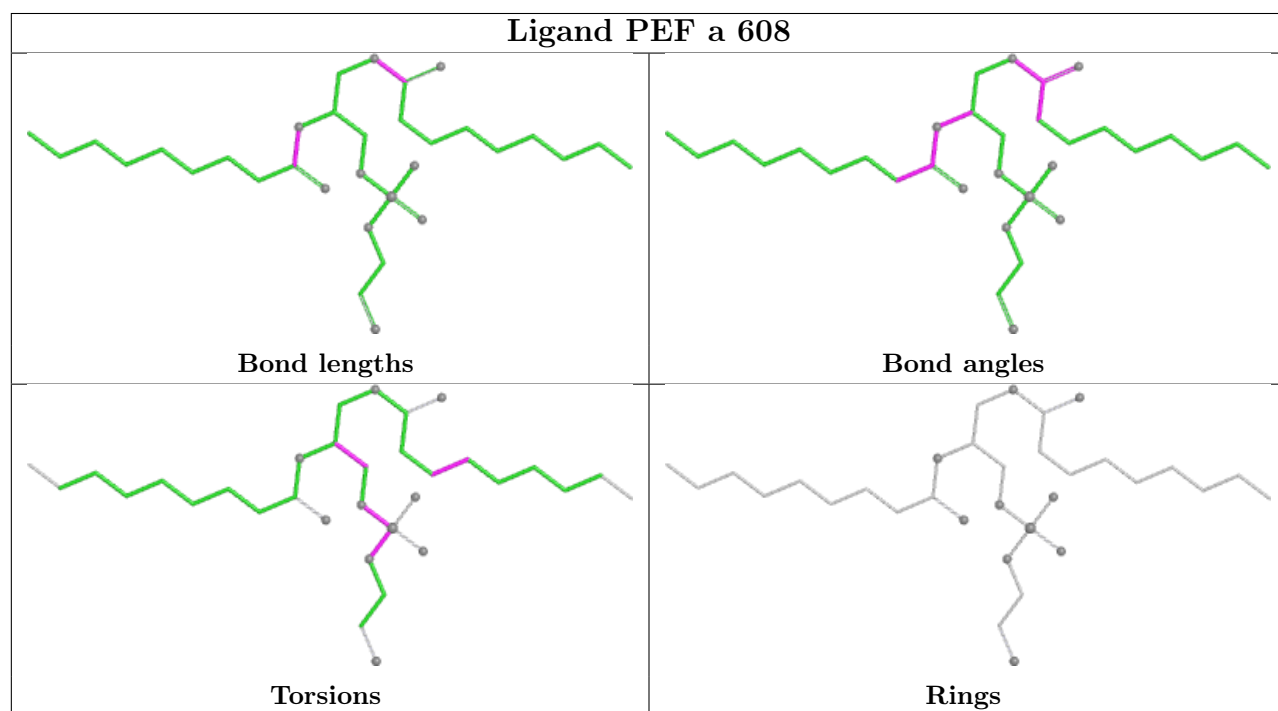
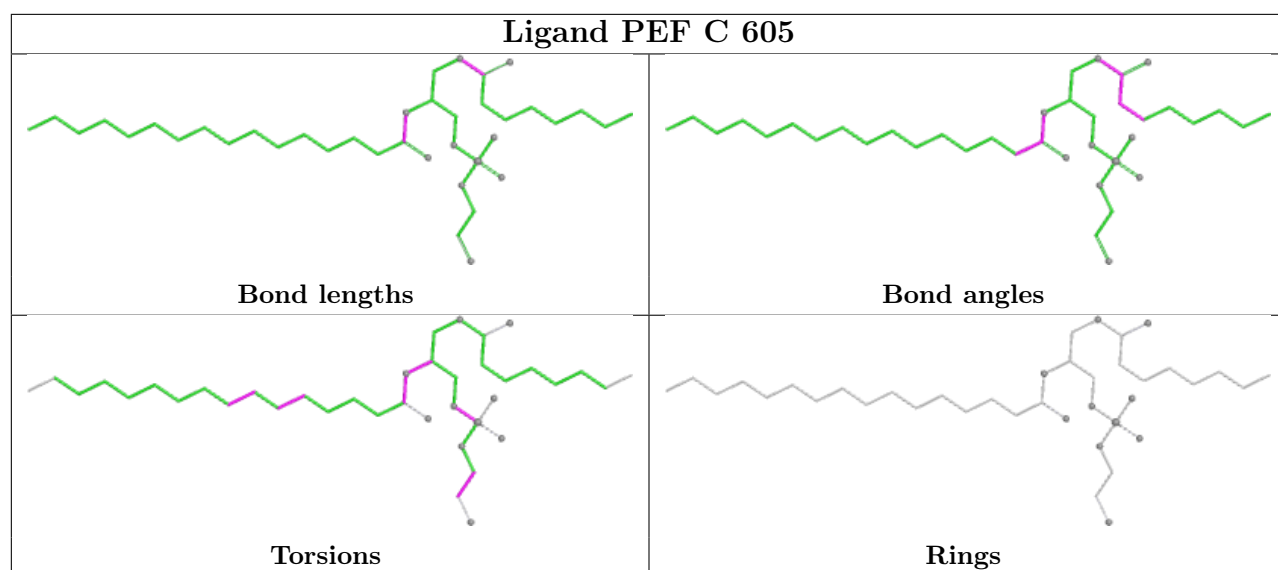




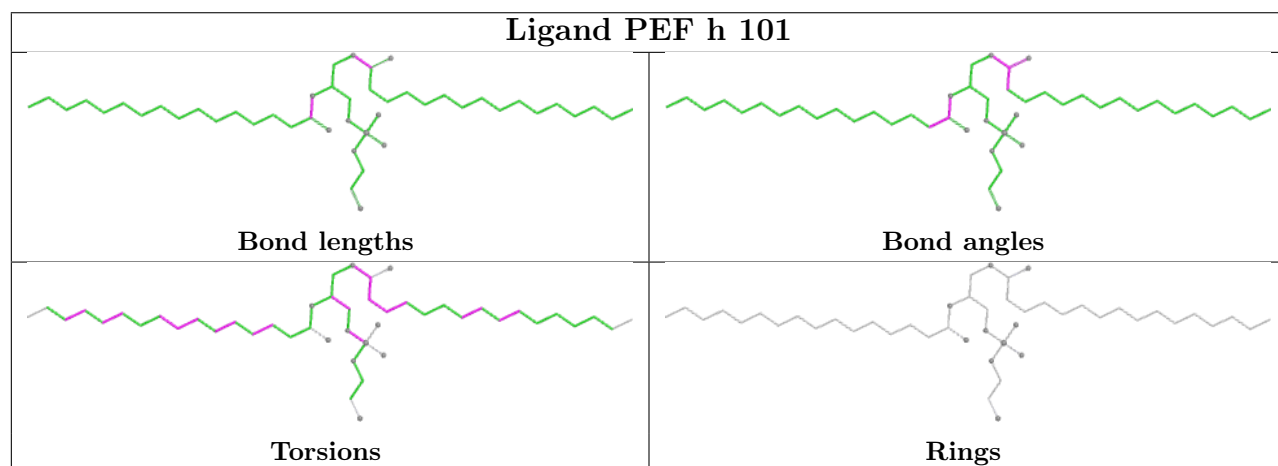
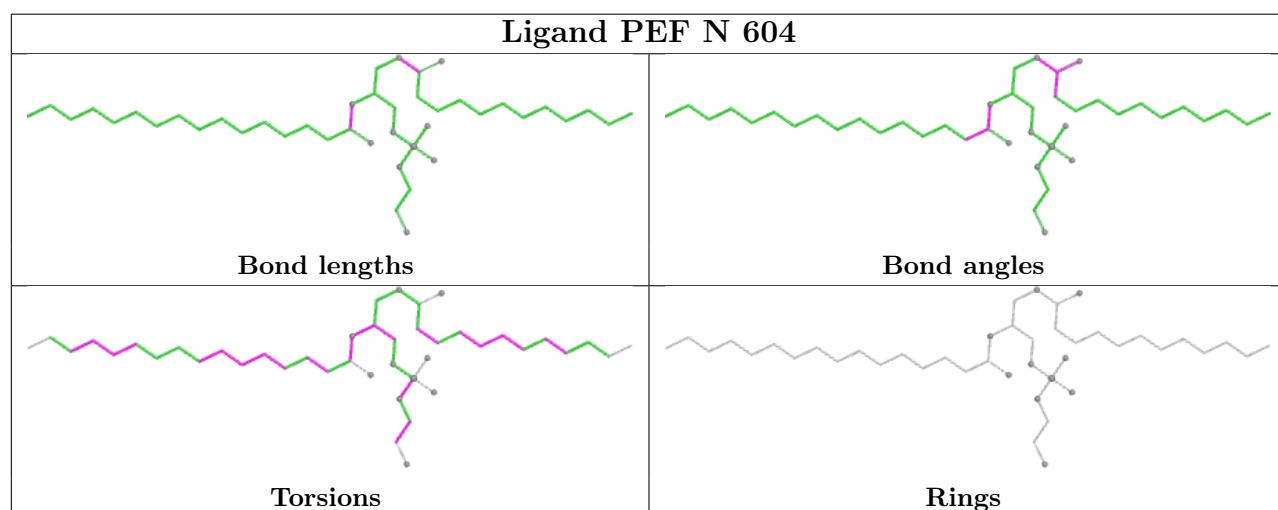
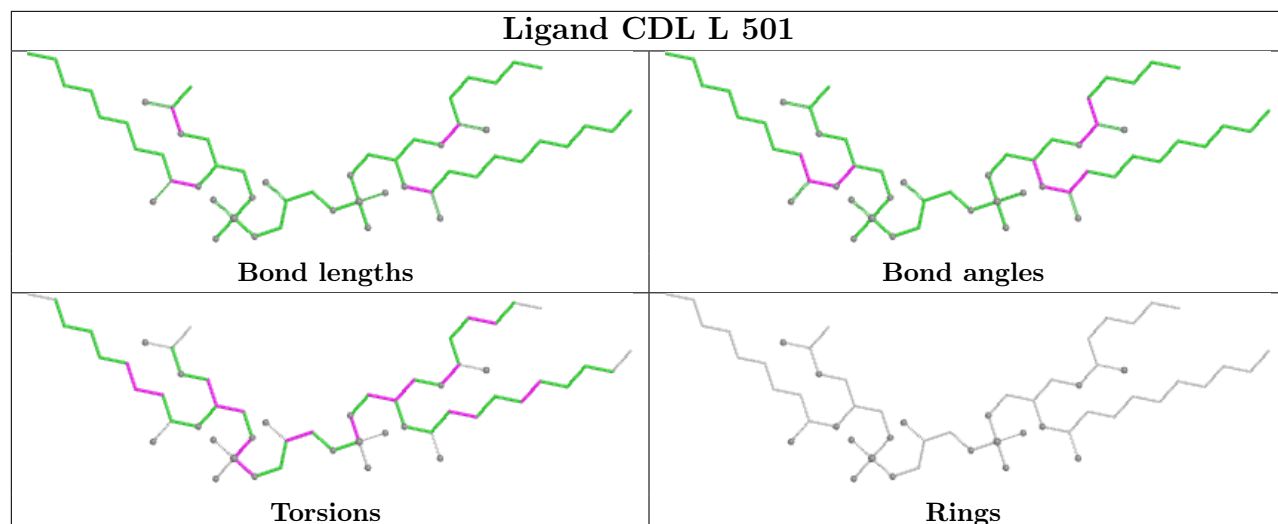


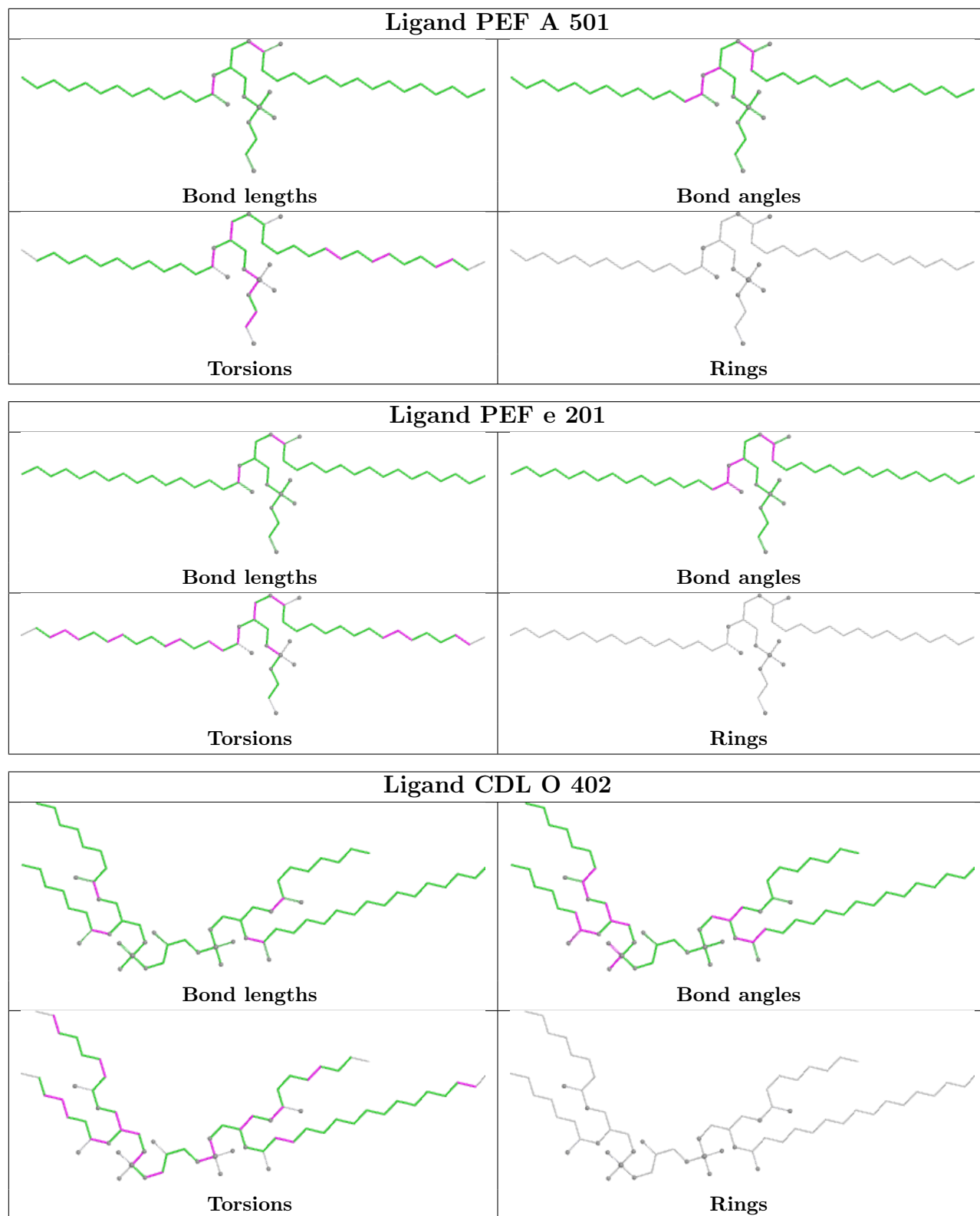


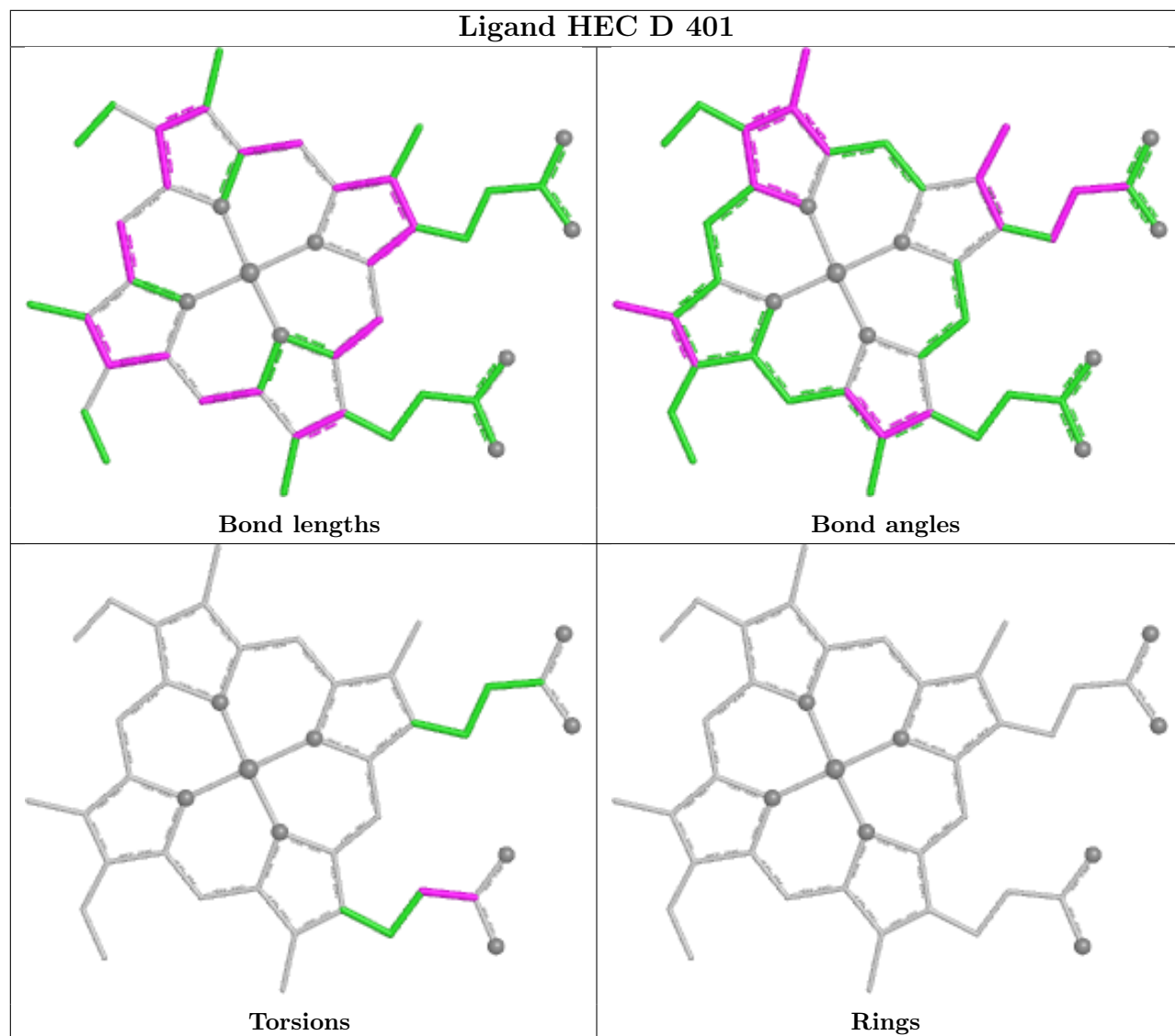


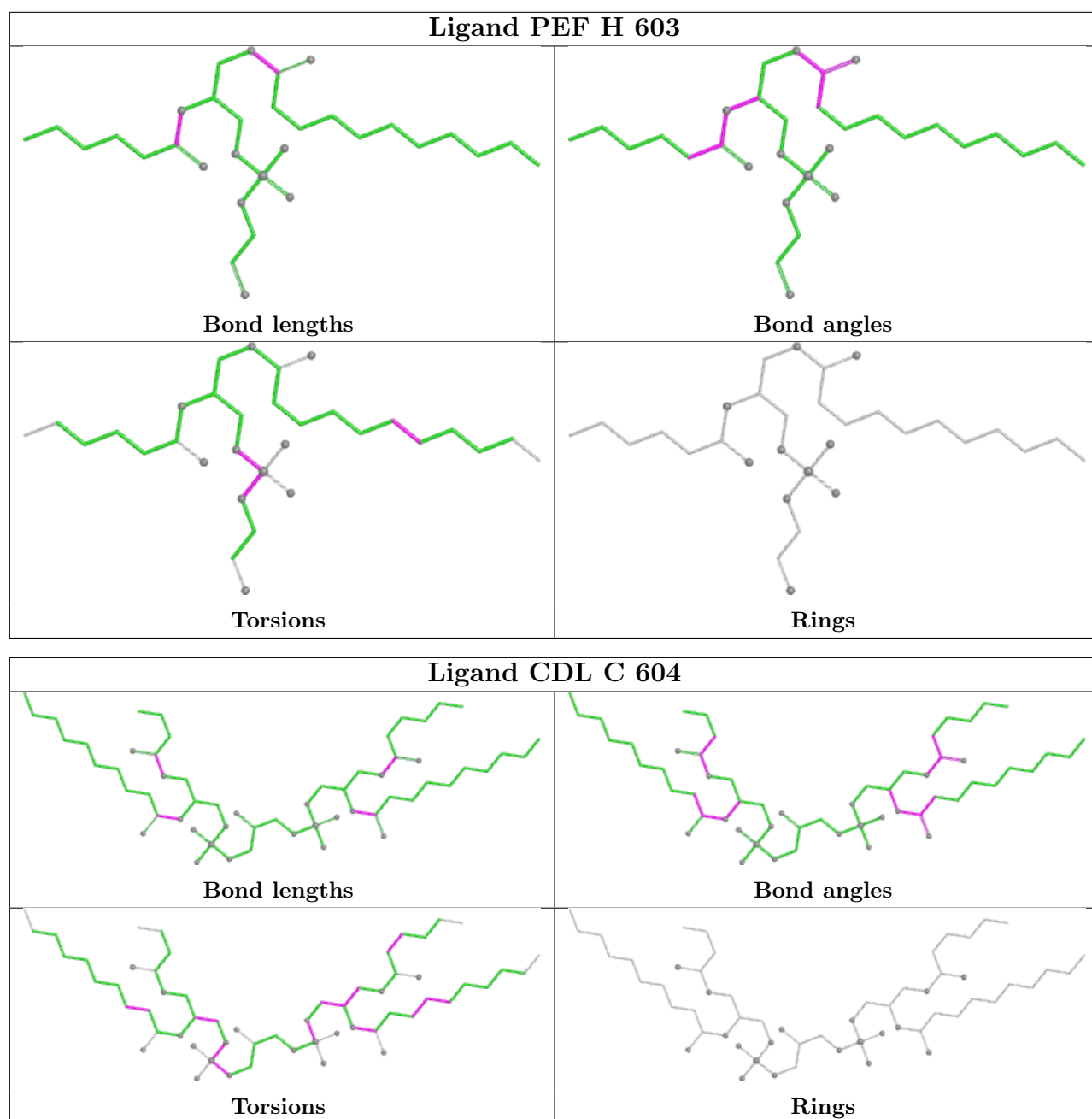


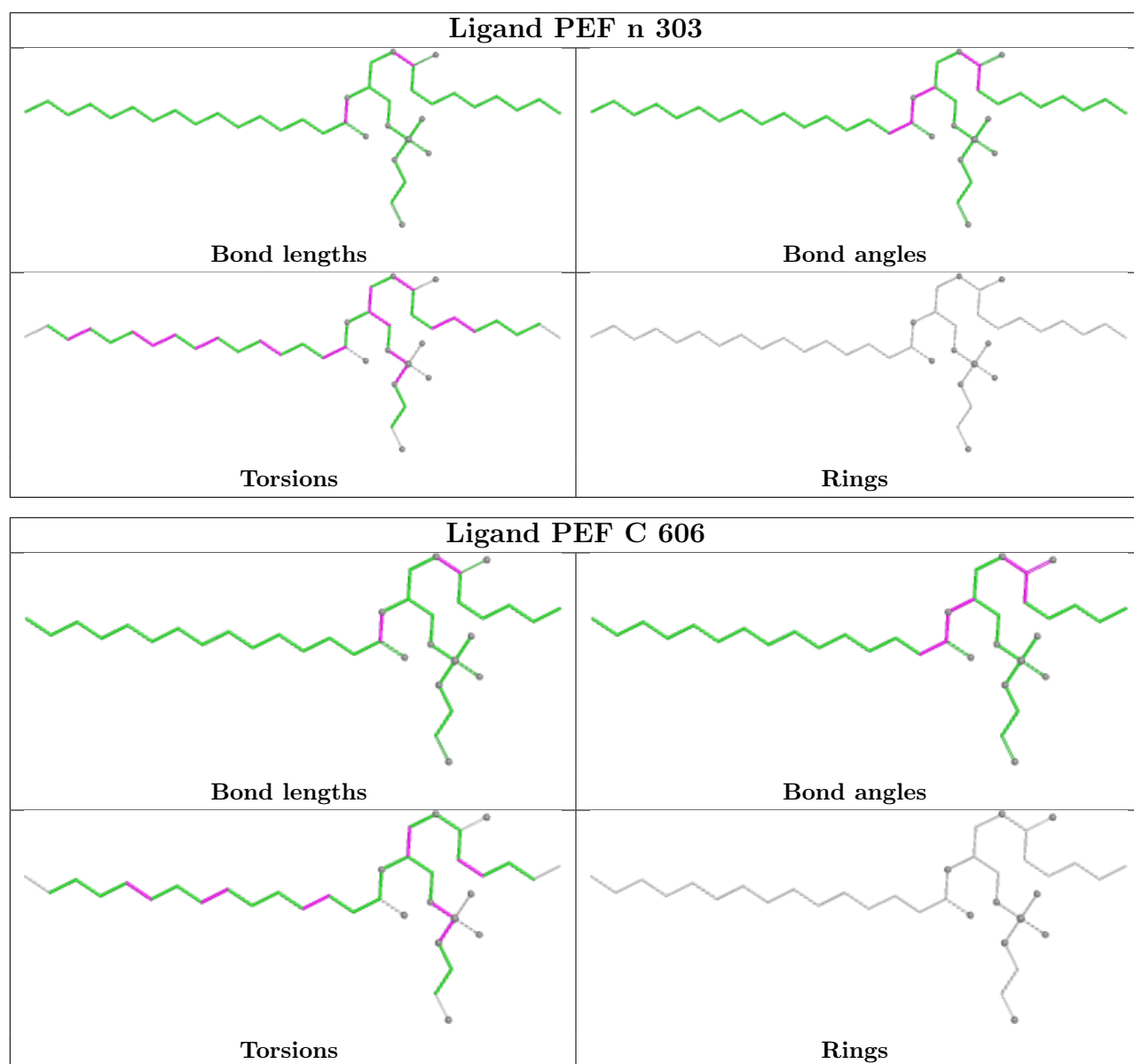


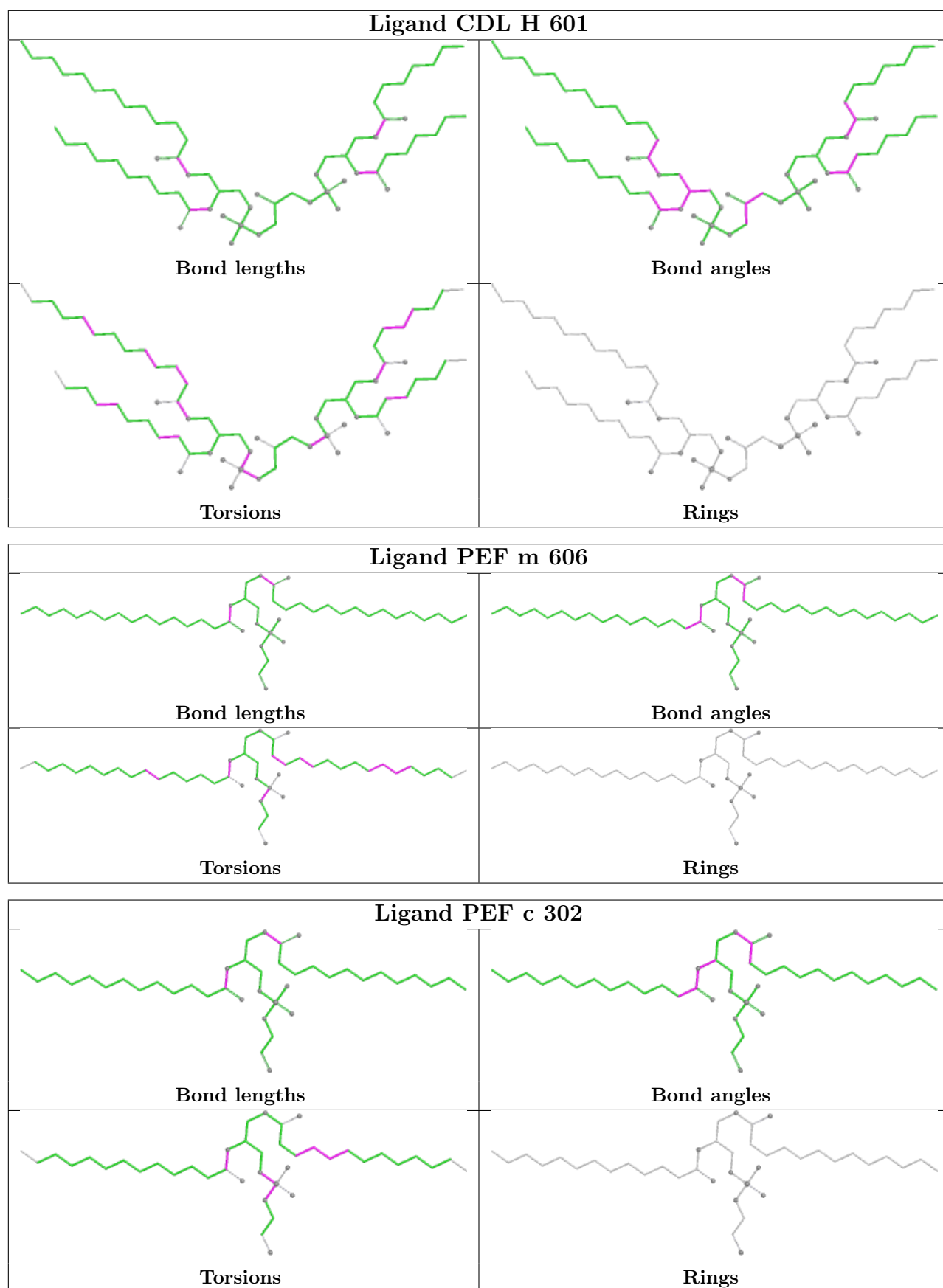


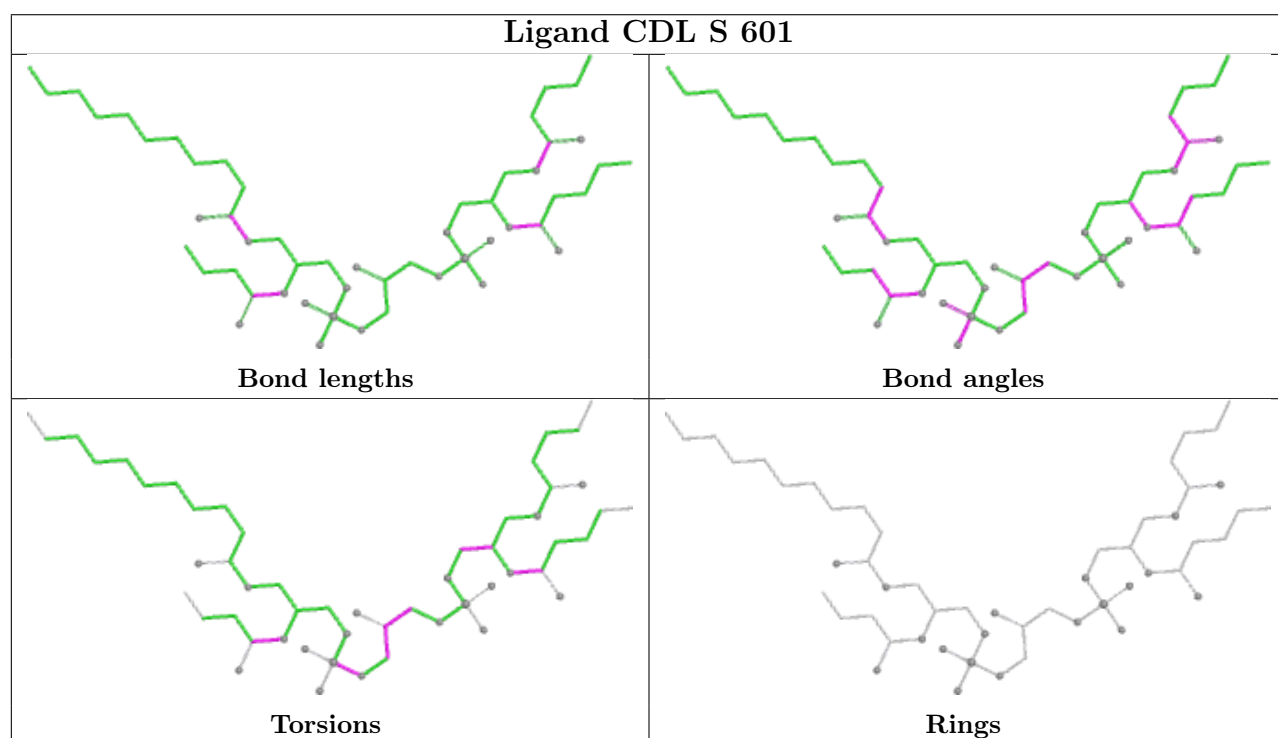
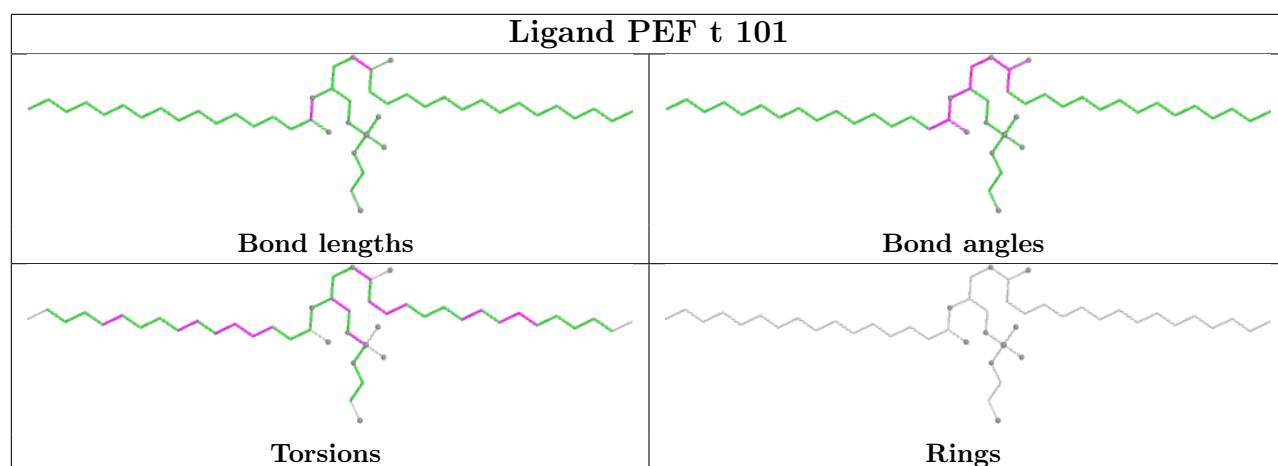


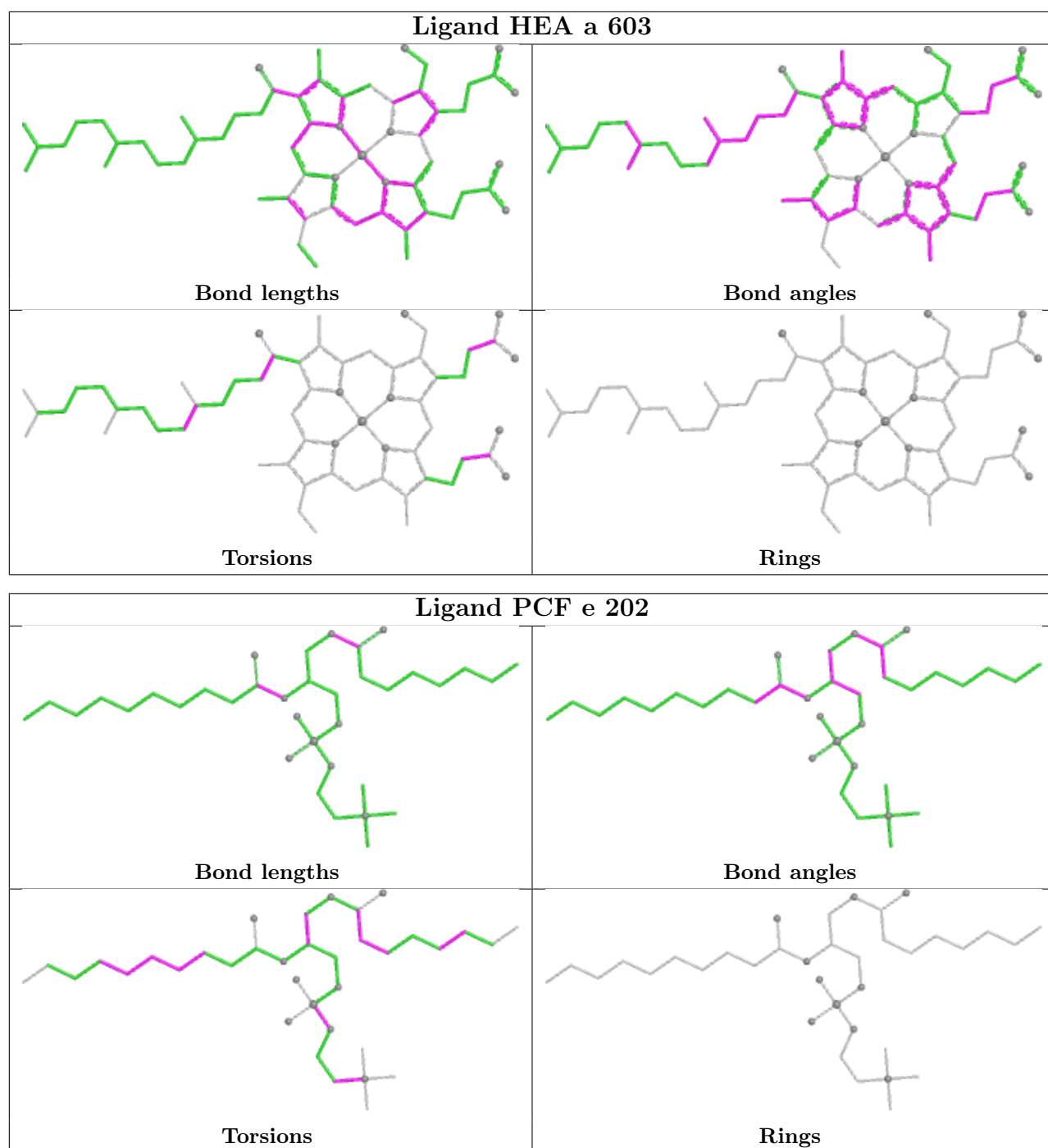




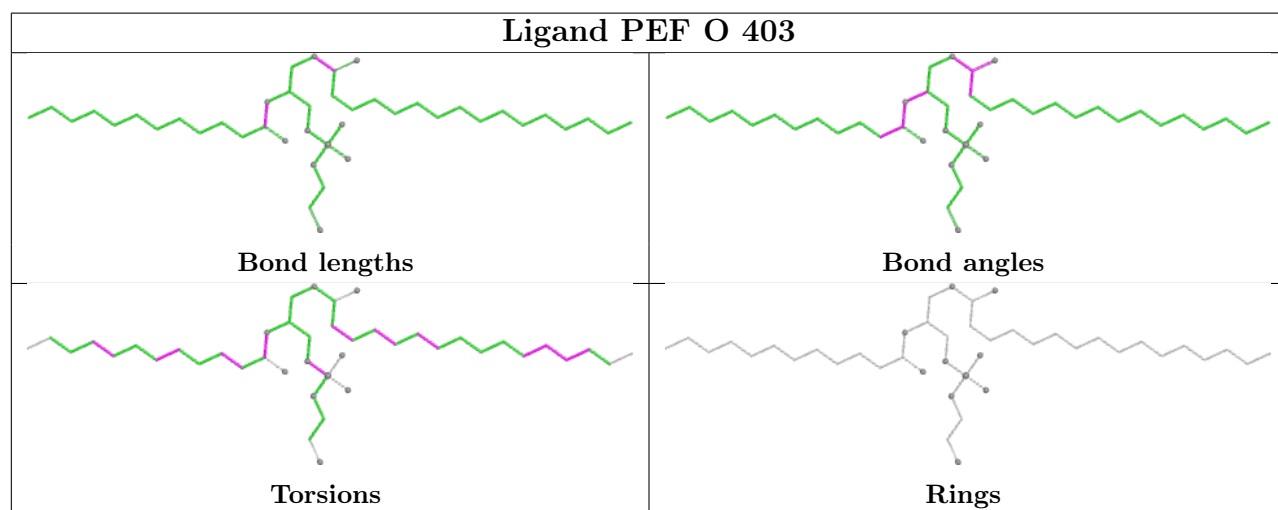
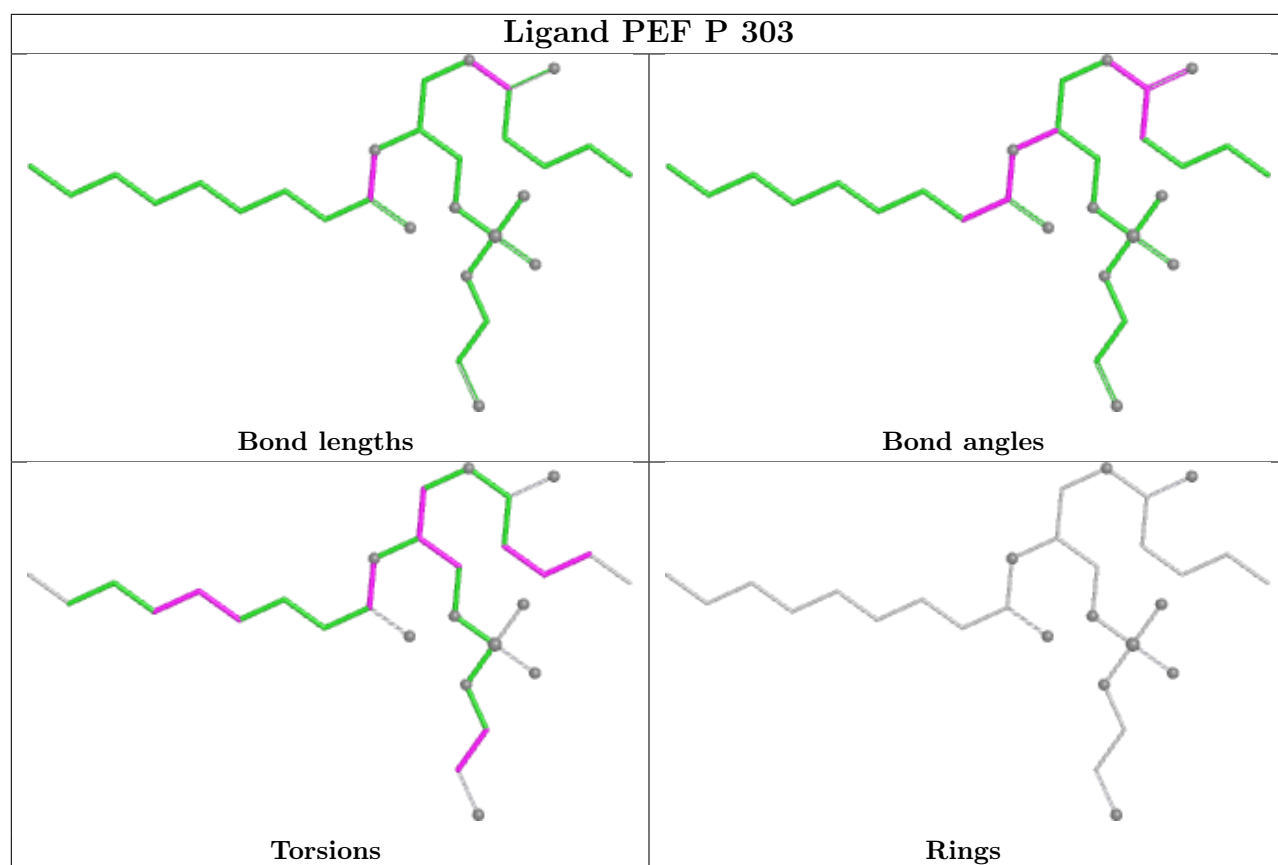


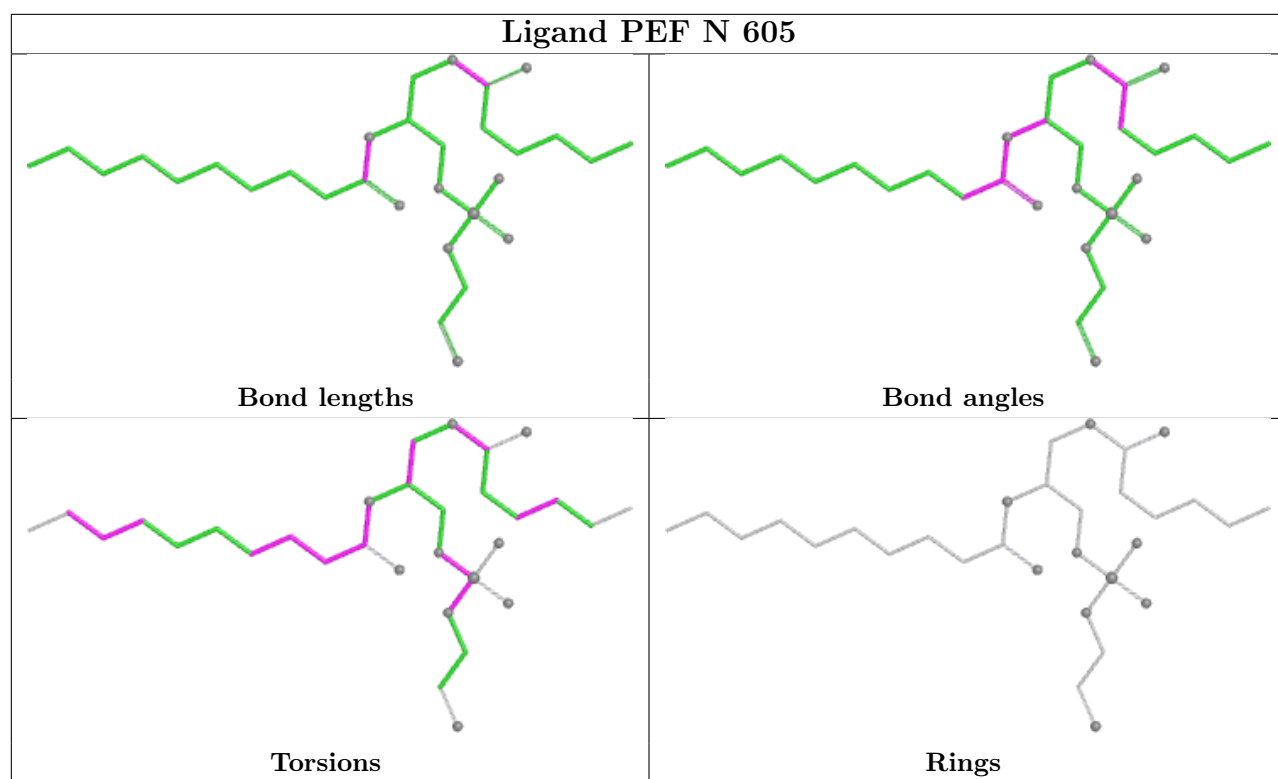


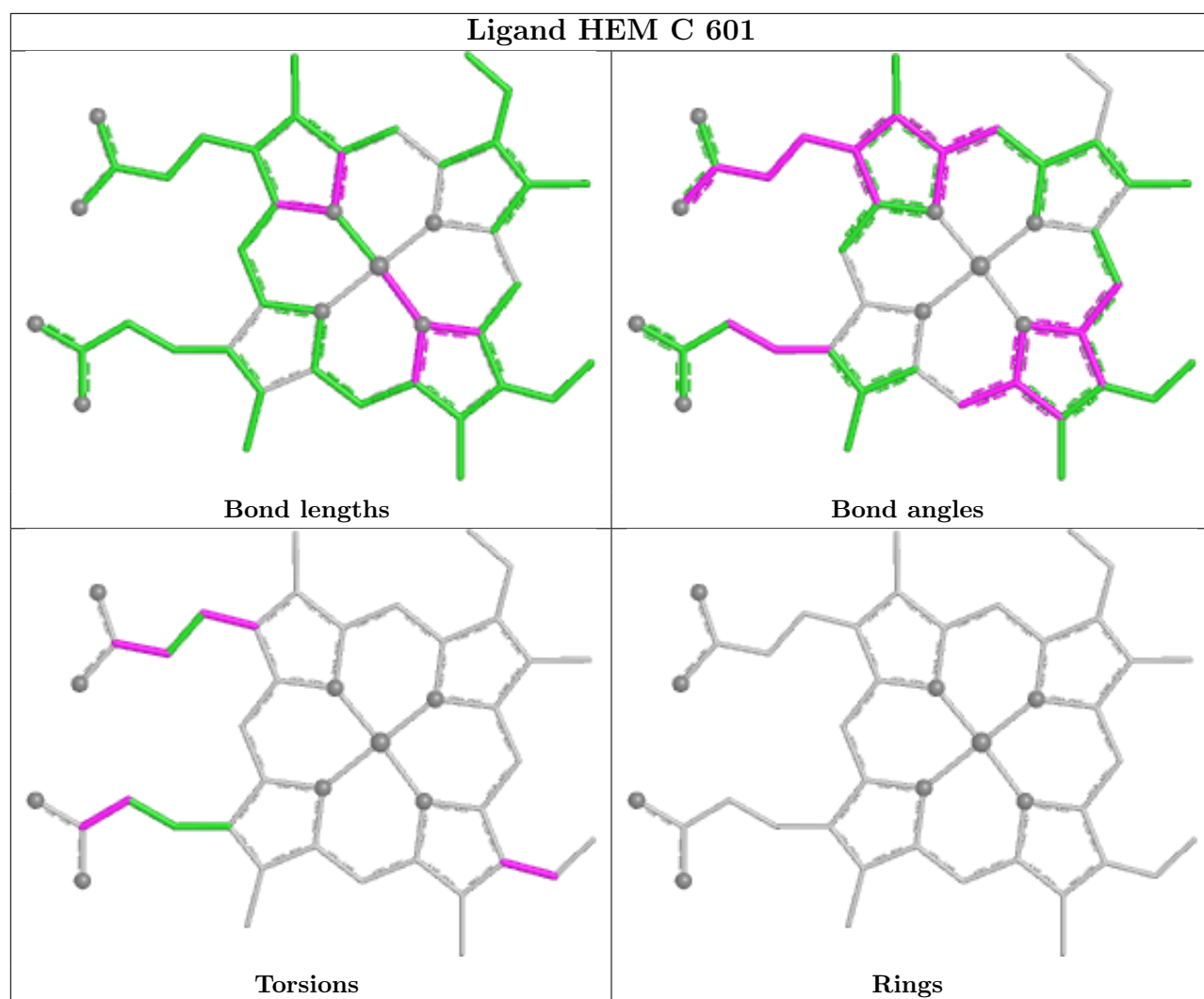


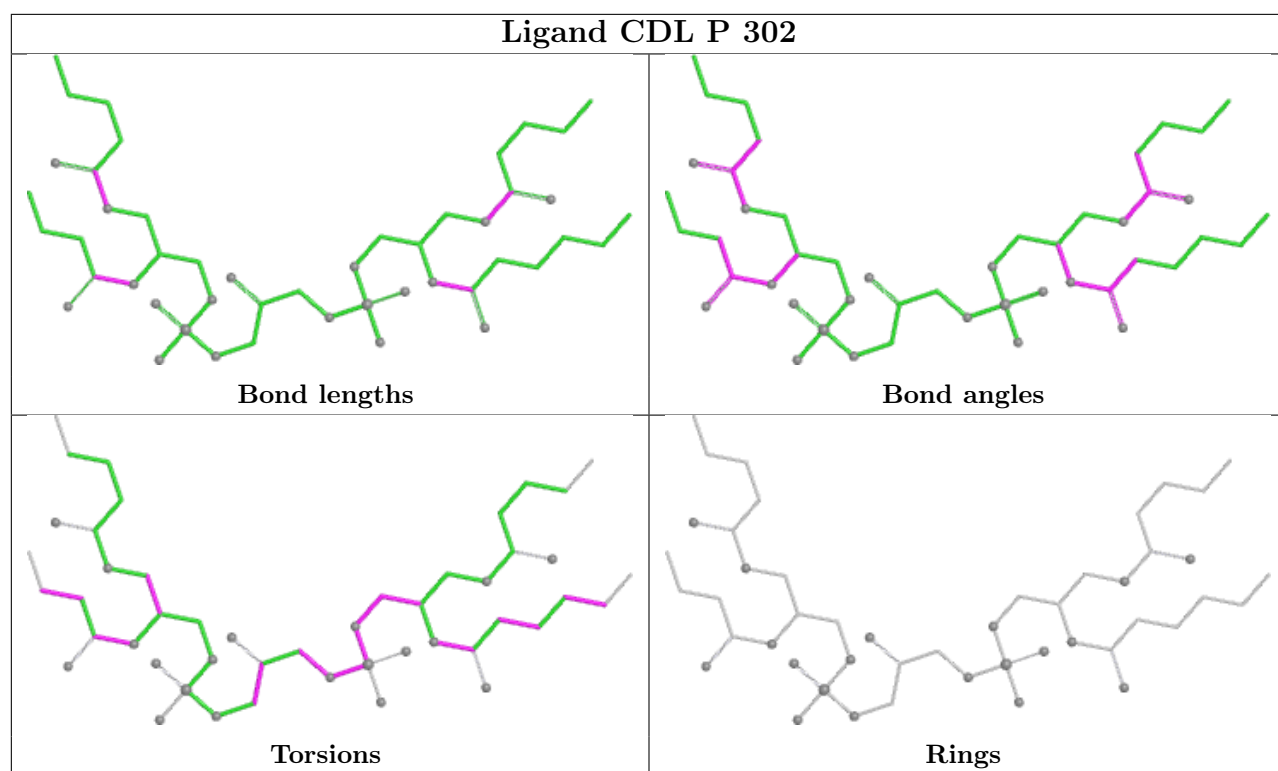


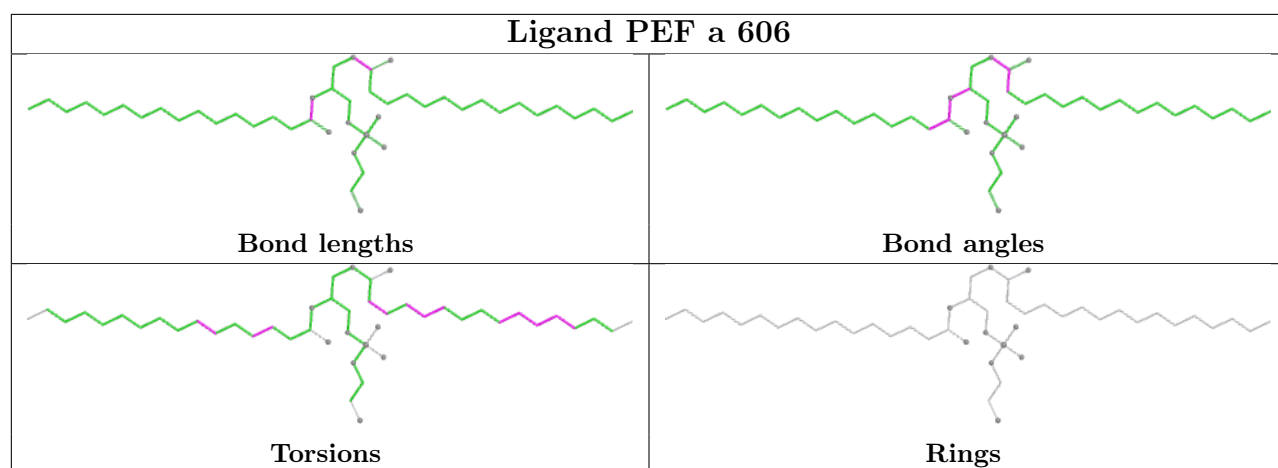
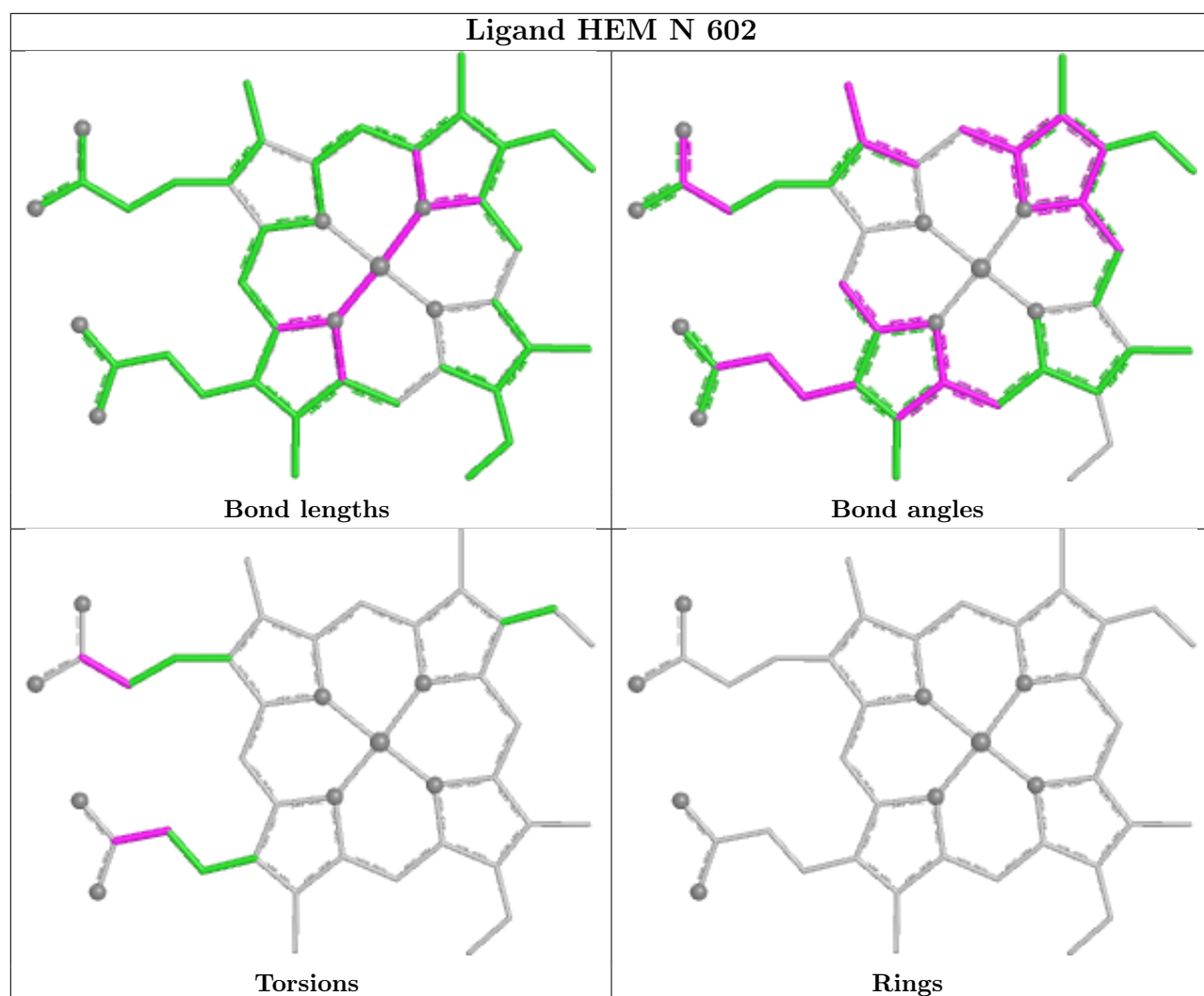


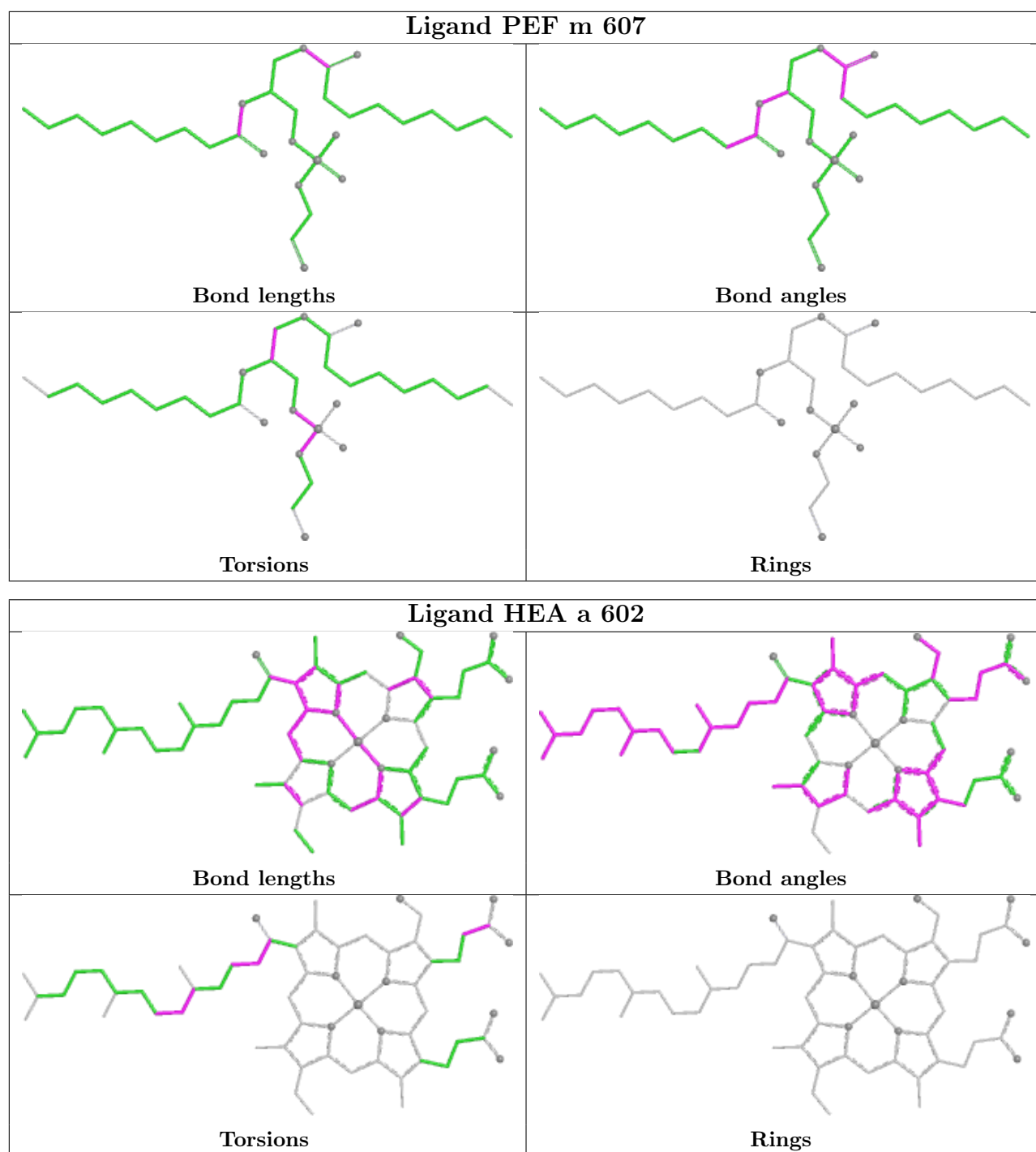












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

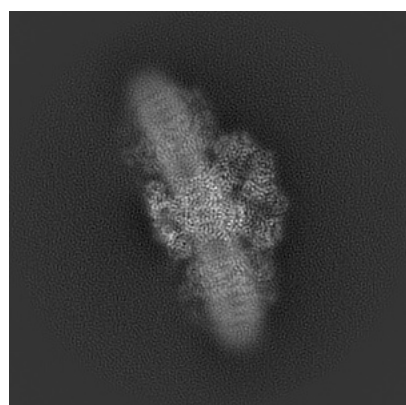
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0262. These allow visual inspection of the internal detail of the map and identification of artifacts.

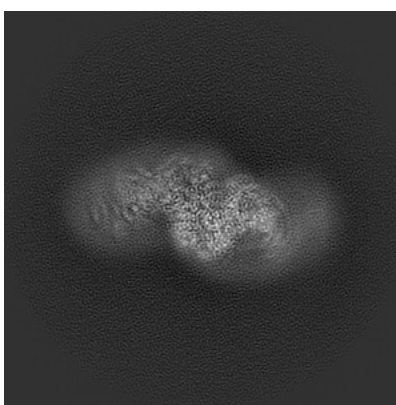
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

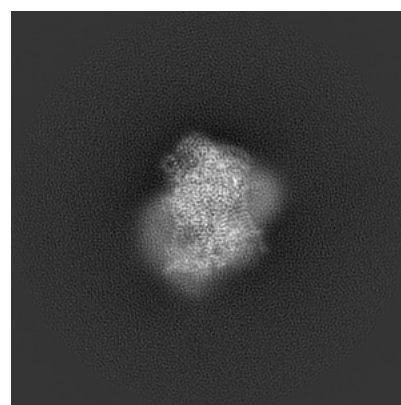
#### 6.1.1 Primary map



X



Y

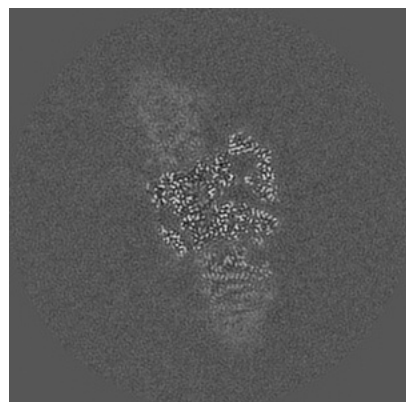


Z

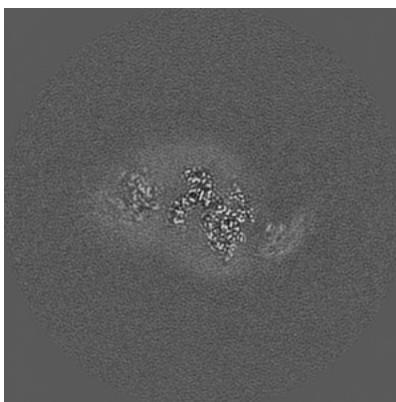
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

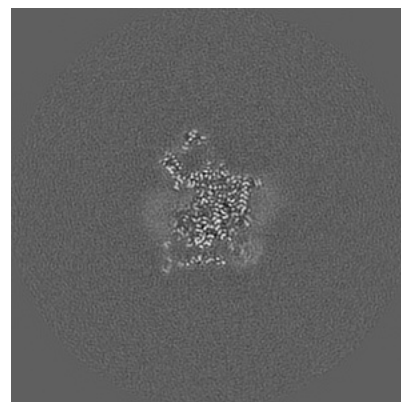
#### 6.2.1 Primary map



X Index: 155



Y Index: 155

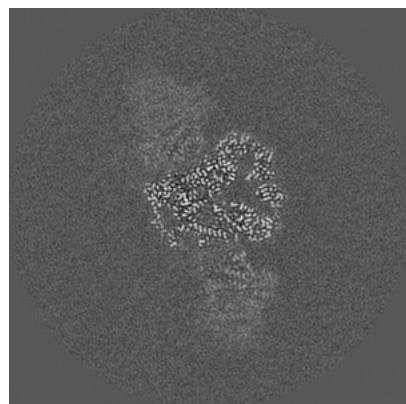


Z Index: 155

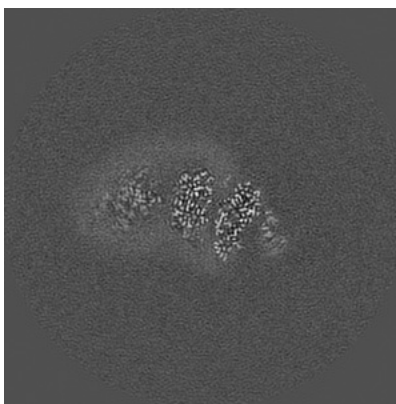
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

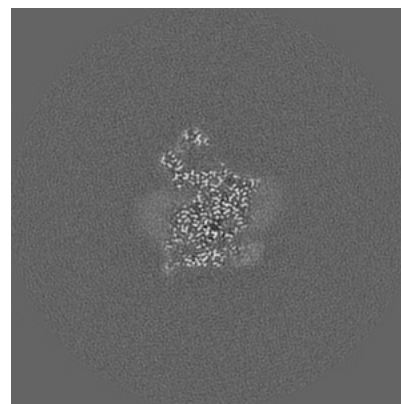
### 6.3.1 Primary map



X Index: 151



Y Index: 163

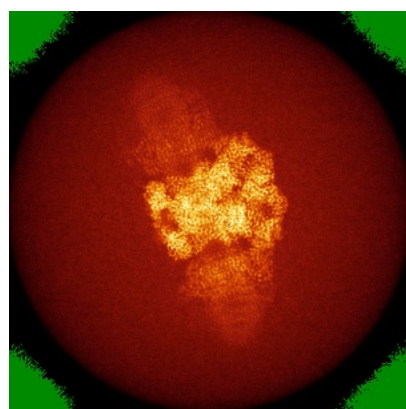


Z Index: 157

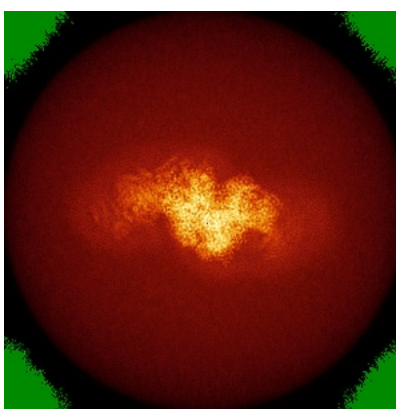
The images above show the largest variance slices of the map in three orthogonal directions.

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

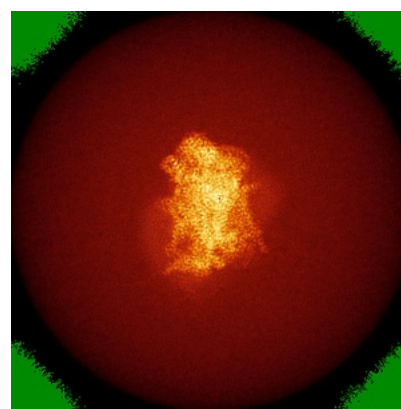
### 6.4.1 Primary map



X



Y



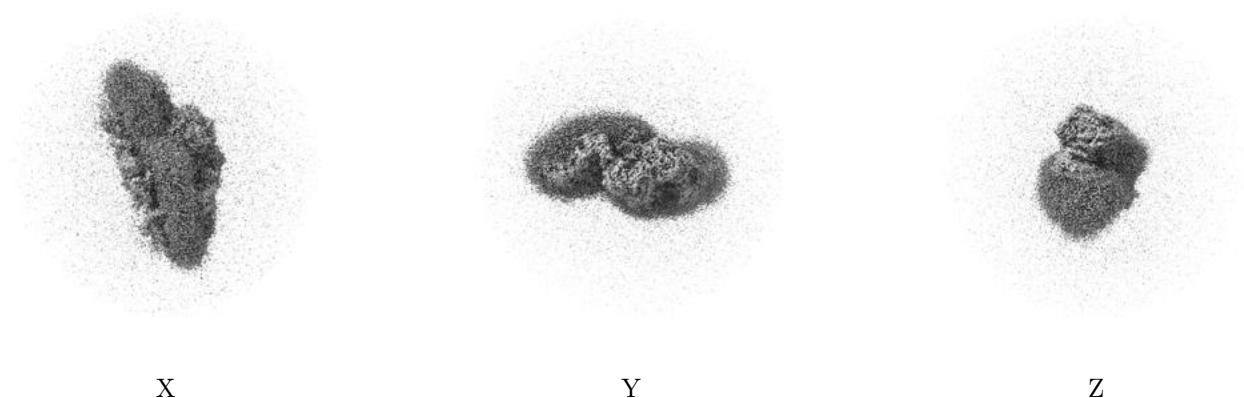
Z

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 0.0263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

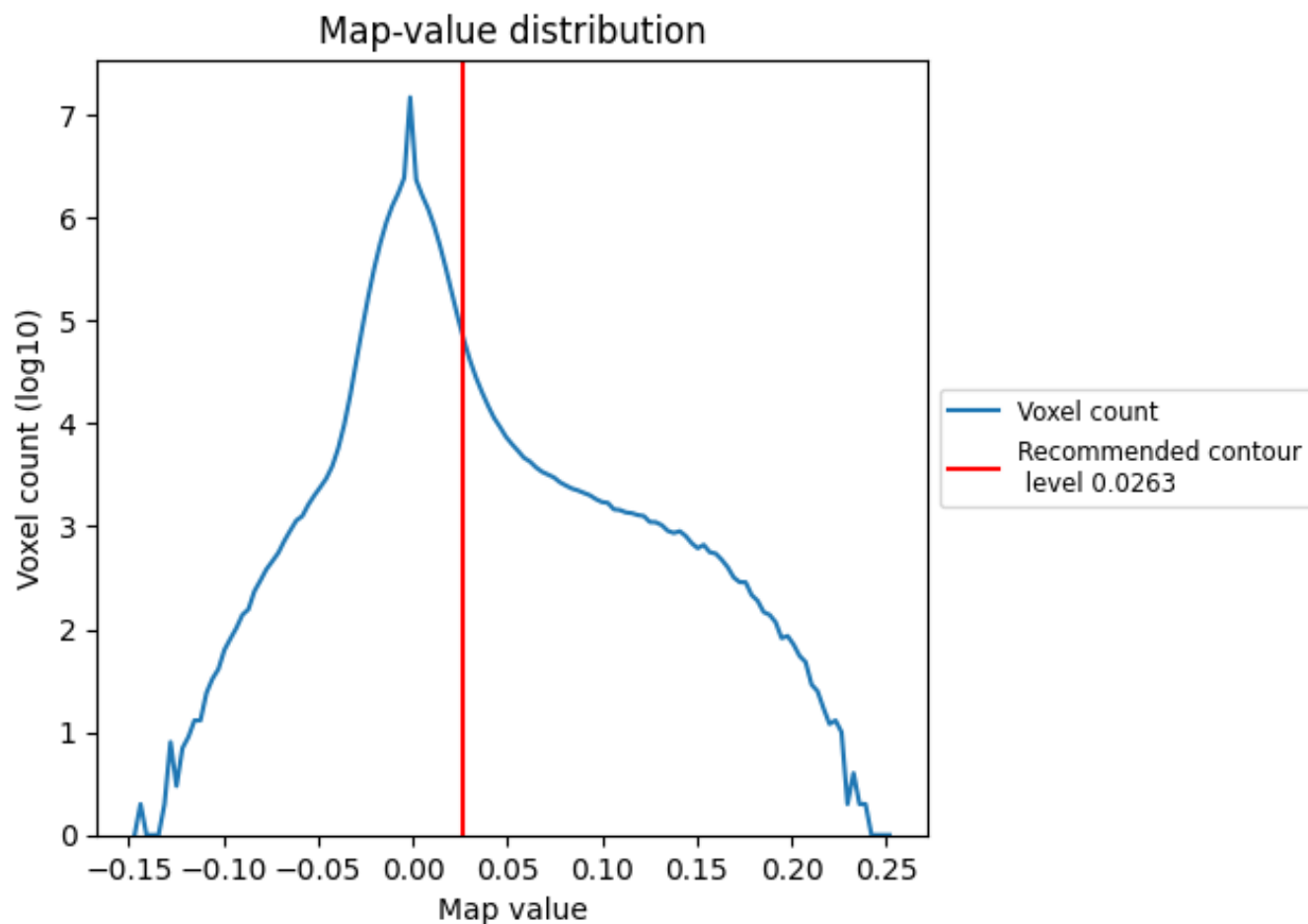
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

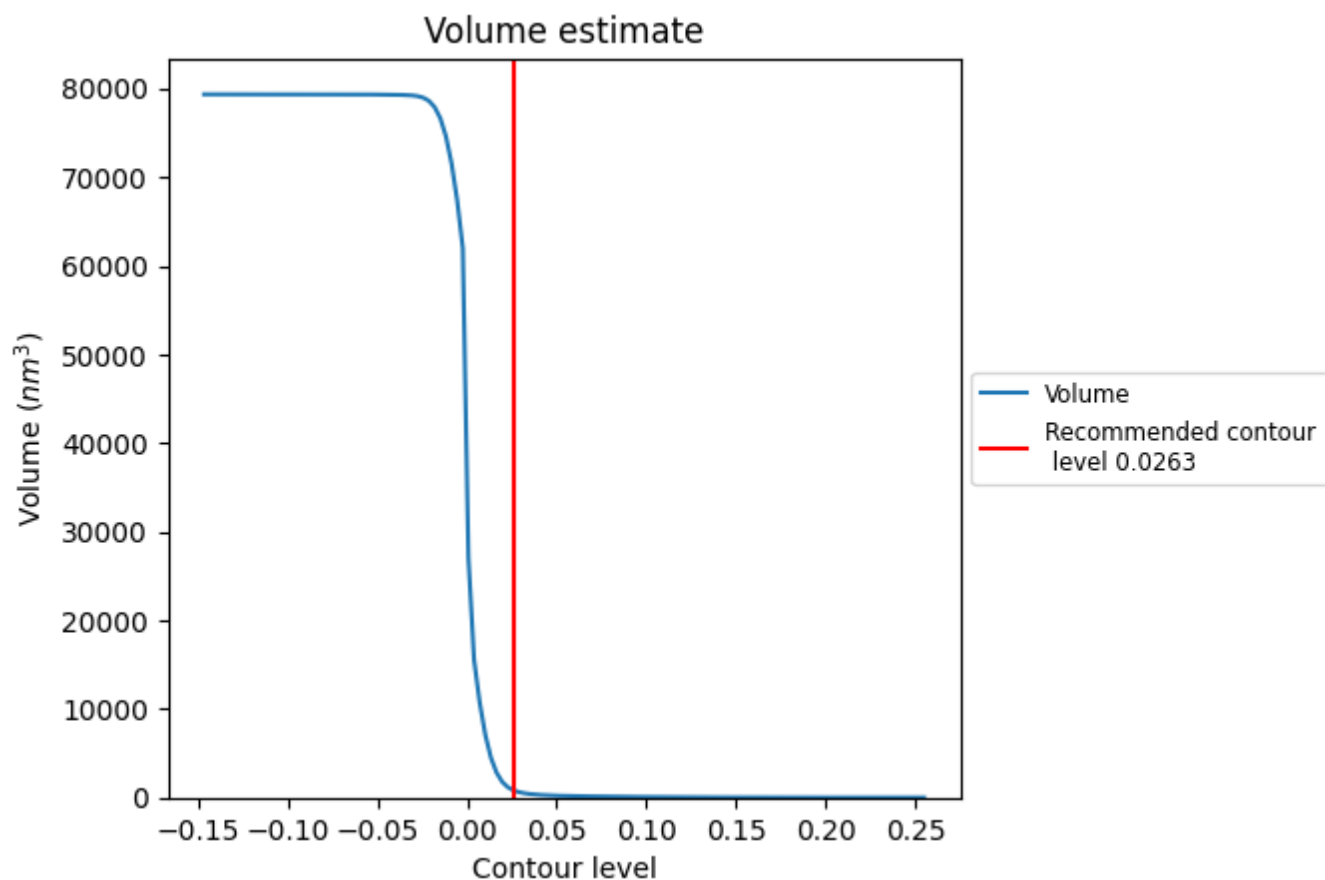
This section contains the results of statistical analysis of the map.

### 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.

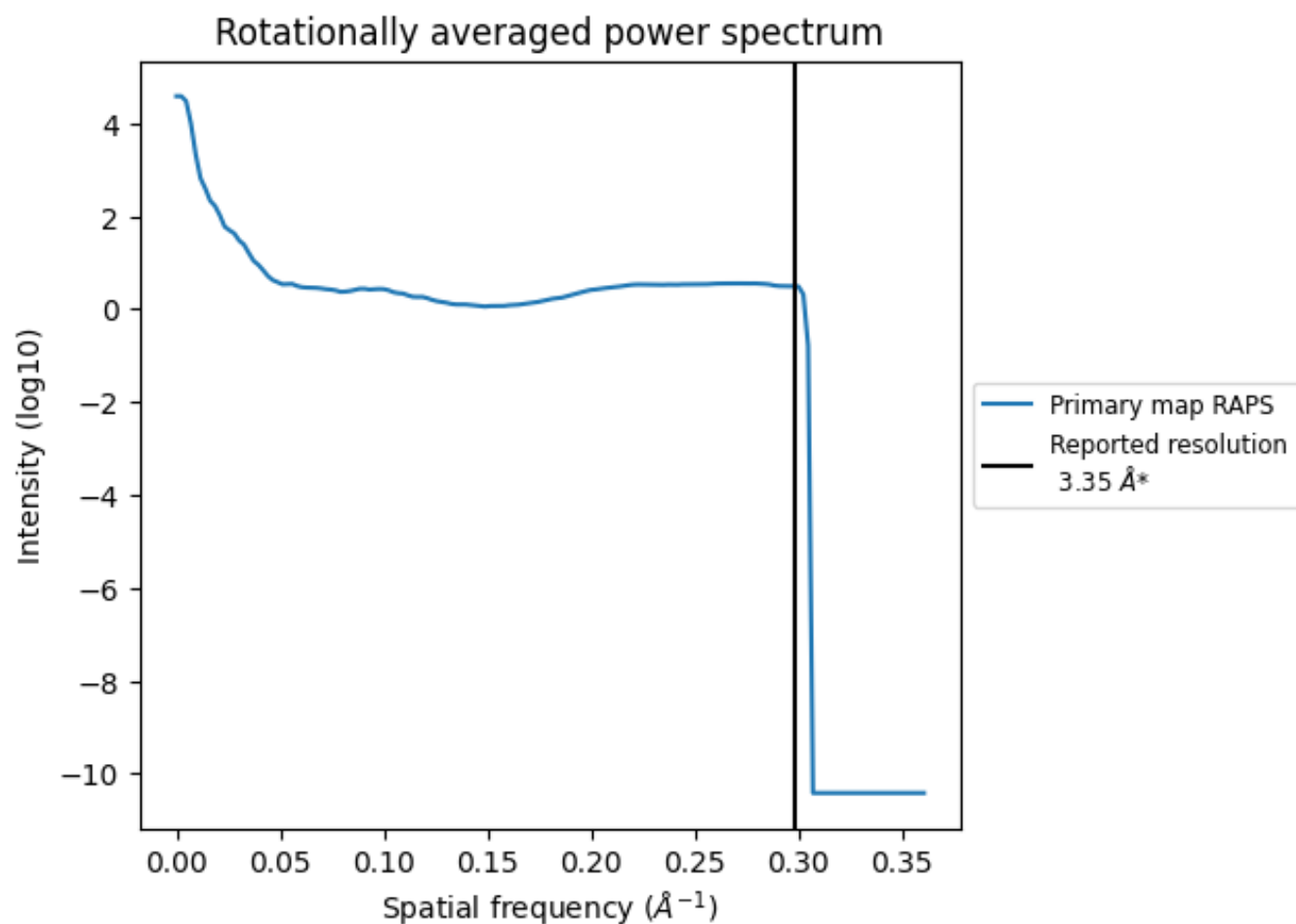
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 786  $\text{nm}^3$ ; this corresponds to an approximate mass of 710 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 ⓘ

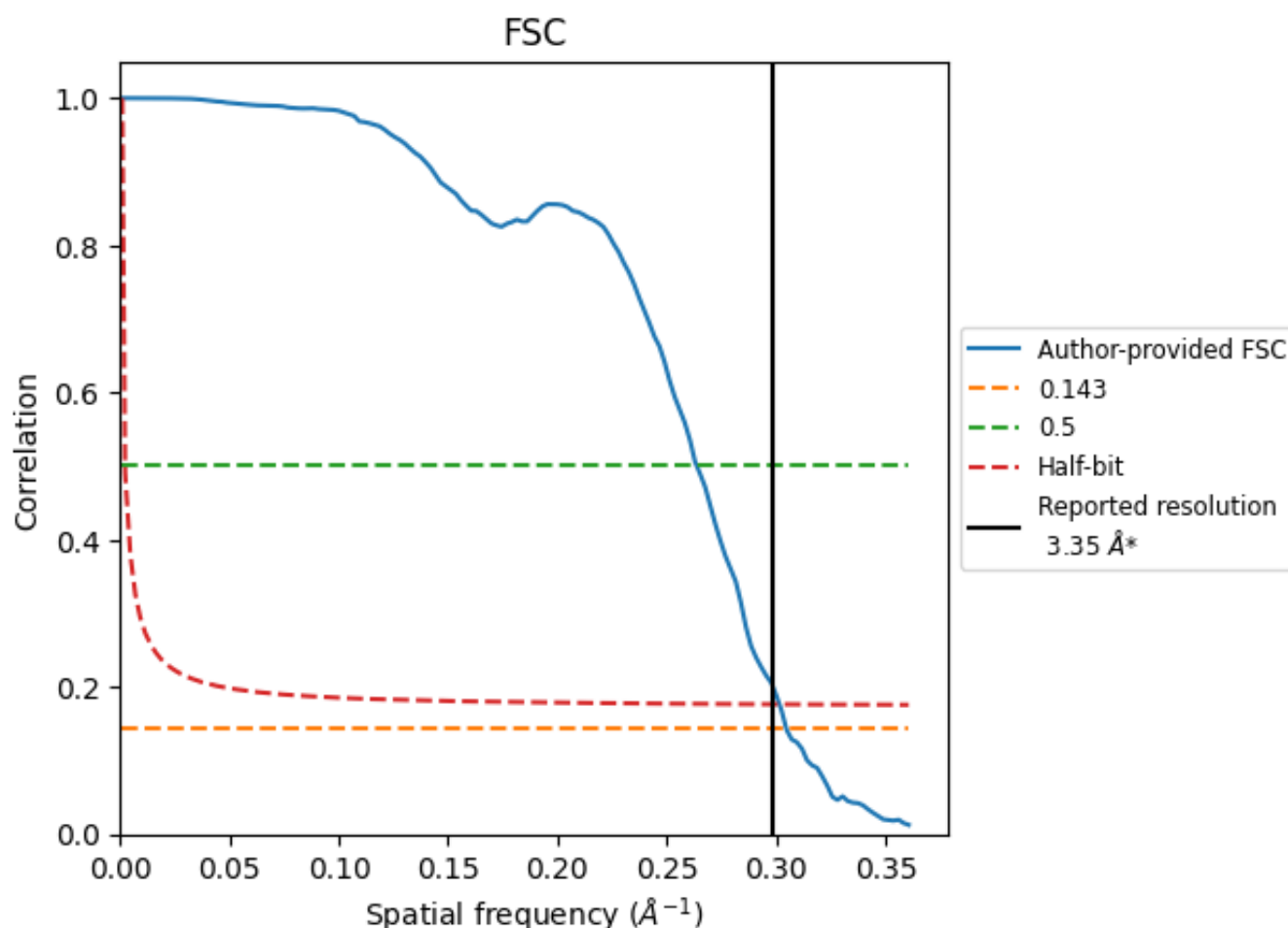


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 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 0.299 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

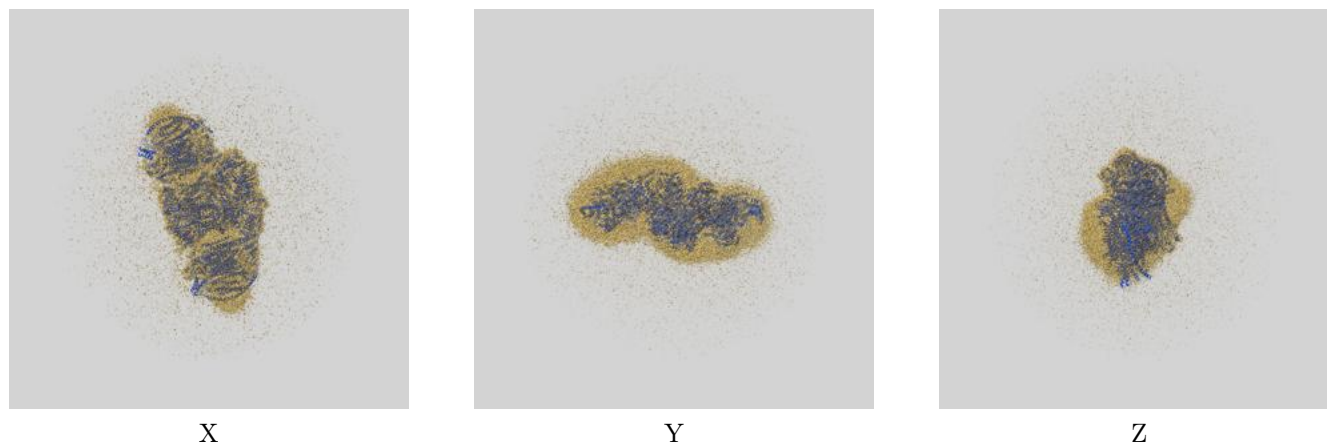
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.35	-
Author-provided FSC curve	3.28	3.79	3.32
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.79 differs from the reported value 3.35 by more than 10 %

## 9 Map-model fit [i](#)

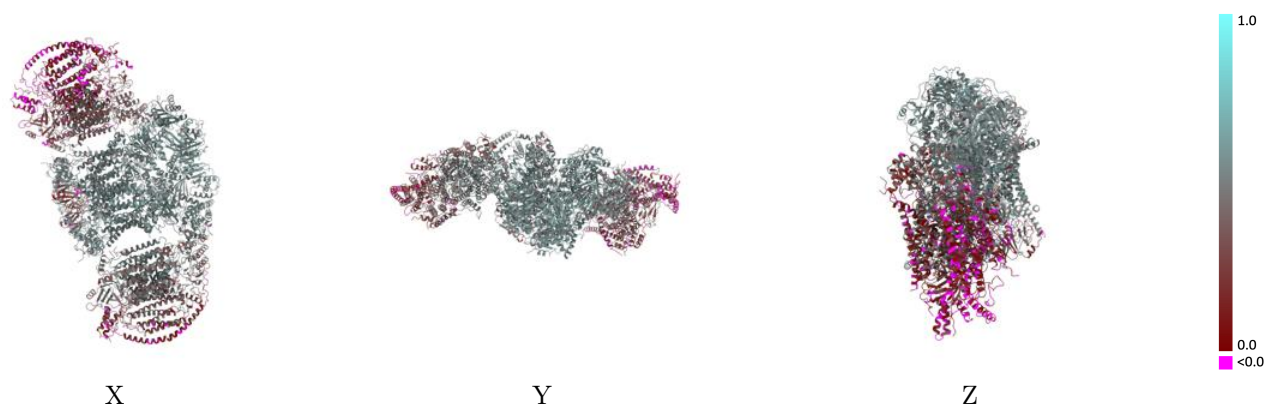
This section contains information regarding the fit between EMDB map EMD-0262 and PDB model 6HU9. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

### 9.1 Map-model overlay [i](#)



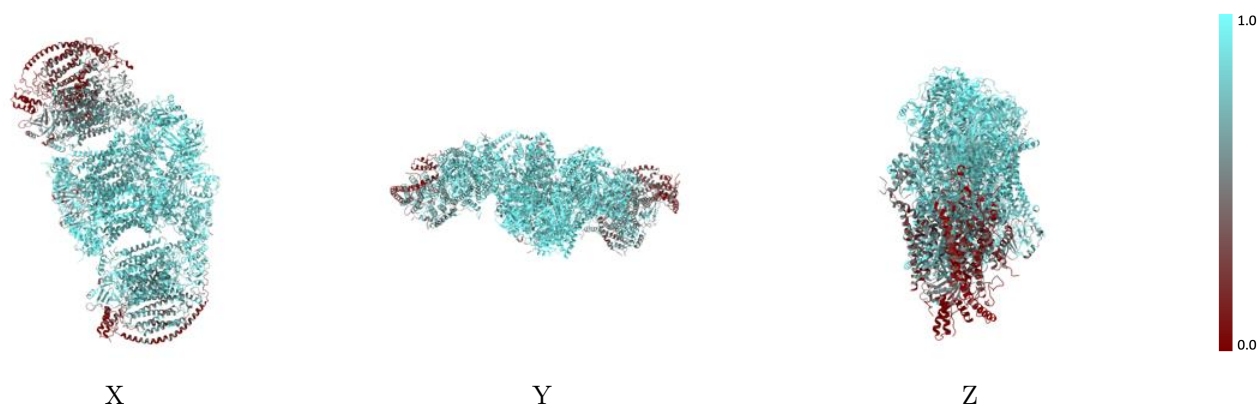
The images above show the 3D surface view of the map at the recommended contour level 0.0263 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

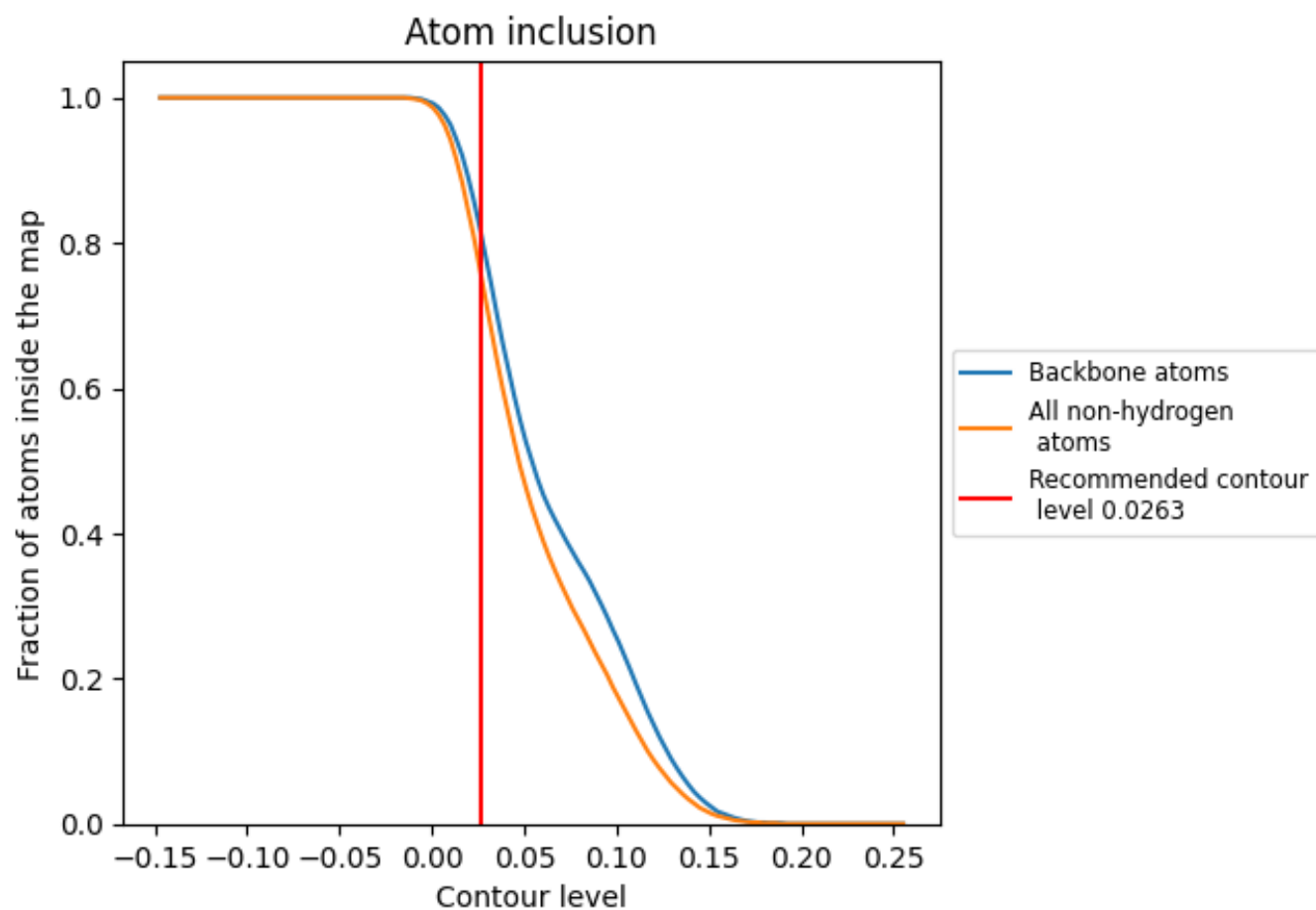
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0263).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.0263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.4310
A	 0.9390	 0.5540
B	 0.9330	 0.5540
C	 0.9370	 0.5660
D	 0.9470	 0.5650
E	 0.7460	 0.3780
F	 0.8970	 0.5060
G	 0.9240	 0.5490
H	 0.9330	 0.5640
I	 0.9200	 0.5460
J	 0.7610	 0.4780
L	 0.9390	 0.5520
M	 0.9300	 0.5520
N	 0.9450	 0.5730
O	 0.9450	 0.5670
P	 0.7520	 0.3860
Q	 0.8990	 0.5040
R	 0.9300	 0.5520
S	 0.9430	 0.5620
T	 0.9230	 0.5450
U	 0.7020	 0.4510
a	 0.8470	 0.4880
b	 0.8150	 0.4450
c	 0.6390	 0.3240
d	 0.7340	 0.3770
e	 0.8490	 0.4970
f	 0.8420	 0.4330
g	 0.6690	 0.3190
h	 0.7720	 0.4330
i	 0.7630	 0.3980
j	 0.1160	 0.1890
k	 0.1900	 0.1450
l	 0.7710	 0.4200
m	 0.5870	 0.2920
n	 0.5130	 0.2370



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
o	 0.2810	 0.1300
p	 0.4110	 0.1980
q	 0.7110	 0.3710
r	 0.6160	 0.2490
s	 0.2650	 0.1390
t	 0.4890	 0.2530
u	 0.4880	 0.1720
v	 0.0430	 0.0320
w	 0.0710	 0.0140
x	 0.5130	 0.2290