



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 09:34 AM EST

PDB ID : 8B6J
EMDB ID : EMD-15868
Title : Cryo-EM structure of cytochrome bc1 complex (complex-III) from respiratory supercomplex of *Tetrahymena thermophila*
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2022-09-27
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:

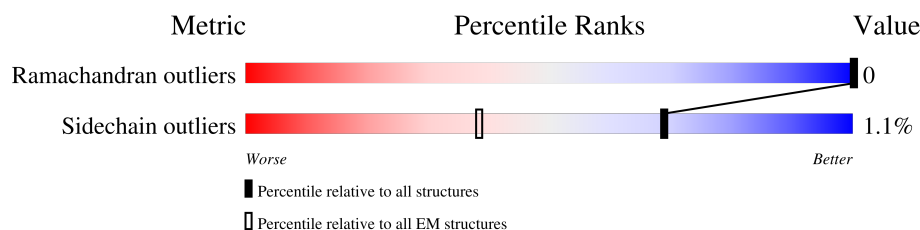
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	 12% 93% 6%
1	a	513	 12% 93% 6%
2	B	482	 7% 95% 5%
2	b	482	 9% 94% 5%
3	C	426	 8% 99% .
3	c	426	 8% 98% .
4	D	319	 8% 92% 8%
4	d	319	 6% 92% 8%
5	E	269	 55% 90% 9%

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Mol	Chain	Length	Quality of chain
5	e	269	
6	F	86	
6	f	86	
7	G	328	
7	g	328	
8	H	130	
8	h	130	
9	I	119	
9	i	119	
10	J	66	
10	j	66	
11	K	62	
11	k	62	
12	L	41	
12	l	41	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 94062 atoms, of which 47043 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 Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	482	Total	C	H	N	O	S	0	0
			7587	2437	3740	671	734	5		
1	a	482	Total	C	H	N	O	S	0	0
			7587	2437	3740	671	734	5		

- Molecule 2 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	460	Total	C	H	N	O	S	0	0
			7118	2240	3555	609	708	6		
2	b	460	Total	C	H	N	O	S	0	0
			7118	2240	3555	609	708	6		

- Molecule 3 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	426	Total	C	H	N	O	S	0	0
			7075	2417	3485	541	610	22		
3	c	426	Total	C	H	N	O	S	0	0
			7074	2417	3484	541	610	22		

- Molecule 4 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	295	Total	C	H	N	O	S	0	0
			4832	1627	2343	418	431	13		
4	d	295	Total	C	H	N	O	S	0	0
			4832	1627	2343	418	431	13		

- Molecule 5 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	245	Total	C	H	N	O	S	0	0
			3893	1251	1927	344	362	9		
5	e	245	Total	C	H	N	O	S	0	0
			3891	1251	1925	344	362	9		

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	86	Total	C	H	N	O	S	0	0
			1372	432	686	116	128	10		
6	f	85	Total	C	H	N	O	S	0	0
			1352	427	674	115	127	9		

- Molecule 7 is a protein called UQCRTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	327	Total	C	H	N	O	S	0	0
			5474	1789	2706	482	491	6		
7	g	327	Total	C	H	N	O	S	0	0
			5474	1789	2706	482	491	6		

- Molecule 8 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	129	Total	C	H	N	O	S	0	0
			2138	708	1040	195	187	8		
8	h	129	Total	C	H	N	O	S	0	0
			2138	708	1040	195	187	8		

- Molecule 9 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1998	664	1003	164	166	1		
9	i	117	Total	C	H	N	O	S	0	0
			1998	664	1003	164	166	1		

- Molecule 10 is a protein called UQCRTT3/UP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	66	Total	C	H	N	O		0	0
			596	198	266	66	66			

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	66	Total	C	H	N	O	0	0
			596	198	266	66	66		

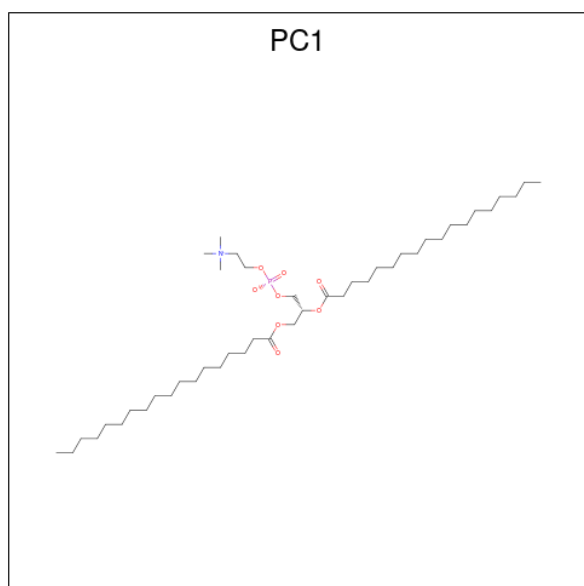
- Molecule 11 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	58	Total	C	H	N	O	S	0	0
			1004	341	503	79	79	2		
11	k	58	Total	C	H	N	O	S	0	0
			1004	341	503	79	79	2		

- Molecule 12 is a protein called UQCRTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	l	32	Total	C	H	N	O	S	0	0
			535	178	273	41	42	1		
12	L	32	Total	C	H	N	O	S	0	0
			535	178	273	41	42	1		

- Molecule 13 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



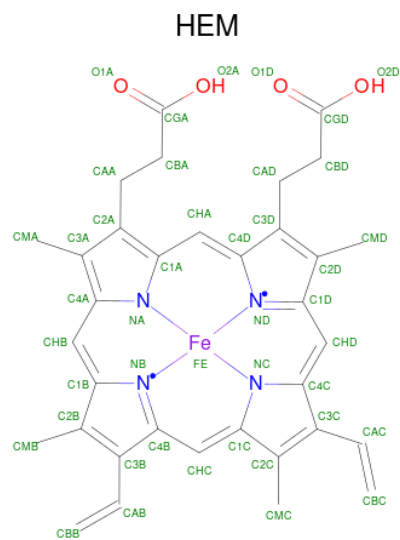
Mol	Chain	Residues	Atoms					AltConf	
13	A	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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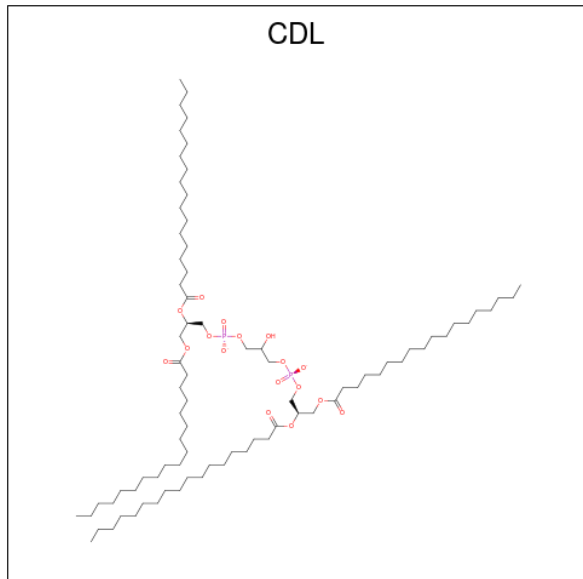
Mol	Chain	Residues	Atoms						AltConf
13	A	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	C	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	C	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	C	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	E	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	E	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	K	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	d	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	g	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
13	k	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



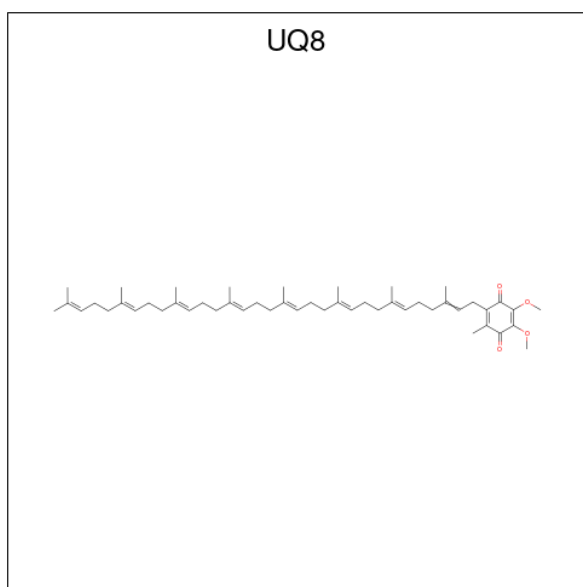
Mol	Chain	Residues	Atoms						AltConf
14	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
14	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
14	c	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
14	c	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



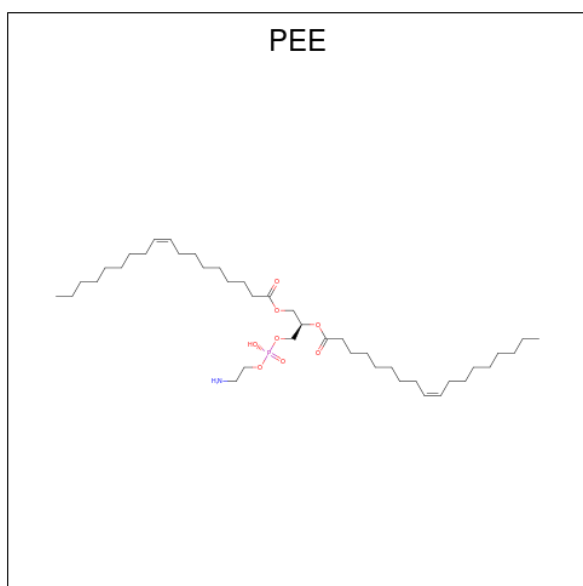
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	C	1	Total 256	C 81	H 156	O 17	P 2	0
15	D	1	Total 256	C 81	H 156	O 17	P 2	0
15	E	1	Total 256	C 81	H 156	O 17	P 2	0
15	H	1	Total 256	C 81	H 156	O 17	P 2	0
15	H	1	Total 256	C 81	H 156	O 17	P 2	0
15	a	1	Total 256	C 81	H 156	O 17	P 2	0
15	c	1	Total 256	C 81	H 156	O 17	P 2	0
15	c	1	Total 256	C 81	H 156	O 17	P 2	0
15	c	1	Total 256	C 81	H 156	O 17	P 2	0
15	g	1	Total 256	C 81	H 156	O 17	P 2	0
15	h	1	Total 256	C 81	H 156	O 17	P 2	0
15	h	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 16 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



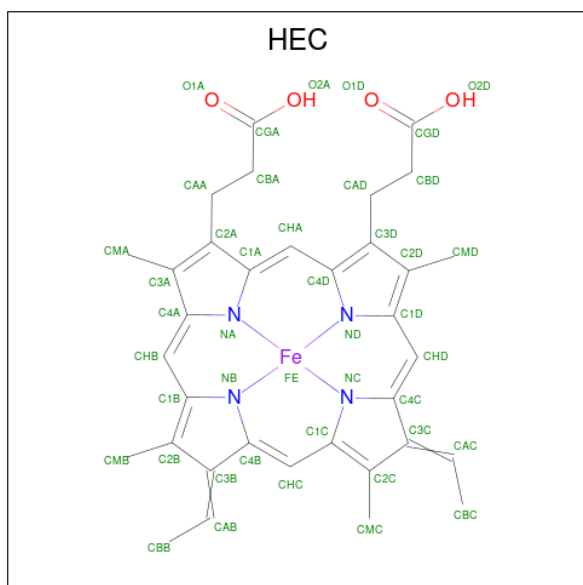
Mol	Chain	Residues	Atoms			AltConf
16	C	1	Total	C	O	0
			53	49	4	
16	C	1	Total	C	O	0
			53	49	4	
16	c	1	Total	C	O	0
			53	49	4	

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
17	C	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
17	L	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
18	D	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
18	d	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

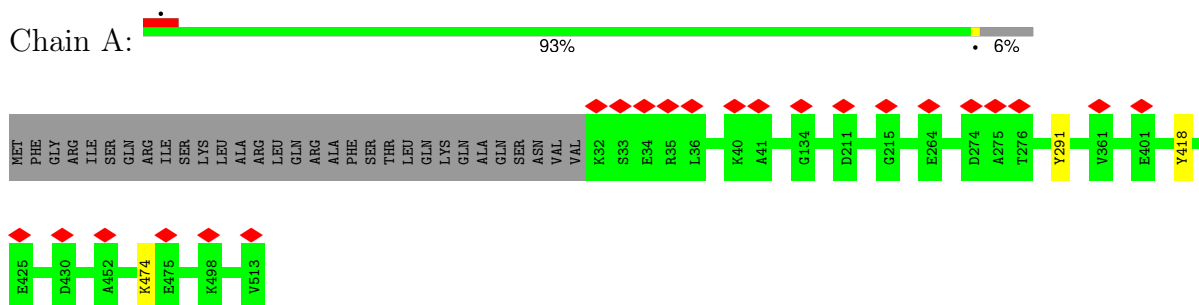


Mol	Chain	Residues	Atoms			AltConf
19	E	1	Total	Fe	S	0
			4	2	2	
19	e	1	Total	Fe	S	0
			4	2	2	

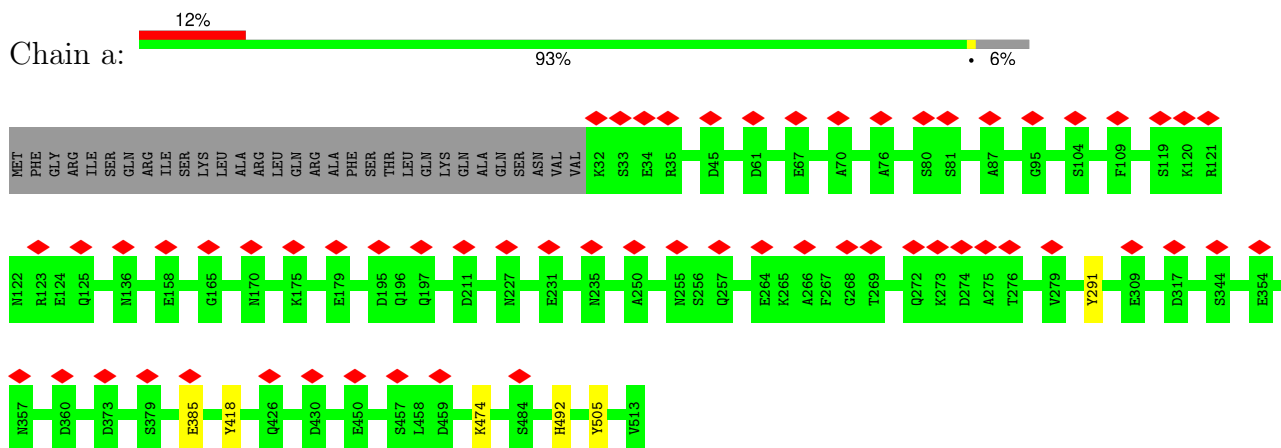
3 Residue-property plots [i](#)

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.

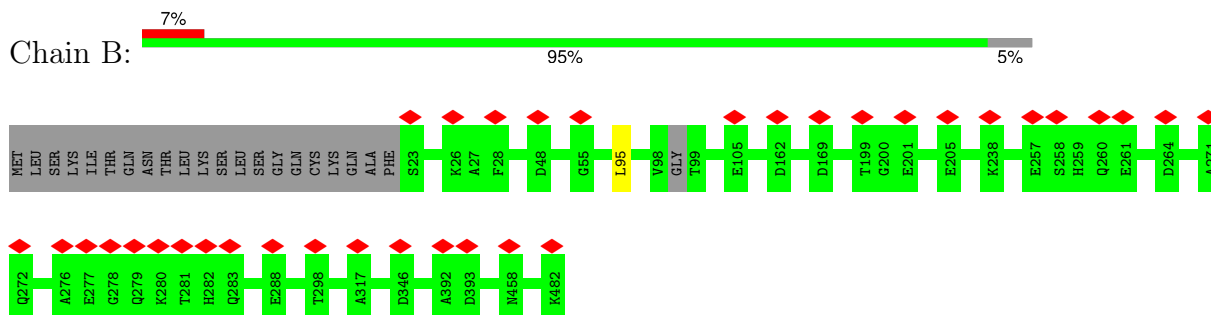
- Molecule 1: Peptidase M16 inactive domain protein



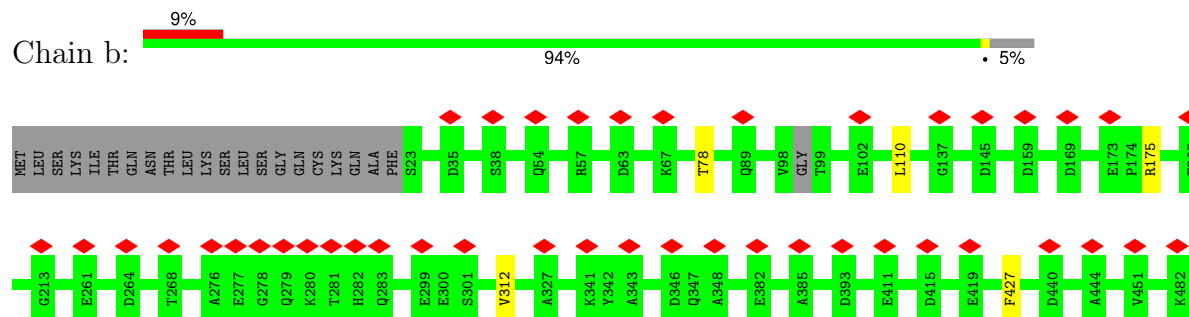
- Molecule 1: Peptidase M16 inactive domain protein



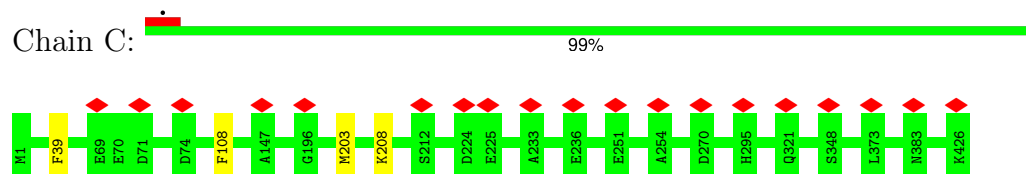
- Molecule 2: M16 family peptidase, putative



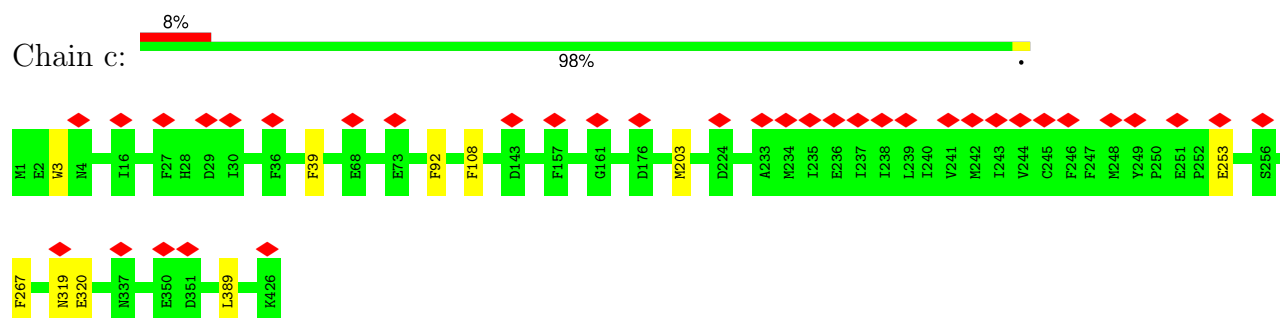
- Molecule 2: M16 family peptidase, putative



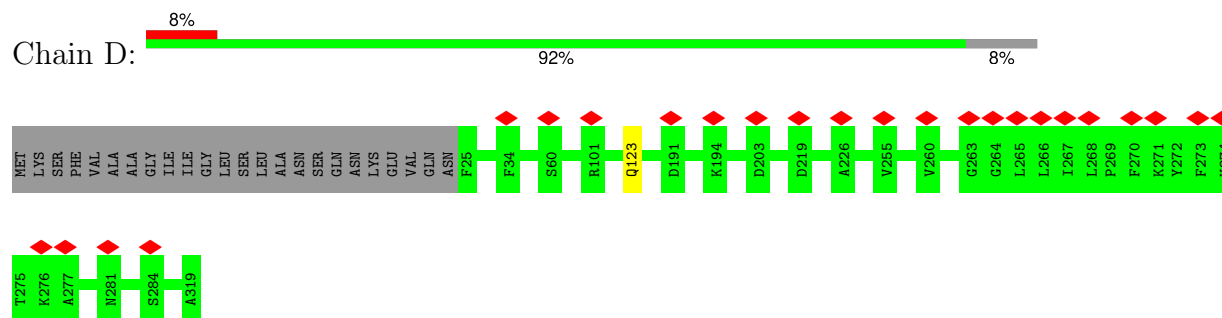
- Molecule 3: Apocytochrome b



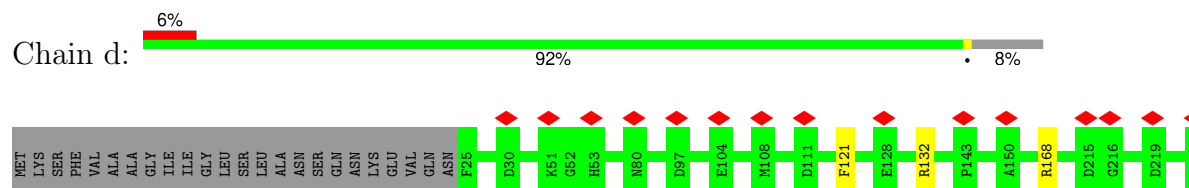
- Molecule 3: Apocytochrome b

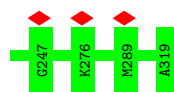


- Molecule 4: Cytochrome protein c1



- Molecule 4: Cytochrome protein c1

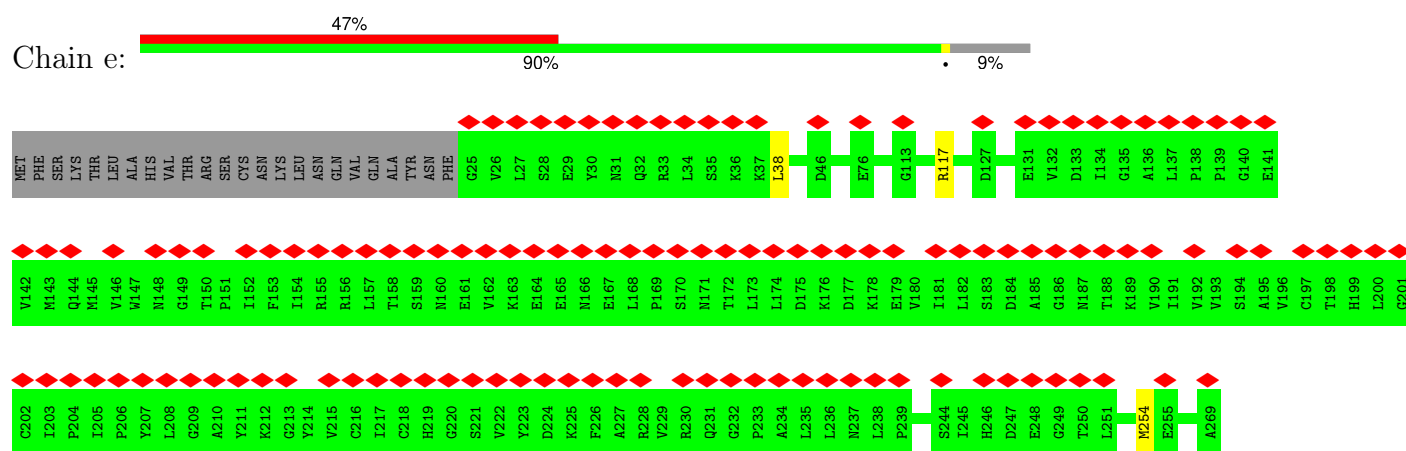




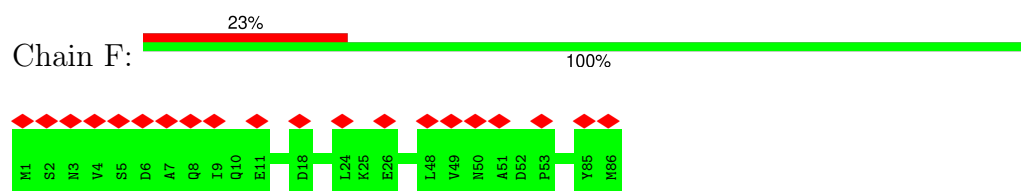
- Molecule 5: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit



- Molecule 5: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

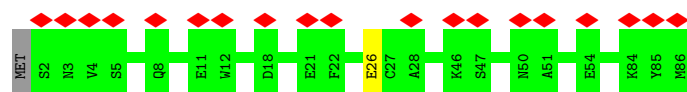


- Molecule 6: Ubiquinol-cytochrome C reductase hinge protein

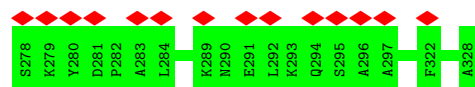
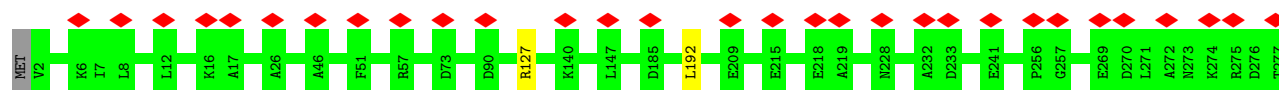


- Molecule 6: Ubiquinol-cytochrome C reductase hinge protein

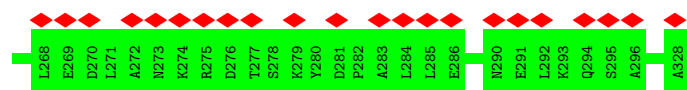




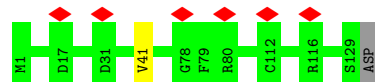
- Molecule 7: UQCRTT1



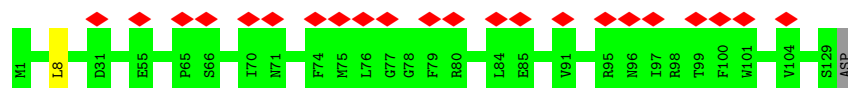
- Molecule 7: UQCRTT1



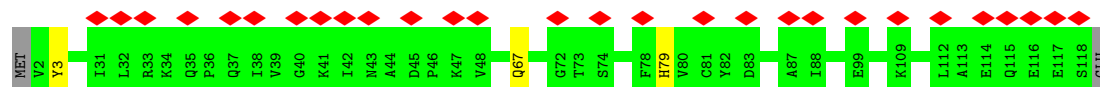
- Molecule 8: Transmembrane protein, putative



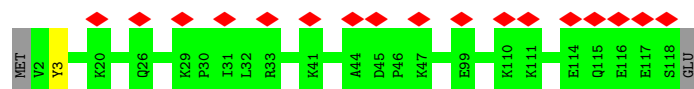
- Molecule 8: Transmembrane protein, putative



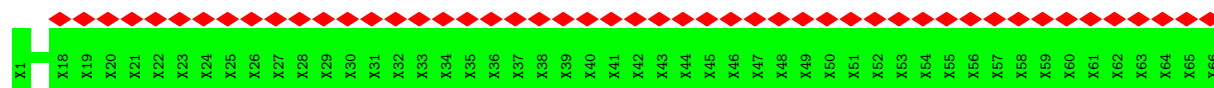
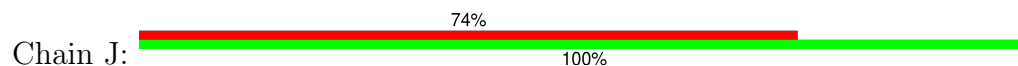
- Molecule 9: Transmembrane protein, putative



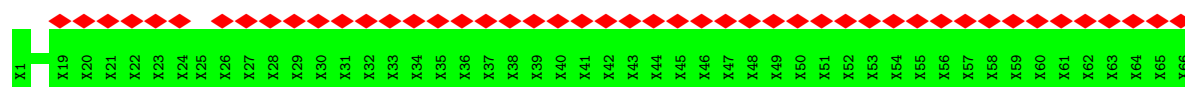
- Molecule 9: Transmembrane protein, putative



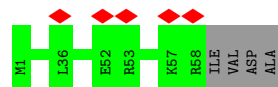
- Molecule 10: UQCRTT3/UP1



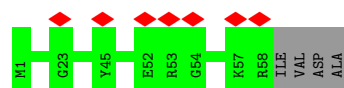
- Molecule 10: UQCRTT3/UP1



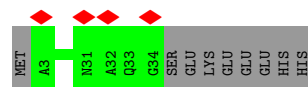
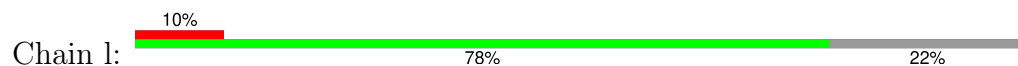
- Molecule 11: Transmembrane protein, putative



- Molecule 11: Transmembrane protein, putative



- Molecule 12: UQCRTT2



- Molecule 12: UQCRTT2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138746	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 ($e^-/\text{\AA}^2$)	25.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.090	Depositor
Minimum map value	-2.921	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, HEC, UQ8, CDL, PC1, PEE

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	0.25	0/3933	0.49	0/5338
1	a	0.25	0/3933	0.47	0/5338
2	B	0.25	0/3616	0.45	0/4897
2	b	0.24	0/3616	0.44	0/4897
3	C	0.26	0/3716	0.42	0/5046
3	c	0.26	0/3716	0.42	0/5046
4	D	0.27	0/2580	0.47	0/3491
4	d	0.27	0/2580	0.47	0/3491
5	E	0.24	0/2015	0.47	0/2732
5	e	0.24	0/2015	0.47	0/2732
6	F	0.25	0/700	0.45	0/942
6	f	0.25	0/692	0.45	0/932
7	G	0.25	0/2846	0.48	0/3839
7	g	0.25	0/2846	0.48	0/3839
8	H	0.26	0/1133	0.49	0/1524
8	h	0.27	0/1133	0.51	0/1524
9	I	0.25	0/1029	0.40	0/1397
9	i	0.25	0/1029	0.40	0/1397
11	K	0.27	0/522	0.43	0/712
11	k	0.26	0/522	0.43	0/712
12	L	0.27	0/269	0.40	0/366
12	l	0.27	0/269	0.40	0/366
All	All	0.25	0/44710	0.46	0/60558

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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	480/513 (94%)	465 (97%)	15 (3%)	0	100	100
1	a	480/513 (94%)	466 (97%)	14 (3%)	0	100	100
2	B	456/482 (95%)	447 (98%)	9 (2%)	0	100	100
2	b	456/482 (95%)	447 (98%)	9 (2%)	0	100	100
3	C	424/426 (100%)	405 (96%)	19 (4%)	0	100	100
3	c	424/426 (100%)	414 (98%)	10 (2%)	0	100	100
4	D	293/319 (92%)	288 (98%)	5 (2%)	0	100	100
4	d	293/319 (92%)	290 (99%)	3 (1%)	0	100	100
5	E	243/269 (90%)	237 (98%)	6 (2%)	0	100	100
5	e	243/269 (90%)	240 (99%)	3 (1%)	0	100	100
6	F	84/86 (98%)	84 (100%)	0	0	100	100
6	f	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
7	G	325/328 (99%)	320 (98%)	5 (2%)	0	100	100
7	g	325/328 (99%)	322 (99%)	3 (1%)	0	100	100
8	H	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
8	h	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	I	115/119 (97%)	115 (100%)	0	0	100	100
9	i	115/119 (97%)	115 (100%)	0	0	100	100
11	K	56/62 (90%)	55 (98%)	1 (2%)	0	100	100
11	k	56/62 (90%)	56 (100%)	0	0	100	100
12	L	30/41 (73%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	30/41 (73%)	30 (100%)	0	0	100	100
All	All	5265/5550 (95%)	5158 (98%)	107 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	411/440 (93%)	408 (99%)	3 (1%)	81	94
1	a	411/440 (93%)	405 (98%)	6 (2%)	60	86
2	B	389/409 (95%)	388 (100%)	1 (0%)	91	97
2	b	389/409 (95%)	384 (99%)	5 (1%)	65	88
3	C	386/386 (100%)	382 (99%)	4 (1%)	73	91
3	c	386/386 (100%)	376 (97%)	10 (3%)	41	75
4	D	255/274 (93%)	254 (100%)	1 (0%)	89	96
4	d	255/274 (93%)	252 (99%)	3 (1%)	67	89
5	E	215/237 (91%)	213 (99%)	2 (1%)	75	92
5	e	215/237 (91%)	212 (99%)	3 (1%)	62	87
6	F	76/76 (100%)	76 (100%)	0	100	100
6	f	75/76 (99%)	74 (99%)	1 (1%)	65	88
7	G	288/289 (100%)	286 (99%)	2 (1%)	81	94
7	g	288/289 (100%)	283 (98%)	5 (2%)	56	84
8	H	117/118 (99%)	116 (99%)	1 (1%)	75	92
8	h	117/118 (99%)	116 (99%)	1 (1%)	75	92
9	I	107/109 (98%)	104 (97%)	3 (3%)	38	72
9	i	107/109 (98%)	106 (99%)	1 (1%)	75	92
11	K	53/56 (95%)	53 (100%)	0	100	100
11	k	53/56 (95%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	27/36 (75%)	26 (96%)	1 (4%)	29	63
12	l	27/36 (75%)	27 (100%)	0	100	100
All	All	4647/4860 (96%)	4594 (99%)	53 (1%)	69	90

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	3	TRP
3	c	319	ASN
7	g	192	LEU
3	c	39	PHE
3	c	203	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

43 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CDL	H	1301	-	99,99,99	0.29	0	105,111,111	0.24	0
15	CDL	C	505	-	99,99,99	0.29	0	105,111,111	0.26	0
13	PC1	E	303	-	53,53,53	0.28	0	59,61,61	0.27	0
14	HEM	C	501	3	42,50,50	1.46	4 (9%)	46,82,82	1.33	6 (13%)
13	PC1	c	505	-	53,53,53	0.28	0	59,61,61	0.28	0
15	CDL	c	503	-	99,99,99	0.30	0	105,111,111	0.25	0
17	PEE	C	512	-	50,50,50	0.78	2 (4%)	53,55,55	0.45	0
14	HEM	c	502	3	42,50,50	1.45	5 (11%)	46,82,82	1.27	4 (8%)
13	PC1	k	301	-	53,53,53	0.39	0	59,61,61	0.36	0
15	CDL	h	401	-	99,99,99	0.29	0	105,111,111	0.26	0
17	PEE	L	401	-	50,50,50	0.78	2 (4%)	53,55,55	0.46	0
14	HEM	c	501	3	42,50,50	1.47	5 (11%)	46,82,82	1.32	7 (15%)
15	CDL	E	304	-	99,99,99	0.29	0	105,111,111	0.25	0
15	CDL	a	1201	-	99,99,99	0.29	0	105,111,111	0.24	0
19	FES	e	301	5	0,4,4	-	-	-	-	-
15	CDL	D	402	-	99,99,99	0.29	0	105,111,111	0.24	0
13	PC1	C	509	-	53,53,53	0.28	0	59,61,61	0.29	0
13	PC1	E	302	-	53,53,53	0.28	0	59,61,61	0.27	0
13	PC1	c	504	-	53,53,53	0.28	0	59,61,61	0.27	0
15	CDL	C	503	-	99,99,99	0.29	0	105,111,111	0.25	0
15	CDL	C	504	-	99,99,99	0.29	0	105,111,111	0.25	0
13	PC1	g	802	-	53,53,53	0.29	0	59,61,61	0.26	0
13	PC1	c	506	-	53,53,53	0.28	0	59,61,61	0.29	0
16	UQ8	C	511	-	53,53,53	0.52	0	66,67,67	0.68	2 (3%)
15	CDL	C	506	-	99,99,99	0.29	0	105,111,111	0.25	0
13	PC1	K	901	-	53,53,53	0.28	0	59,61,61	0.29	0
18	HEC	D	401	4	32,50,50	2.14	3 (9%)	30,82,82	2.41	7 (23%)
15	CDL	h	402	-	99,99,99	0.29	0	105,111,111	0.24	0
16	UQ8	c	508	-	53,53,53	0.52	0	66,67,67	0.71	3 (4%)
18	HEC	d	802	4	32,50,50	2.14	3 (9%)	30,82,82	2.40	5 (16%)
13	PC1	A	1201	-	53,53,53	0.28	0	59,61,61	0.28	0
13	PC1	C	508	-	53,53,53	0.28	0	59,61,61	0.29	0
13	PC1	d	801	-	53,53,53	0.28	0	59,61,61	0.27	0
14	HEM	C	502	3	42,50,50	1.45	5 (11%)	46,82,82	1.22	4 (8%)
16	UQ8	C	510	-	53,53,53	0.55	0	66,67,67	0.76	3 (4%)
13	PC1	A	1202	-	53,53,53	0.28	0	59,61,61	0.29	0
15	CDL	c	509	-	99,99,99	0.29	0	105,111,111	0.26	0
15	CDL	c	507	-	99,99,99	0.29	0	105,111,111	0.25	0
13	PC1	C	507	-	53,53,53	0.29	0	59,61,61	0.27	0
15	CDL	g	801	-	99,99,99	0.29	0	105,111,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PC1	c	510	-	53,53,53	0.28	0	59,61,61	0.29	0
19	FES	E	301	5	0,4,4	-	-	-		
15	CDL	H	1302	-	99,99,99	0.29	0	105,111,111	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	H	1301	-	-	24/110/110/110	-
15	CDL	C	505	-	-	25/110/110/110	-
13	PC1	E	303	-	-	10/57/57/57	-
14	HEM	C	501	3	-	5/12/54/54	-
13	PC1	c	505	-	-	8/57/57/57	-
15	CDL	c	503	-	-	30/110/110/110	-
17	PEE	C	512	-	-	17/54/54/54	-
14	HEM	c	502	3	-	0/12/54/54	-
13	PC1	k	301	-	-	24/57/57/57	-
15	CDL	h	401	-	-	22/110/110/110	-
17	PEE	L	401	-	-	11/54/54/54	-
14	HEM	c	501	3	-	0/12/54/54	-
15	CDL	E	304	-	-	25/110/110/110	-
15	CDL	a	1201	-	-	32/110/110/110	-
19	FES	e	301	5	-	-	0/1/1/1
15	CDL	D	402	-	-	19/110/110/110	-
13	PC1	C	509	-	-	12/57/57/57	-
13	PC1	E	302	-	-	19/57/57/57	-
13	PC1	c	504	-	-	18/57/57/57	-
15	CDL	C	503	-	-	28/110/110/110	-
15	CDL	C	504	-	-	30/110/110/110	-
13	PC1	g	802	-	-	12/57/57/57	-
13	PC1	c	506	-	-	12/57/57/57	-
16	UQ8	C	511	-	-	8/51/75/75	0/1/1/1
15	CDL	C	506	-	-	23/110/110/110	-
13	PC1	K	901	-	-	11/57/57/57	-
18	HEC	D	401	4	-	0/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	h	402	-	-	21/110/110/110	-
16	UQ8	c	508	-	-	13/51/75/75	0/1/1/1
18	HEC	d	802	4	-	2/10/54/54	-
13	PC1	A	1201	-	-	12/57/57/57	-
13	PC1	C	508	-	-	23/57/57/57	-
13	PC1	d	801	-	-	15/57/57/57	-
14	HEM	C	502	3	-	6/12/54/54	-
16	UQ8	C	510	-	-	14/51/75/75	0/1/1/1
13	PC1	A	1202	-	-	15/57/57/57	-
15	CDL	c	509	-	-	20/110/110/110	-
15	CDL	c	507	-	-	28/110/110/110	-
13	PC1	C	507	-	-	20/57/57/57	-
15	CDL	g	801	-	-	22/110/110/110	-
13	PC1	c	510	-	-	15/57/57/57	-
19	FES	E	301	5	-	-	0/1/1/1
15	CDL	H	1302	-	-	20/110/110/110	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	401	HEC	C2B-C3B	-6.19	1.33	1.40
18	d	802	HEC	C2B-C3B	-6.18	1.33	1.40
18	D	401	HEC	C3C-C2C	-6.14	1.33	1.40
18	d	802	HEC	C3C-C2C	-6.08	1.33	1.40
18	d	802	HEC	C3D-C2D	5.38	1.53	1.37

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	401	HEC	CBB-CAB-C3B	-7.81	109.22	127.49
18	d	802	HEC	CBC-CAC-C3C	-7.76	109.32	127.49
18	D	401	HEC	CBC-CAC-C3C	-7.74	109.37	127.49
18	d	802	HEC	CBB-CAB-C3B	-7.73	109.40	127.49
16	c	508	UQ8	C8-C7-C6	2.75	118.86	112.08

There are no chirality outliers.

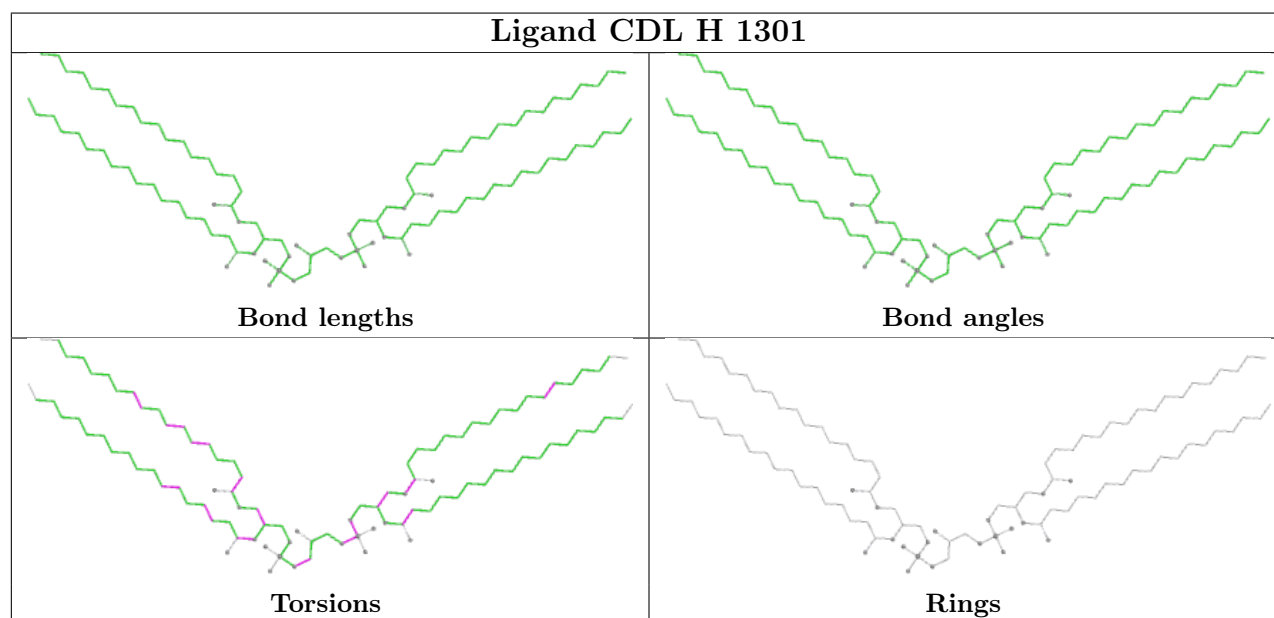
5 of 671 torsion outliers are listed below:

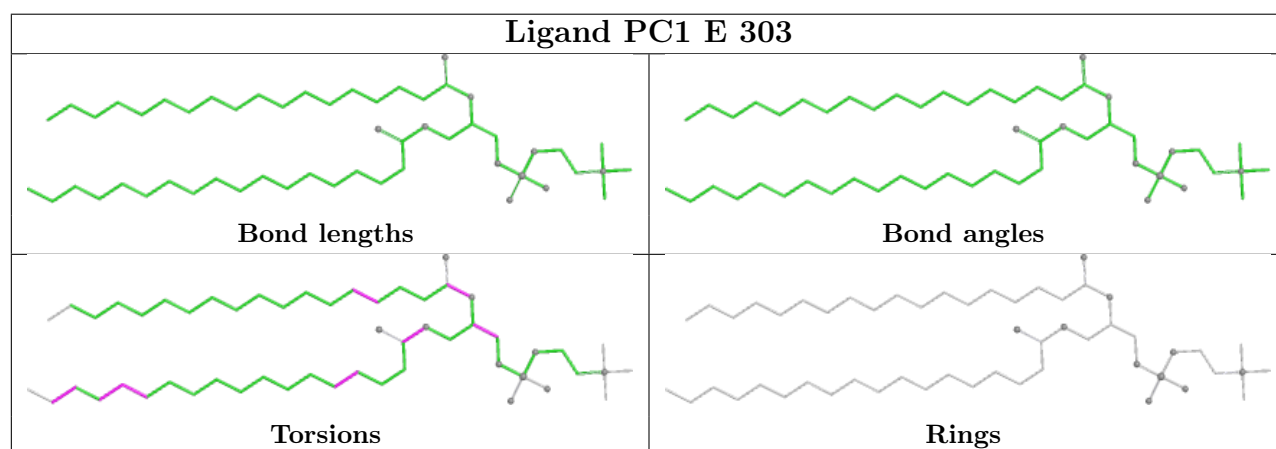
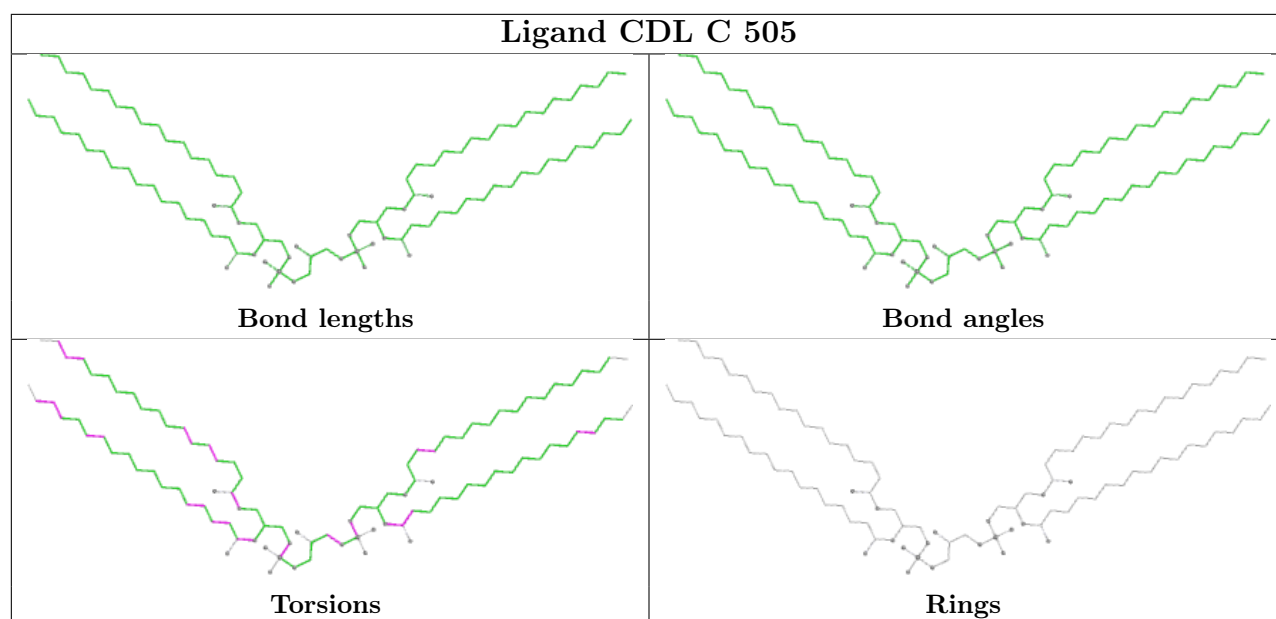
Mol	Chain	Res	Type	Atoms
13	A	1201	PC1	C11-O13-P-O14
13	A	1202	PC1	C11-O13-P-O14
13	A	1202	PC1	C1-O11-P-O14
13	A	1202	PC1	C1-O11-P-O13
13	A	1202	PC1	O13-C11-C12-N

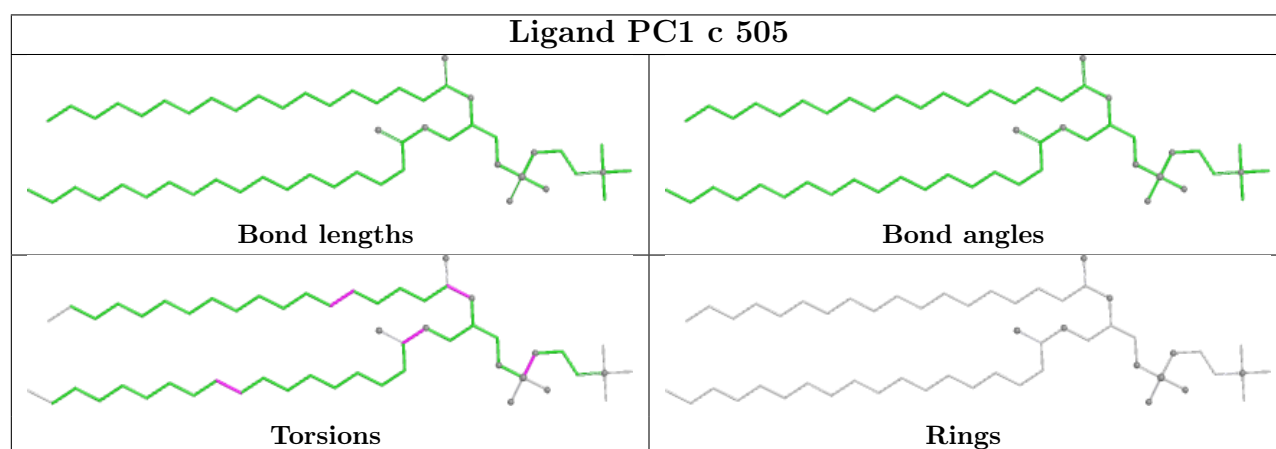
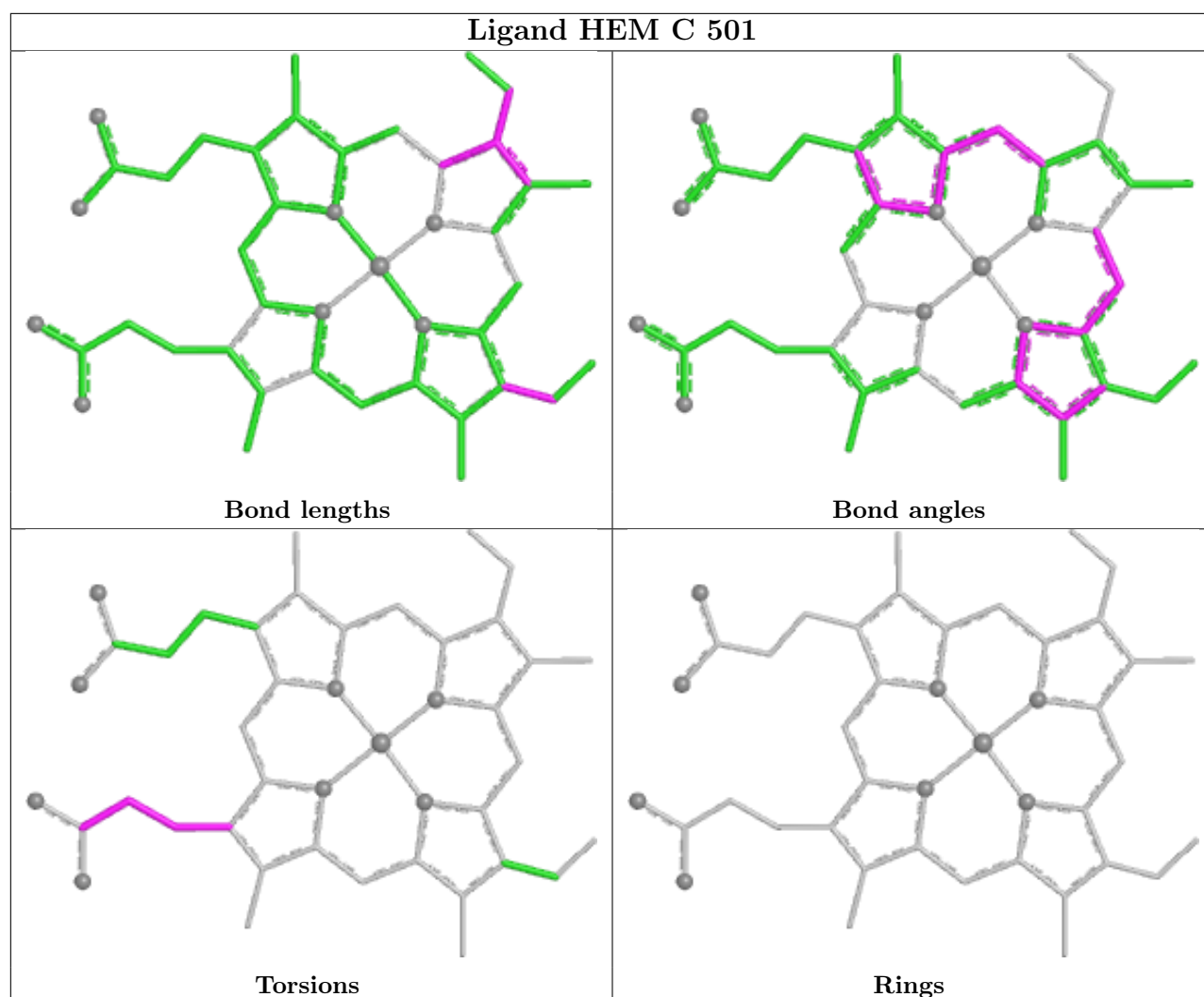
There are no ring outliers.

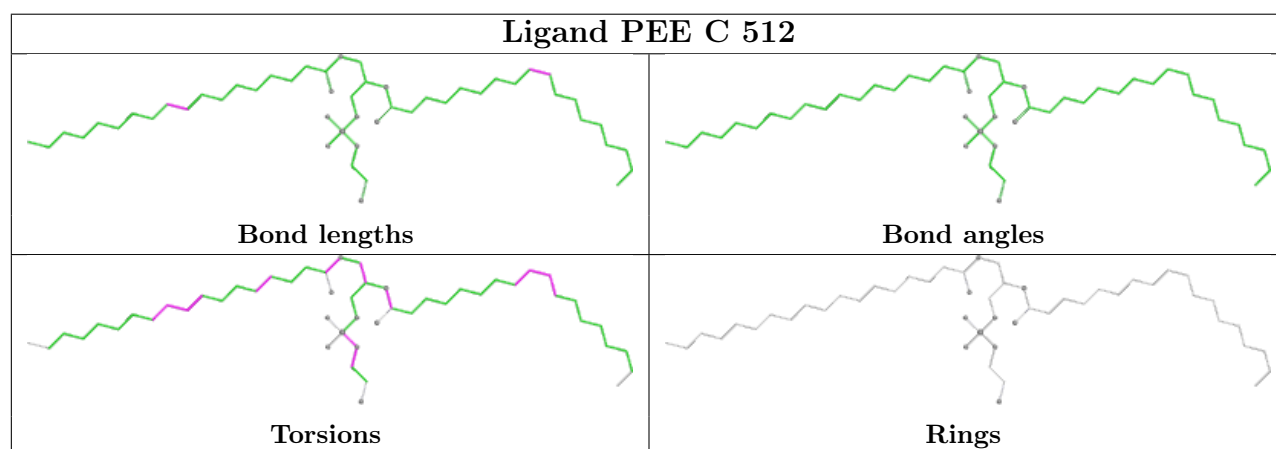
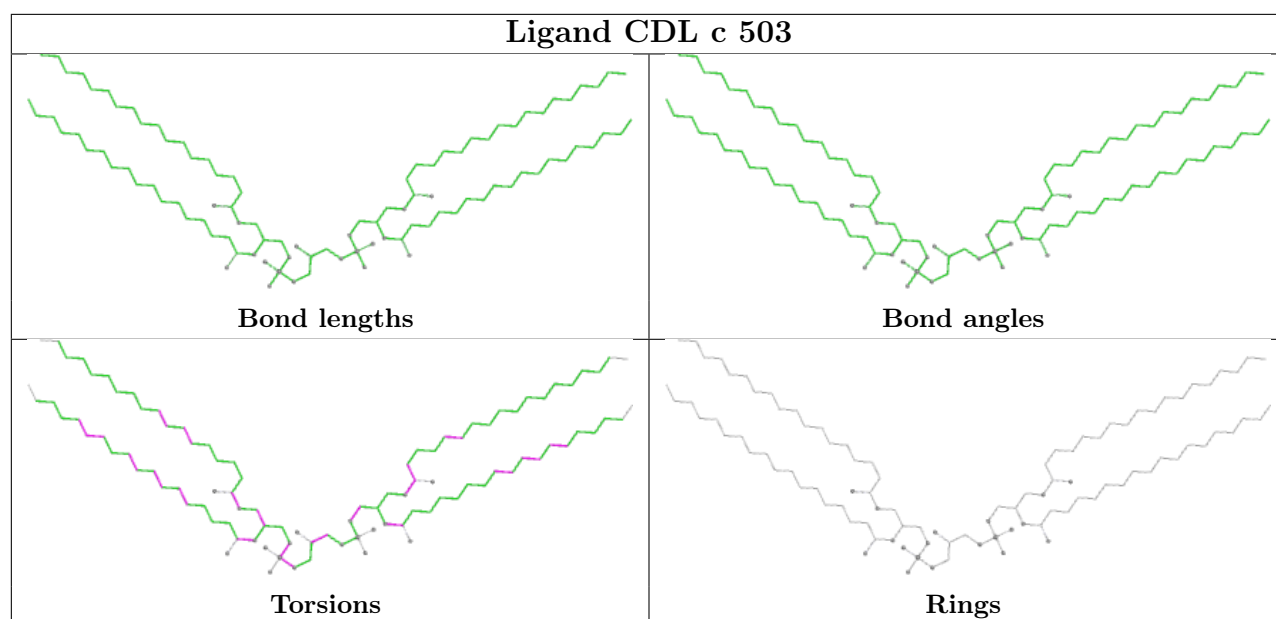
No monomer is involved in short contacts.

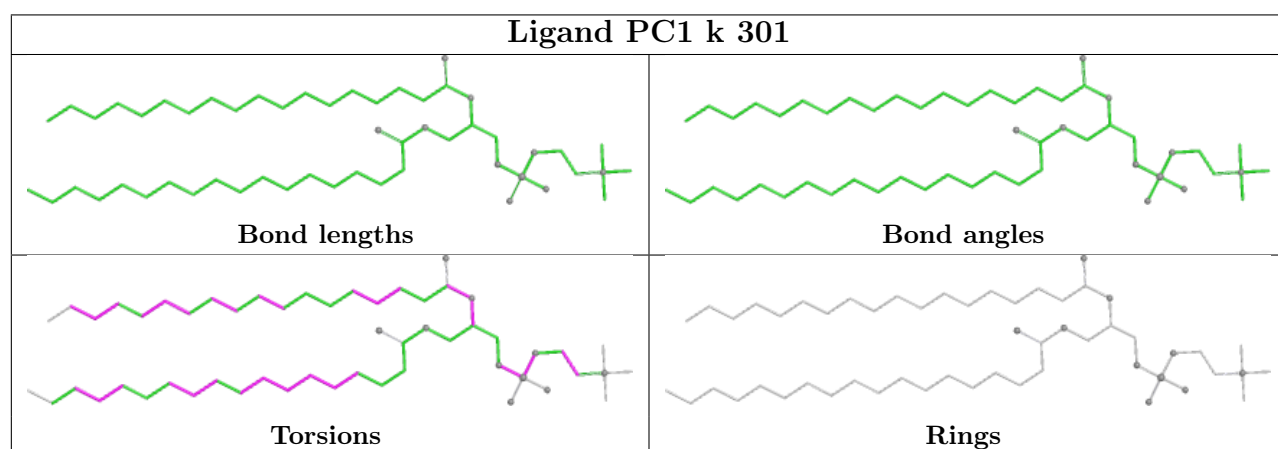
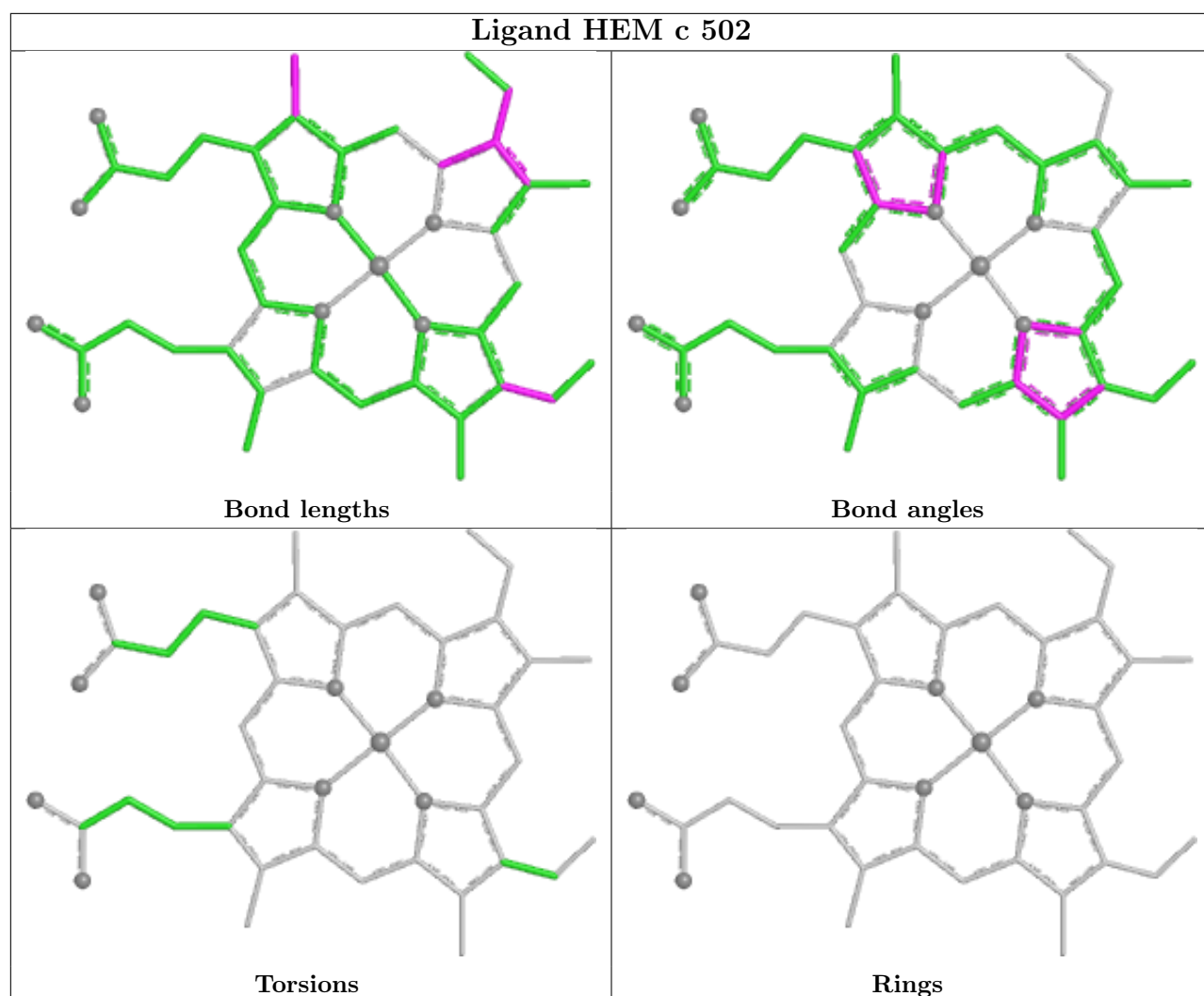
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

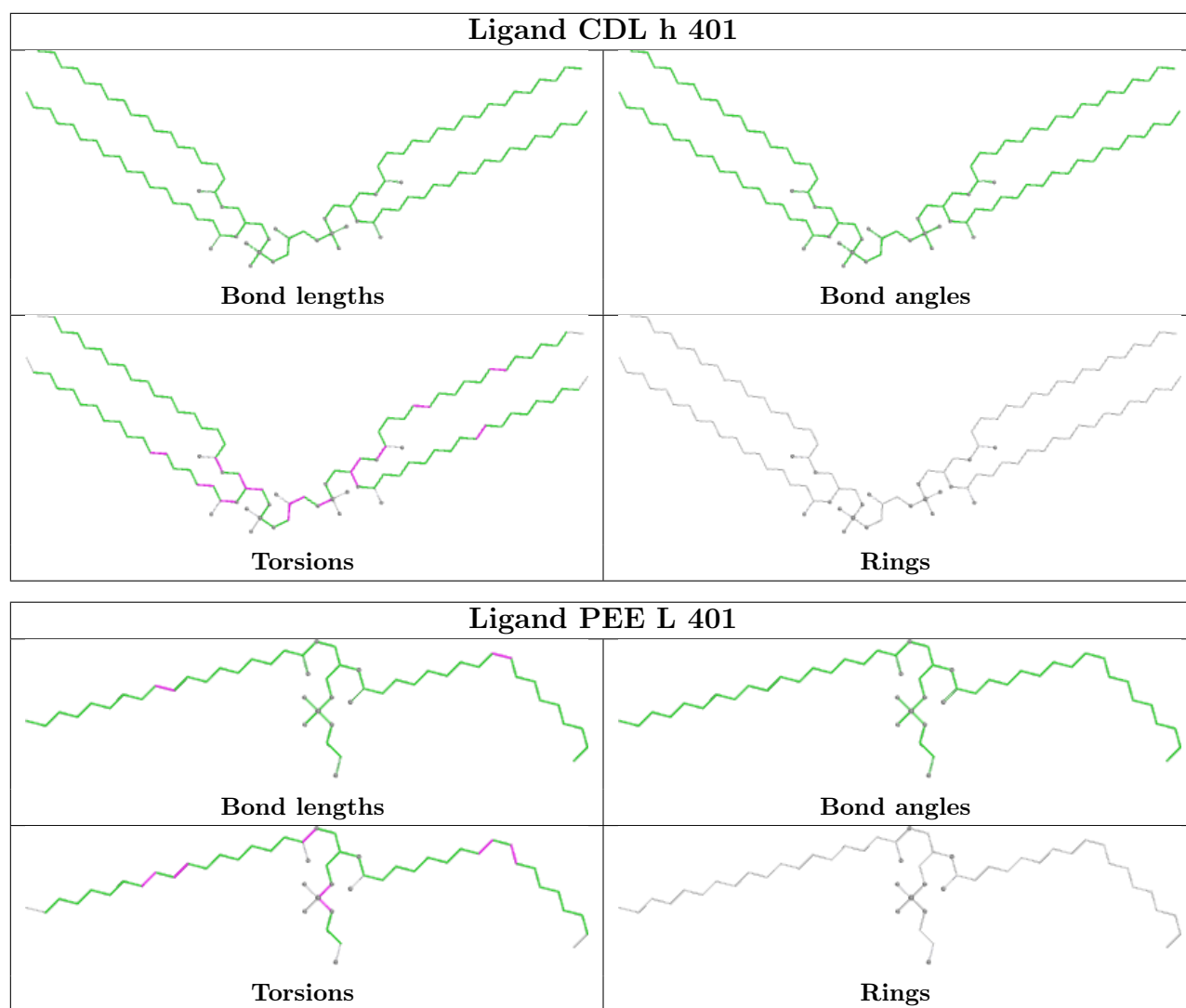


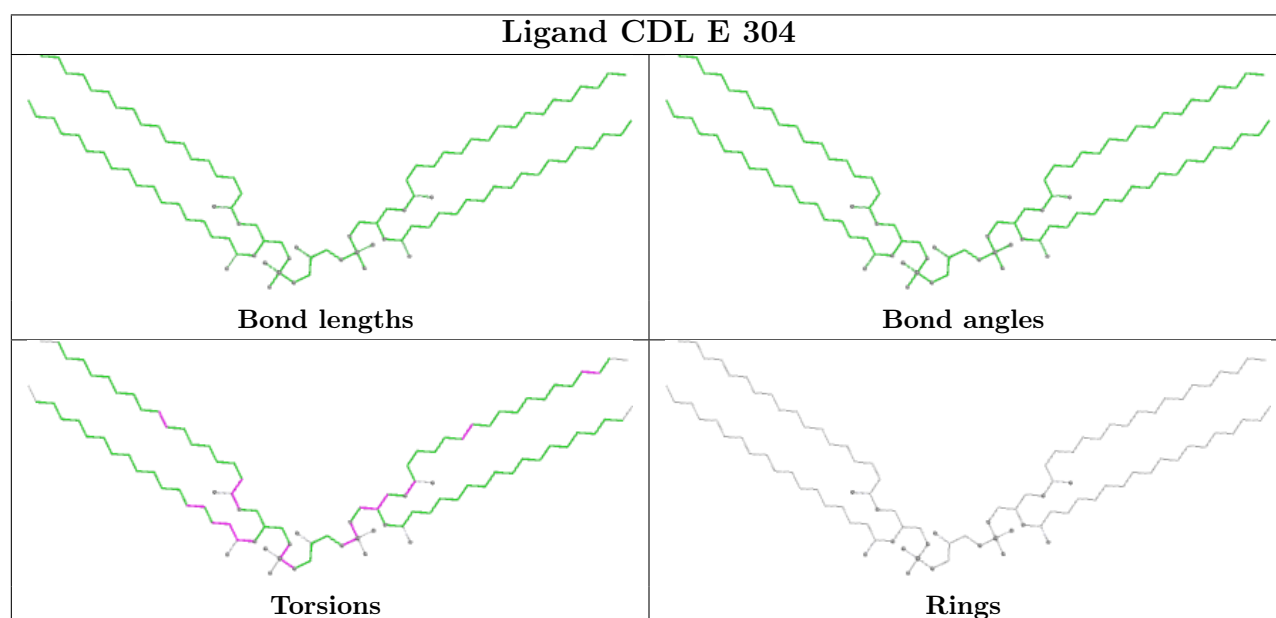
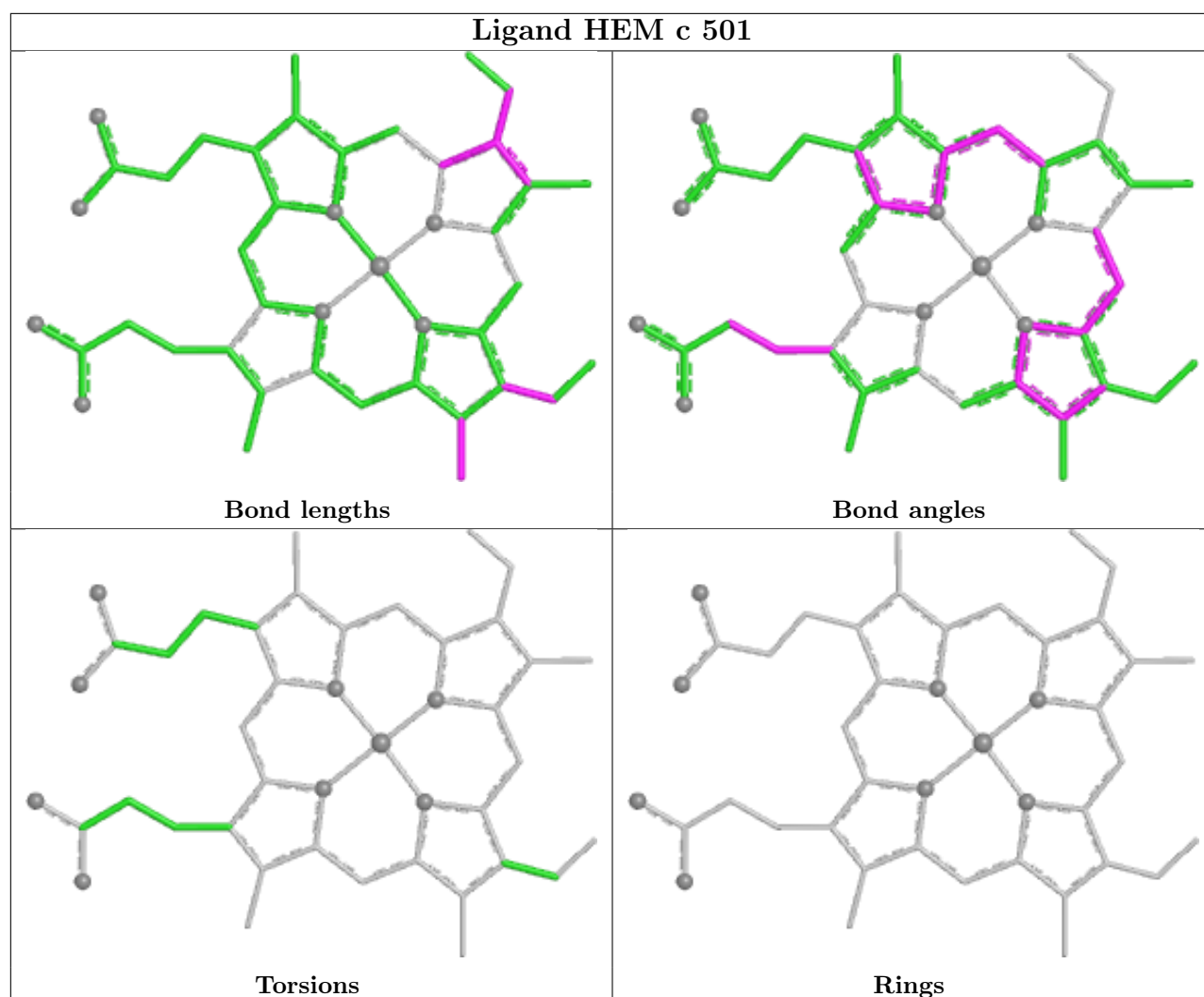


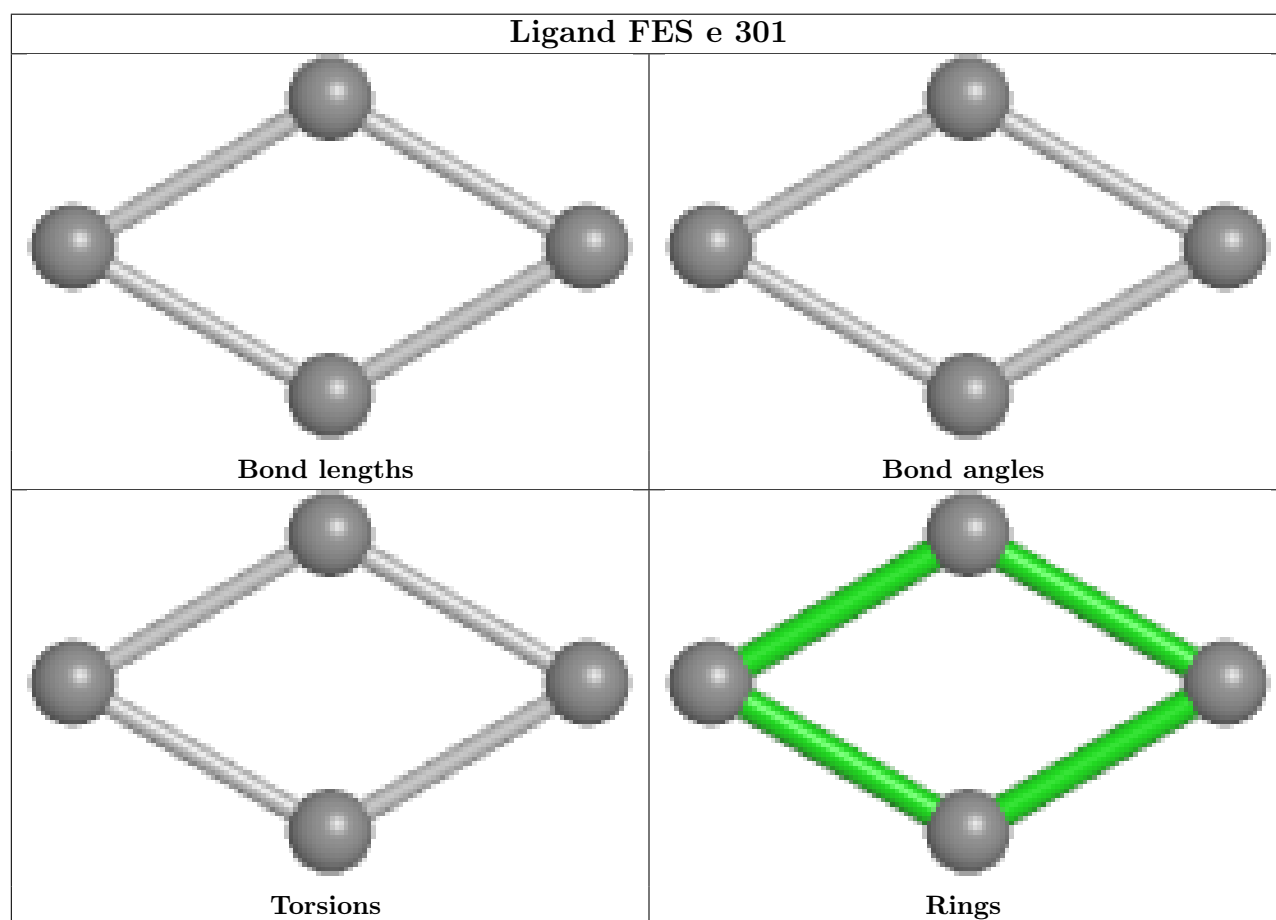
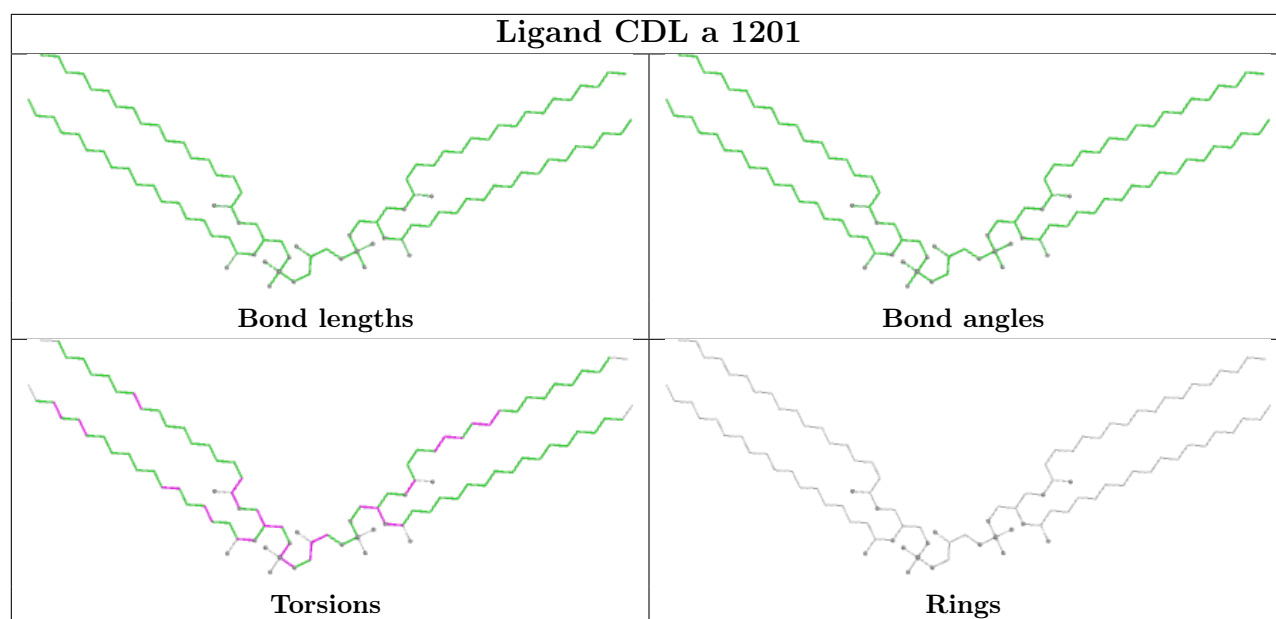


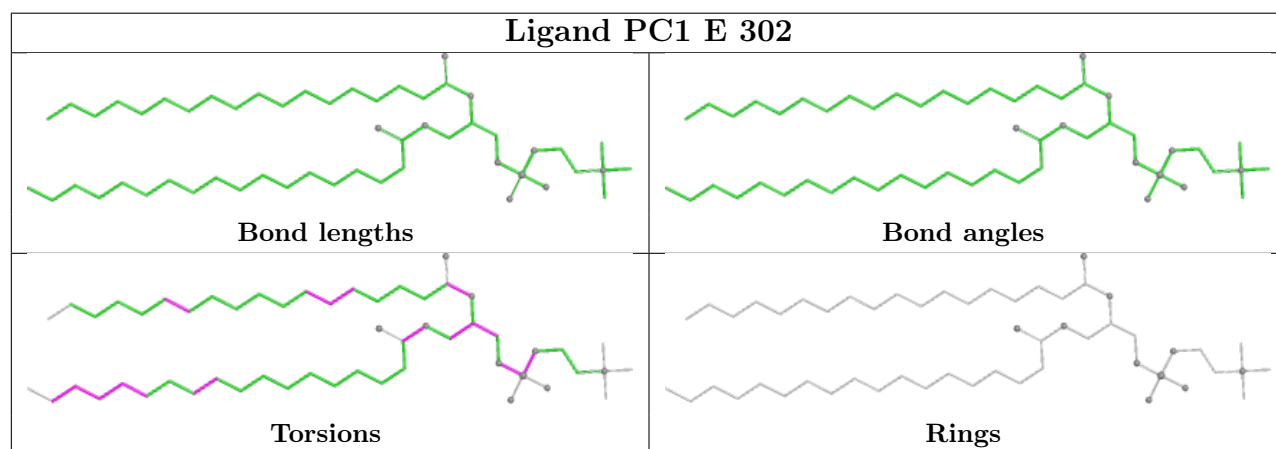
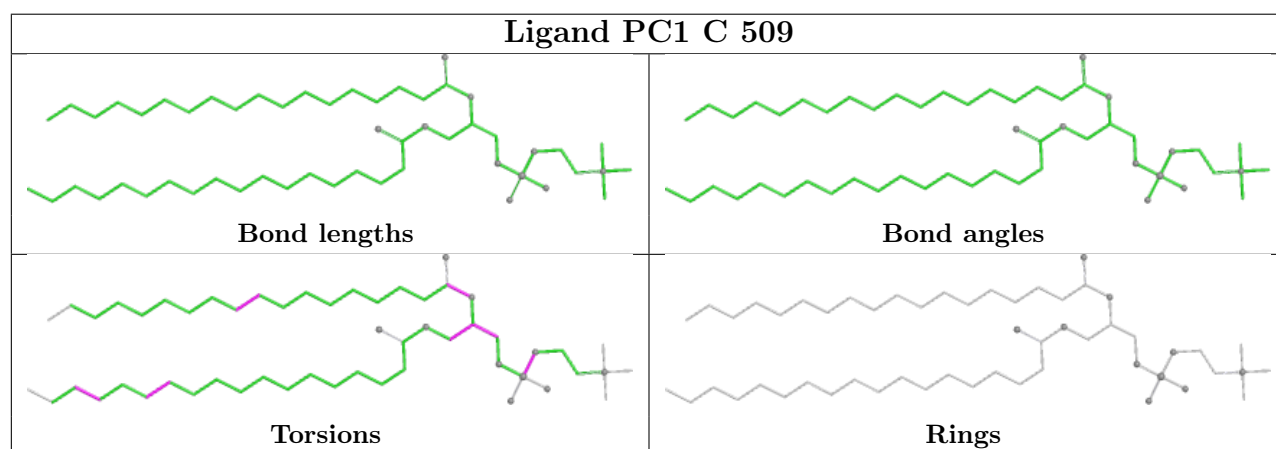
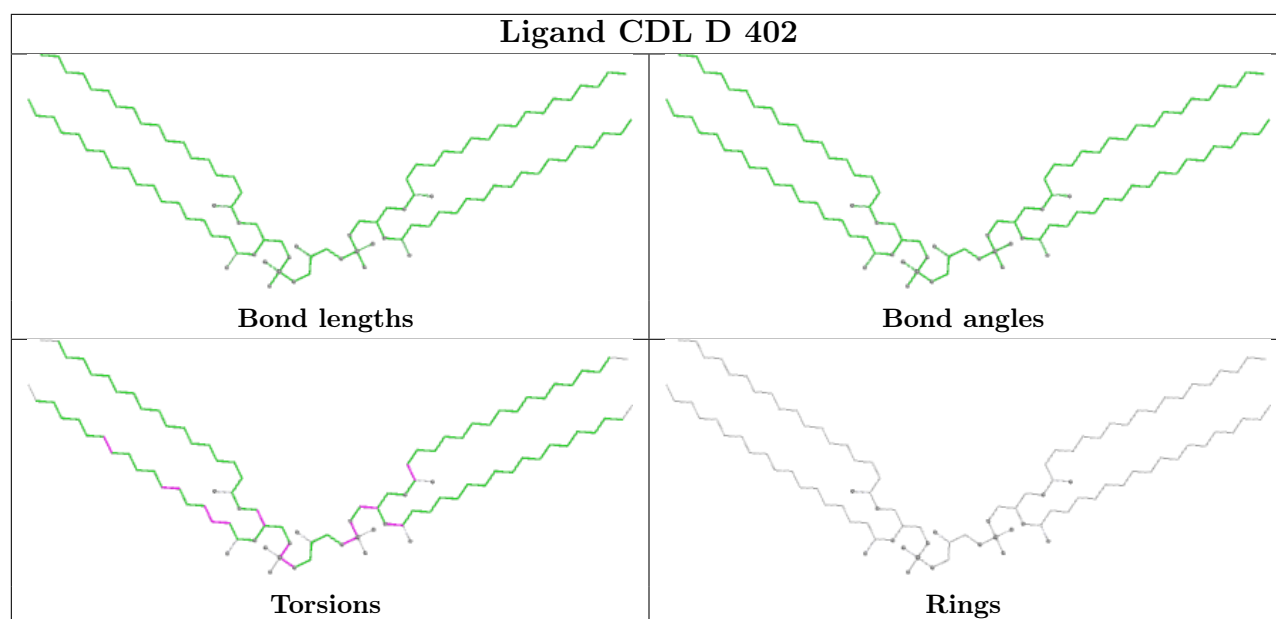


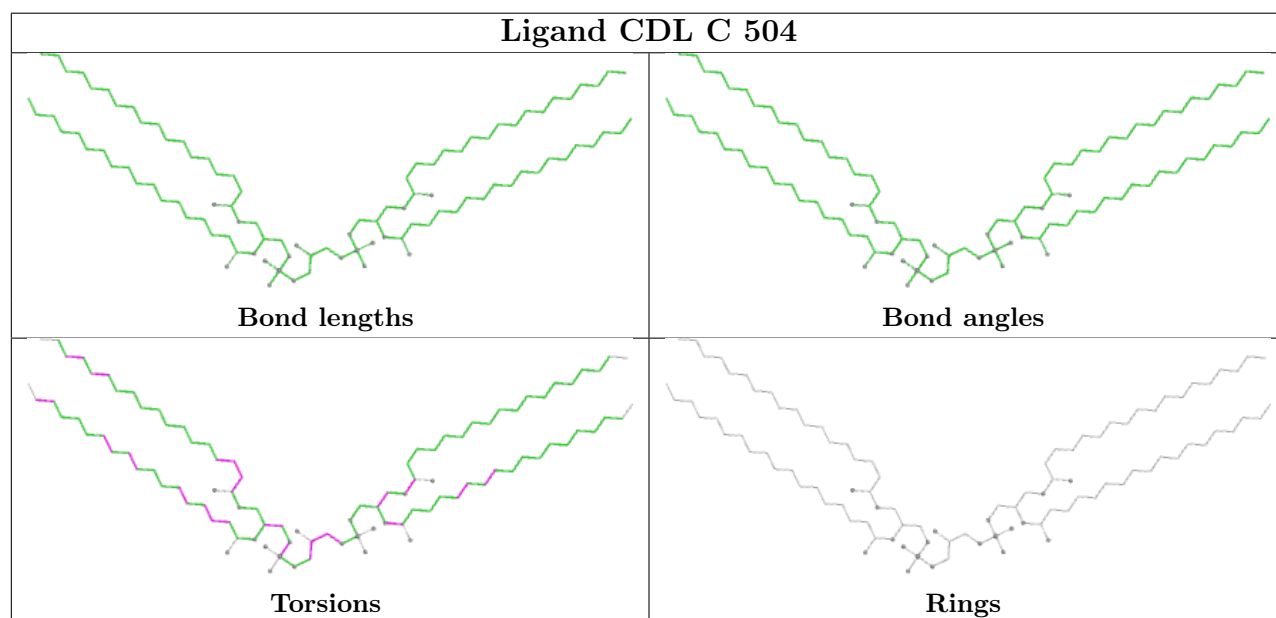
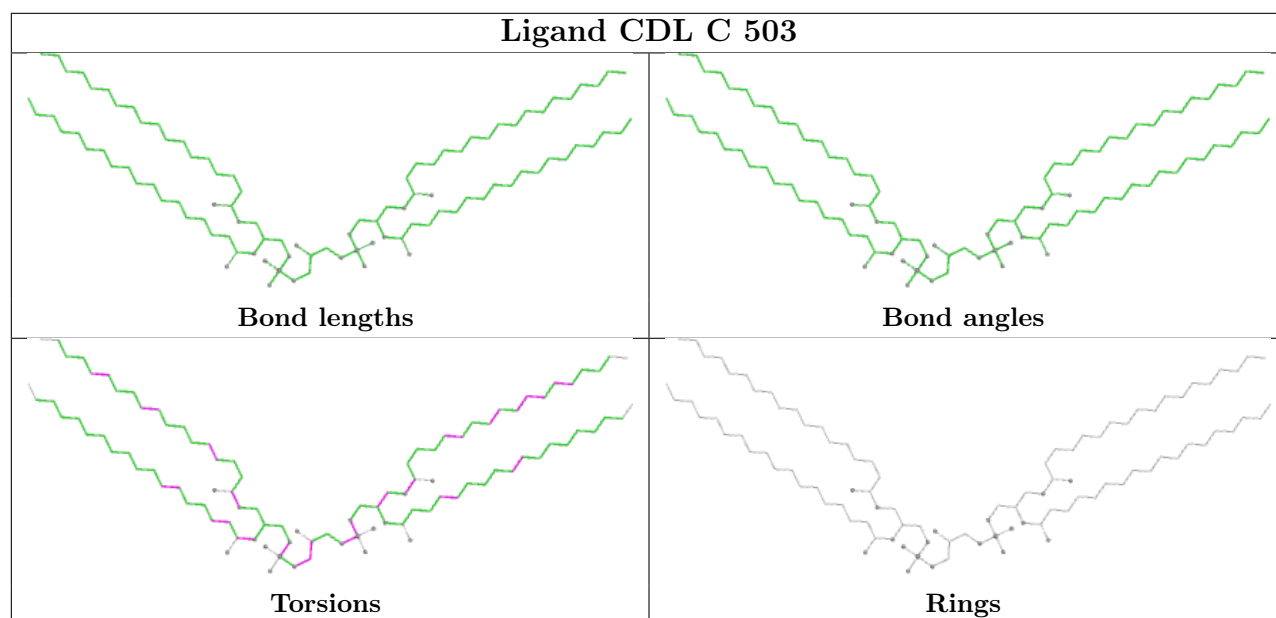
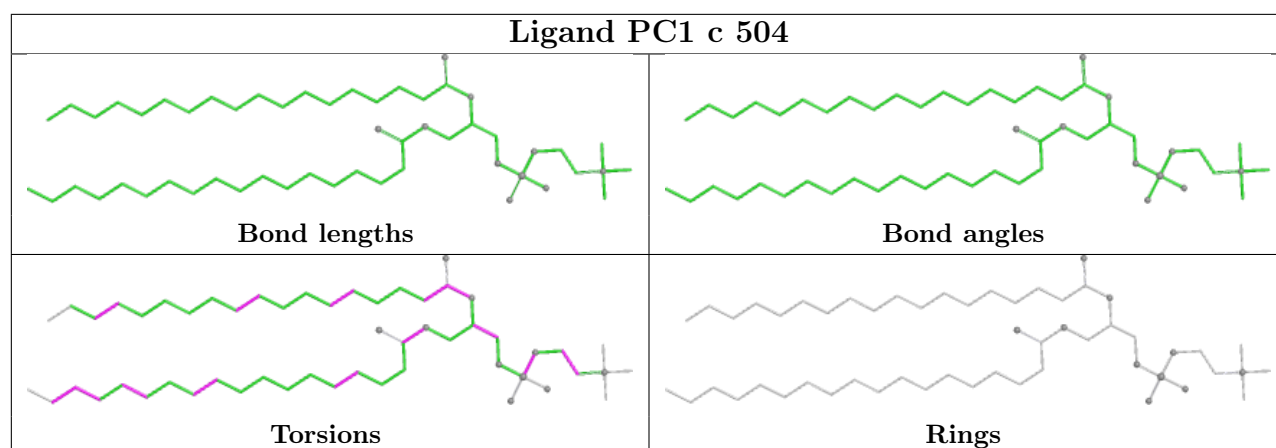


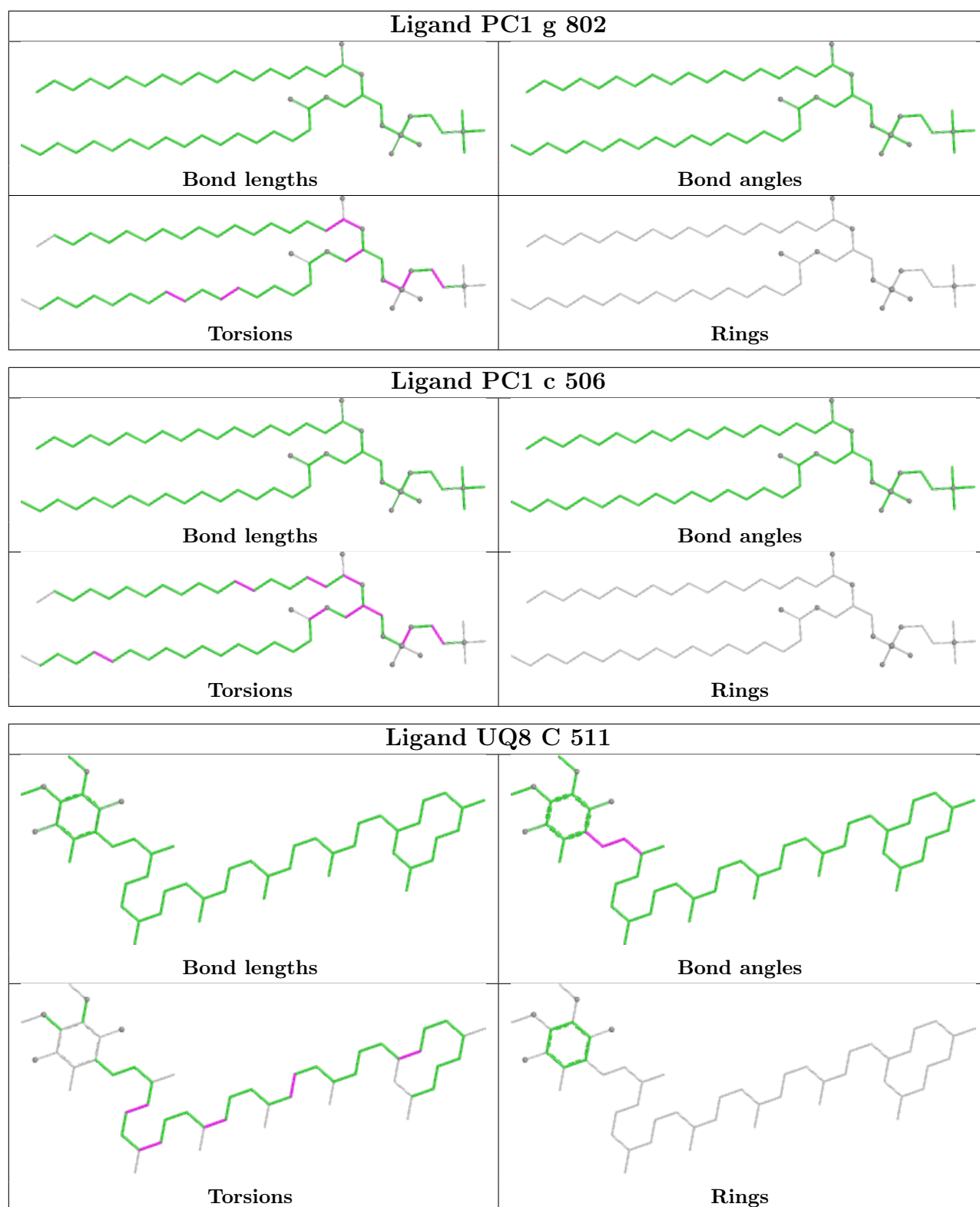


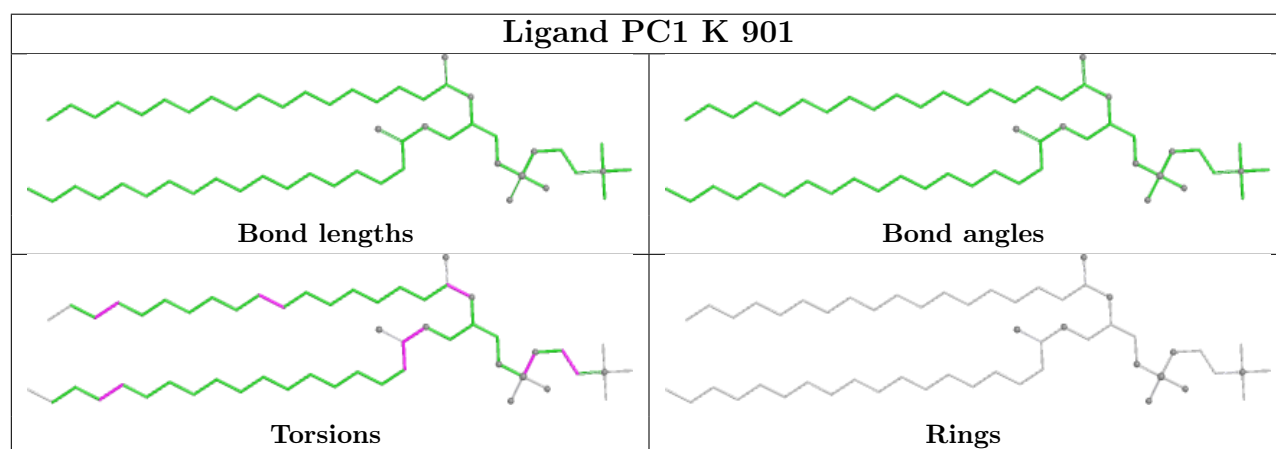
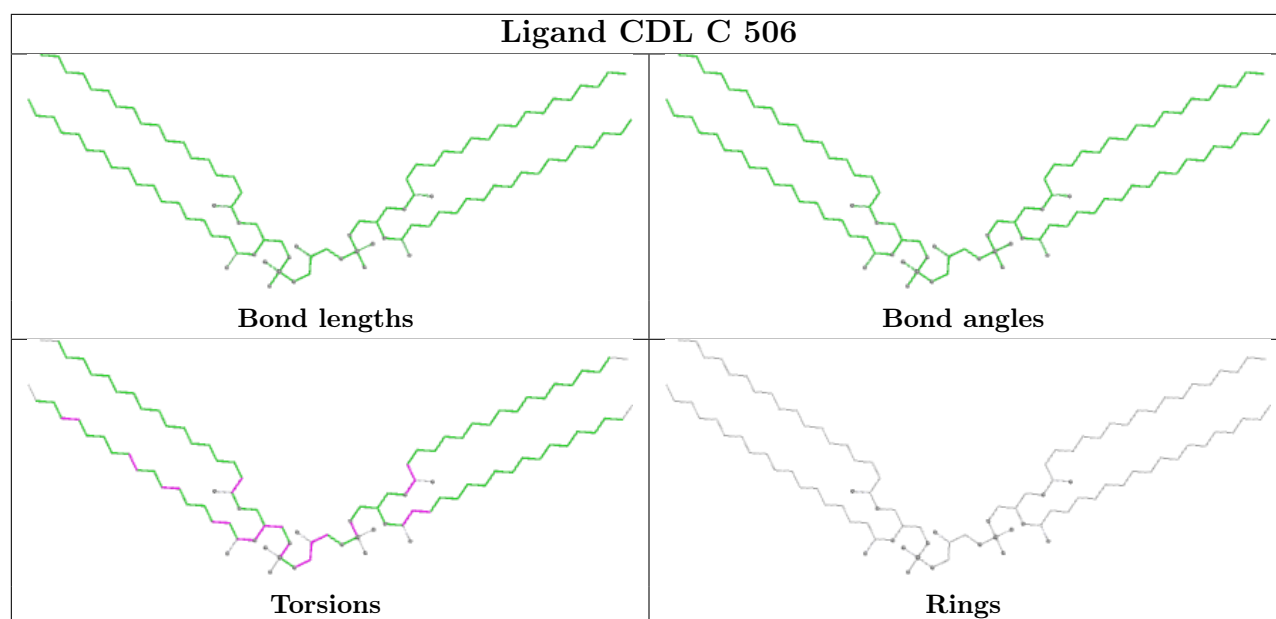


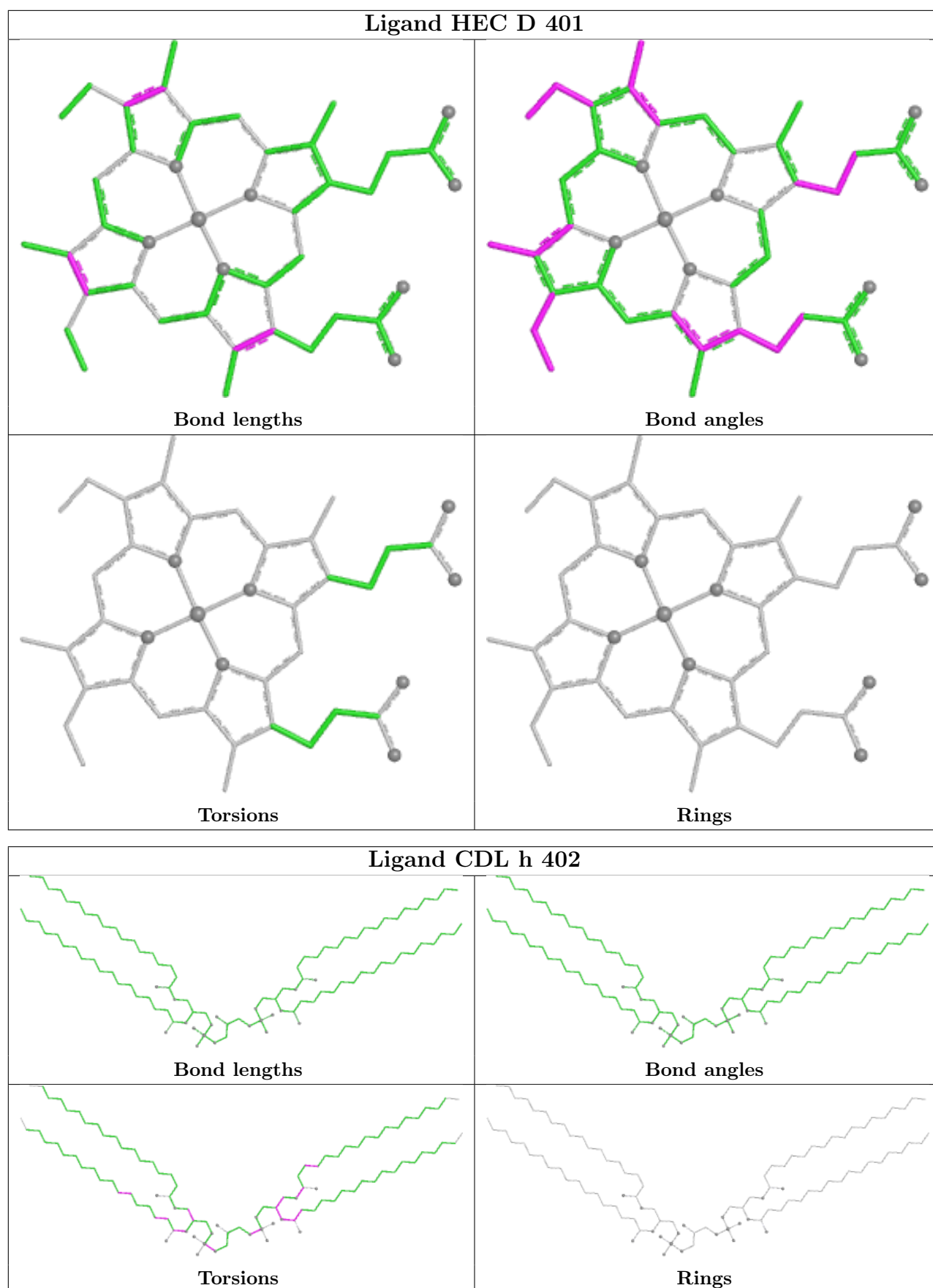


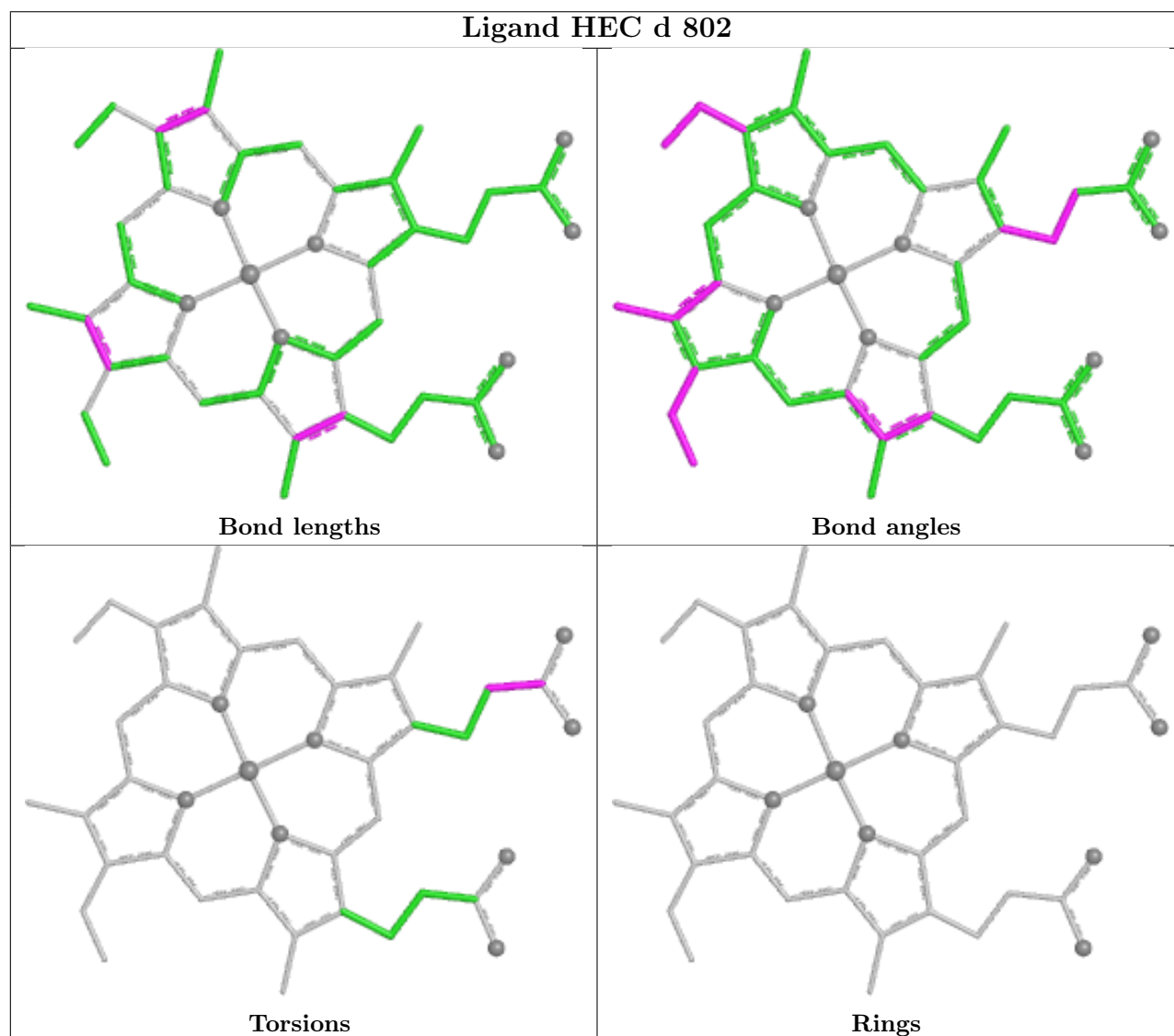
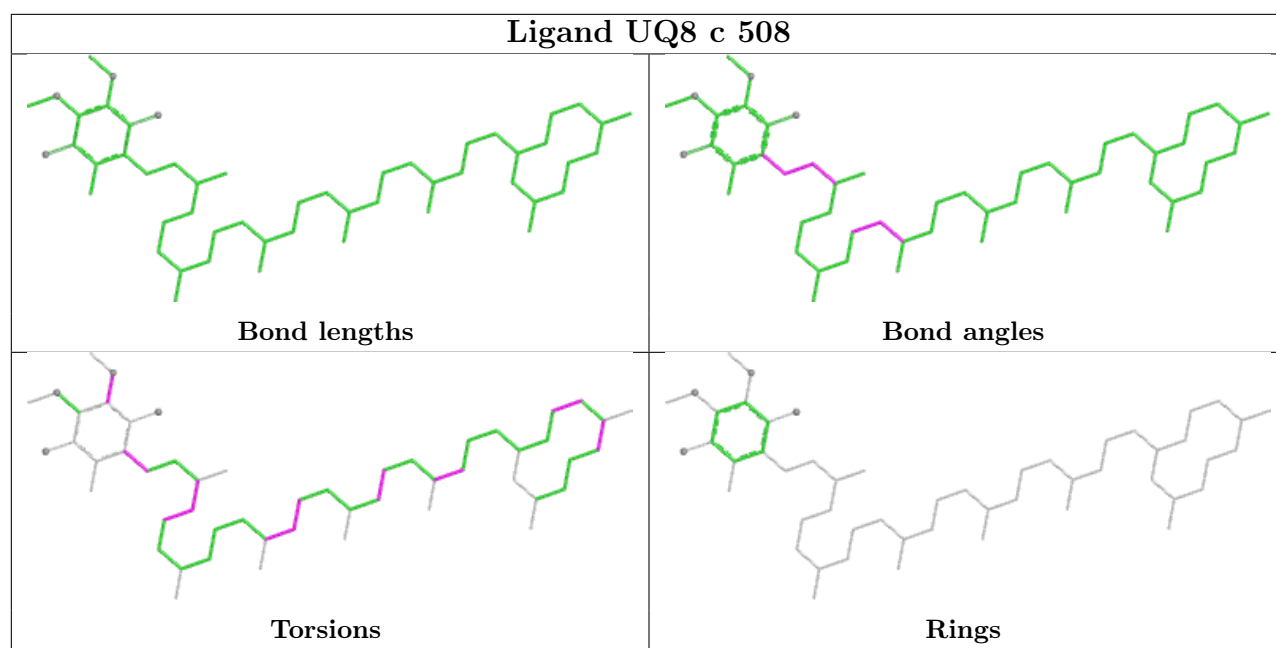


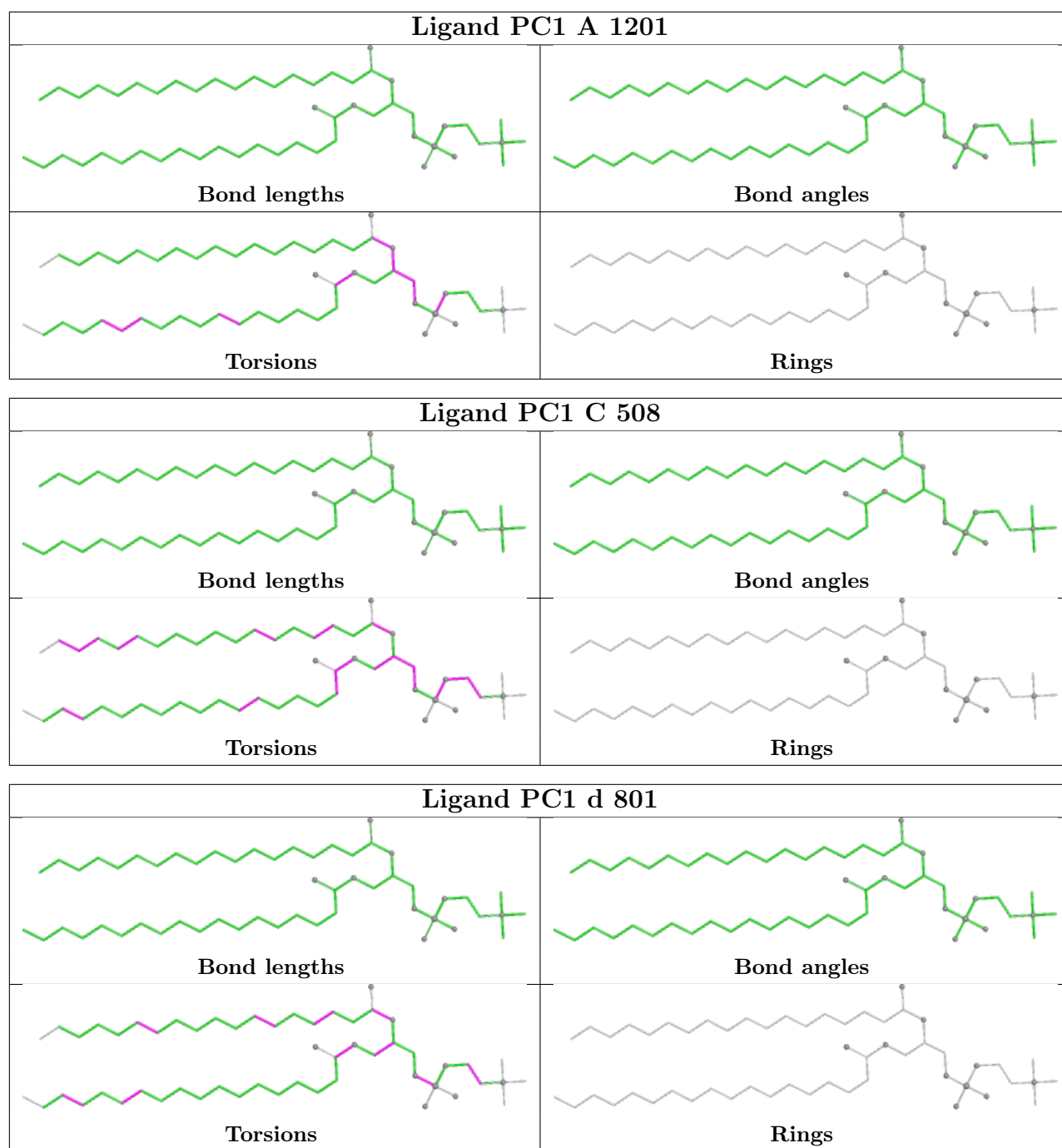


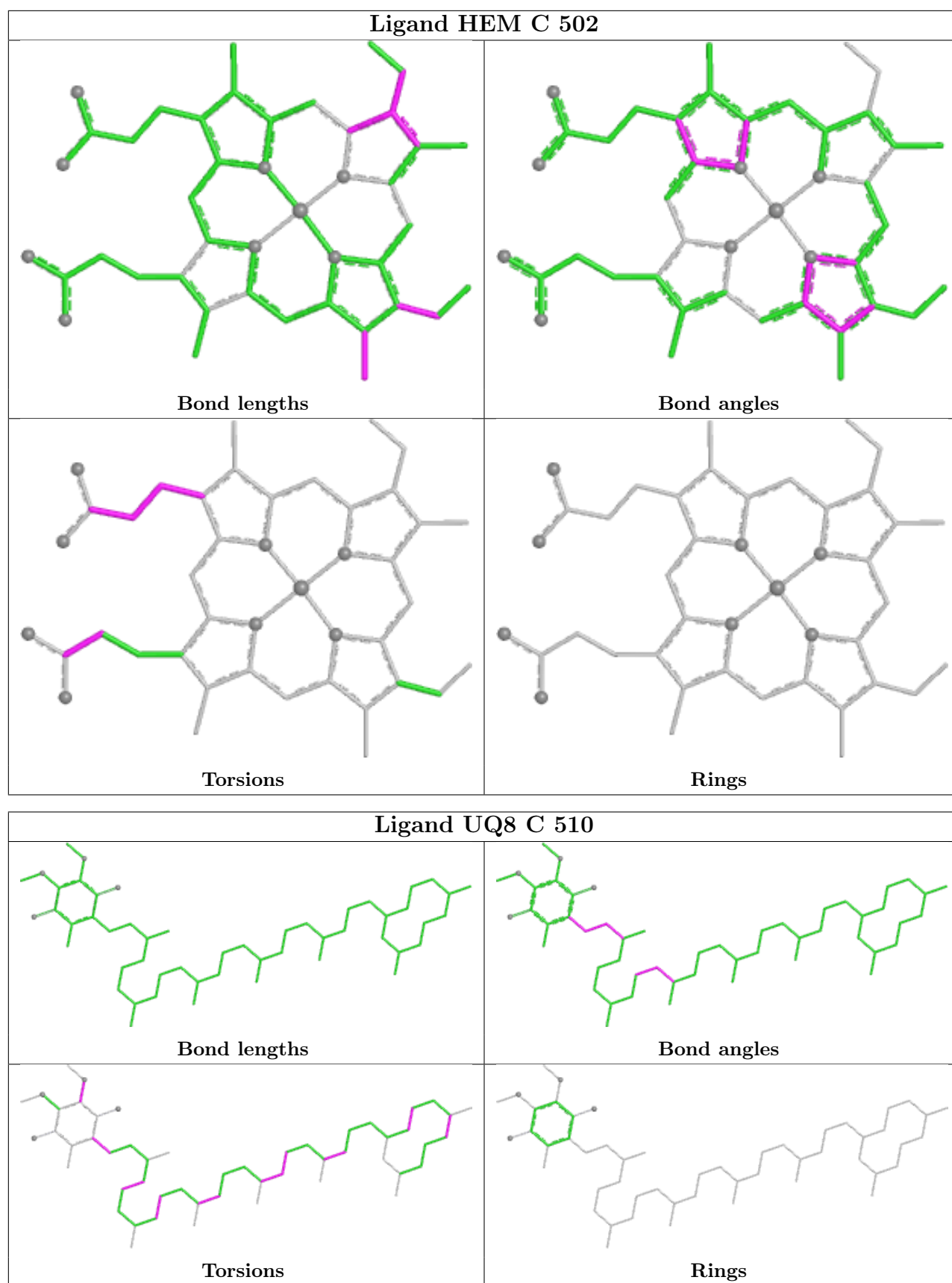


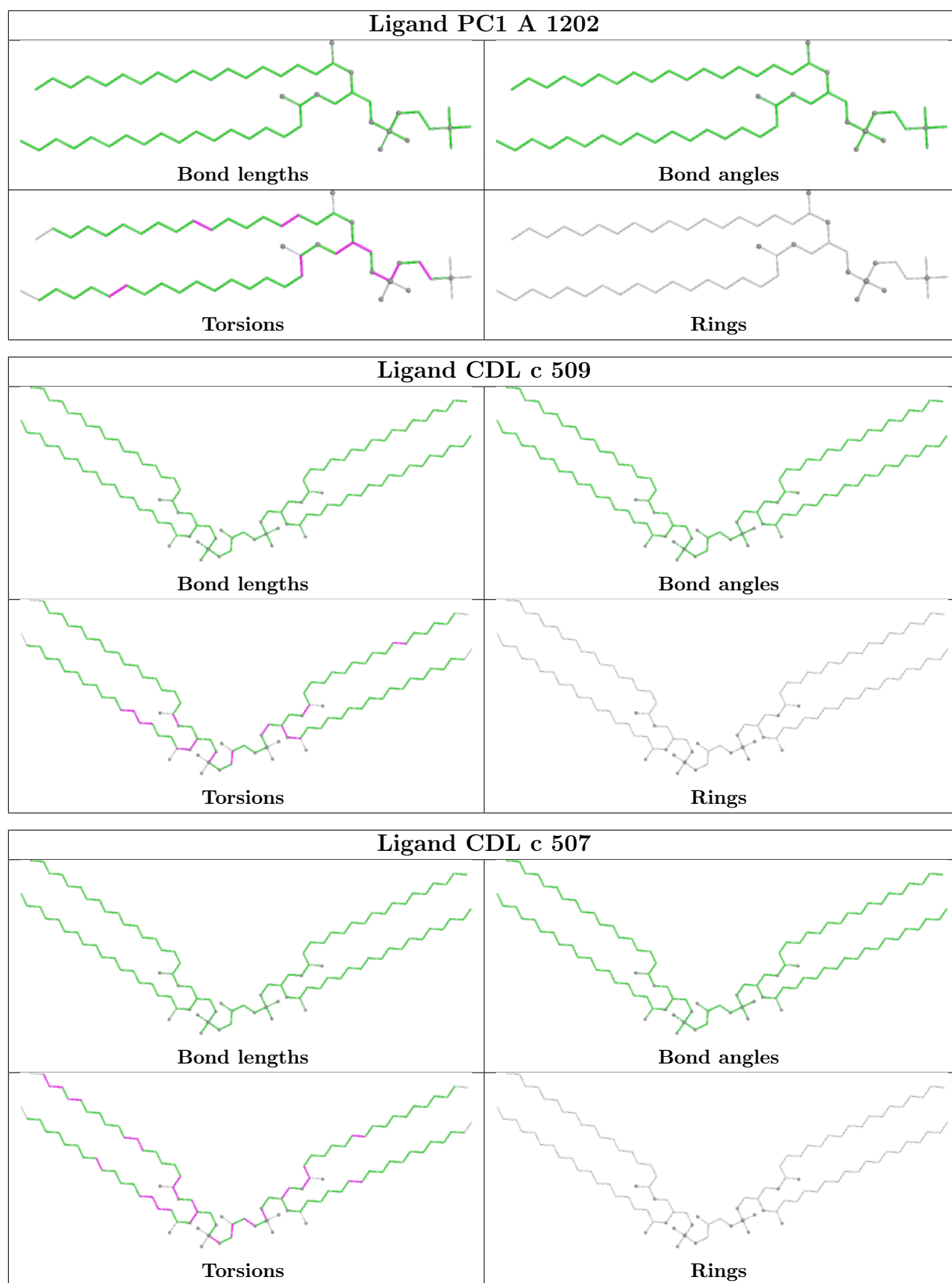


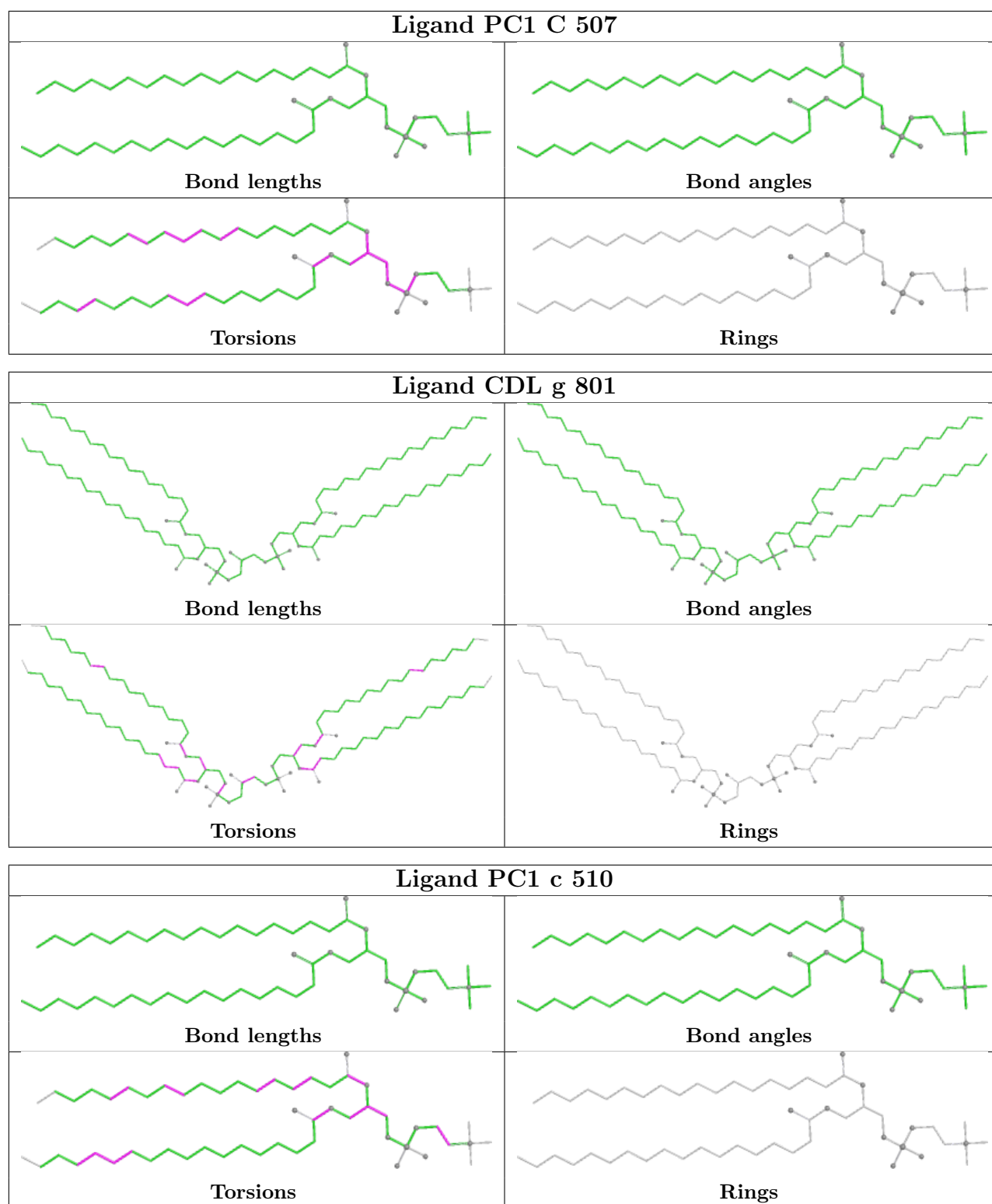


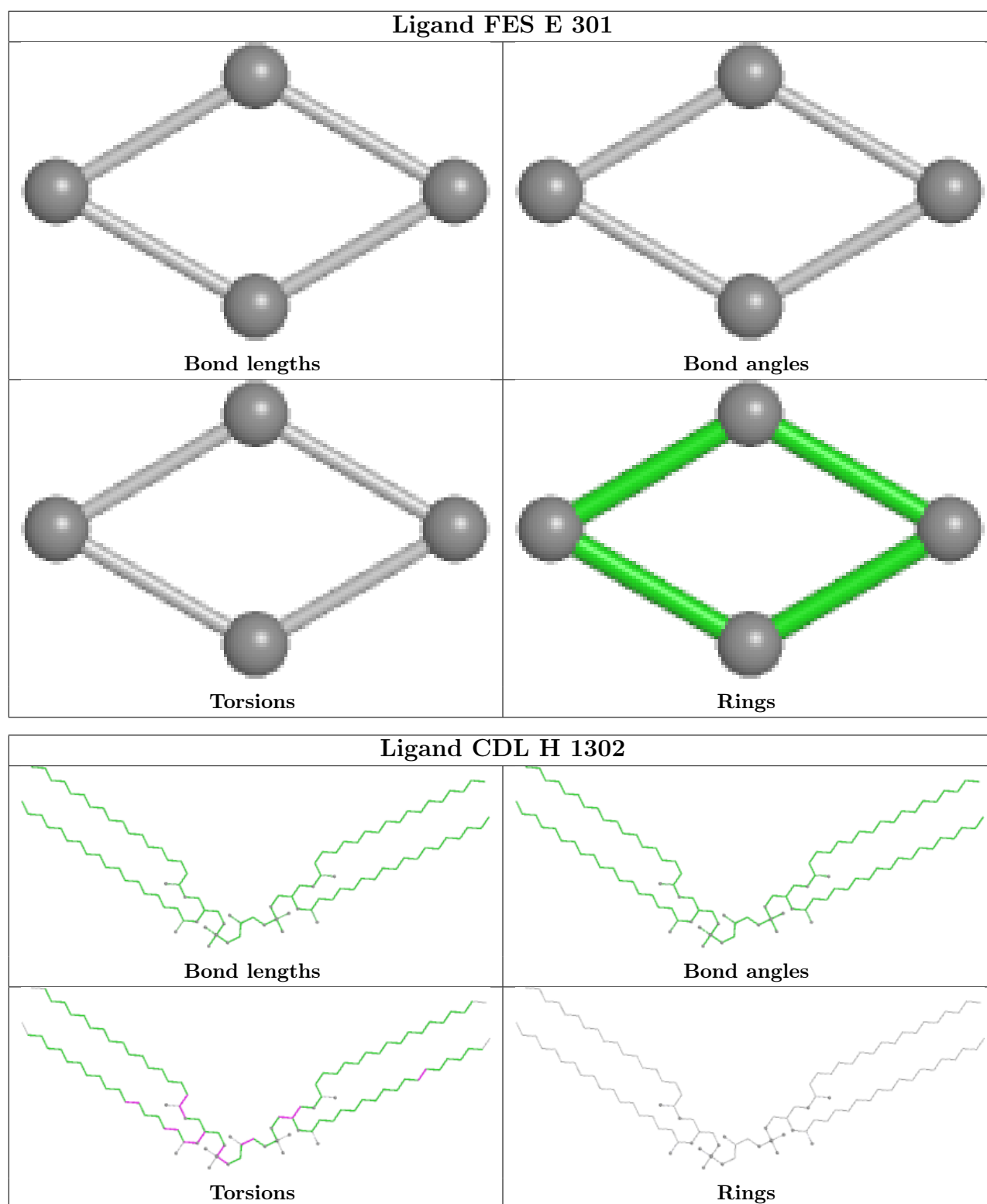












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

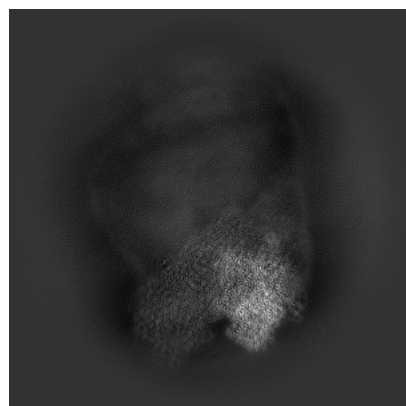
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15868. These allow visual inspection of the internal detail of the map and identification of artifacts.

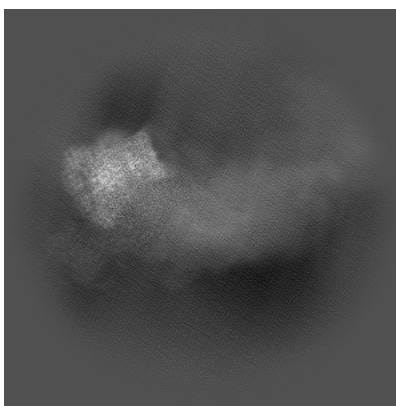
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

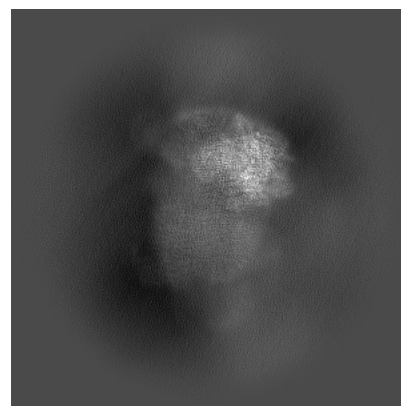
6.1.1 Primary map



X

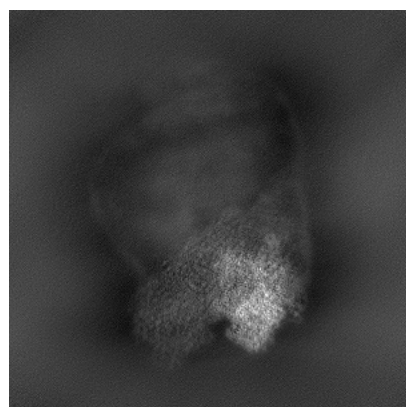


Y

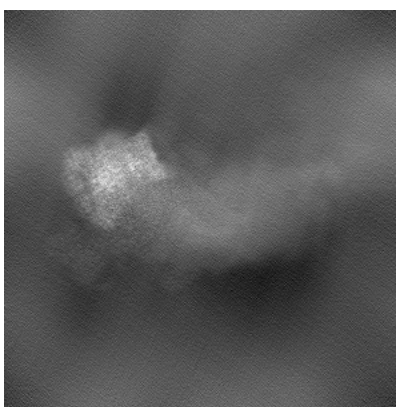


Z

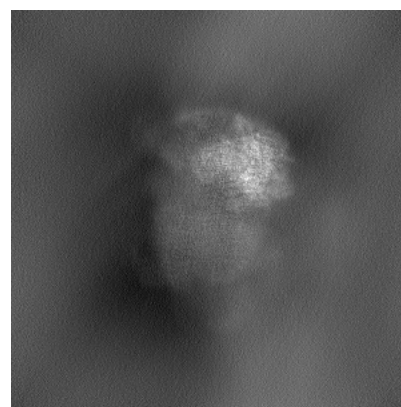
6.1.2 Raw map



X



Y

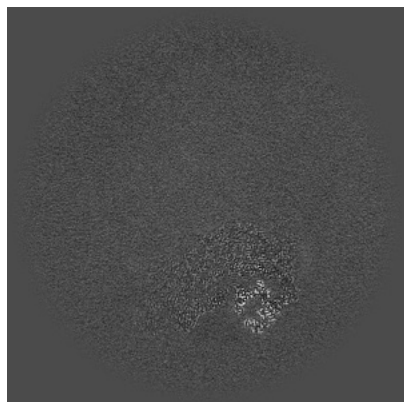


Z

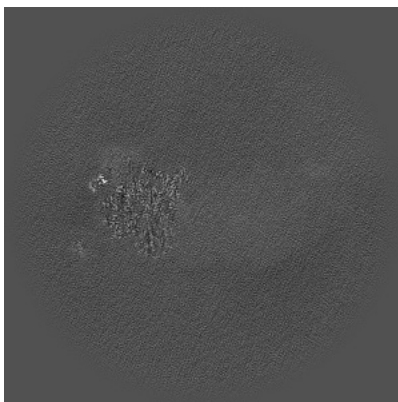
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

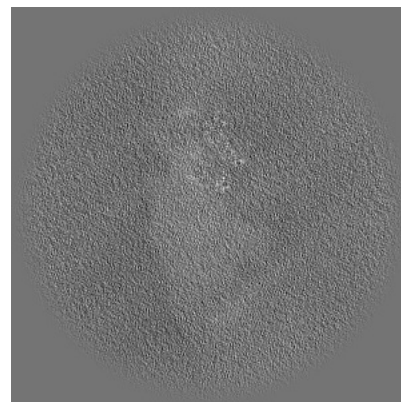
6.2.1 Primary map



X Index: 240

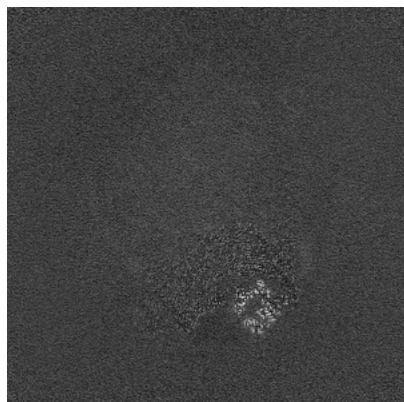


Y Index: 240

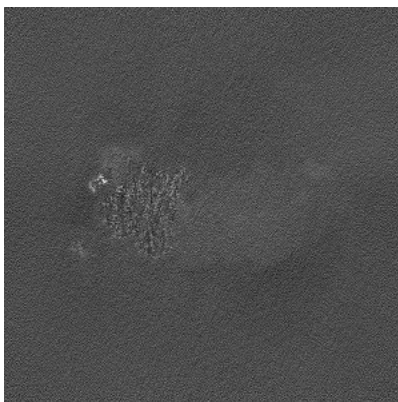


Z Index: 240

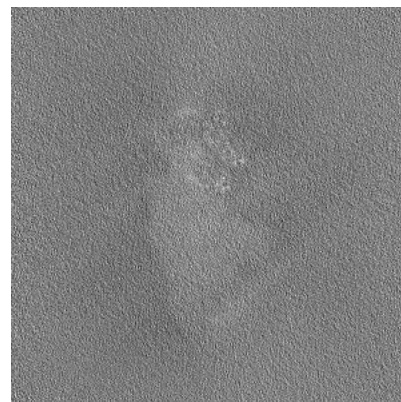
6.2.2 Raw map



X Index: 240



Y Index: 240

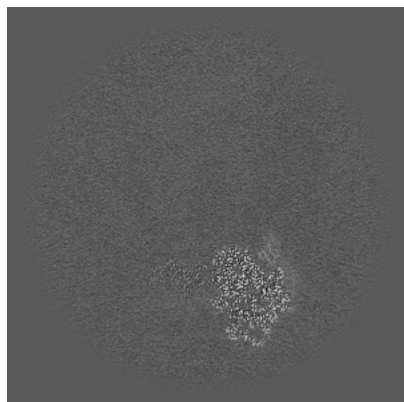


Z Index: 240

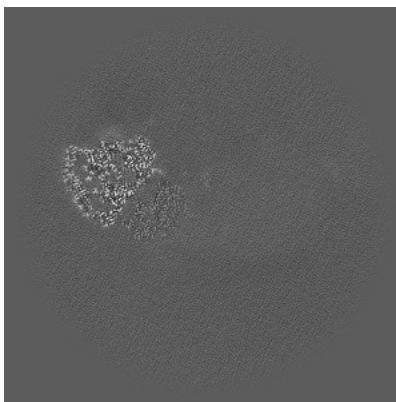
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

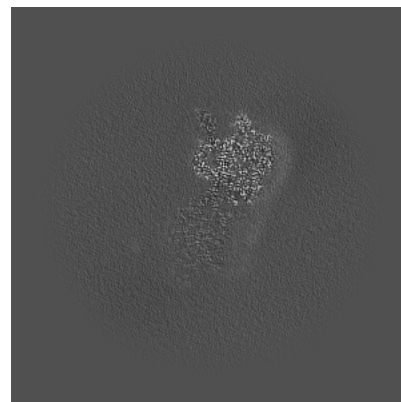
6.3.1 Primary map



X Index: 289

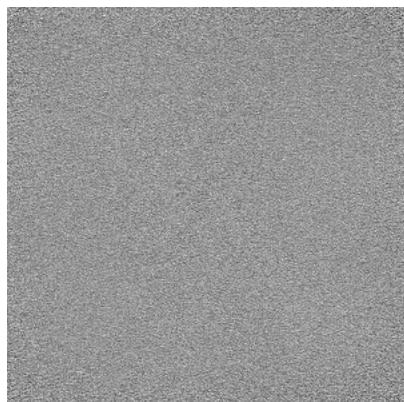


Y Index: 295

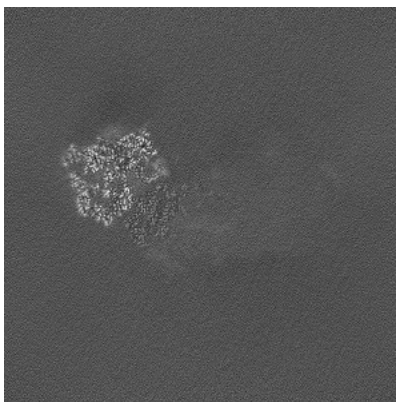


Z Index: 125

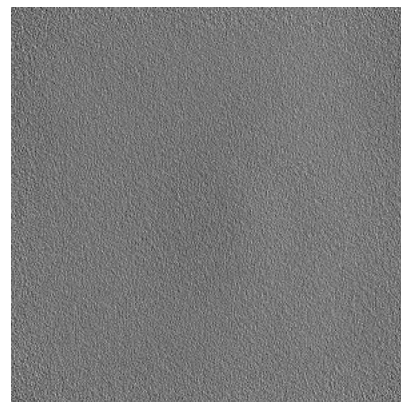
6.3.2 Raw map



X Index: 0



Y Index: 304

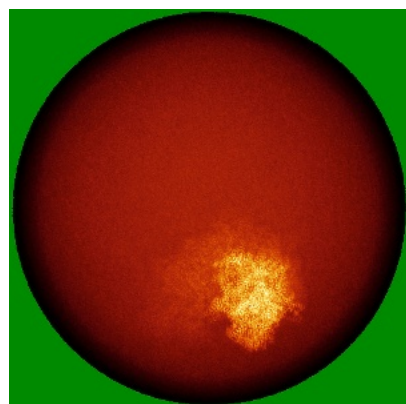


Z Index: 0

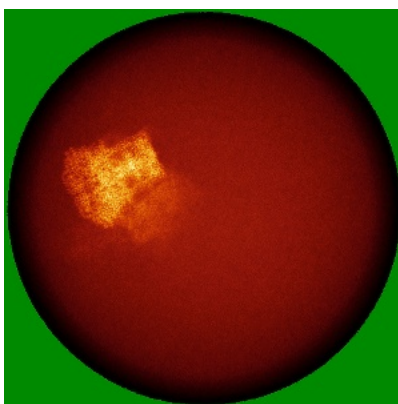
The images above show the largest variance slices of the map in three orthogonal directions.

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

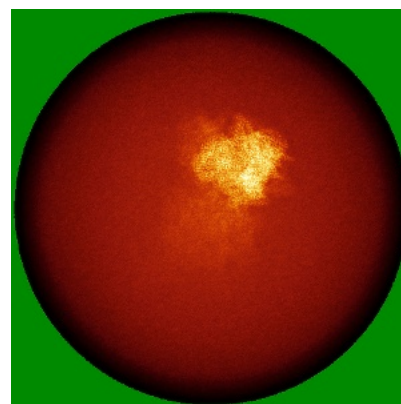
6.4.1 Primary map



X

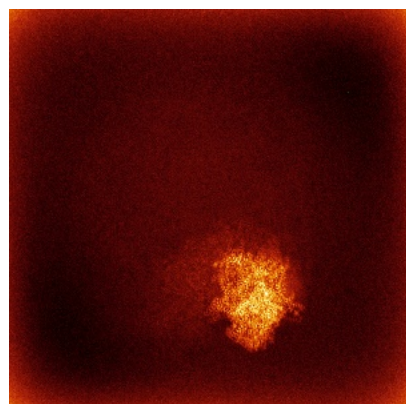


Y

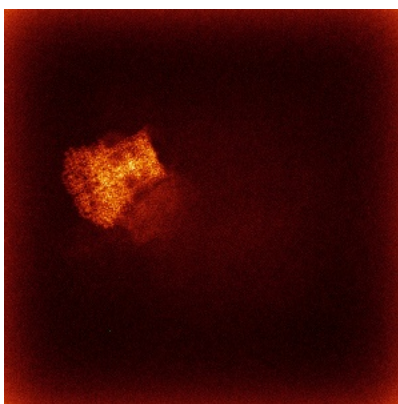


Z

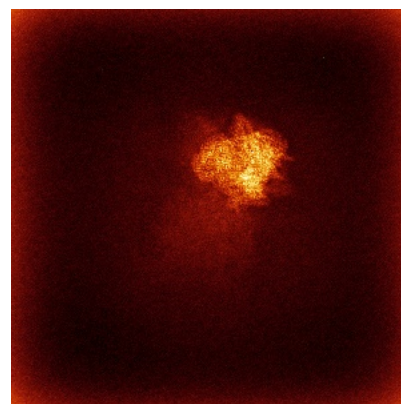
6.4.2 Raw map



X



Y

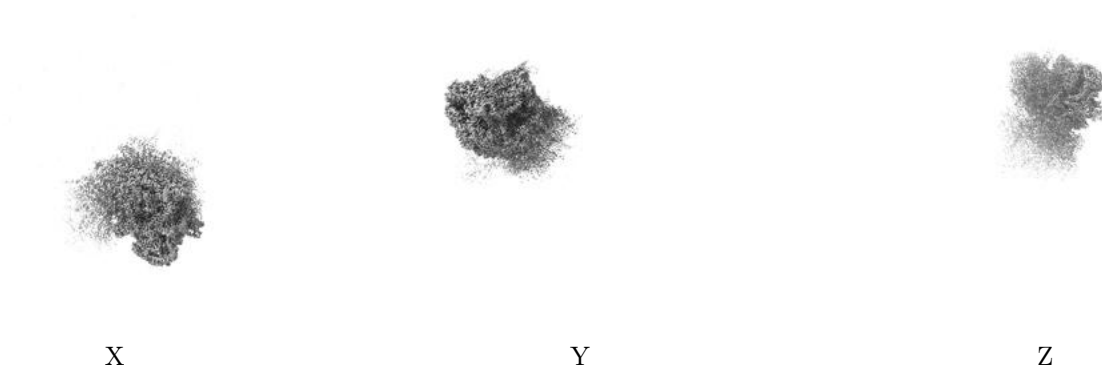


Z

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

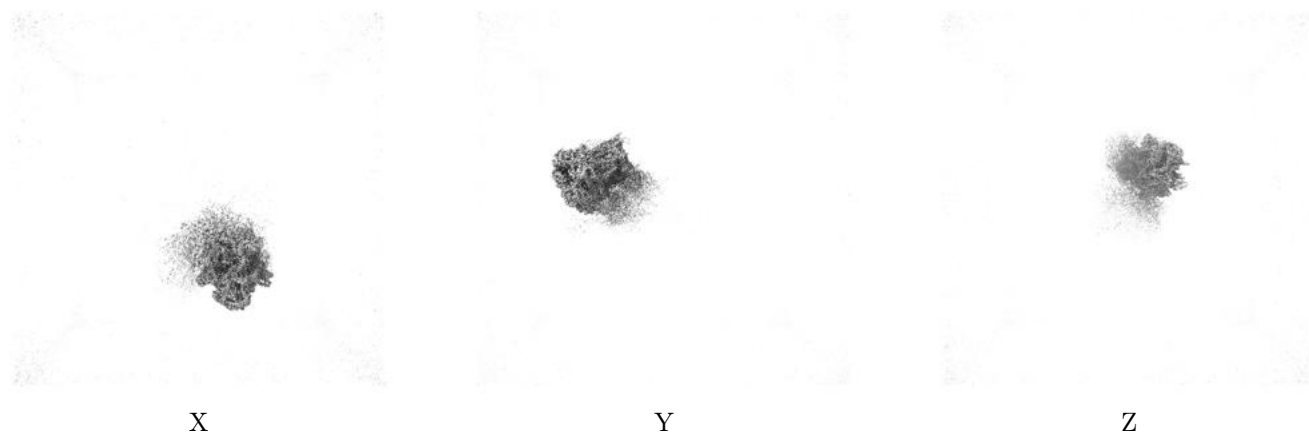
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

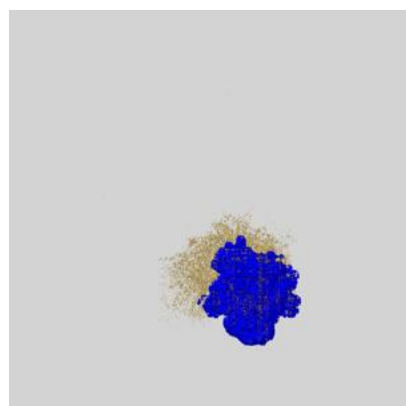
6.6 Mask visualisation [i](#)

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

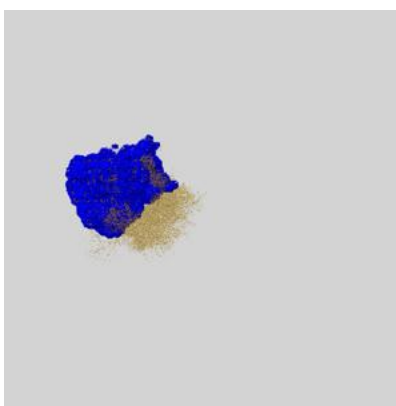
A mask typically either:

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

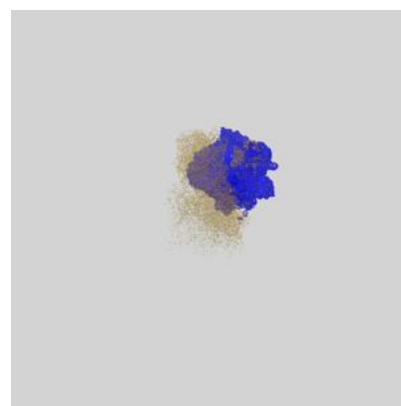
6.6.1 emd_15868_msk_1.map [i](#)



X



Y

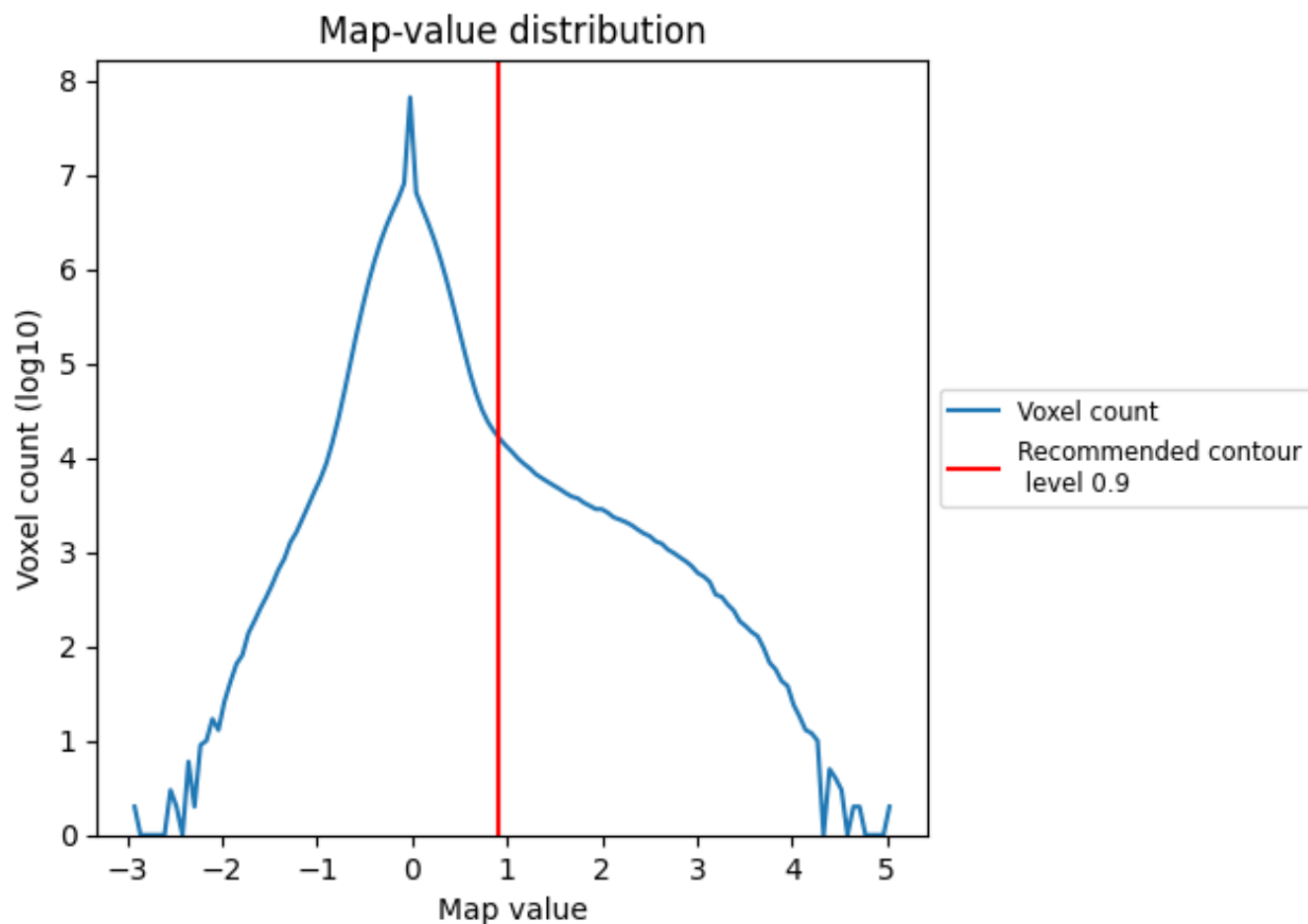


Z

7 Map analysis [i](#)

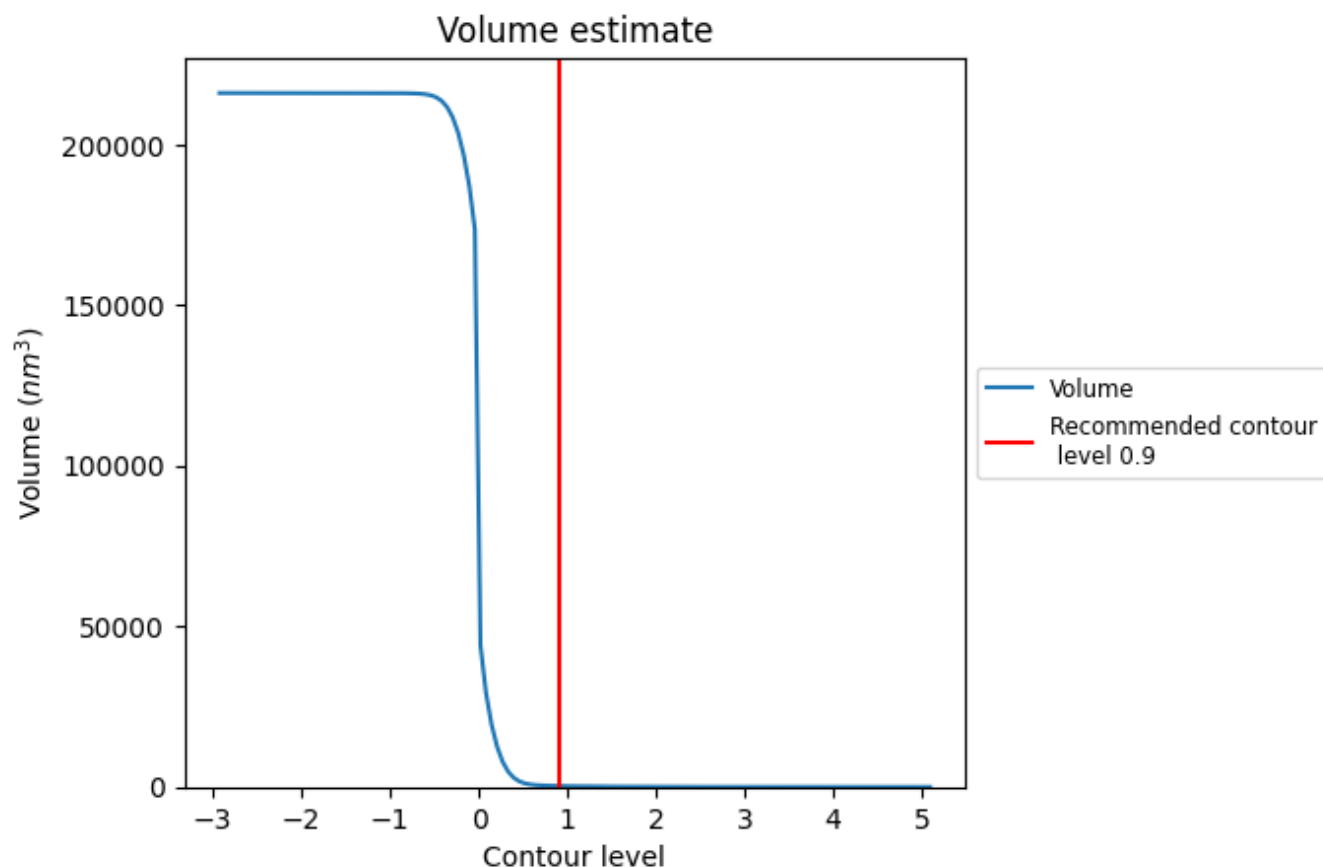
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

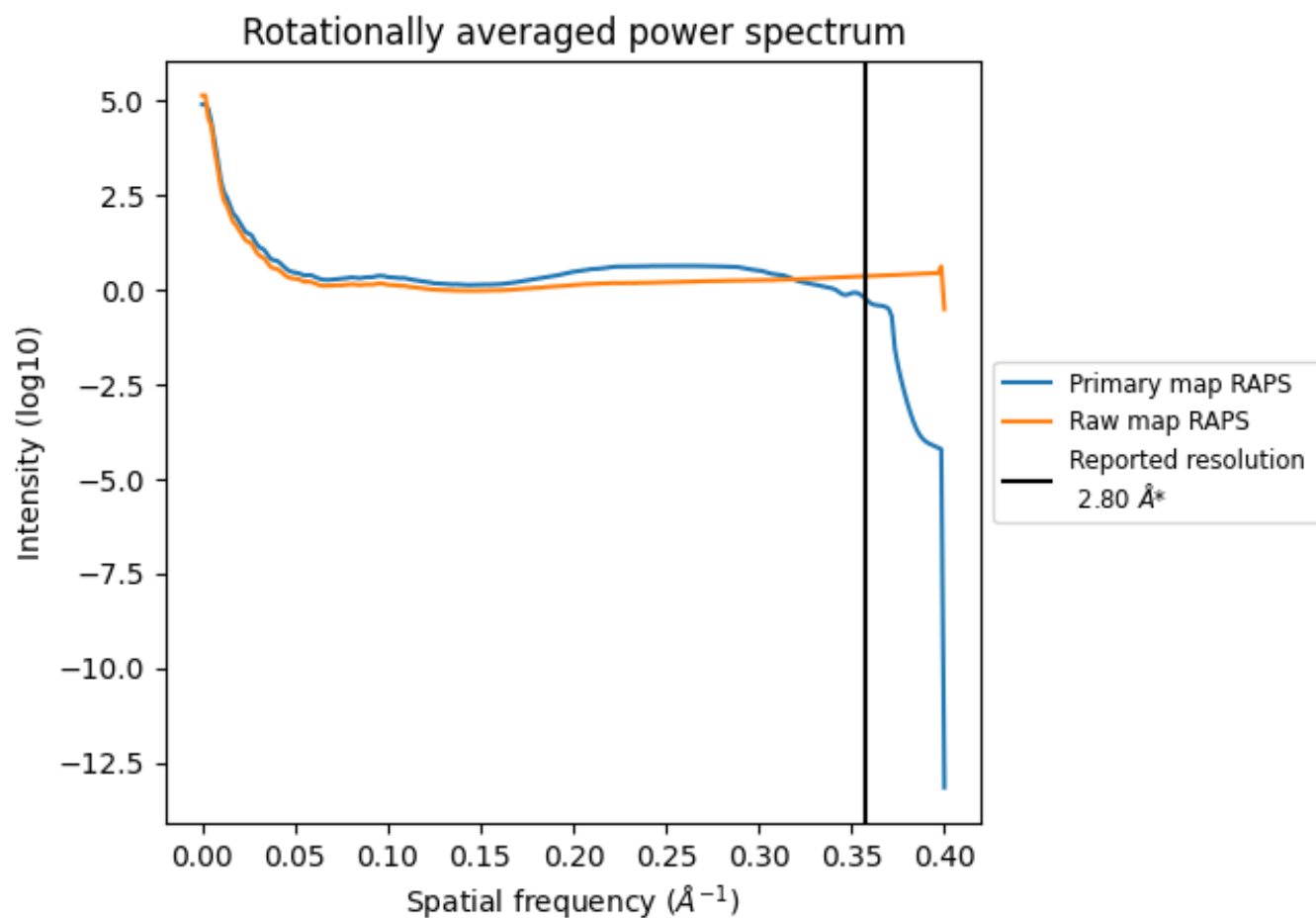
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm^3 ; this corresponds to an approximate mass of 270 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 ⓘ

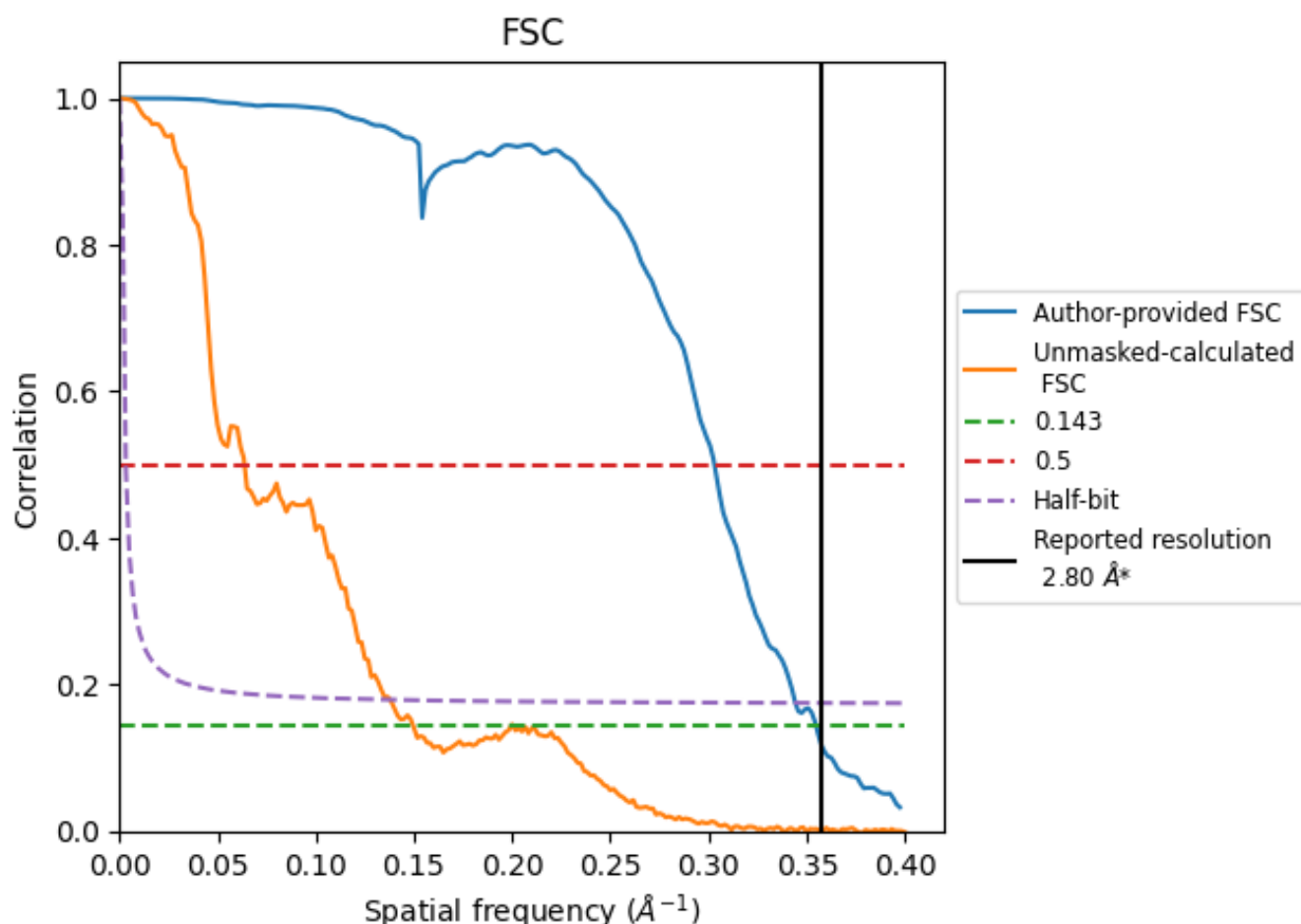


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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](#)

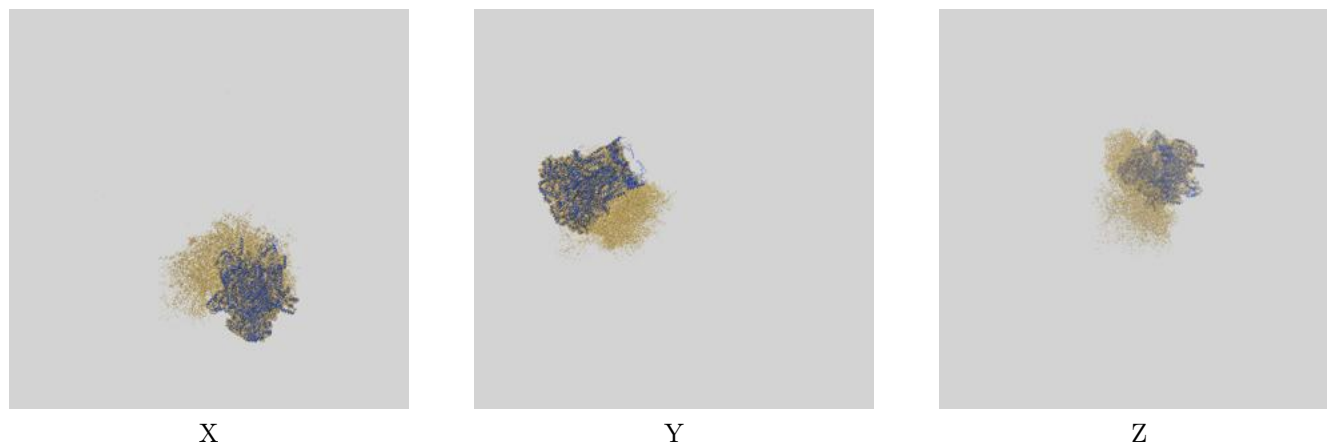
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.30	2.91
Unmasked-calculated*	6.68	15.70	7.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.68 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

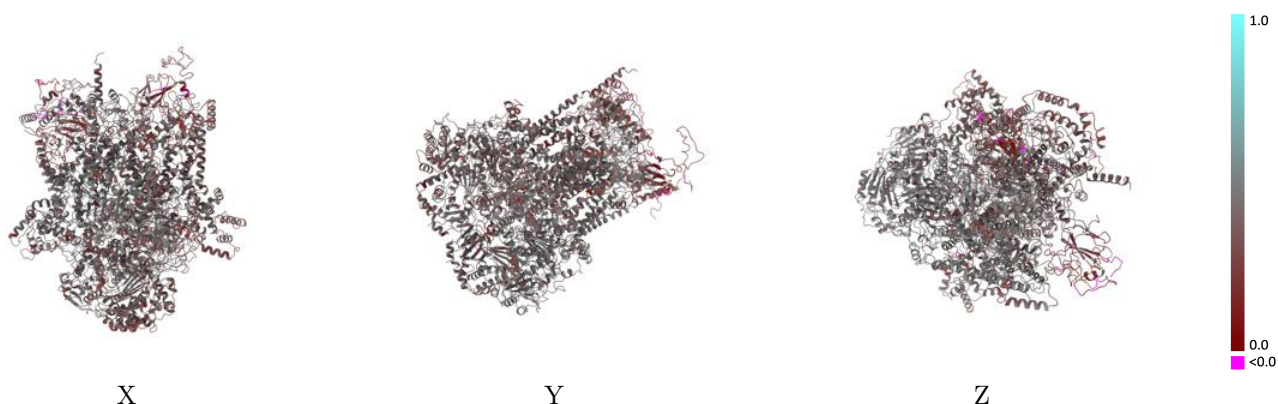
This section contains information regarding the fit between EMDB map EMD-15868 and PDB model 8B6J. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



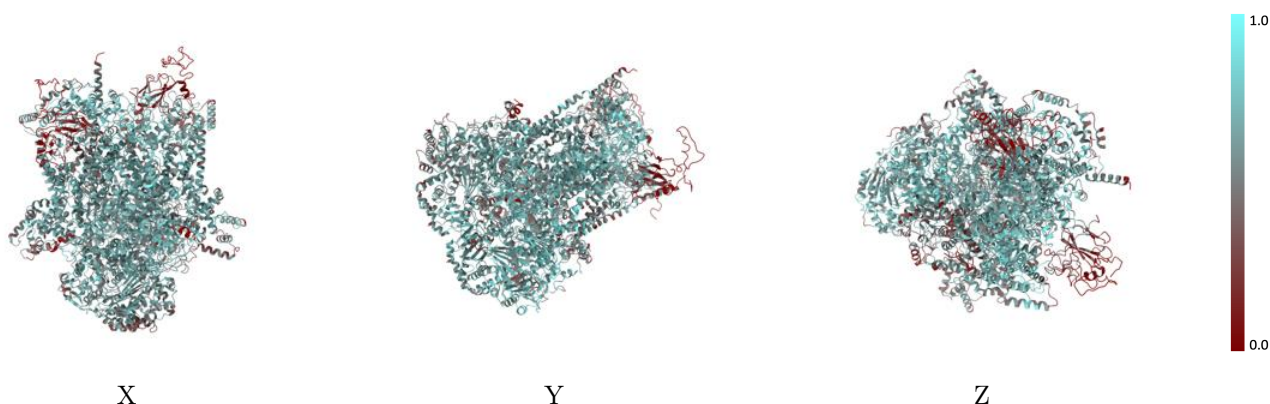
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



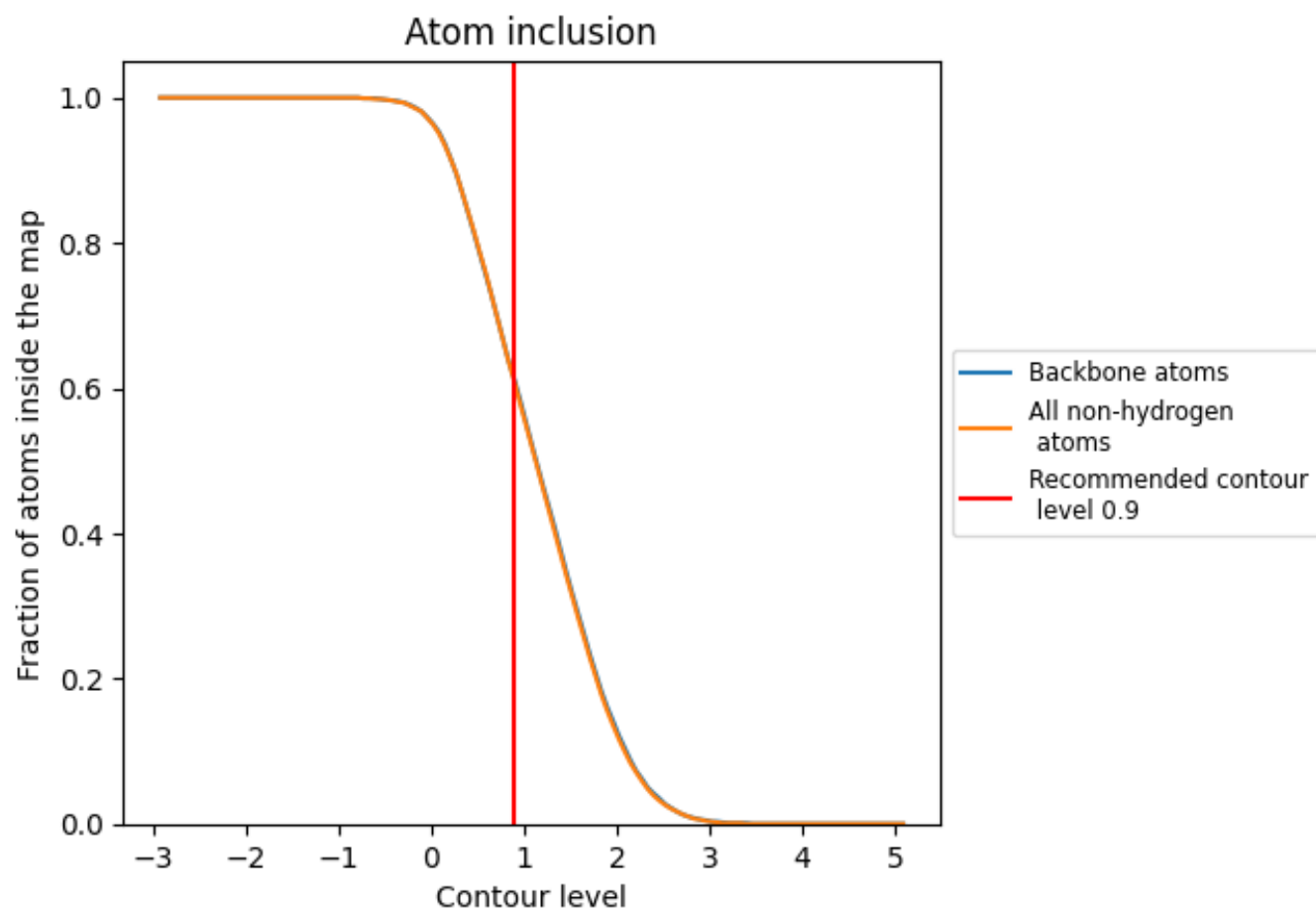
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 61% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6080	 0.4020
A	 0.7270	 0.4460
B	 0.6740	 0.4180
C	 0.6400	 0.3960
D	 0.6820	 0.4350
E	 0.3410	 0.3480
F	 0.5350	 0.3750
G	 0.6460	 0.3970
H	 0.6190	 0.3890
I	 0.5680	 0.4450
J	 0.2210	 0.2880
K	 0.6530	 0.4010
L	 0.6240	 0.3650
a	 0.6270	 0.3940
b	 0.6430	 0.4060
c	 0.6280	 0.4190
d	 0.7050	 0.4080
e	 0.4070	 0.3300
f	 0.5410	 0.3350
g	 0.5910	 0.4150
h	 0.5160	 0.4320
i	 0.6070	 0.3770
j	 0.2330	 0.2250
k	 0.6180	 0.3910
l	 0.6590	 0.4440

