



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 02:25 AM JST

PDB ID : 8IUJ / pdb_00008iuj
EMDB ID : EMD-35723
Title : Cryo-EM structure of Euglena gracilis super-complex III2+IV2, composite
Authors : Wu, M.C.; Tian, H.T.; He, Z.X.; Hu, Y.Q.; Zhou, L.
Deposited on : 2023-03-24
Resolution : 3.06 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:

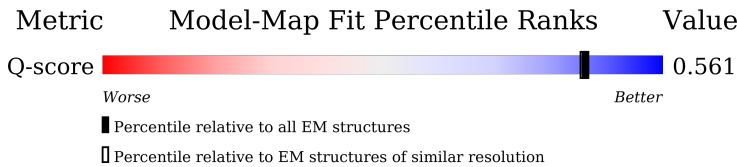
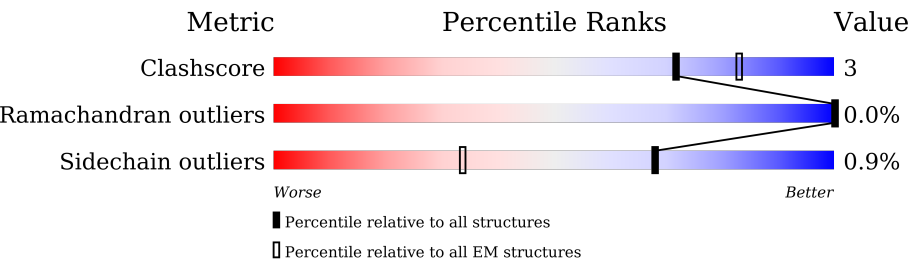
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.06 Å.

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



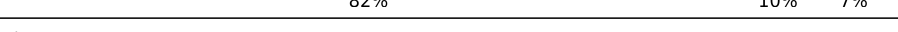
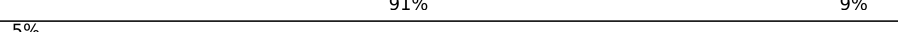
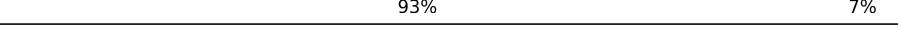
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	QA	479	92% 8%
1	Qa	479	94% 6%
2	QC	368	91% 8%
2	Qc	368	91% 8%

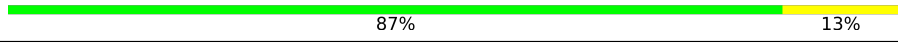
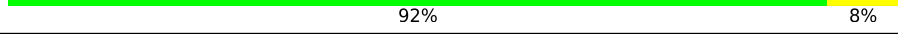
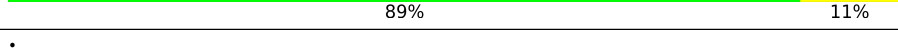
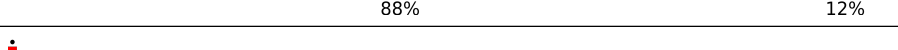
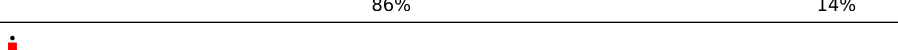
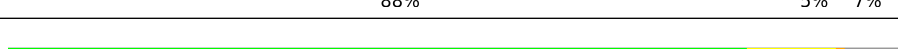
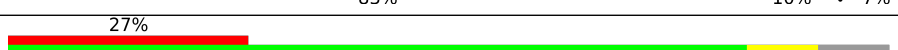
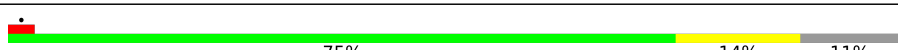
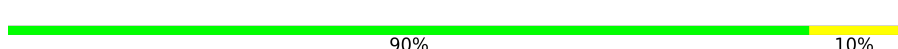
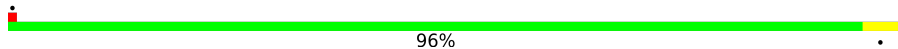
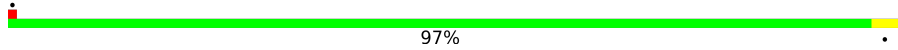
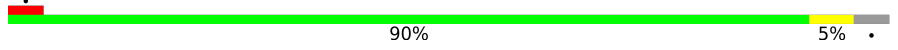
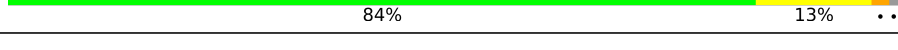
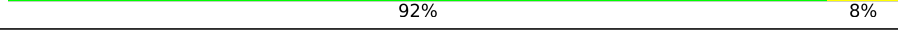
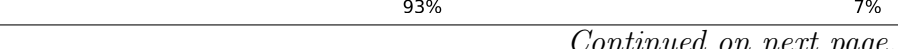
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Mol	Chain	Length	Quality of chain
3	QD	243	 91% 8%
3	Qd	243	 91% 9%
4	QH	86	 92% 7%
4	Qh	86	 85% 14%
5	QJ	154	 88% 8%
5	Qj	154	 88% 8%
6	QK	100	 57% 39%
6	Qk	100	 53% 8% 39%
7	4A	246	 79% 17%
7	4a	246	 78% 5% 17%
8	4C	139	 81% 7% 12%
8	4c	139	 81% 8% 12%
9	4E	165	 90% 7%
9	4e	165	 5% 90% 7%
10	4H	221	 88% 5% 7%
10	4h	221	 82% 10% 7%
11	4J	88	 91% 9%
11	4j	88	 5% 93% 7%
12	5C	208	 87% 7% 6%
12	5c	208	 88% 7% 6%
13	6A	112	 15% 88% 12%
13	6a	112	 70% 11% 19%
14	6B	287	 89% 10%
14	6b	287	 90% 9%
15	7C	171	 83% 5% 12%

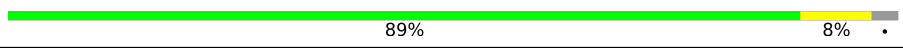
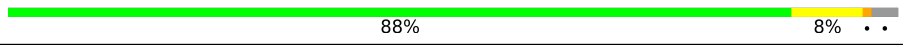
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Mol	Chain	Length	Quality of chain
15	7c	171	
16	C1	495	
16	c1	495	
17	C2	196	
17	c2	196	
18	C3	161	
18	c3	161	
19	DC	179	
19	dc	179	
20	QE	252	
20	Qe	252	
21	QF	72	
21	Qf	72	
22	QG	228	
22	Qg	228	
23	QI	70	
23	Qi	70	
24	QB	474	
24	Qb	474	
25	5B	174	
25	5b	174	
26	4D	174	
26	4d	174	
27	4F	75	
27	4f	75	

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Mol	Chain	Length	Quality of chain
28	4G	315	
28	4g	315	
29	4I	274	
29	4i	274	
30	7A	178	
30	7a	178	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	HEC	QD	301	X	-	-	-
33	HEC	Qd	301	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 200404 atoms, of which 99661 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 MPP-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	QA	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		
1	Qa	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	QC	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		
2	Qc	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		

- Molecule 3 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	QD	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		
3	Qd	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		

- Molecule 4 is a protein called UQCRQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	QH	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		
4	Qh	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		

- Molecule 5 is a protein called UQCR10.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	QJ	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		
5	Qj	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		

- Molecule 6 is a protein called Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	QK	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		
6	Qk	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

- Molecule 7 is a protein called COXEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	4a	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		
7	4A	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		

- Molecule 8 is a protein called COXEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	4c	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		
8	4C	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		

- Molecule 9 is a protein called COXEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4e	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		
9	4E	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		

- Molecule 10 is a protein called COXEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4h	205	Total	C	H	N	O		0	0
			3250	1040	1644	260	306			

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	4H	205	Total	C	H	N	O	0	0
			3250	1040	1644	260	306		

- Molecule 11 is a protein called COXEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	4j	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		
11	4J	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		

- Molecule 12 is a protein called COX5c.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	5c	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		
12	5C	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		

- Molecule 13 is a protein called COX6a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	6a	91	Total	C	H	N	O	S	0	0
			1497	498	747	128	120	4		
13	6A	111	Total	C	H	N	O	S	0	0
			1829	608	909	157	150	5		

- Molecule 14 is a protein called COX6b-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	6b	282	Total	C	H	N	O	S	0	0
			4512	1455	2227	396	427	7		
14	6B	282	Total	C	H	N	O	S	0	0
			4514	1455	2229	396	427	7		

- Molecule 15 is a protein called COX7c.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	7c	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		
15	7C	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	c1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		
16	C1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	c2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		
17	C2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		

- Molecule 18 is a protein called Putative NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		
18	C3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		

- Molecule 19 is a protein called COX4.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	dc	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		
19	DC	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		

- Molecule 20 is a protein called UQCRFS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	QE	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		
20	Qe	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		

- Molecule 21 is a protein called UQCRH.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	QF	64	Total	C	H	N	O	S	0	0
			1016	325	501	91	93	6		
21	Qf	64	Total	C	H	N	O	S	0	0
			1016	325	501	91	93	6		

- Molecule 22 is a protein called UQCRB.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	QG	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		
22	Qg	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		

- Molecule 23 is a protein called UQCR9.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	QI	70	Total	C	H	N	O	S	0	0
			741	290	292	77	81	1		
23	Qi	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		

- Molecule 24 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Qb	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		
24	QB	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		

- Molecule 25 is a protein called COX5b-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	5B	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		
25	5b	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		

- Molecule 26 is a protein called COXEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	4D	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	4d	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

- Molecule 27 is a protein called COXEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	4F	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		
27	4f	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		

- Molecule 28 is a protein called COXEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	4G	297	Total	C	H	N	O	S	0	0
			4690	1478	2339	408	457	8		
28	4g	297	Total	C	H	N	O	S	0	0
			4690	1478	2339	408	457	8		

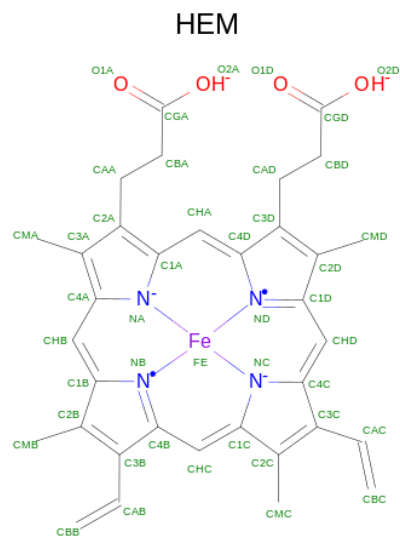
- Molecule 29 is a protein called COXEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4I	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		
29	4i	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		

- Molecule 30 is a protein called COX7a.

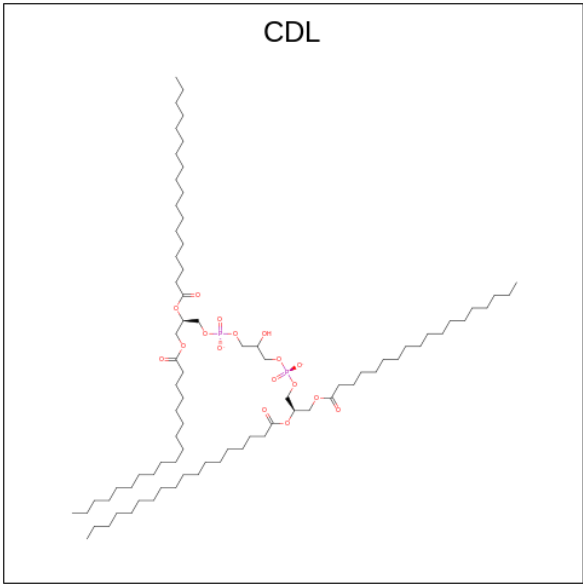
Mol	Chain	Residues	Atoms						AltConf	Trace
30	7a	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		
30	7A	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



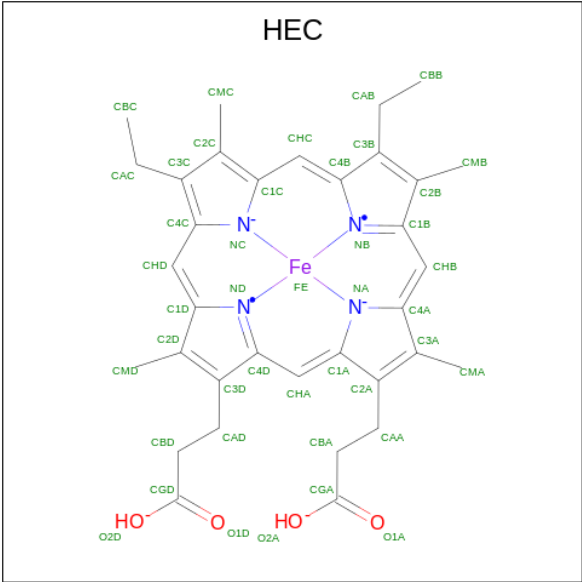
Mol	Chain	Residues	Atoms					AltConf
31	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
31	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 32 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



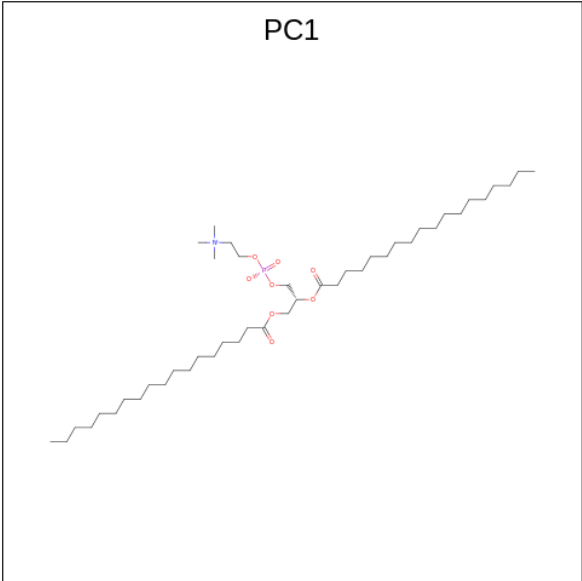
Mol	Chain	Residues	Atoms					AltConf
32	QC	1	Total	C	H	O	P	0
			112	37	56	17	2	
32	QD	1	Total	C	H	O	P	0
			151	50	82	17	2	
32	QH	1	Total	C	H	O	P	0
			175	57	99	17	2	
32	QJ	1	Total	C	H	O	P	0
			118	39	60	17	2	
32	Qc	1	Total	C	H	O	P	0
			106	35	52	17	2	
32	Qd	1	Total	C	H	O	P	0
			256	81	156	17	2	
32	Qh	1	Total	C	H	O	P	0
			139	46	74	17	2	
32	Qh	1	Total	C	H	O	P	0
			124	41	64	17	2	
32	Qj	1	Total	C	H	O	P	0
			88	29	40	17	2	
32	4c	1	Total	C	H	O	P	0
			157	51	87	17	2	
32	4e	1	Total	C	H	O	P	0
			163	53	91	17	2	
32	7c	1	Total	C	H	O	P	0
			220	71	130	17	2	
32	4E	1	Total	C	H	O	P	0
			163	53	91	17	2	
32	C1	1	Total	C	H	O	P	0
			220	71	130	17	2	
32	QE	1	Total	C	H	O	P	0
			124	41	64	17	2	

- Molecule 33 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
33	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 34 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



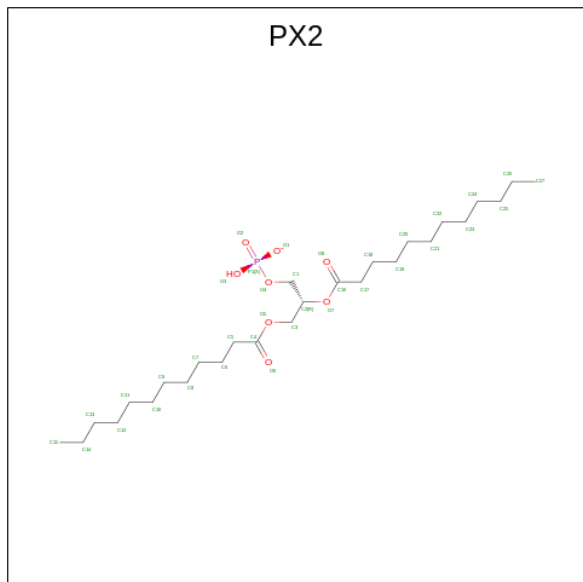
Mol	Chain	Residues	Atoms						AltConf
34	QD	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	

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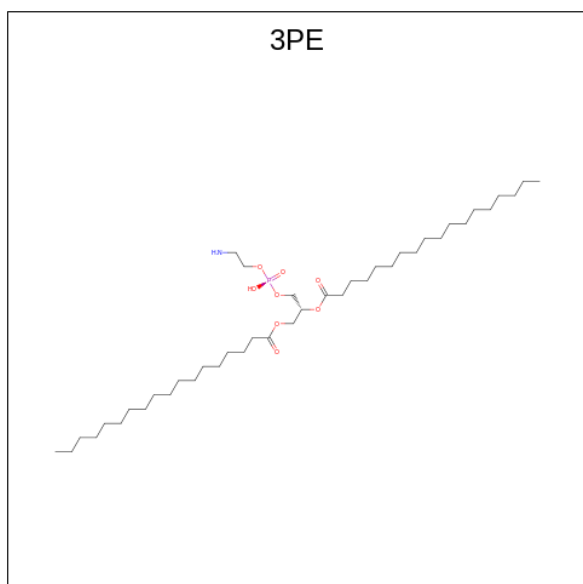
Mol	Chain	Residues	Atoms						AltConf
34	Qc	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
34	Qd	1	Total 67	C 21	H 36	N 1	O 8	P 1	0
34	Qj	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
34	4a	1	Total 118	C 37	H 71	N 1	O 8	P 1	0
34	4e	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
34	7c	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
34	c1	1	Total 127	C 40	H 77	N 1	O 8	P 1	0
34	c1	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
34	c3	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
34	4A	1	Total 118	C 37	H 71	N 1	O 8	P 1	0
34	4A	1	Total 112	C 36	H 66	N 1	O 8	P 1	0
34	4E	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
34	C1	1	Total 127	C 40	H 77	N 1	O 8	P 1	0
34	C1	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
34	C3	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
34	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
34	QE	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
34	Qe	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
34	Qe	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
34	Qe	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
34	Qg	1	Total 58	C 18	H 30	N 1	O 8	P 1	0

- Molecule 35 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



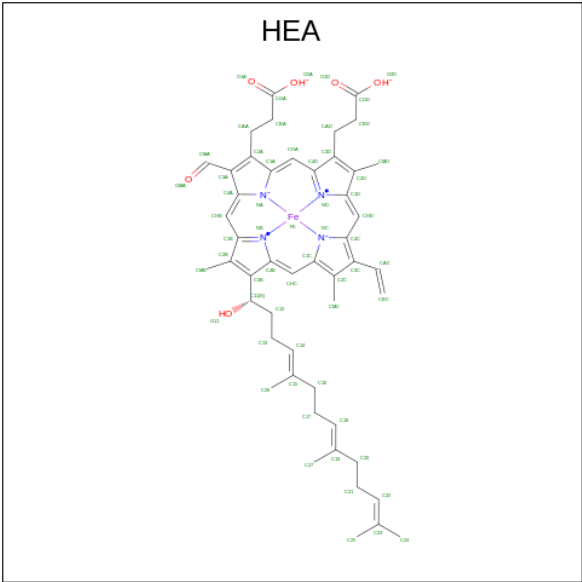
Mol	Chain	Residues	Atoms				AltConf
35	QD	1	Total	C	O	P	0
			36	27	8	1	
35	QJ	1	Total	C	O	P	0
			36	27	8	1	
35	4C	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 36 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
36	4a	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	c1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	c1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	C1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	C1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
36	4D	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
36	4F	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	7a	1	Total 100	C 31	H 59	N 1	O 8	P 1	0
36	4d	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
36	4d	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	7A	1	Total 100	C 31	H 59	N 1	O 8	P 1	0

- Molecule 37 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
37	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
37	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
37	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
37	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

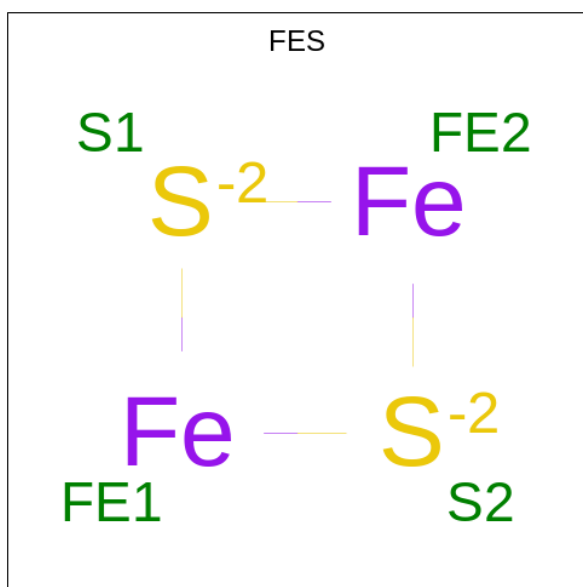
- Molecule 38 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	c1	1	Total	Cu	0
			1	1	
38	c2	2	Total	Cu	0
			2	2	
38	C1	1	Total	Cu	0
			1	1	
38	C2	2	Total	Cu	0
			2	2	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
39	c1	1	Total	Mg	0
			1	1	
39	C1	1	Total	Mg	0
			1	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	QE	1	Total	Fe	S	0
			4	2	2	
40	Qe	1	Total	Fe	S	0
			4	2	2	

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	5B	1	Total	Zn	0
			1	1	
41	5b	1	Total	Zn	0
			1	1	

- Molecule 42 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (CCD ID: S12) (formula: C₂₄H₄₆NO₉P).

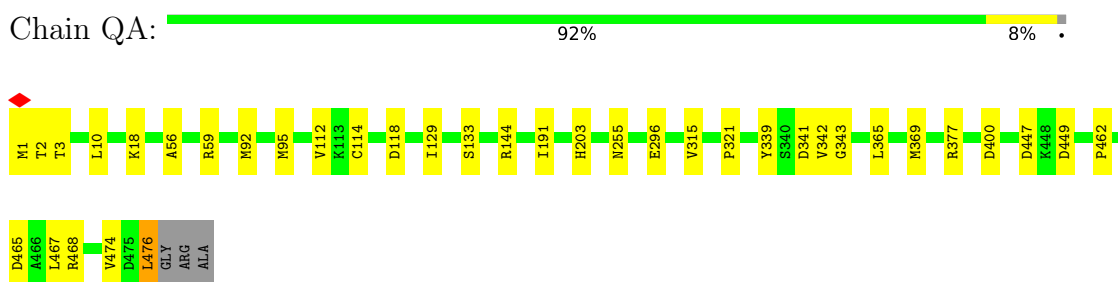


Mol	Chain	Residues	Atoms						AltConf
42	4F	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	
42	4d	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	

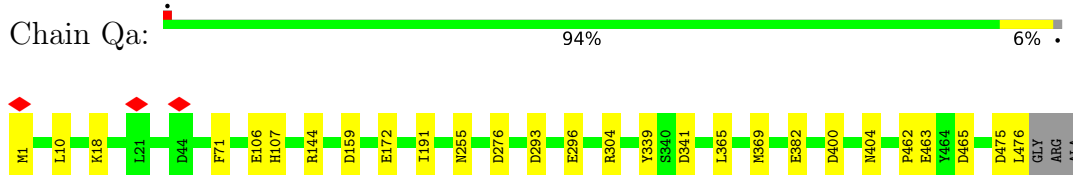
3 Residue-property plots [i](#)

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.

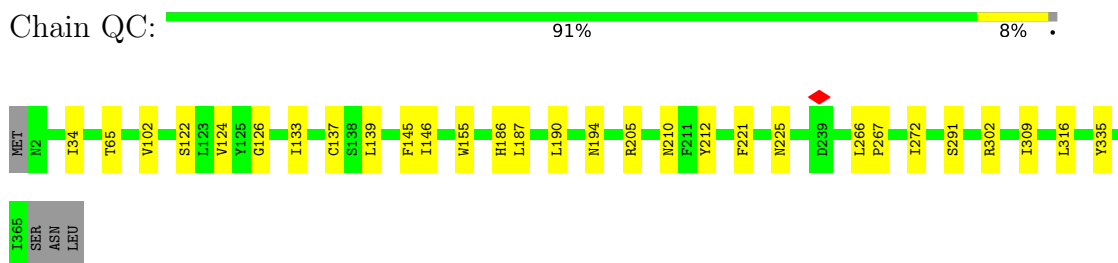
- Molecule 1: MPP-beta



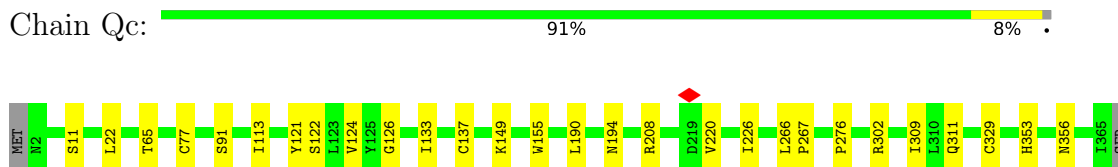
- Molecule 1: MPP-beta



- Molecule 2: Cytochrome b



- Molecule 2: Cytochrome b



ASN
LEU

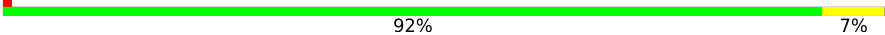
- Molecule 3: Cytochrome c1, heme protein

Chain QD:  91% 8%

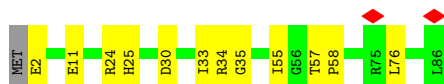
- Molecule 3: Cytochrome c1, heme protein

Chain Qd:  91% 9%

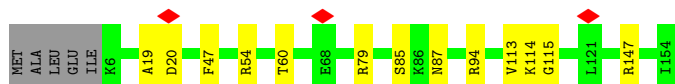
- Molecule 4: UQCRQ

Chain QH:  92% 7%

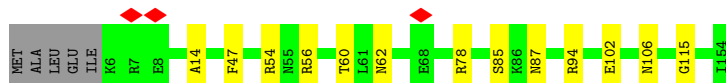
- Molecule 4: UQCRQ

Chain Qh:  85% 14%

- Molecule 5: UQCR10

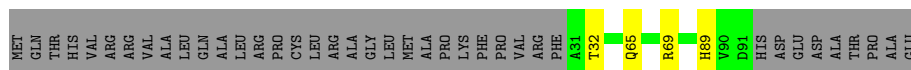
Chain QJ:  88% 8%

- Molecule 5: UQCR10

Chain Qj:  88% 8%

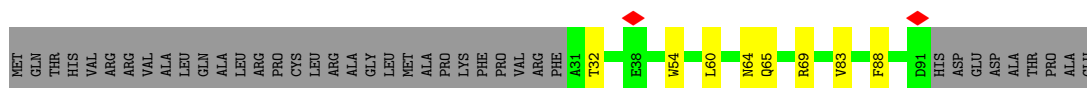
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain QK:  57% 39%



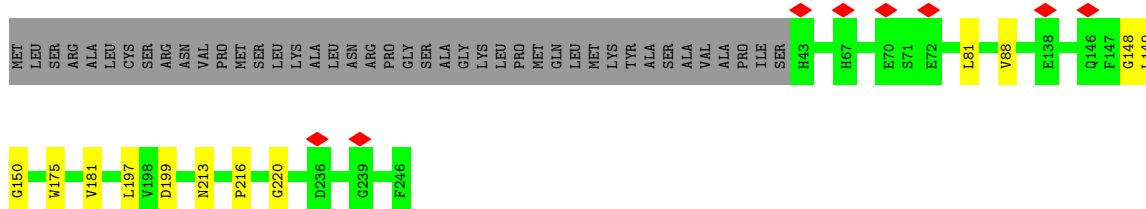
- Molecule 6: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain Qk:  53% 8% 39%



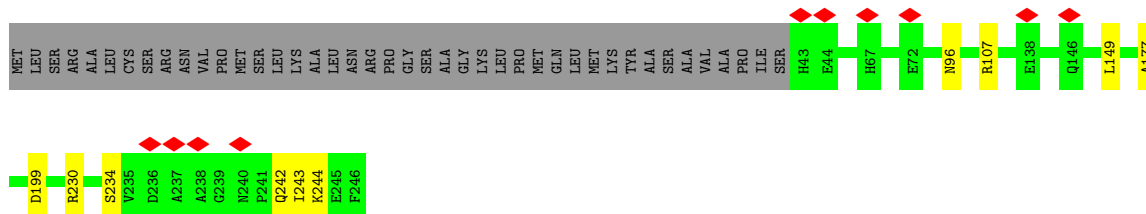
- Molecule 7: COXEG1

Chain 4a:  78% 5% 17%



- Molecule 7: COXEG1

Chain 4A:  79% 1% 17%



- Molecule 8: COXEG3

Chain 4c:  81% 8% 12%

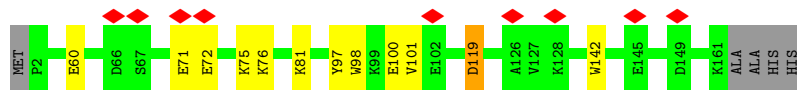
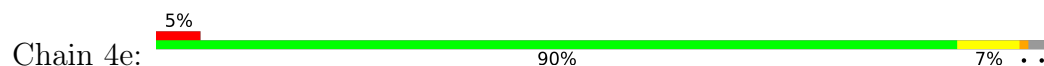


- Molecule 8: COXEG3

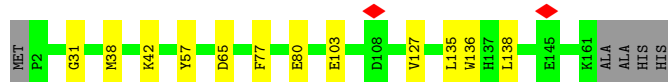
Chain 4C:  81% 7% 12%



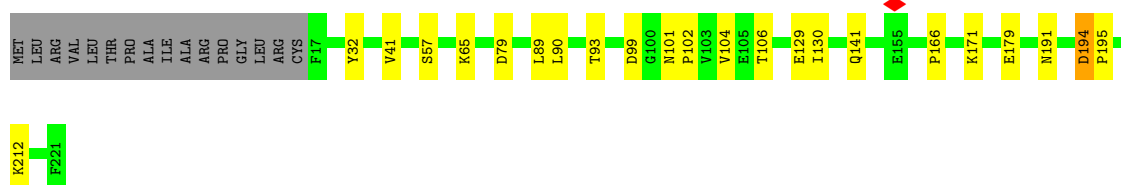
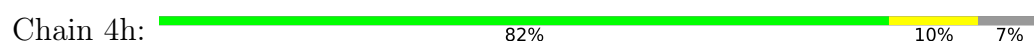
- Molecule 9: COXEG5



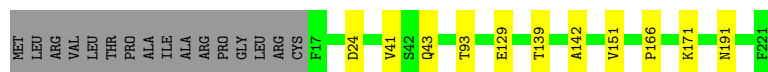
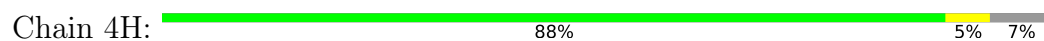
- Molecule 9: COXEG5



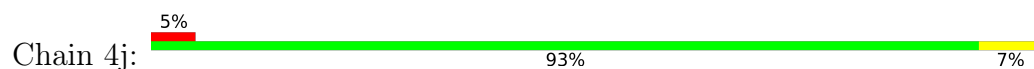
- Molecule 10: COXEG8



- Molecule 10: COXEG8



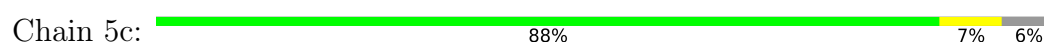
- Molecule 11: COXEG10



- Molecule 11: COXEG10

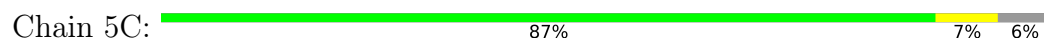


- Molecule 12: COX5c

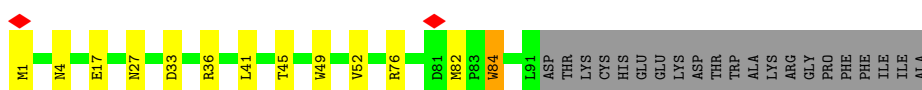




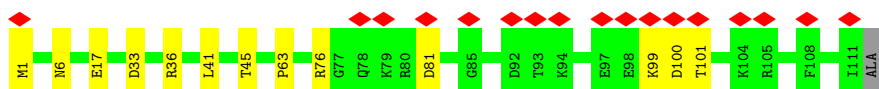
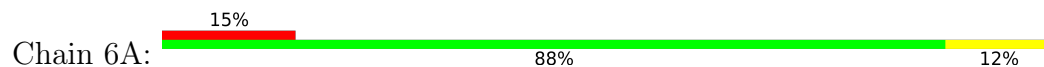
- Molecule 12: COX5c



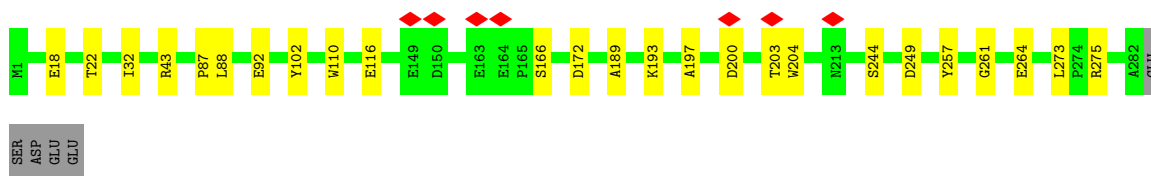
- Molecule 13: COX6a



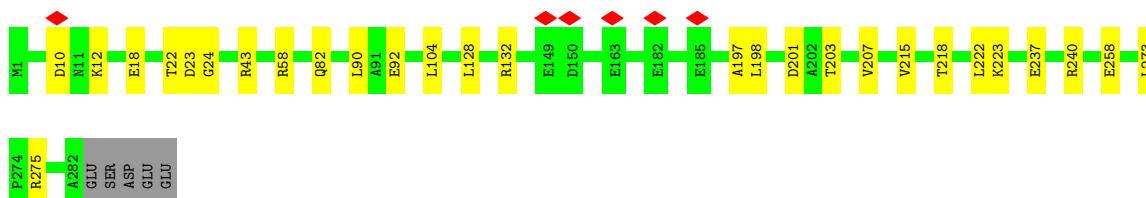
- Molecule 13: COX6a



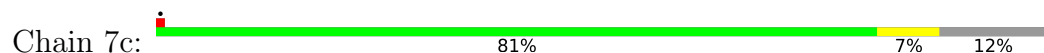
- Molecule 14: COX6b-1

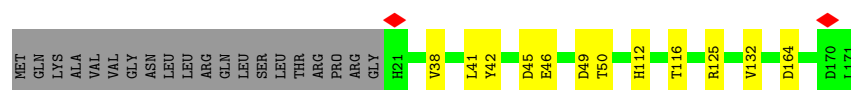


- Molecule 14: COX6b-1

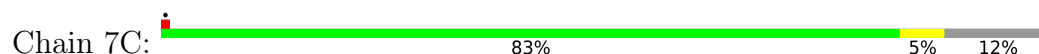


- Molecule 15: COX7c

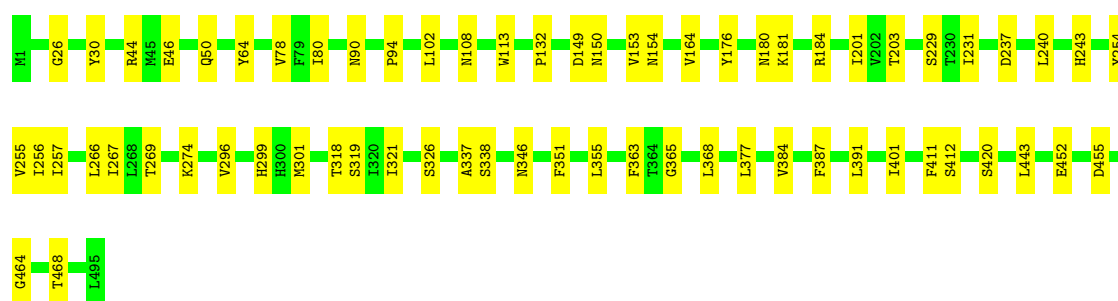




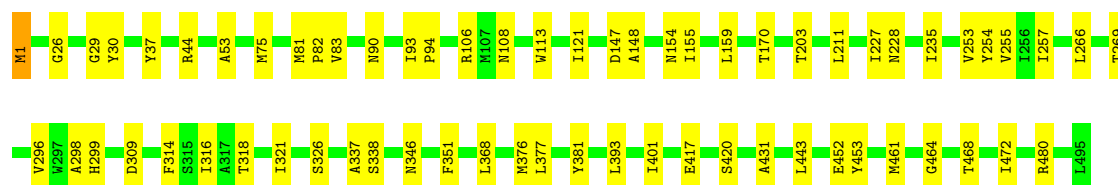
- Molecule 15: COX7c



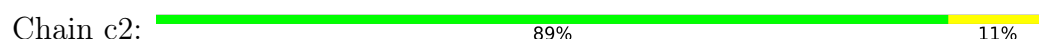
- Molecule 16: Cytochrome c oxidase subunit 1



- Molecule 16: Cytochrome c oxidase subunit 1



- Molecule 17: Cytochrome c oxidase subunit 2



- Molecule 17: Cytochrome c oxidase subunit 2



- Molecule 18: Putative NADH dehydrogenase subunit 6

Chain c3:  86% 14%



- Molecule 18: Putative NADH dehydrogenase subunit 6

Chain C3:  88% 12%

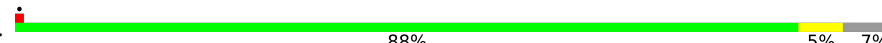


- Molecule 19: COX4

Chain dc:  83% 10% 7%



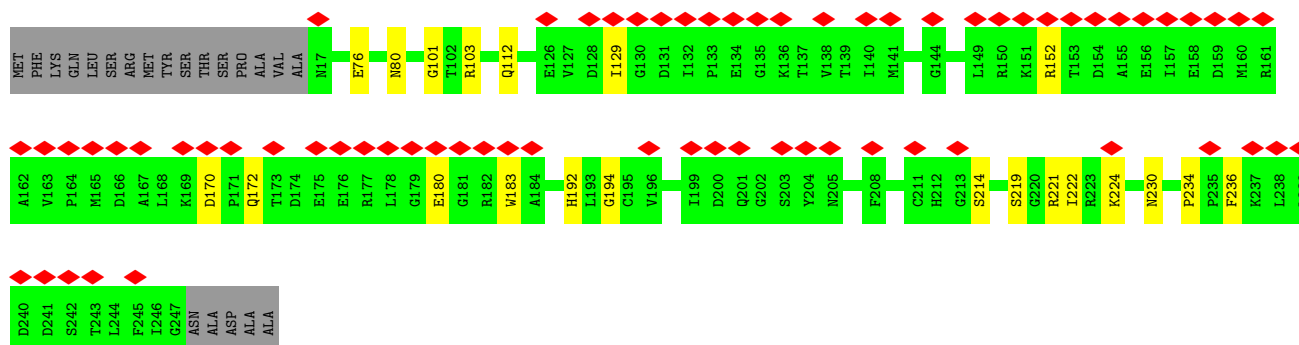
- Molecule 19: COX4

Chain DC:  88% 5% 7%



- Molecule 20: UQCRFS1

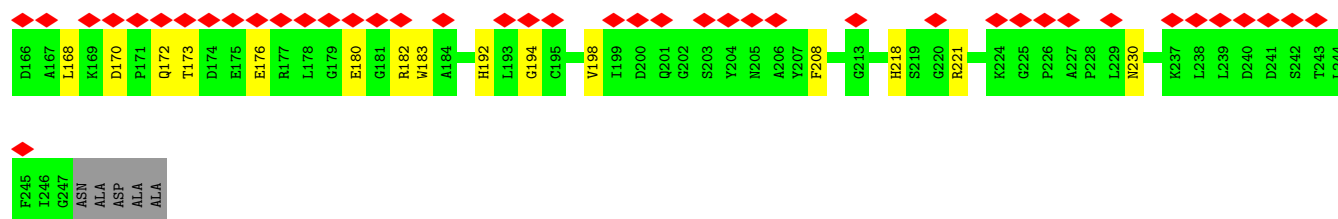
Chain QE:  27% 83% 8% 8%



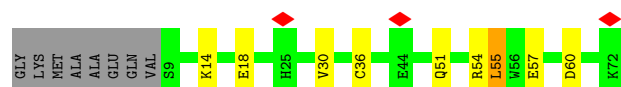
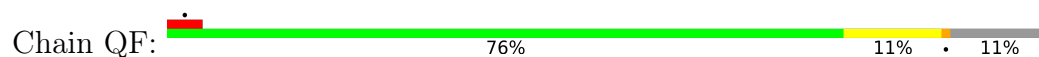
- Molecule 20: UQCRFS1

Chain Qe:  30% 81% 11% 8%

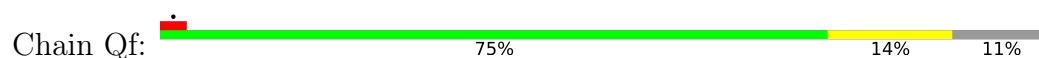




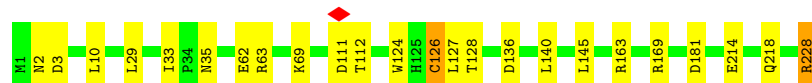
• Molecule 21: UQCRH



• Molecule 21: UQCRH



• Molecule 22: UQCRB



• Molecule 22: UQCRB



• Molecule 23: UQCR9

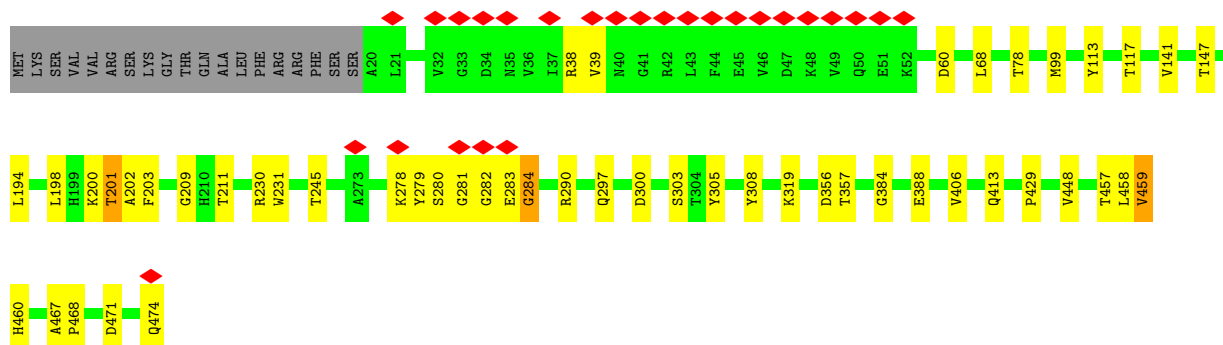
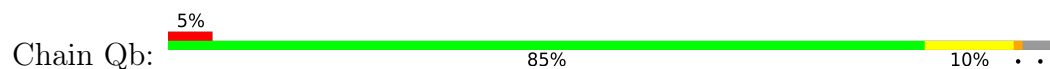


• Molecule 23: UQCR9

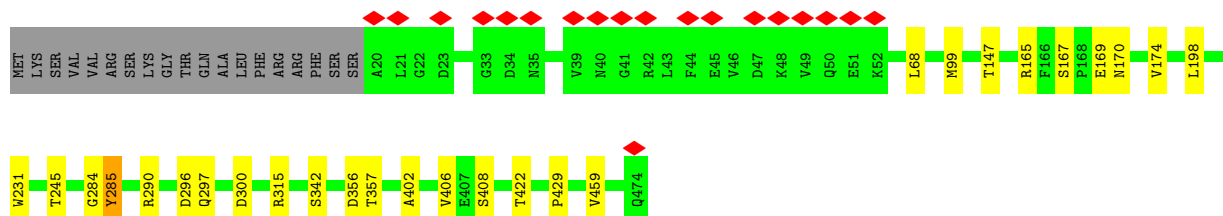




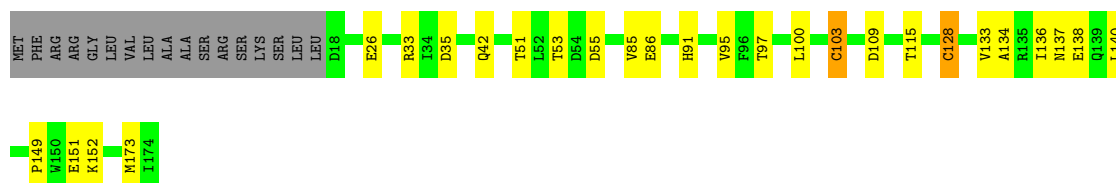
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



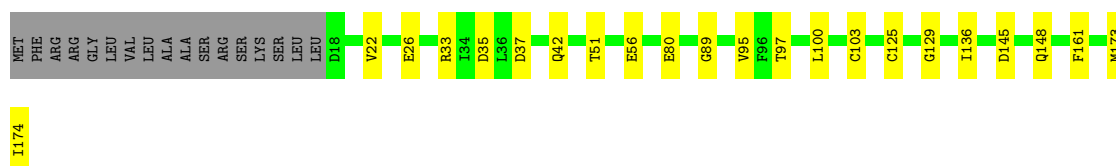
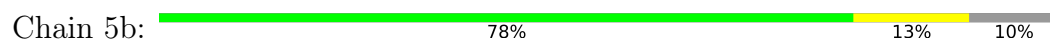
- Molecule 24: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



- Molecule 25: COX5b-2



- Molecule 25: COX5b-2



- Molecule 26: COXEG4

Chain 4D:  89% 10% ..

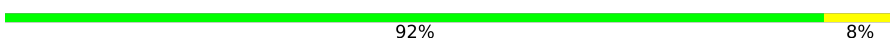


• Molecule 26: COXEG4

Chain 4d:  84% 13% ..



• Molecule 27: COXEG6

Chain 4F:  92% 8%



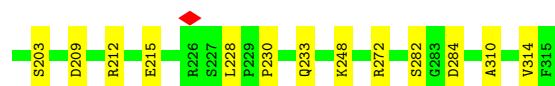
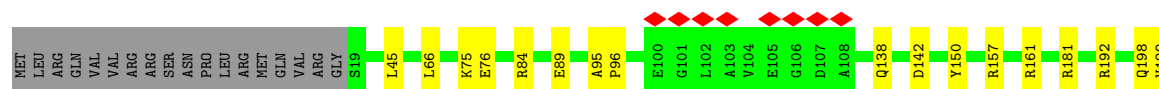
• Molecule 27: COXEG6

Chain 4f:  93% 7%



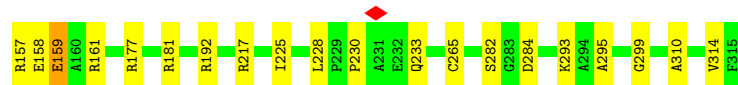
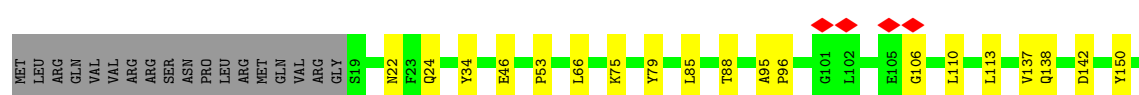
• Molecule 28: COXEG7

Chain 4G:  85% 10% 6%



• Molecule 28: COXEG7

Chain 4g:  82% 12% 6%



• Molecule 29: COXEG9

Chain 4I:  89% 8% .



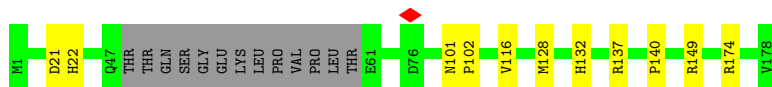
• Molecule 29: COXEG9

Chain 4i:  88% 8% . .



• Molecule 30: COX7a

Chain 7a:  87% 6% 7%



• Molecule 30: COX7a

Chain 7A:  84% 8% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135598	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 ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	39.138	Depositor
Minimum map value	-21.701	Depositor
Average map value	-0.023	Depositor
Map value standard deviation	1.026	Depositor
Recommended contour level	4.8	Depositor
Map size (Å)	537.60004, 537.60004, 537.60004	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, HEA, HEM, CU, MG, CDL, 3PE, S12, FES, ZN, HEC, PX2

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	QA	0.21	0/3838	0.30	0/5193
1	Qa	0.21	0/3838	0.30	0/5193
2	QC	0.24	0/3058	0.31	0/4178
2	Qc	0.25	0/3058	0.33	0/4178
3	QD	0.24	0/2027	0.30	0/2760
3	Qd	0.24	0/2027	0.31	0/2760
4	QH	0.22	0/717	0.28	0/966
4	Qh	0.22	0/717	0.30	0/966
5	QJ	0.18	0/1243	0.26	0/1693
5	Qj	0.19	0/1243	0.26	0/1693
6	QK	0.20	0/498	0.27	0/677
6	Qk	0.19	0/498	0.25	0/677
7	4A	0.17	0/1650	0.25	0/2235
7	4a	0.18	0/1650	0.27	0/2235
8	4C	0.19	0/1051	0.27	0/1432
8	4c	0.19	0/1051	0.28	0/1432
9	4E	0.18	0/1376	0.25	0/1864
9	4e	0.16	0/1376	0.26	0/1864
10	4H	0.20	0/1640	0.29	0/2224
10	4h	0.18	0/1640	0.27	0/2224
11	4J	0.21	0/736	0.26	0/1008
11	4j	0.21	0/736	0.27	0/1008
12	5C	0.23	0/1616	0.29	0/2192
12	5c	0.23	0/1616	0.29	0/2192
13	6A	0.18	0/953	0.27	0/1292
13	6a	0.17	0/777	0.28	0/1055
14	6B	0.21	0/2343	0.26	0/3174
14	6b	0.21	0/2343	0.27	0/3174
15	7C	0.23	0/1299	0.28	0/1777
15	7c	0.23	0/1299	0.29	0/1777
16	C1	0.26	0/4054	0.36	0/5516
16	c1	0.29	0/4054	0.38	0/5516

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C2	0.24	0/1620	0.34	0/2207
17	c2	0.26	0/1620	0.36	0/2207
18	C3	0.22	0/1416	0.30	0/1945
18	c3	0.23	0/1416	0.34	0/1945
19	DC	0.23	0/1410	0.29	0/1914
19	dc	0.23	0/1410	0.29	0/1914
20	QE	0.17	0/1842	0.28	0/2502
20	Qe	0.16	0/1842	0.28	0/2502
21	QF	0.16	0/526	0.25	0/702
21	Qf	0.17	0/526	0.26	0/702
22	QG	0.24	0/1987	0.33	0/2696
22	Qg	0.24	0/1987	0.32	0/2696
23	QI	0.21	0/251	0.25	0/340
23	Qi	0.21	0/251	0.26	0/340
24	QB	0.22	0/3532	0.31	0/4805
24	Qb	0.24	0/3532	0.37	0/4805
25	5B	0.25	0/1294	0.36	0/1759
25	5b	0.26	0/1294	0.32	0/1759
26	4D	0.22	0/1379	0.32	0/1867
26	4d	0.21	0/1379	0.33	0/1867
27	4F	0.19	0/641	0.28	0/867
27	4f	0.19	0/641	0.30	0/867
28	4G	0.20	0/2391	0.28	0/3240
28	4g	0.20	0/2391	0.28	0/3240
29	4I	0.25	0/2255	0.26	0/3059
29	4i	0.25	0/2255	0.28	0/3059
30	7A	0.20	0/1359	0.28	0/1835
30	7a	0.18	0/1359	0.29	0/1835
All	All	0.22	0/99828	0.30	0/135601

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
24	Qb	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	Qb	283	GLU	Peptide
24	Qb	284	GLY	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	QA	3750	3658	3668	28	0
1	Qa	3750	3658	3668	19	0
2	QC	2975	3064	3076	19	0
2	Qc	2975	3064	3076	24	0
3	QD	1959	1858	1864	16	0
3	Qd	1959	1858	1864	15	0
4	QH	701	692	694	6	0
4	Qh	701	692	694	11	0
5	QJ	1206	1212	1216	10	0
5	Qj	1206	1212	1216	11	0
6	QK	485	499	500	3	0
6	Qk	485	499	500	7	0
7	4A	1612	1608	1617	6	0
7	4a	1612	1608	1617	12	0
8	4C	1022	1027	1029	8	0
8	4c	1022	1027	1029	9	0
9	4E	1333	1279	1283	9	0
9	4e	1333	1279	1283	5	0
10	4H	1606	1644	1648	7	0
10	4h	1606	1644	1648	16	0
11	4J	711	688	689	4	0
11	4j	711	688	689	5	0
12	5C	1571	1546	1550	11	0
12	5c	1571	1546	1550	11	0
13	6A	920	909	912	16	0
13	6a	750	747	749	13	0
14	6B	2285	2229	2239	23	0
14	6b	2285	2227	2237	18	0
15	7C	1254	1183	1190	7	0
15	7c	1254	1183	1190	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C1	3938	3980	3999	44	0
16	c1	3938	3980	3999	47	0
17	C2	1585	1647	1652	13	0
17	c2	1585	1647	1652	16	0
18	C3	1378	1413	1419	15	0
18	c3	1378	1413	1419	19	0
19	DC	1366	1362	1366	8	0
19	dc	1366	1362	1366	13	0
20	QE	1795	1776	1780	14	0
20	Qe	1795	1776	1780	17	0
21	QF	515	501	507	5	0
21	Qf	515	501	507	5	0
22	QG	1932	1870	1880	18	0
22	Qg	1932	1870	1880	14	0
23	QI	449	292	292	2	0
23	Qi	449	293	294	1	0
24	QB	3458	3431	3443	20	0
24	Qb	3458	3431	3443	40	0
25	5B	1258	1184	1192	22	0
25	5b	1258	1184	1192	18	0
26	4D	1349	1359	1363	14	0
26	4d	1349	1359	1363	19	0
27	4F	620	626	627	3	0
27	4f	620	626	627	3	0
28	4G	2351	2339	2343	18	0
28	4g	2351	2339	2343	27	0
29	4I	2178	2046	2058	17	0
29	4i	2178	2046	2058	19	0
30	7A	1319	1284	1295	11	0
30	7a	1319	1284	1295	9	0
31	QC	86	0	60	4	0
31	Qc	86	0	60	7	0
32	4E	72	91	91	0	0
32	4c	70	87	87	0	0
32	4e	72	91	91	0	0
32	7c	90	130	130	0	0
32	C1	90	130	130	0	0
32	QC	56	56	56	1	0
32	QD	69	82	82	1	0
32	QE	60	64	64	0	0
32	QH	76	99	99	0	0
32	QJ	58	60	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Qc	54	52	52	2	0
32	Qd	100	156	156	2	0
32	Qh	125	138	138	0	0
32	Qj	48	40	40	1	0
33	QD	43	0	31	6	0
33	Qd	43	0	31	2	0
34	4A	93	137	137	0	0
34	4E	35	44	44	1	0
34	4a	47	71	71	0	0
34	4e	35	44	44	1	0
34	7c	54	88	88	0	0
34	C1	86	123	123	1	0
34	C3	51	79	79	0	0
34	DC	54	88	88	1	0
34	QD	31	36	36	0	0
34	QE	36	46	46	1	0
34	Qc	36	46	46	0	0
34	Qd	31	36	36	0	0
34	Qe	144	222	222	4	0
34	Qg	28	30	30	0	0
34	Qj	54	88	88	0	0
34	c1	86	123	123	1	0
34	c3	51	79	79	0	0
35	4C	36	0	52	4	0
35	QD	36	0	52	3	0
35	QJ	36	0	52	2	0
36	4D	35	44	44	0	0
36	4F	51	82	82	1	0
36	4a	51	82	82	0	0
36	4d	86	126	126	0	0
36	7A	41	59	59	0	0
36	7a	41	59	59	0	0
36	C1	80	108	108	1	0
36	c1	80	108	108	1	0
37	C1	120	0	108	10	0
37	c1	120	0	108	18	0
38	C1	1	0	0	0	0
38	C2	2	0	0	0	0
38	c1	1	0	0	0	0
38	c2	2	0	0	0	0
39	C1	1	0	0	0	0
39	c1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	QE	4	0	0	1	0
40	Qe	4	0	0	0	0
41	5B	1	0	0	0	0
41	5b	1	0	0	0	0
42	4F	35	44	44	1	0
42	4d	35	44	44	0	0
All	All	100743	99661	100585	689	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 3.

The worst 5 of 689 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)
3:QD:40:CYS:SG	33:QD:301:HEC:CAC	2.02	1.48
2:QC:291:SER:OG	22:QG:35:ASN:O	1.89	0.89
24:Qb:460:HIS:NE2	24:Qb:468:PRO:O	2.06	0.88
5:Qj:54:ARG:NH2	32:Qj:202:CDL:OB3	2.08	0.85
13:6a:4:ASN:ND2	25:5b:148:GLN:OE1	2.08	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	QA	476/479 (99%)	460 (97%)	16 (3%)	0	100	100
1	Qa	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
2	QC	362/368 (98%)	354 (98%)	7 (2%)	1 (0%)	36	63
2	Qc	362/368 (98%)	350 (97%)	12 (3%)	0	100	100
3	QD	239/243 (98%)	225 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Qd	239/243 (98%)	218 (91%)	21 (9%)	0	100	100
4	QH	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
4	Qh	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
5	QJ	147/154 (96%)	141 (96%)	6 (4%)	0	100	100
5	Qj	147/154 (96%)	139 (95%)	8 (5%)	0	100	100
6	QK	59/100 (59%)	59 (100%)	0	0	100	100
6	Qk	59/100 (59%)	59 (100%)	0	0	100	100
7	4A	202/246 (82%)	195 (96%)	7 (4%)	0	100	100
7	4a	202/246 (82%)	191 (95%)	11 (5%)	0	100	100
8	4C	121/139 (87%)	115 (95%)	6 (5%)	0	100	100
8	4c	121/139 (87%)	118 (98%)	3 (2%)	0	100	100
9	4E	158/165 (96%)	154 (98%)	4 (2%)	0	100	100
9	4e	158/165 (96%)	154 (98%)	4 (2%)	0	100	100
10	4H	203/221 (92%)	200 (98%)	3 (2%)	0	100	100
10	4h	203/221 (92%)	197 (97%)	6 (3%)	0	100	100
11	4J	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
11	4j	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
12	5C	194/208 (93%)	189 (97%)	5 (3%)	0	100	100
12	5c	194/208 (93%)	185 (95%)	9 (5%)	0	100	100
13	6A	109/112 (97%)	101 (93%)	7 (6%)	1 (1%)	14	39
13	6a	89/112 (80%)	86 (97%)	3 (3%)	0	100	100
14	6B	280/287 (98%)	274 (98%)	6 (2%)	0	100	100
14	6b	280/287 (98%)	271 (97%)	9 (3%)	0	100	100
15	7C	149/171 (87%)	143 (96%)	6 (4%)	0	100	100
15	7c	149/171 (87%)	142 (95%)	7 (5%)	0	100	100
16	C1	493/495 (100%)	479 (97%)	14 (3%)	0	100	100
16	c1	493/495 (100%)	473 (96%)	20 (4%)	0	100	100
17	C2	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
17	c2	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
18	C3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
18	c3	159/161 (99%)	151 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	DC	165/179 (92%)	159 (96%)	6 (4%)	0	100	100
19	dc	165/179 (92%)	157 (95%)	8 (5%)	0	100	100
20	QE	229/252 (91%)	219 (96%)	10 (4%)	0	100	100
20	Qe	229/252 (91%)	216 (94%)	13 (6%)	0	100	100
21	QF	62/72 (86%)	62 (100%)	0	0	100	100
21	Qf	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
22	QG	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
22	Qg	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
23	QI	28/70 (40%)	28 (100%)	0	0	100	100
23	Qi	28/70 (40%)	27 (96%)	1 (4%)	0	100	100
24	QB	453/474 (96%)	438 (97%)	15 (3%)	0	100	100
24	Qb	453/474 (96%)	429 (95%)	24 (5%)	0	100	100
25	5B	155/174 (89%)	149 (96%)	6 (4%)	0	100	100
25	5b	155/174 (89%)	148 (96%)	7 (4%)	0	100	100
26	4D	171/174 (98%)	157 (92%)	14 (8%)	0	100	100
26	4d	171/174 (98%)	161 (94%)	10 (6%)	0	100	100
27	4F	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
27	4f	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
28	4G	295/315 (94%)	286 (97%)	9 (3%)	0	100	100
28	4g	295/315 (94%)	283 (96%)	12 (4%)	0	100	100
29	4I	263/274 (96%)	255 (97%)	8 (3%)	0	100	100
29	4i	263/274 (96%)	252 (96%)	11 (4%)	0	100	100
30	7A	161/178 (90%)	155 (96%)	6 (4%)	0	100	100
30	7a	161/178 (90%)	156 (97%)	5 (3%)	0	100	100
All	All	11970/12768 (94%)	11501 (96%)	467 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	6A	100	ASP
2	QC	145	PHE

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	QA	400/401 (100%)	398 (100%)	2 (0%)	81	82
1	Qa	400/401 (100%)	397 (99%)	3 (1%)	73	79
2	QC	337/341 (99%)	335 (99%)	2 (1%)	78	81
2	Qc	337/341 (99%)	336 (100%)	1 (0%)	86	85
3	QD	206/207 (100%)	206 (100%)	0	100	100
3	Qd	206/207 (100%)	206 (100%)	0	100	100
4	QH	71/72 (99%)	71 (100%)	0	100	100
4	Qh	71/72 (99%)	71 (100%)	0	100	100
5	QJ	124/128 (97%)	124 (100%)	0	100	100
5	Qj	124/128 (97%)	123 (99%)	1 (1%)	73	79
6	QK	50/82 (61%)	50 (100%)	0	100	100
6	Qk	50/82 (61%)	50 (100%)	0	100	100
7	4A	173/207 (84%)	171 (99%)	2 (1%)	63	75
7	4a	173/207 (84%)	173 (100%)	0	100	100
8	4C	112/127 (88%)	111 (99%)	1 (1%)	70	78
8	4c	112/127 (88%)	110 (98%)	2 (2%)	51	70
9	4E	142/145 (98%)	142 (100%)	0	100	100
9	4e	142/145 (98%)	138 (97%)	4 (3%)	38	63
10	4H	176/189 (93%)	174 (99%)	2 (1%)	65	76
10	4h	176/189 (93%)	175 (99%)	1 (1%)	78	81
11	4J	75/75 (100%)	74 (99%)	1 (1%)	61	74
11	4j	75/75 (100%)	75 (100%)	0	100	100
12	5C	167/178 (94%)	165 (99%)	2 (1%)	63	75
12	5c	167/178 (94%)	167 (100%)	0	100	100
13	6A	97/97 (100%)	97 (100%)	0	100	100
13	6a	79/97 (81%)	78 (99%)	1 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	6B	238/243 (98%)	237 (100%)	1 (0%)	84	84
14	6b	238/243 (98%)	238 (100%)	0	100	100
15	7C	135/152 (89%)	134 (99%)	1 (1%)	76	80
15	7c	135/152 (89%)	135 (100%)	0	100	100
16	C1	438/438 (100%)	434 (99%)	4 (1%)	70	78
16	c1	438/438 (100%)	437 (100%)	1 (0%)	87	87
17	C2	178/178 (100%)	177 (99%)	1 (1%)	78	81
17	c2	178/178 (100%)	176 (99%)	2 (1%)	65	76
18	C3	155/155 (100%)	154 (99%)	1 (1%)	78	81
18	c3	155/155 (100%)	155 (100%)	0	100	100
19	DC	148/153 (97%)	148 (100%)	0	100	100
19	dc	148/153 (97%)	144 (97%)	4 (3%)	39	64
20	QE	193/209 (92%)	192 (100%)	1 (0%)	81	82
20	Qe	193/209 (92%)	191 (99%)	2 (1%)	68	77
21	QF	58/63 (92%)	56 (97%)	2 (3%)	32	59
21	Qf	58/63 (92%)	55 (95%)	3 (5%)	21	48
22	QG	207/207 (100%)	203 (98%)	4 (2%)	50	69
22	Qg	207/207 (100%)	204 (99%)	3 (1%)	59	73
23	QI	27/27 (100%)	27 (100%)	0	100	100
23	Qi	27/27 (100%)	27 (100%)	0	100	100
24	QB	369/386 (96%)	367 (100%)	2 (0%)	81	82
24	Qb	369/386 (96%)	364 (99%)	5 (1%)	59	73
25	5B	134/148 (90%)	131 (98%)	3 (2%)	45	67
25	5b	134/148 (90%)	133 (99%)	1 (1%)	76	80
26	4D	146/147 (99%)	141 (97%)	5 (3%)	32	59
26	4d	146/147 (99%)	139 (95%)	7 (5%)	23	50
27	4F	62/62 (100%)	62 (100%)	0	100	100
27	4f	62/62 (100%)	61 (98%)	1 (2%)	55	72
28	4G	247/264 (94%)	246 (100%)	1 (0%)	84	84
28	4g	247/264 (94%)	244 (99%)	3 (1%)	63	75
29	4I	230/238 (97%)	230 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	4i	230/238 (97%)	227 (99%)	3 (1%)	61	74
30	7A	138/150 (92%)	136 (99%)	2 (1%)	59	73
30	7a	138/150 (92%)	137 (99%)	1 (1%)	76	80
All	All	10448/10938 (96%)	10359 (99%)	89 (1%)	68	78

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	Qg	16	ASN
30	7a	137	ARG
22	Qg	126	CYS
26	4D	81	ILE
26	4d	166	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 202 such sidechains are listed below:

Mol	Chain	Res	Type
13	6A	68	ASN
24	QB	50	GLN
30	7A	15	HIS
20	Qe	192	HIS
24	Qb	195	GLN

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 75 ligands modelled in this entry, 10 are monoatomic - leaving 65 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
32	CDL	Qd	302	-	99,99,99	0.31	0	105,111,111	0.30	0
33	HEC	QD	301	3	50,50,50	1.30	4 (8%)	68,82,82	1.20	6 (8%)
34	PC1	c1	508	-	35,35,53	0.36	0	41,43,61	0.31	0
34	PC1	QE	303	-	35,35,53	0.35	0	41,43,61	0.37	0
40	FES	Qe	303	20	0,4,4	-	-	-	-	-
31	HEM	QC	402	2	50,50,50	1.34	7 (14%)	66,82,82	1.73	15 (22%)
32	CDL	QE	302	-	59,59,99	0.38	0	65,71,111	0.33	0
34	PC1	4a	301	-	46,46,53	0.32	0	52,54,61	0.31	0
34	PC1	Qe	301	-	53,53,53	0.30	0	59,61,61	0.35	0
36	3PE	C1	507	-	39,39,50	0.36	0	42,44,55	0.35	0
36	3PE	7A	201	-	40,40,50	0.34	0	43,45,55	0.30	0
37	HEA	c1	501	16	66,67,67	2.20	24 (36%)	78,103,103	2.70	31 (39%)
32	CDL	4c	201	-	69,69,99	0.35	0	75,81,111	0.32	0
31	HEM	Qc	402	2	50,50,50	1.33	7 (14%)	66,82,82	1.74	14 (21%)
36	3PE	c1	506	-	39,39,50	0.35	0	42,44,55	0.39	0
37	HEA	c1	502	16	66,67,67	2.24	24 (36%)	78,103,103	2.60	26 (33%)
34	PC1	Qc	403	-	35,35,53	0.36	0	41,43,61	0.34	0
34	PC1	c3	201	-	50,50,53	0.31	0	56,58,61	0.29	0
32	CDL	7c	201	-	89,89,99	0.32	0	95,101,111	0.35	0
34	PC1	Qe	302	-	53,53,53	0.30	0	59,61,61	0.29	0
34	PC1	4E	201	-	34,34,53	0.36	0	40,42,61	0.33	0
40	FES	QE	301	20	0,4,4	-	-	-	-	-
32	CDL	4E	202	-	71,71,99	0.36	0	77,83,111	0.34	0
35	PX2	4C	201	-	35,35,35	0.99	4 (11%)	39,40,40	1.06	2 (5%)
34	PC1	4A	302	-	45,45,53	0.32	0	51,53,61	0.33	0
34	PC1	Qg	301	-	27,27,53	0.40	0	33,35,61	0.35	0
36	3PE	4d	201	-	34,34,50	0.37	0	37,39,55	0.34	0
32	CDL	Qh	102	-	59,59,99	0.38	0	65,71,111	0.37	0
36	3PE	4d	202	-	50,50,50	0.31	0	53,55,55	0.27	0
34	PC1	4A	301	-	46,46,53	0.32	0	52,54,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	HEA	C1	501	16	66,67,67	2.22	25 (37%)	78,103,103	2.69	28 (35%)
36	3PE	7a	201	-	40,40,50	0.34	0	43,45,55	0.29	0
32	CDL	Qj	202	-	47,47,99	0.43	0	53,59,111	0.37	0
36	3PE	C1	508	-	39,39,50	0.35	0	42,44,55	0.34	0
34	PC1	Qd	303	-	30,30,53	0.38	0	36,38,61	0.34	0
42	S12	4F	102	-	33,34,34	0.79	0	36,40,40	1.18	2 (5%)
35	PX2	QJ	201	-	35,35,35	0.98	3 (8%)	39,40,40	1.11	2 (5%)
32	CDL	QH	101	-	75,75,99	0.34	0	81,87,111	0.32	0
34	PC1	C3	201	-	50,50,53	0.32	0	56,58,61	0.30	0
34	PC1	Qe	304	-	35,35,53	0.35	0	41,43,61	0.36	0
36	3PE	4a	302	-	50,50,50	0.31	0	53,55,55	0.42	0
31	HEM	QC	401	2	50,50,50	1.33	8 (16%)	66,82,82	1.74	14 (21%)
34	PC1	C1	505	-	49,49,53	0.32	0	55,57,61	0.32	0
34	PC1	4e	201	-	34,34,53	0.36	0	40,42,61	0.32	0
32	CDL	C1	506	-	89,89,99	0.32	0	95,101,111	0.28	0
34	PC1	C1	509	-	35,35,53	0.37	0	41,43,61	0.32	0
36	3PE	4F	101	-	50,50,50	0.31	0	53,55,55	0.32	0
37	HEA	C1	502	16	66,67,67	2.23	24 (36%)	78,103,103	2.57	29 (37%)
31	HEM	Qc	401	2	50,50,50	1.34	8 (16%)	66,82,82	1.79	15 (22%)
35	PX2	QD	304	-	35,35,35	0.99	4 (11%)	39,40,40	1.02	2 (5%)
42	S12	4d	203	-	33,34,34	0.77	0	36,40,40	1.10	3 (8%)
32	CDL	Qc	404	-	53,53,99	0.40	0	59,65,111	0.34	0
34	PC1	QD	303	-	30,30,53	0.38	0	36,38,61	0.37	0
32	CDL	Qh	101	-	64,64,99	0.37	0	70,76,111	0.32	0
32	CDL	QJ	202	-	57,57,99	0.39	0	63,69,111	0.33	0
32	CDL	QD	302	-	68,68,99	0.38	0	74,80,111	0.37	0
33	HEC	Qd	301	3	50,50,50	1.31	5 (10%)	68,82,82	1.19	4 (5%)
34	PC1	c1	505	-	49,49,53	0.31	0	55,57,61	0.31	0
36	3PE	c1	507	-	39,39,50	0.34	0	42,44,55	0.33	0
32	CDL	4e	202	-	71,71,99	0.36	0	77,83,111	0.33	0
34	PC1	Qj	201	-	53,53,53	0.30	0	59,61,61	0.28	0
34	PC1	7c	202	-	53,53,53	0.30	0	59,61,61	0.30	0
34	PC1	DC	201	-	53,53,53	0.32	0	59,61,61	0.51	1 (1%)
32	CDL	QC	403	-	55,55,99	0.40	0	61,67,111	0.33	0
36	3PE	4D	201	-	34,34,50	0.37	0	37,39,55	0.34	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
32	CDL	Qd	302	-	-	28/110/110/110	-
33	HEC	QD	301	3	1/1/3/7	2/14/54/54	-
34	PC1	c1	508	-	-	6/39/39/57	-
34	PC1	QE	303	-	-	10/39/39/57	-
40	FES	Qe	303	20	-	-	0/1/1/1
31	HEM	QC	402	2	-	6/14/54/54	-
32	CDL	QE	302	-	-	24/70/70/110	-
34	PC1	4a	301	-	-	14/50/50/57	-
34	PC1	Qe	301	-	-	17/57/57/57	-
36	3PE	C1	507	-	-	17/43/43/54	-
36	3PE	7A	201	-	-	8/44/44/54	-
37	HEA	c1	501	16	-	13/36/76/76	-
32	CDL	4c	201	-	-	25/80/80/110	-
31	HEM	Qc	402	2	-	6/14/54/54	-
36	3PE	c1	506	-	-	19/43/43/54	-
37	HEA	c1	502	16	-	15/36/76/76	-
34	PC1	Qc	403	-	-	12/39/39/57	-
34	PC1	c3	201	-	-	16/54/54/57	-
32	CDL	7c	201	-	-	18/100/100/110	-
34	PC1	Qe	302	-	-	15/57/57/57	-
34	PC1	4E	201	-	-	5/38/38/57	-
40	FES	QE	301	20	-	-	0/1/1/1
32	CDL	4E	202	-	-	24/82/82/110	-
35	PX2	4C	201	-	-	16/37/37/37	-
34	PC1	4A	302	-	-	15/49/49/57	-
34	PC1	Qg	301	-	-	5/31/31/57	-
36	3PE	4d	201	-	-	5/38/38/54	-
32	CDL	Qh	102	-	-	15/70/70/110	-
36	3PE	4d	202	-	-	19/54/54/54	-
34	PC1	4A	301	-	-	12/50/50/57	-
37	HEA	C1	501	16	-	15/36/76/76	-
36	3PE	7a	201	-	-	9/44/44/54	-
32	CDL	Qj	202	-	-	11/58/58/110	-
36	3PE	C1	508	-	-	6/43/43/54	-
34	PC1	Qd	303	-	-	6/34/34/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	S12	4F	102	-	-	20/38/38/38	-
35	PX2	QJ	201	-	-	18/37/37/37	-
32	CDL	QH	101	-	-	17/86/86/110	-
34	PC1	C3	201	-	-	16/54/54/57	-
34	PC1	Qe	304	-	-	8/39/39/57	-
36	3PE	4a	302	-	-	23/54/54/54	-
31	HEM	QC	401	2	-	5/14/54/54	-
34	PC1	C1	505	-	-	13/53/53/57	-
34	PC1	4e	201	-	-	3/38/38/57	-
32	CDL	C1	506	-	-	19/100/100/110	-
34	PC1	C1	509	-	-	8/39/39/57	-
36	3PE	4F	101	-	-	21/54/54/54	-
37	HEA	C1	502	16	-	13/36/76/76	-
31	HEM	Qc	401	2	-	6/14/54/54	-
35	PX2	QD	304	-	-	15/37/37/37	-
42	S12	4d	203	-	-	24/38/38/38	-
32	CDL	Qc	404	-	-	12/64/64/110	-
34	PC1	QD	303	-	-	17/34/34/57	-
32	CDL	Qh	101	-	-	18/75/75/110	-
32	CDL	QJ	202	-	-	17/68/68/110	-
33	HEC	Qd	301	3	1/1/3/7	3/14/54/54	-
32	CDL	QD	302	-	-	22/79/79/110	-
34	PC1	c1	505	-	-	16/53/53/57	-
36	3PE	c1	507	-	-	14/43/43/54	-
32	CDL	4e	202	-	-	23/82/82/110	-
34	PC1	Qj	201	-	-	8/57/57/57	-
34	PC1	7c	202	-	-	26/57/57/57	-
34	PC1	DC	201	-	-	29/57/57/57	-
32	CDL	QC	403	-	-	13/66/66/110	-
36	3PE	4D	201	-	-	6/38/38/54	-

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c1	502	HEA	C3B-C2B	5.42	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C1	502	HEA	C3B-C2B	5.27	1.46	1.34
37	C1	501	HEA	C3B-C2B	5.12	1.46	1.34
37	c1	501	HEA	C3B-C2B	5.07	1.46	1.34
37	C1	501	HEA	FE-ND	5.02	2.10	1.94

The worst 5 of 194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C1	501	HEA	CAD-CBD-CGD	-8.18	96.01	113.60
37	c1	501	HEA	CAD-CBD-CGD	-7.66	97.11	113.60
37	C1	501	HEA	CAA-CBA-CGA	-7.48	97.52	113.60
37	C1	502	HEA	CAD-CBD-CGD	-7.16	98.20	113.60
37	c1	501	HEA	CAA-CBA-CGA	-7.12	98.27	113.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	QD	301	HEC	NA
33	Qd	301	HEC	NA

5 of 887 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	QC	401	HEM	C2C-C3C-CAC-CBC
31	QC	401	HEM	C4C-C3C-CAC-CBC
31	QC	402	HEM	C2C-C3C-CAC-CBC
31	QC	402	HEM	C4C-C3C-CAC-CBC
32	QC	403	CDL	CA2-OA2-PA1-OA3

There are no ring outliers.

33 monomers are involved in 78 short contacts:

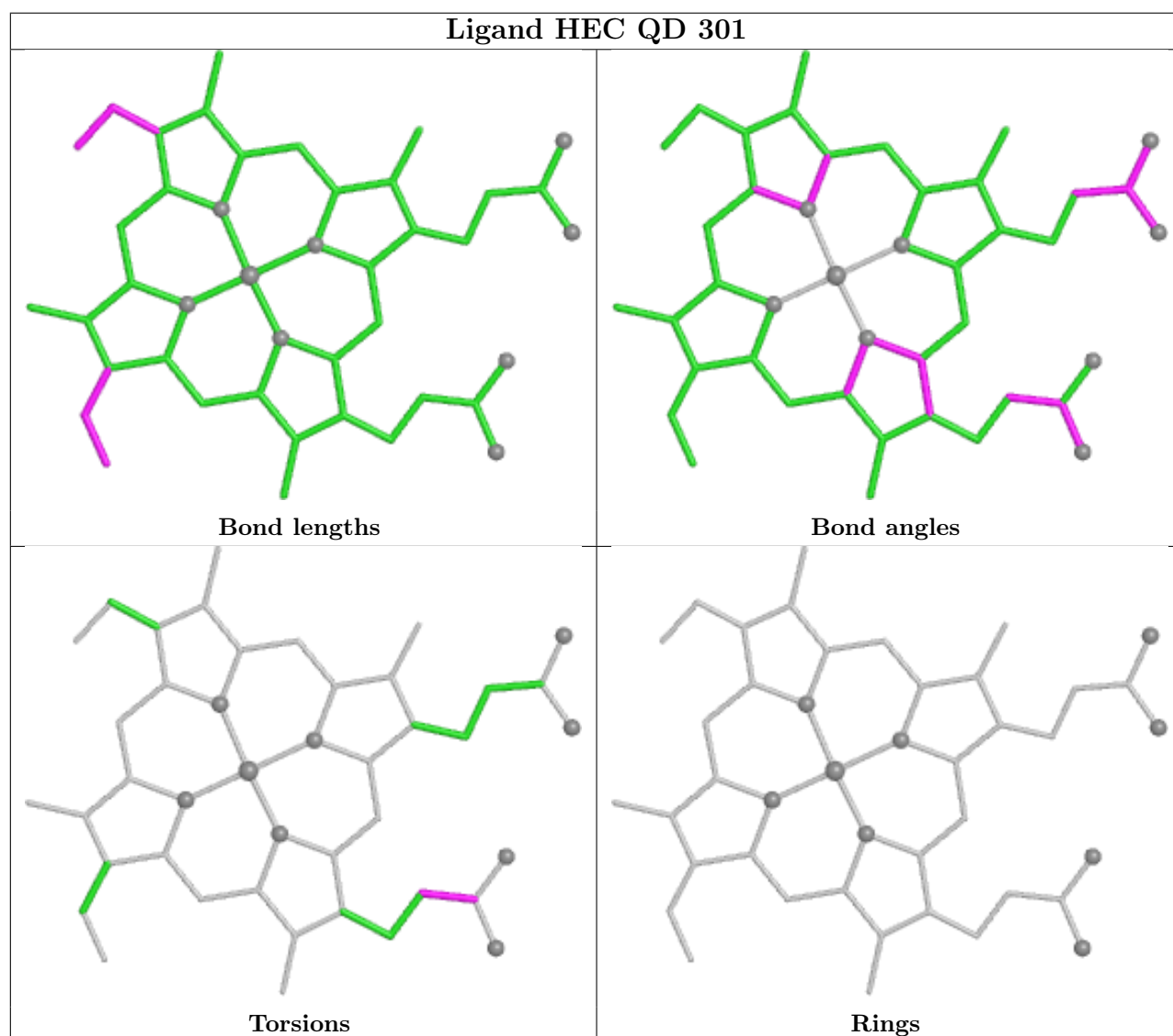
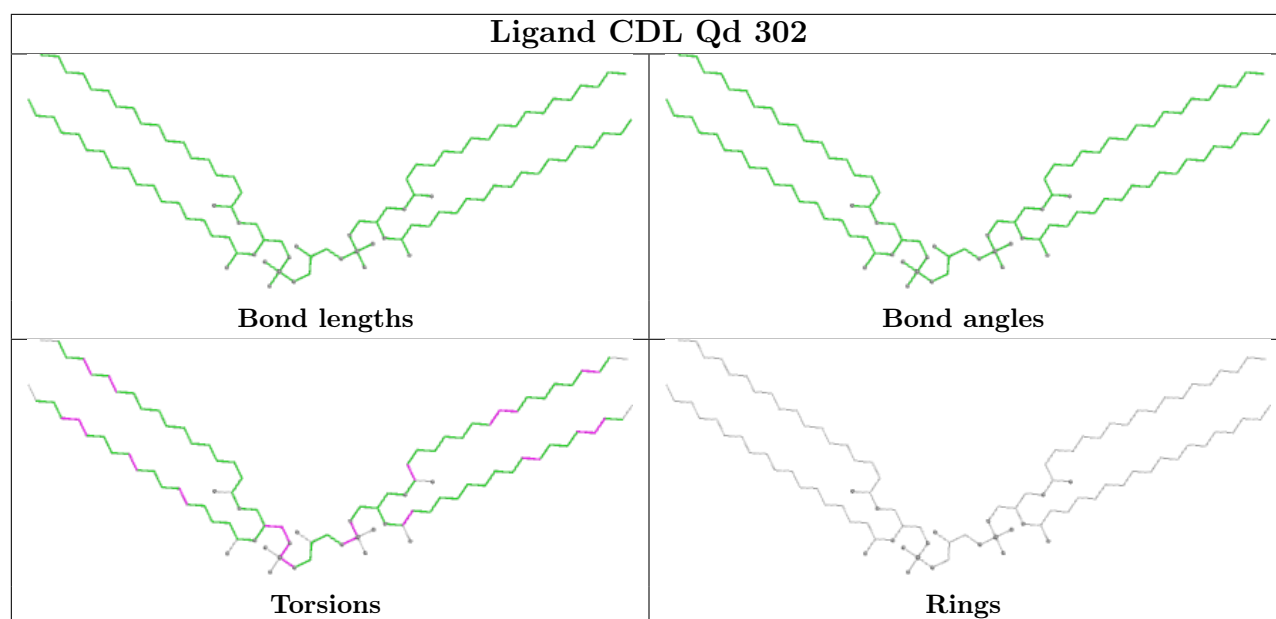
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	Qd	302	CDL	2	0
33	QD	301	HEC	6	0
34	c1	508	PC1	1	0
34	QE	303	PC1	1	0
31	QC	402	HEM	3	0
34	Qe	301	PC1	1	0
36	C1	507	3PE	1	0
37	c1	501	HEA	14	0

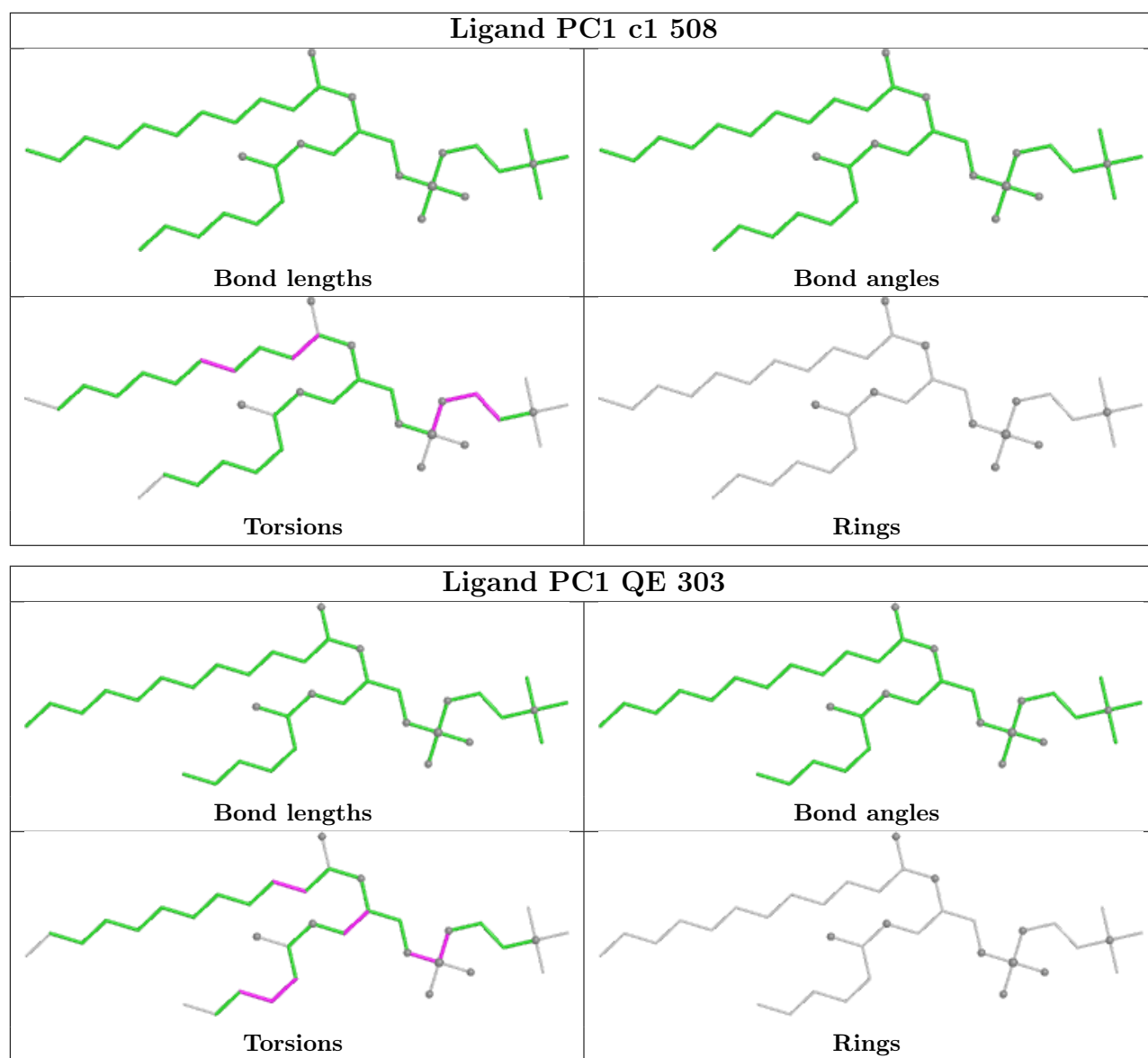
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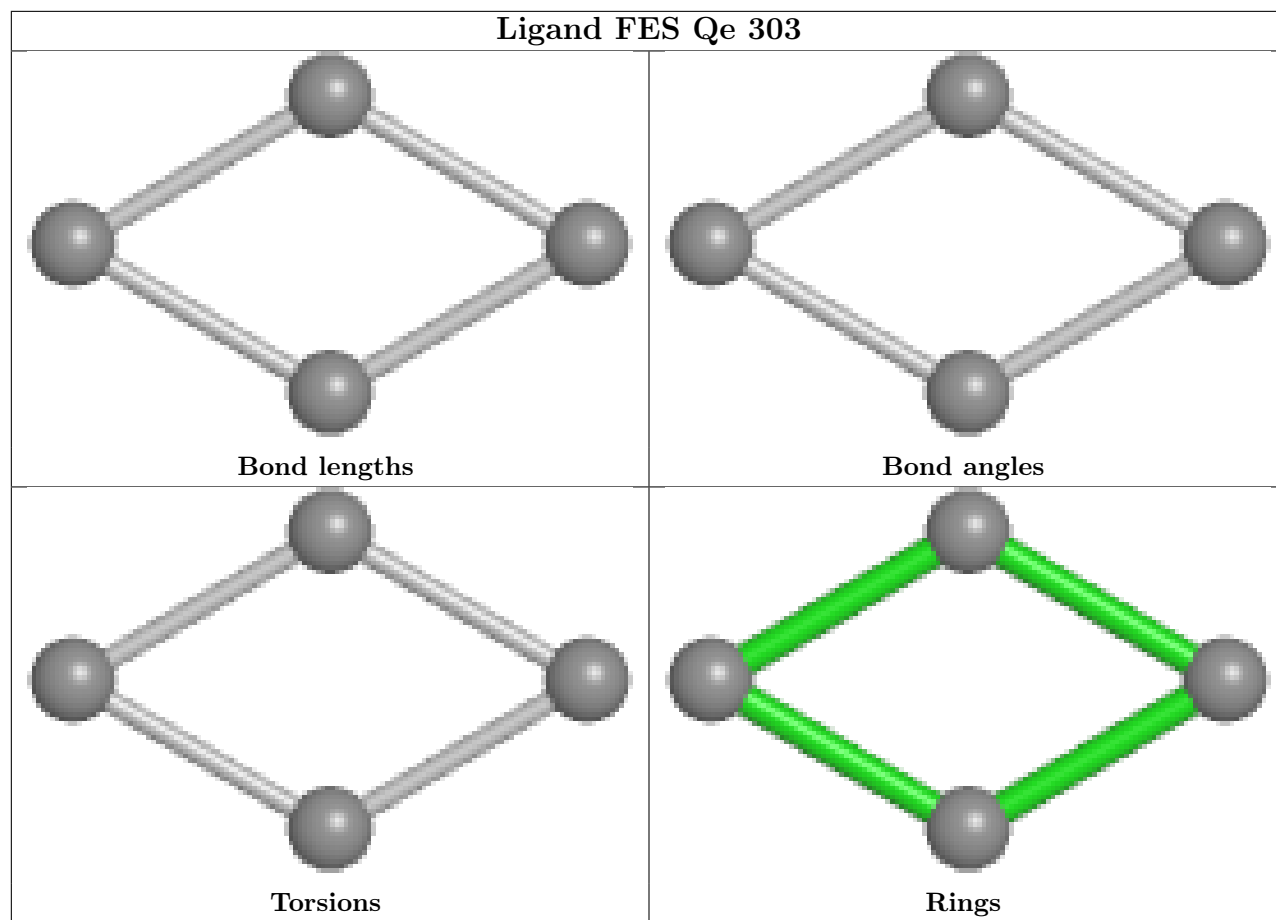
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Qc	402	HEM	3	0
36	c1	506	3PE	1	0
37	c1	502	HEA	4	0
34	Qe	302	PC1	2	0
34	4E	201	PC1	1	0
40	QE	301	FES	1	0
35	4C	201	PX2	4	0
37	C1	501	HEA	6	0
32	Qj	202	CDL	1	0
42	4F	102	S12	1	0
35	QJ	201	PX2	2	0
34	Qe	304	PC1	1	0
31	QC	401	HEM	1	0
34	C1	505	PC1	1	0
34	4e	201	PC1	1	0
36	4F	101	3PE	1	0
37	C1	502	HEA	4	0
31	Qc	401	HEM	4	0
35	QD	304	PX2	3	0
32	Qc	404	CDL	2	0
32	QJ	202	CDL	1	0
32	QD	302	CDL	1	0
33	Qd	301	HEC	2	0
34	DC	201	PC1	1	0
32	QC	403	CDL	1	0

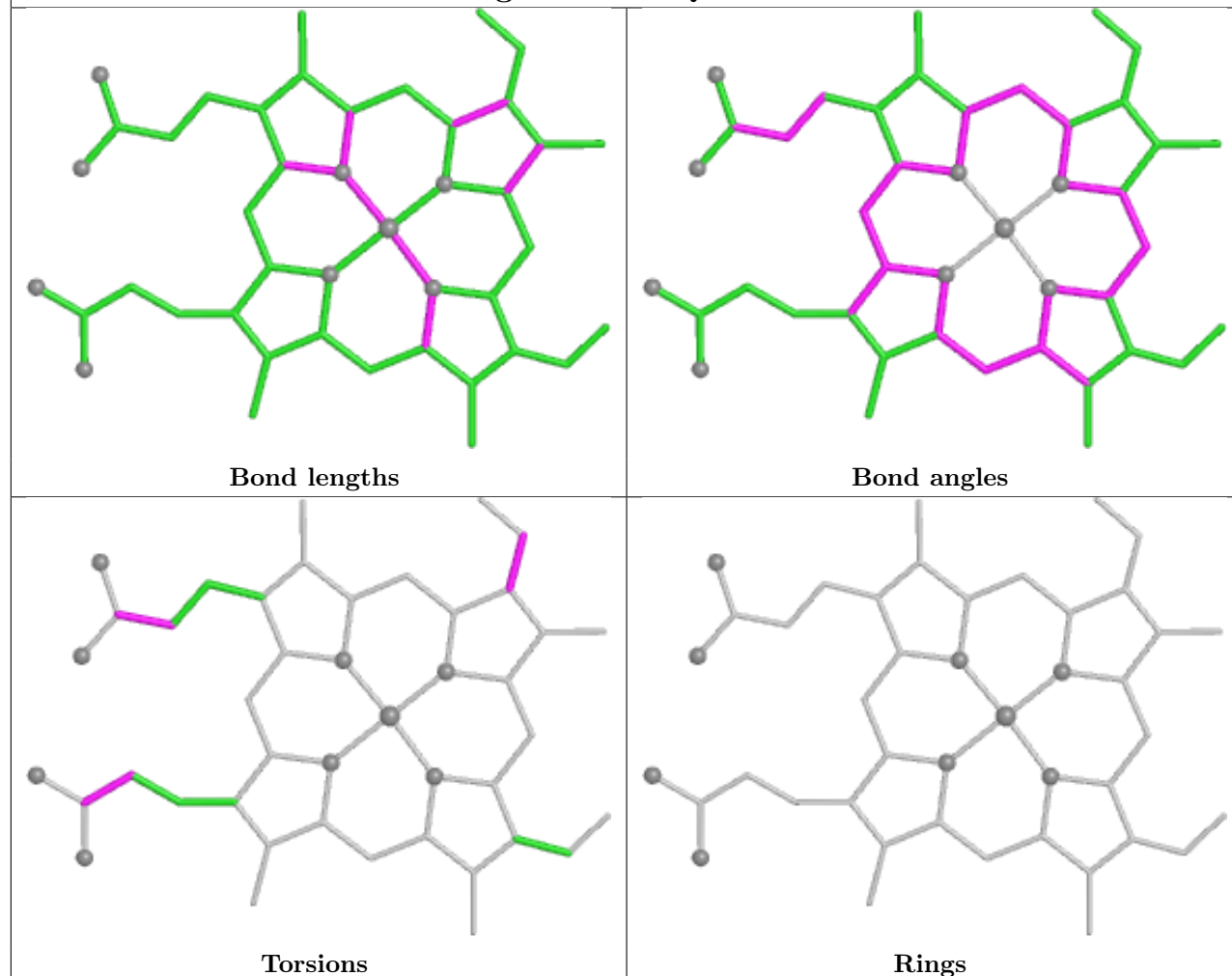
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



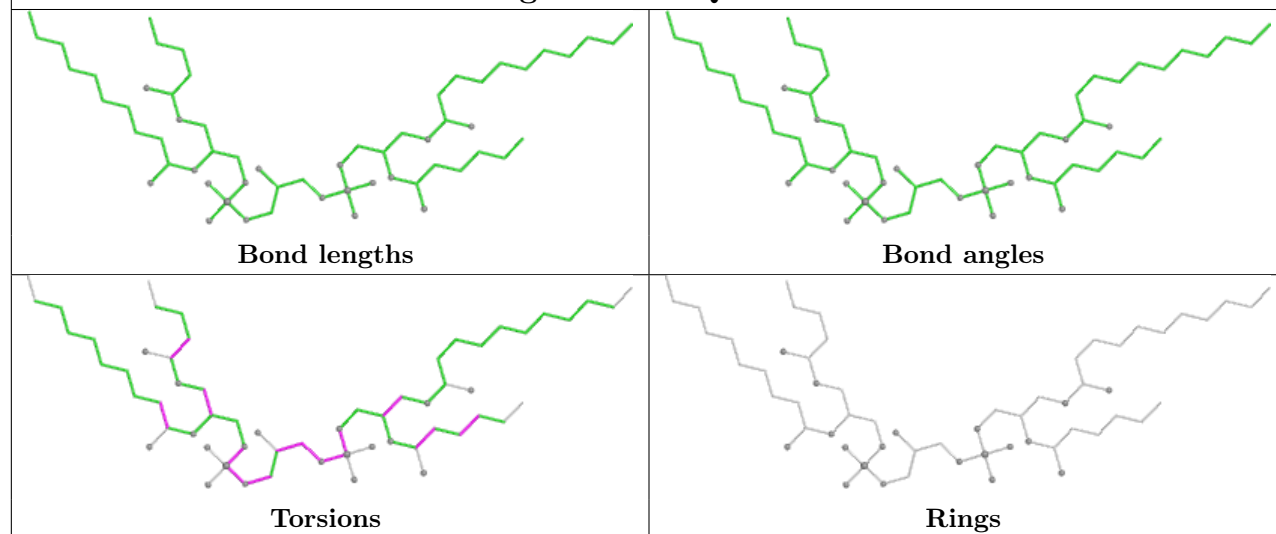


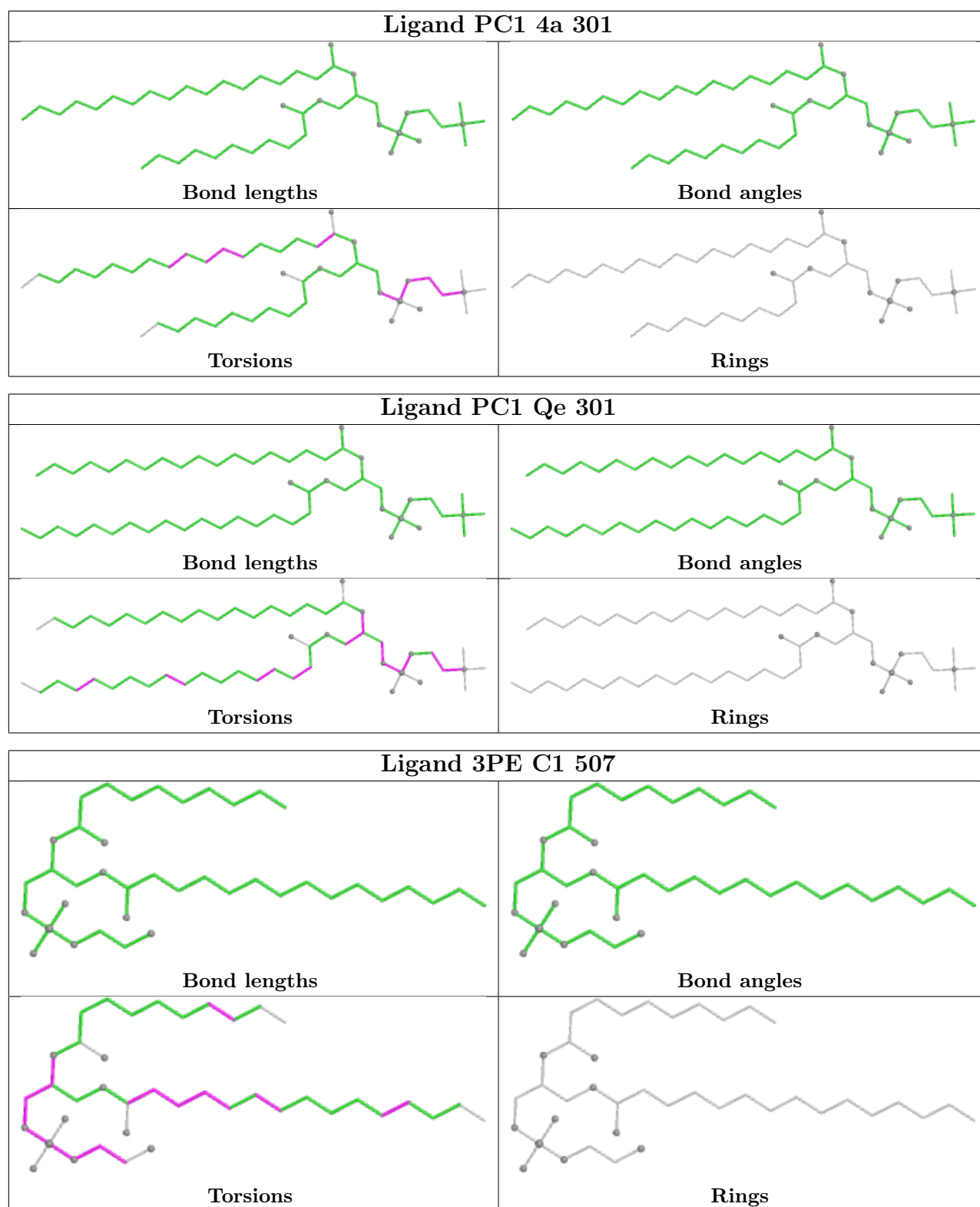


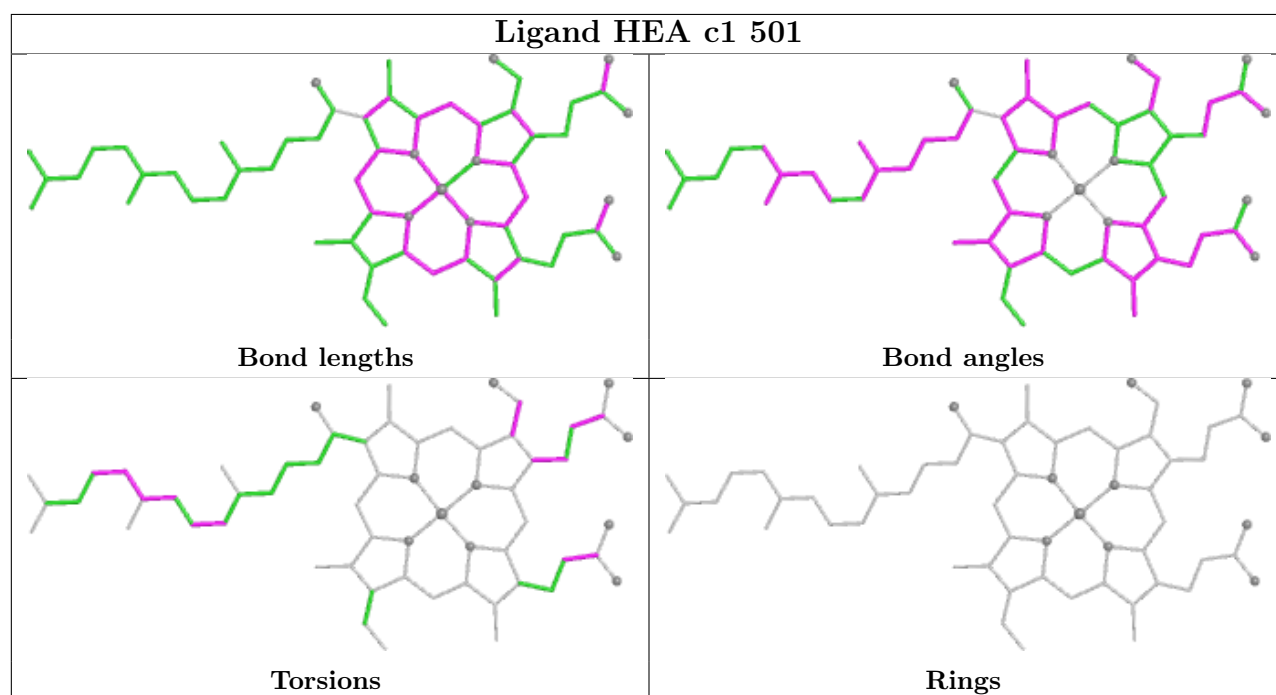
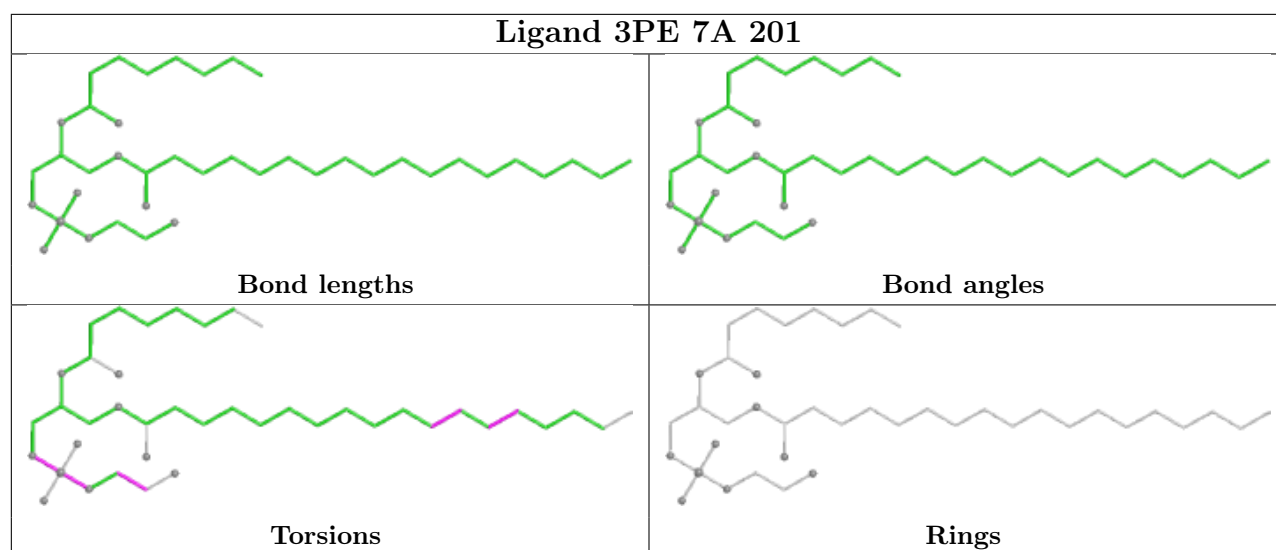
Ligand HEM QC 402

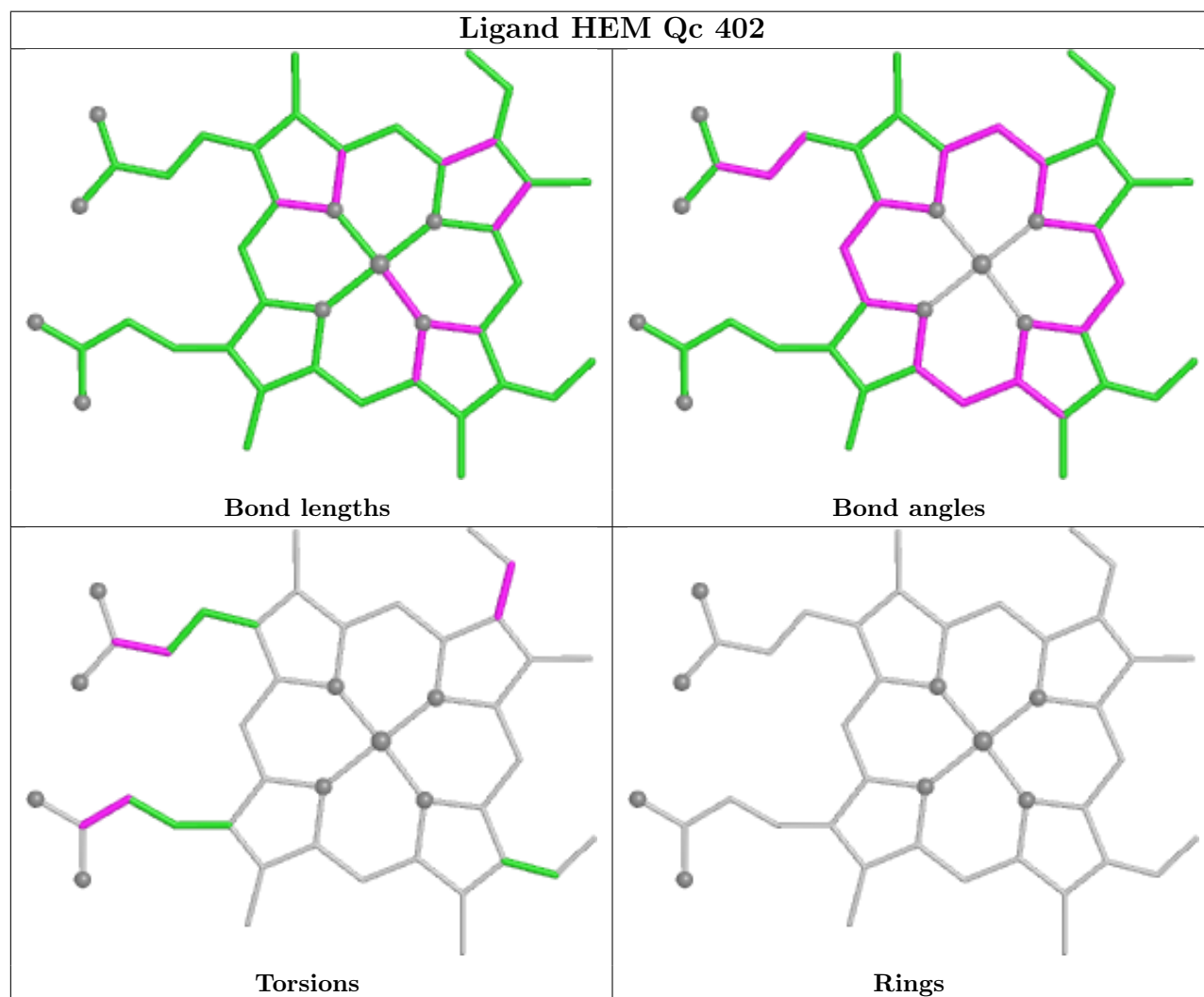
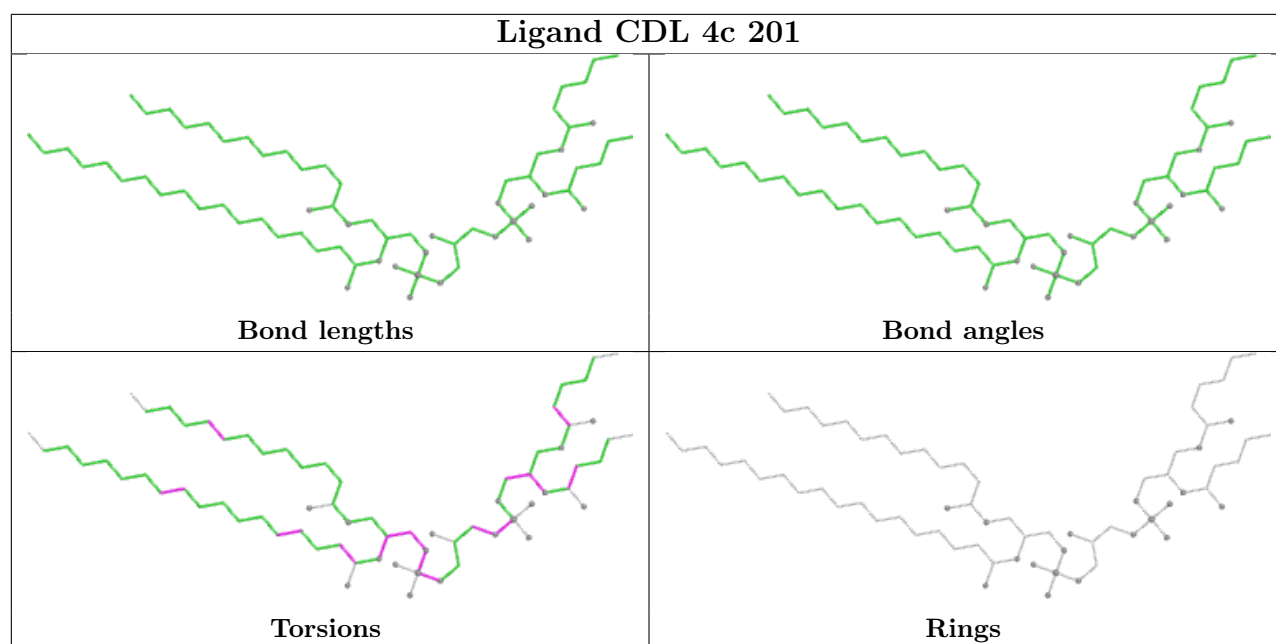


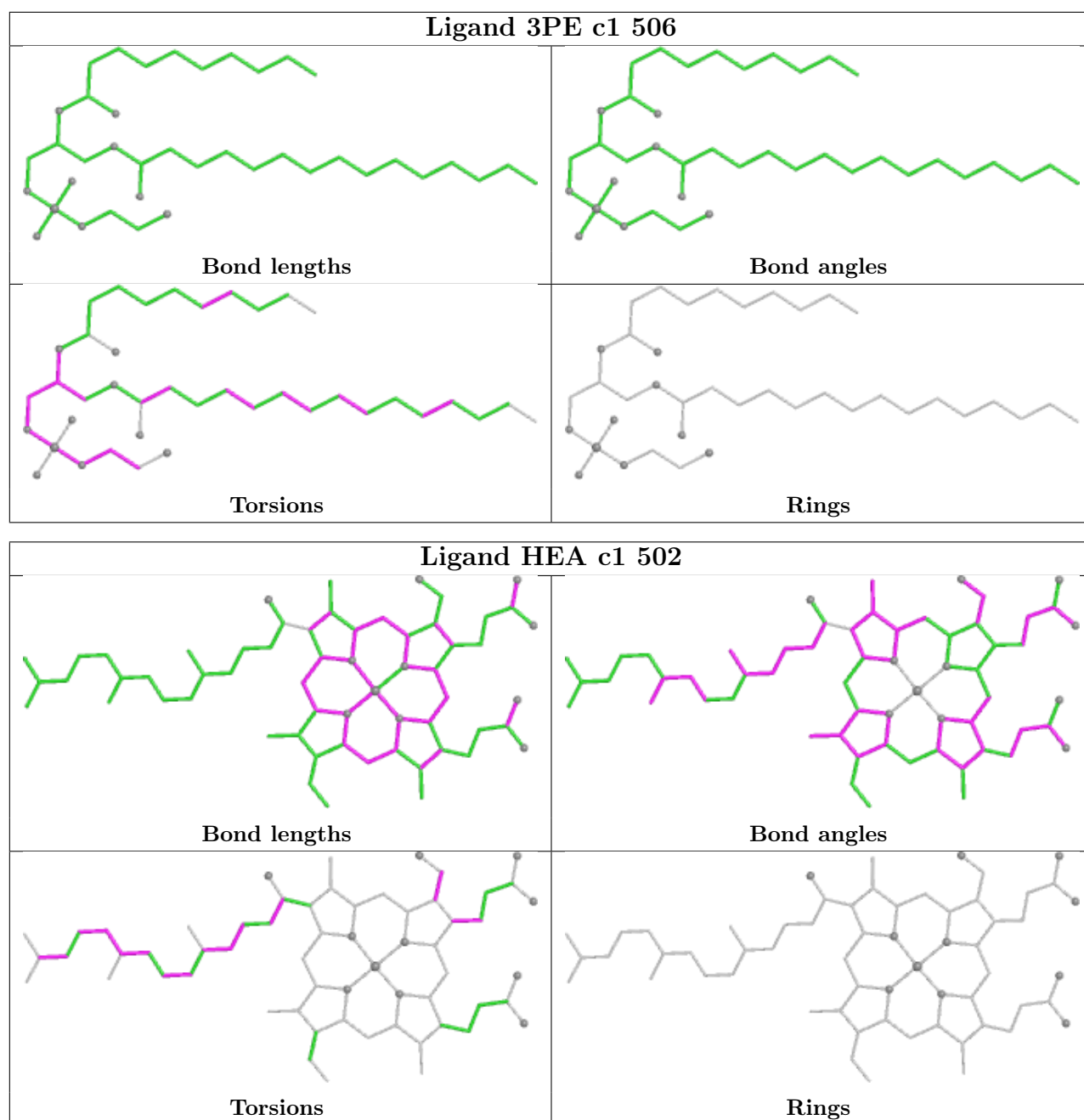
Ligand CDL QE 302

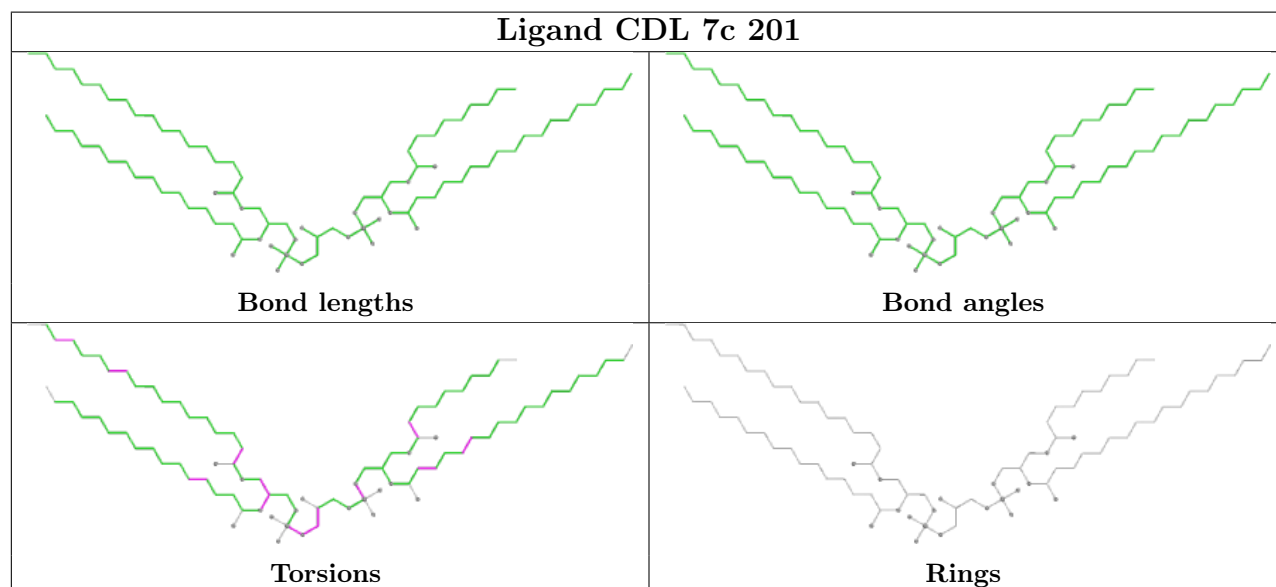
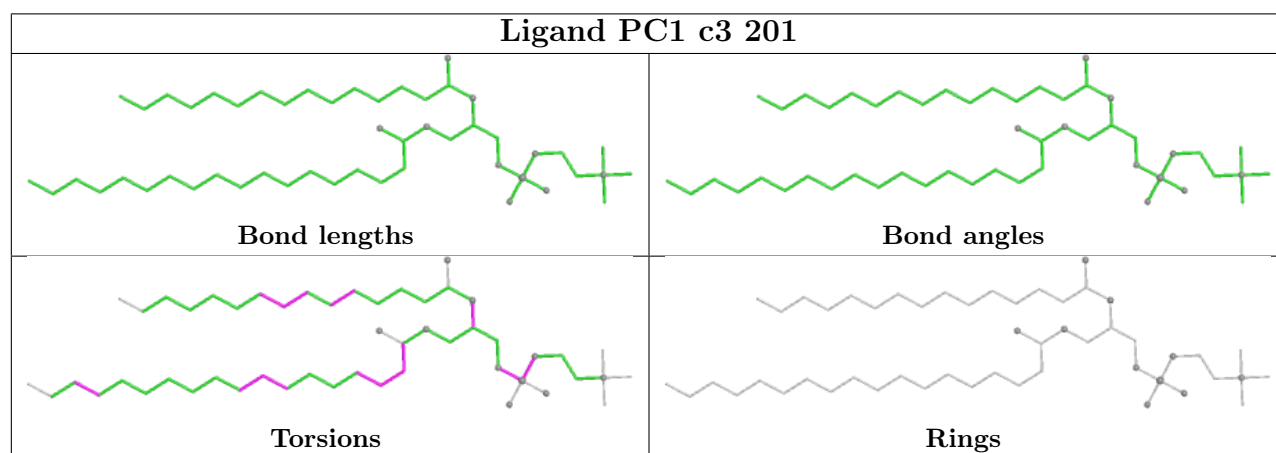
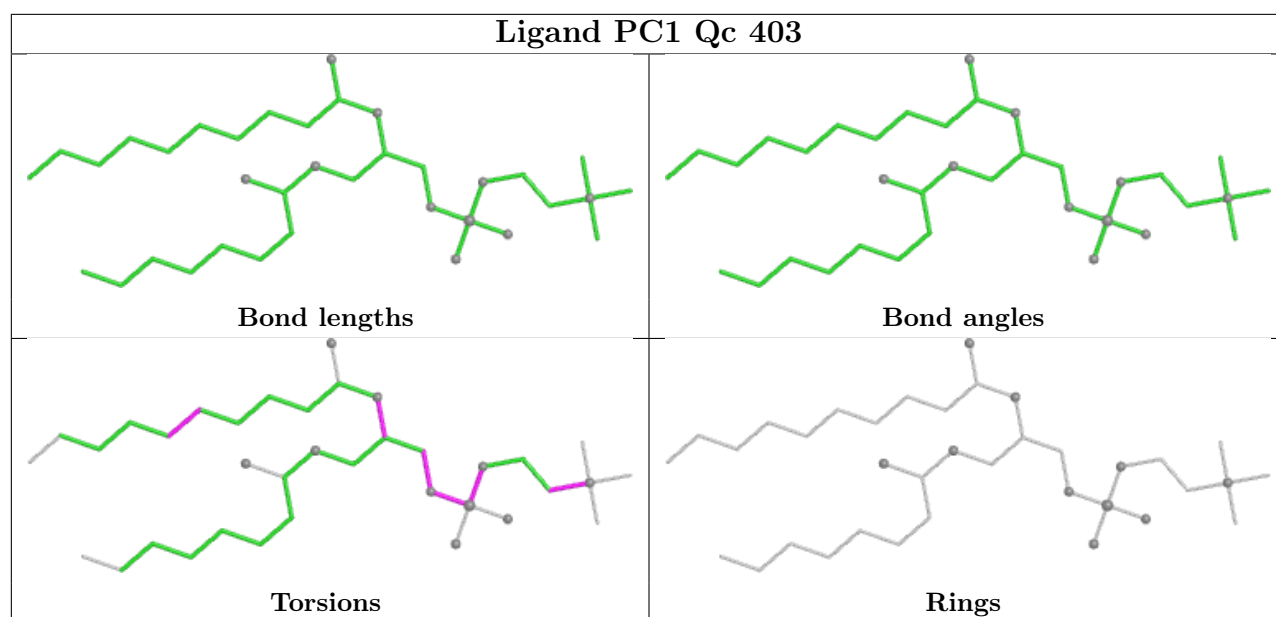


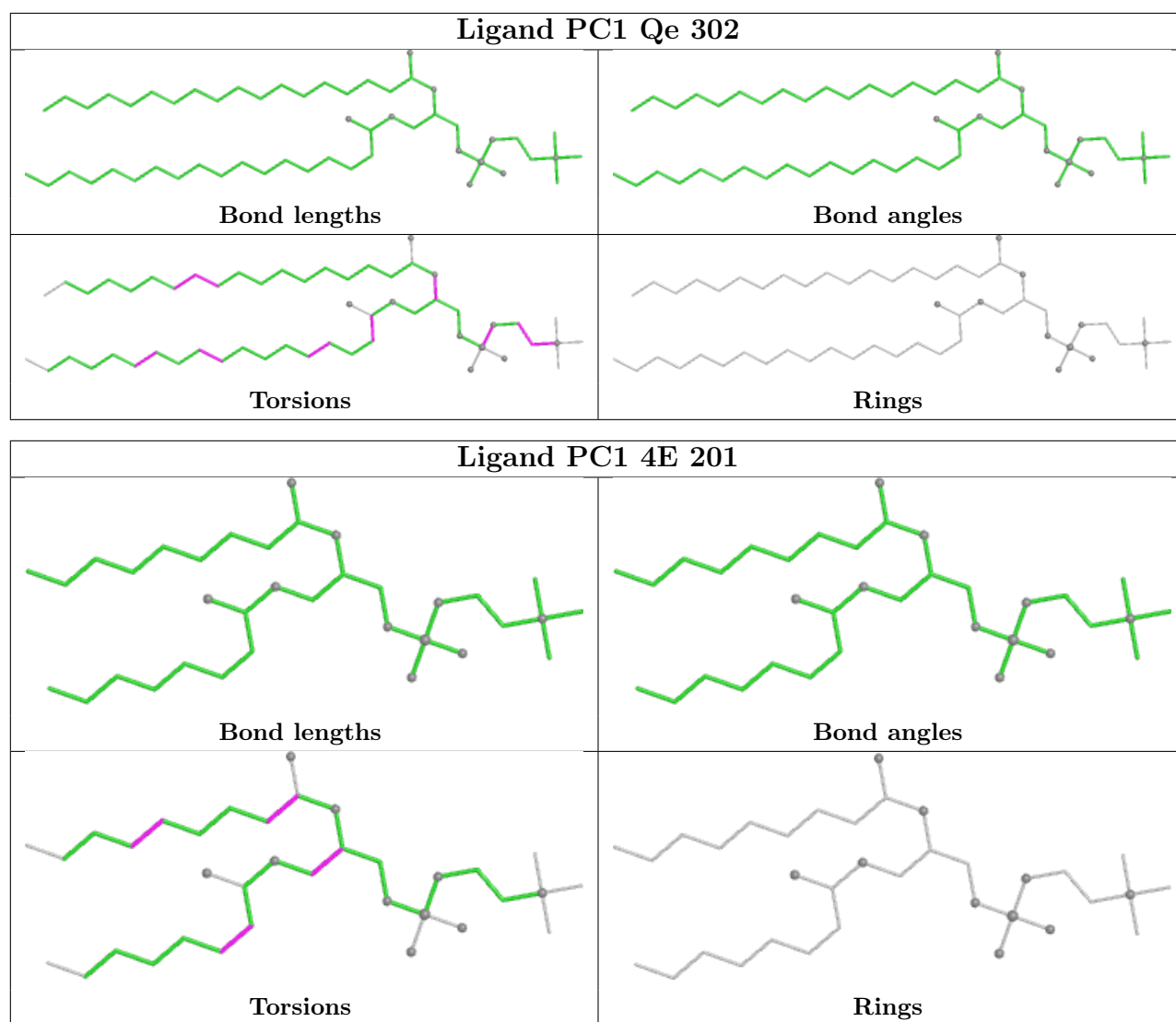


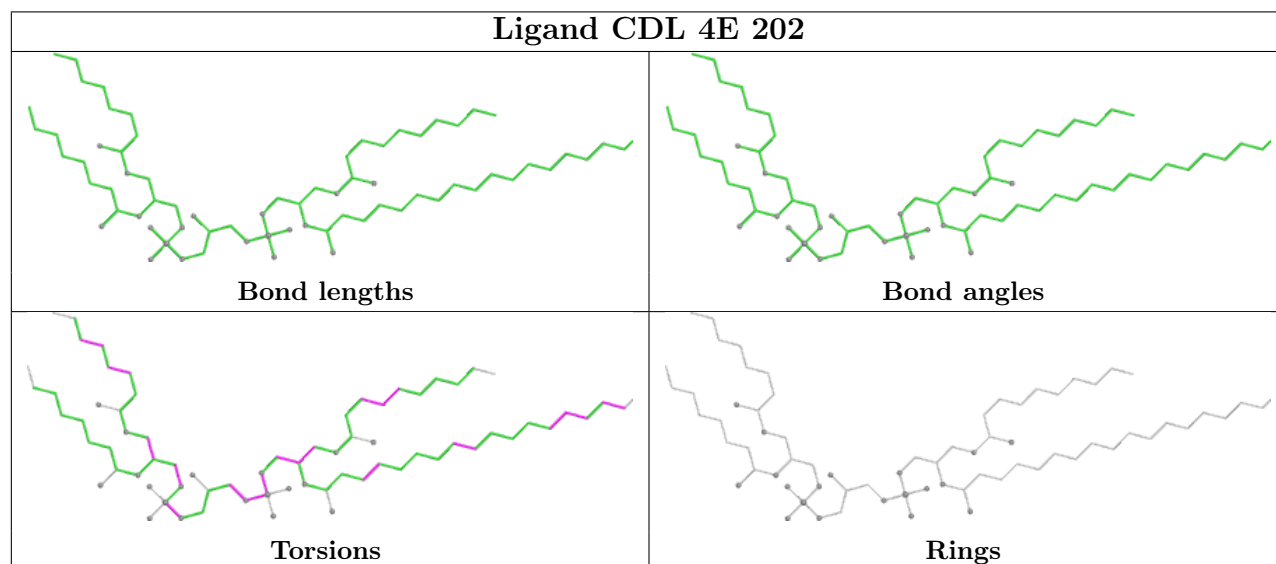
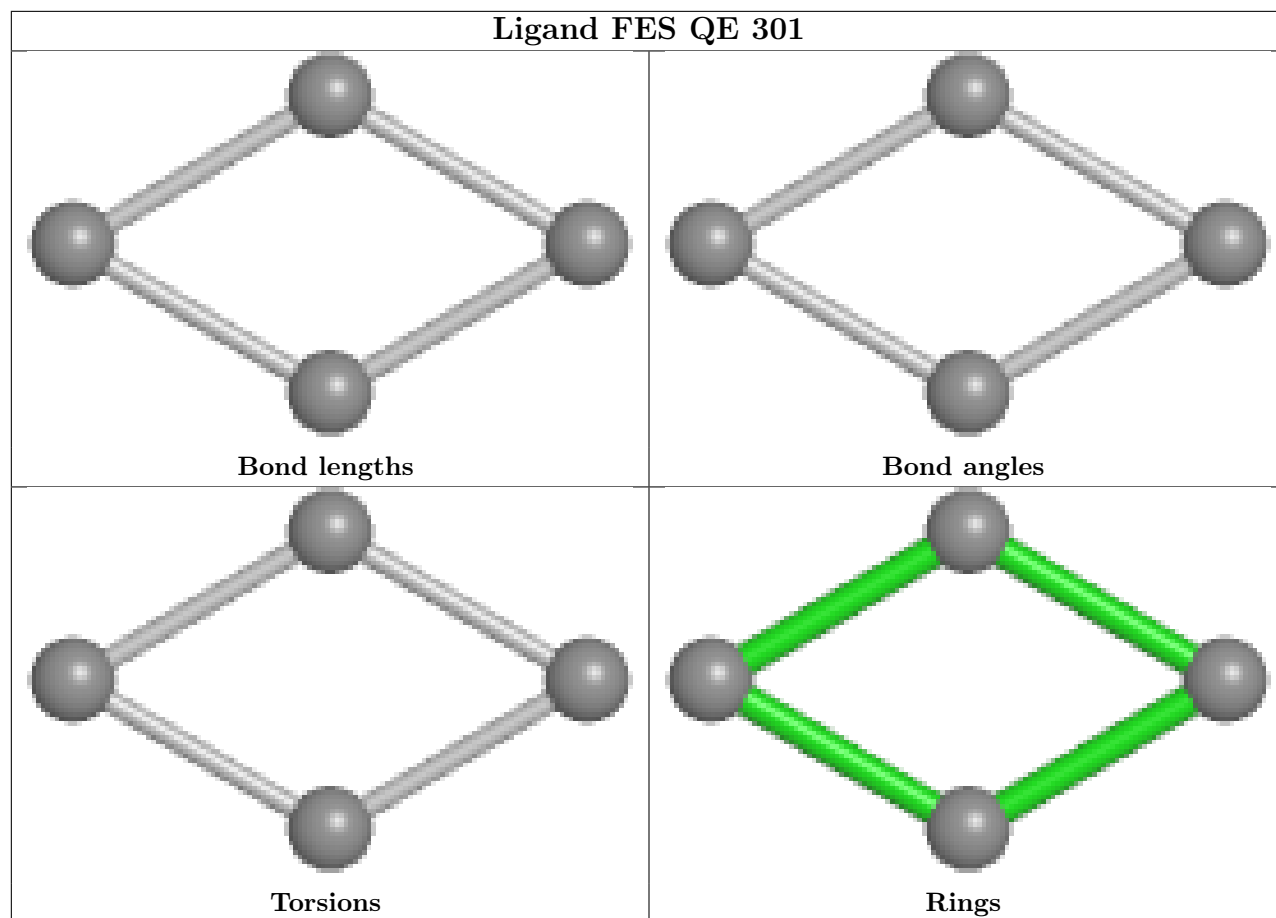


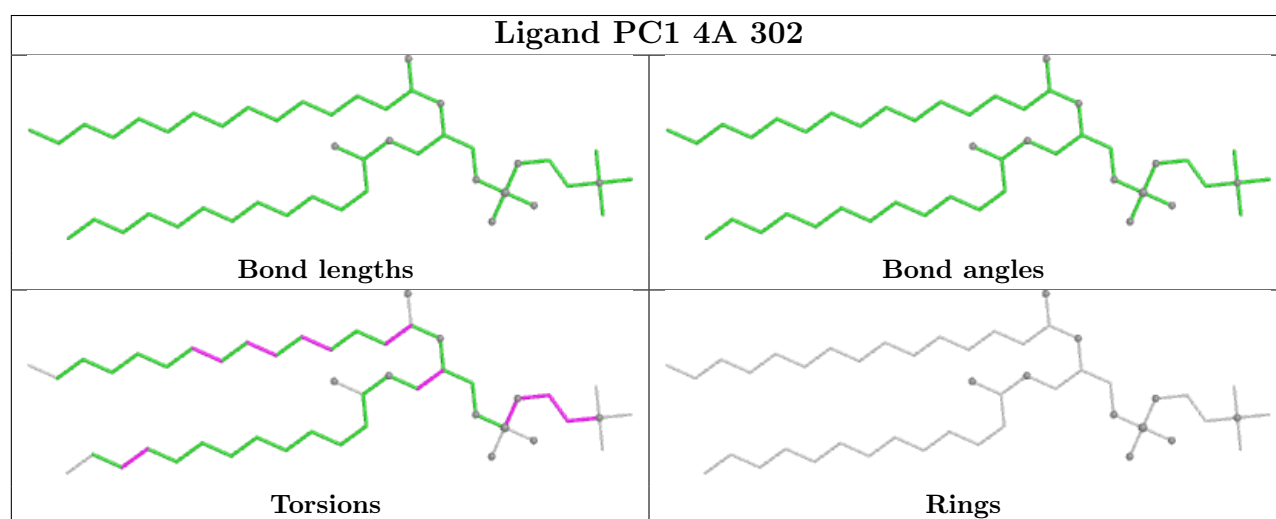
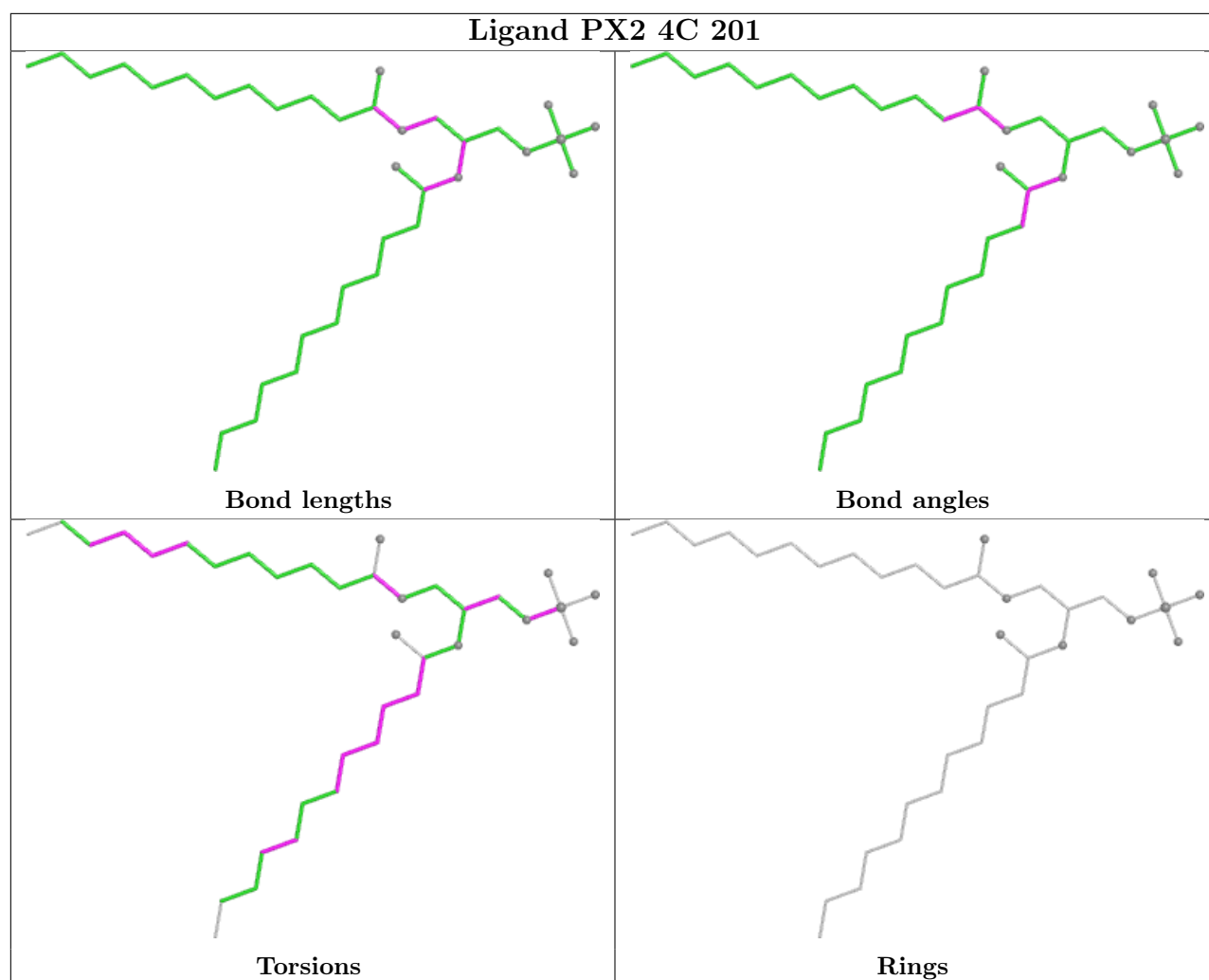


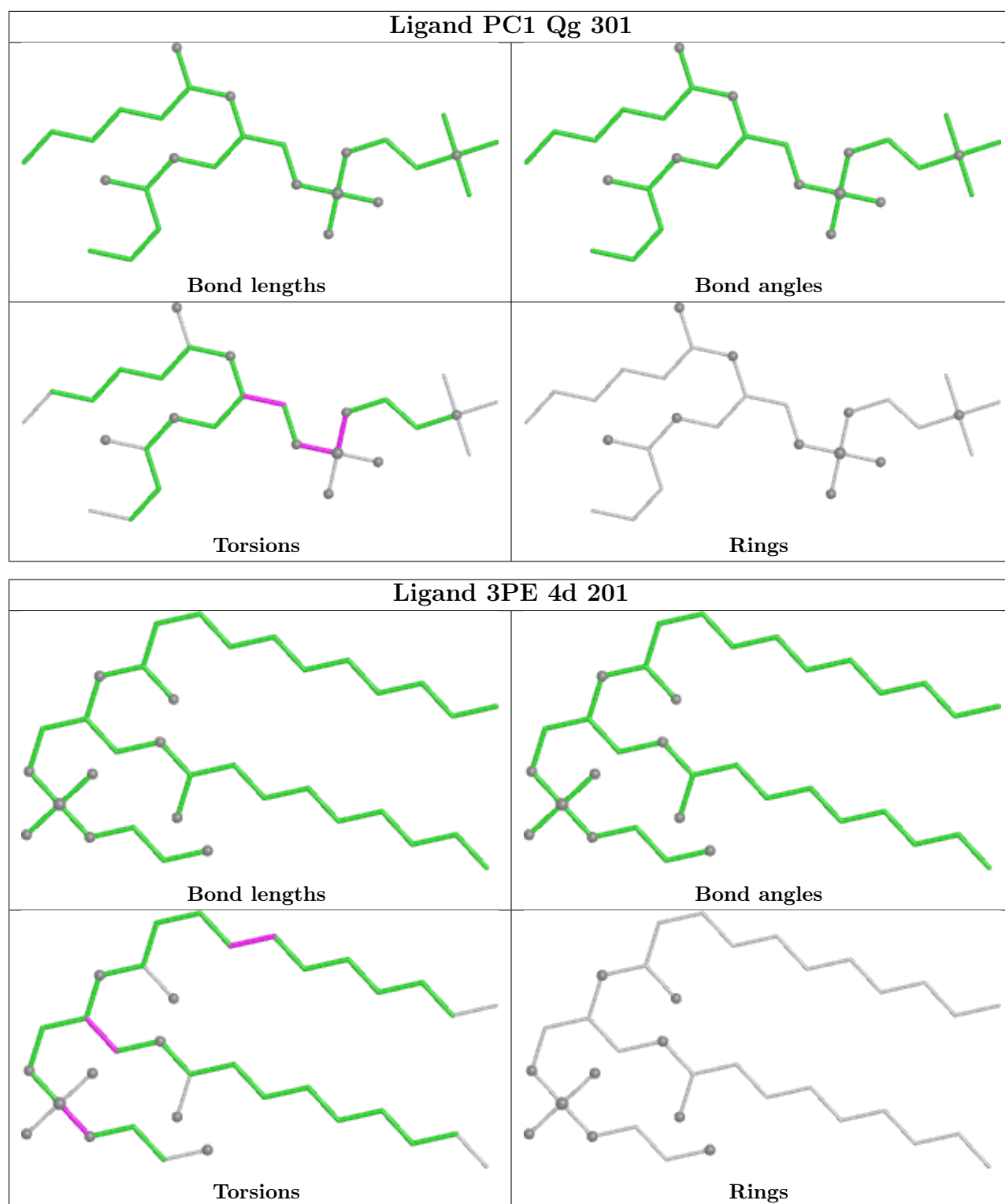


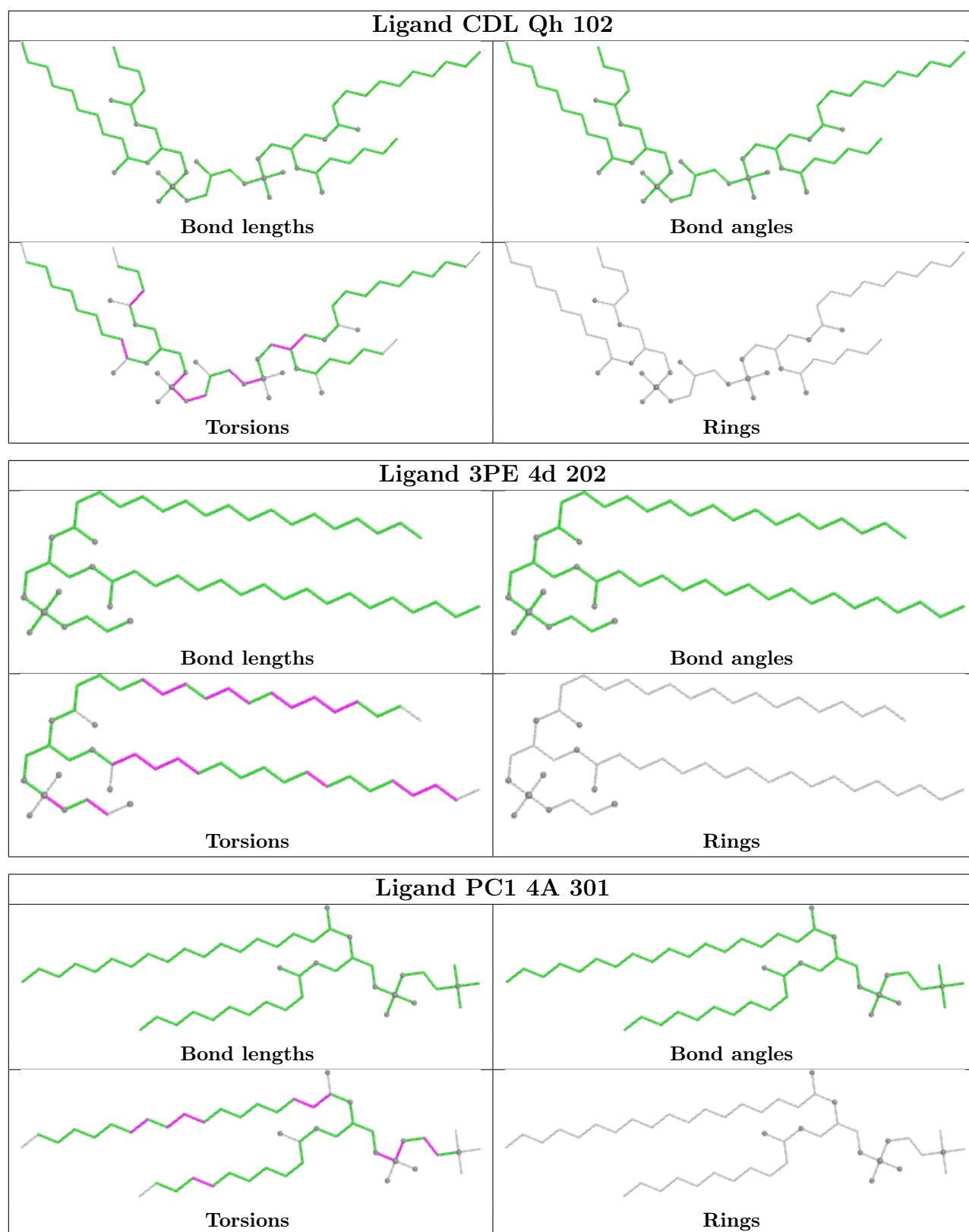


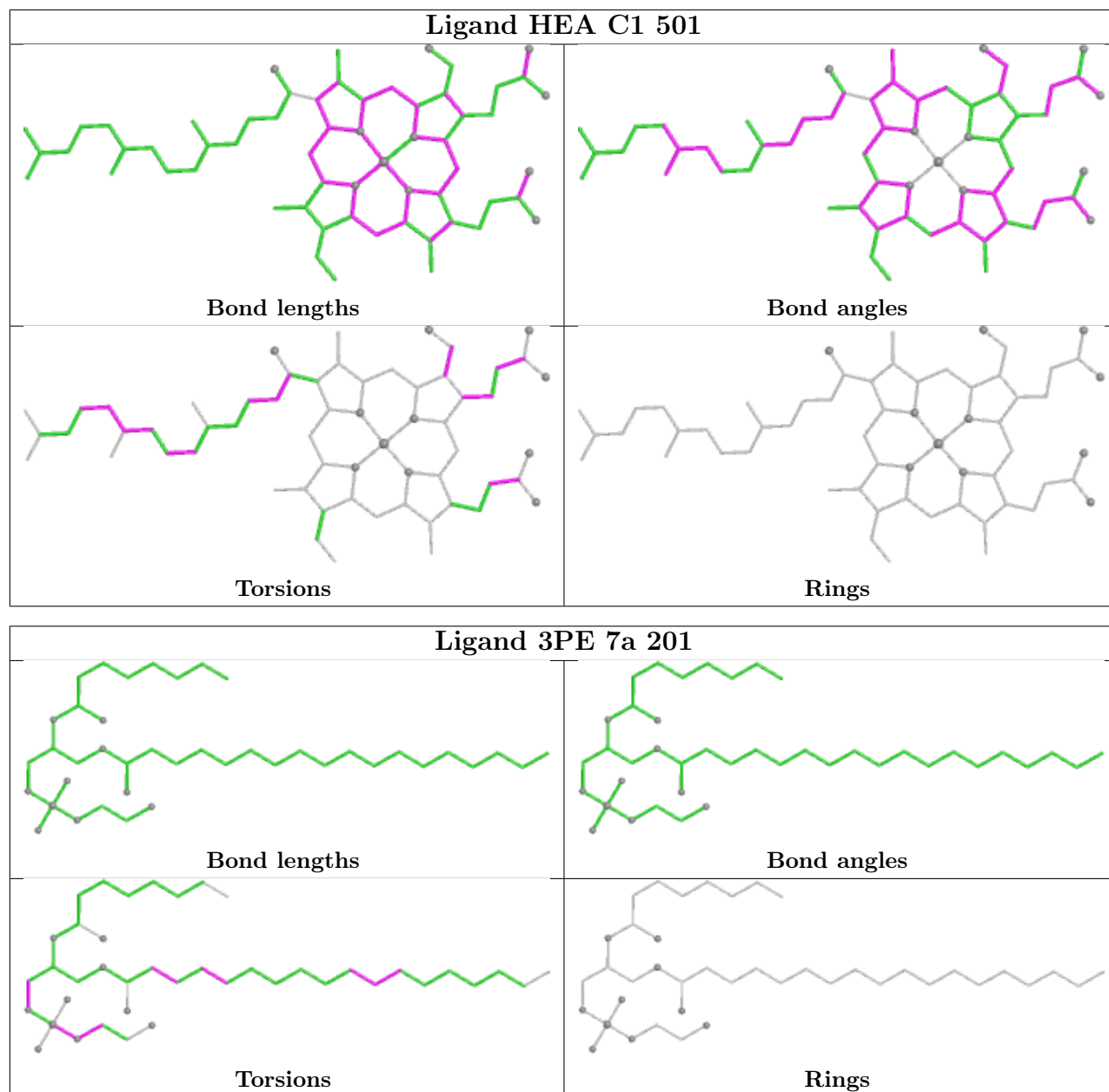


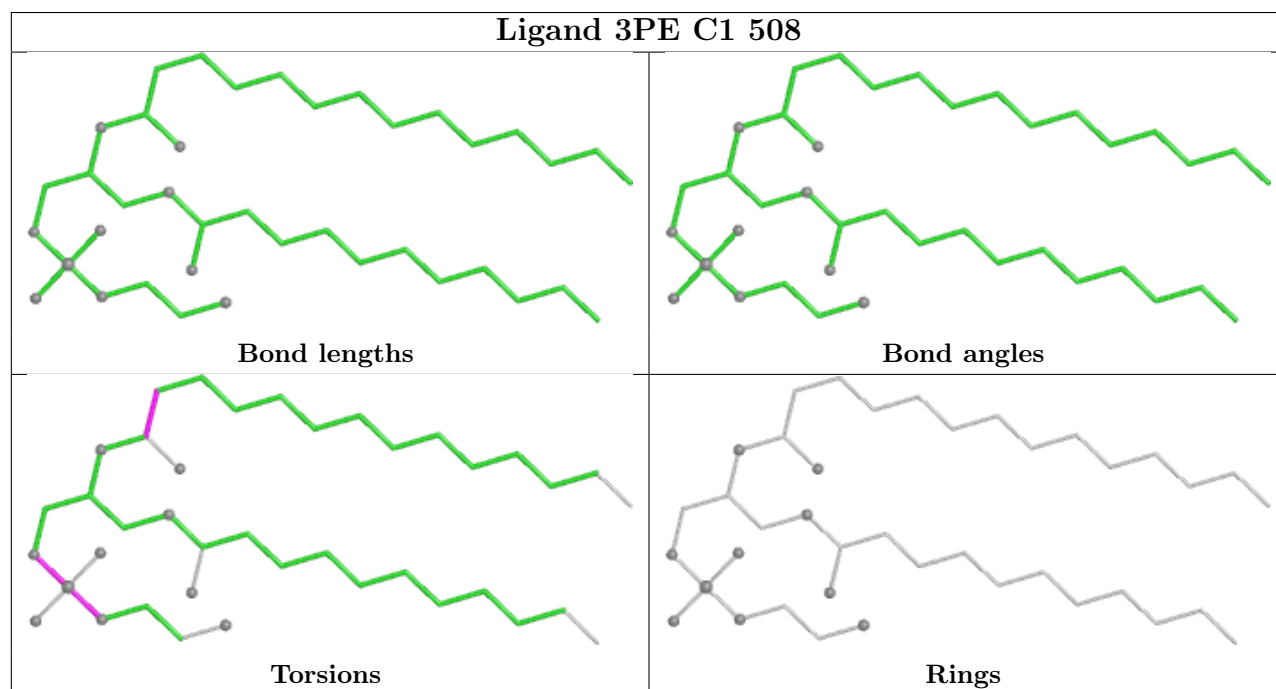
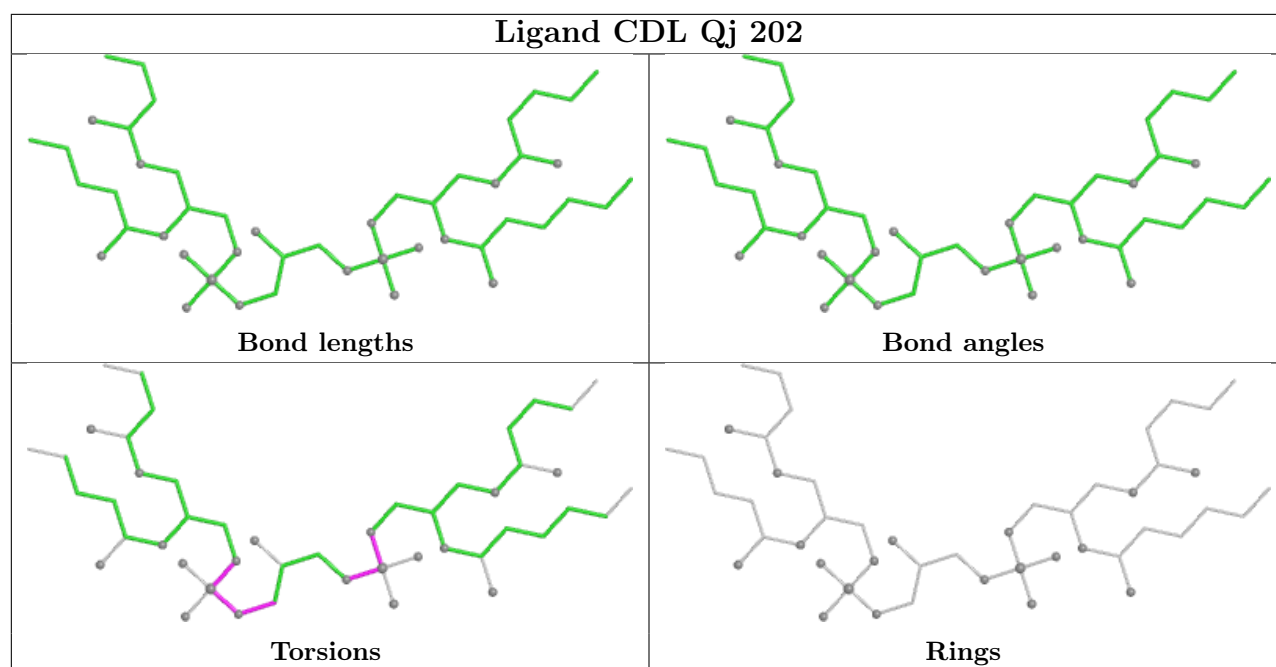


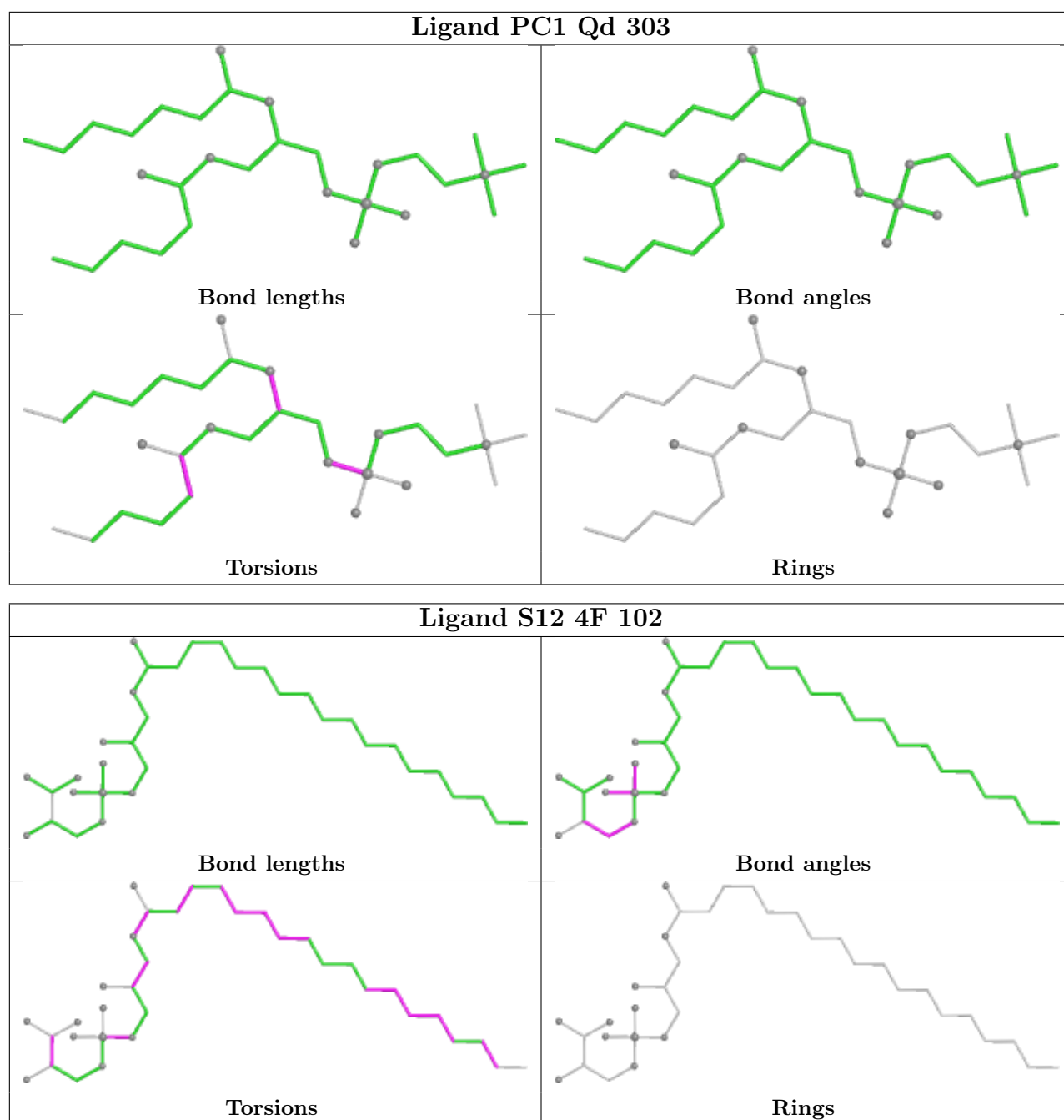


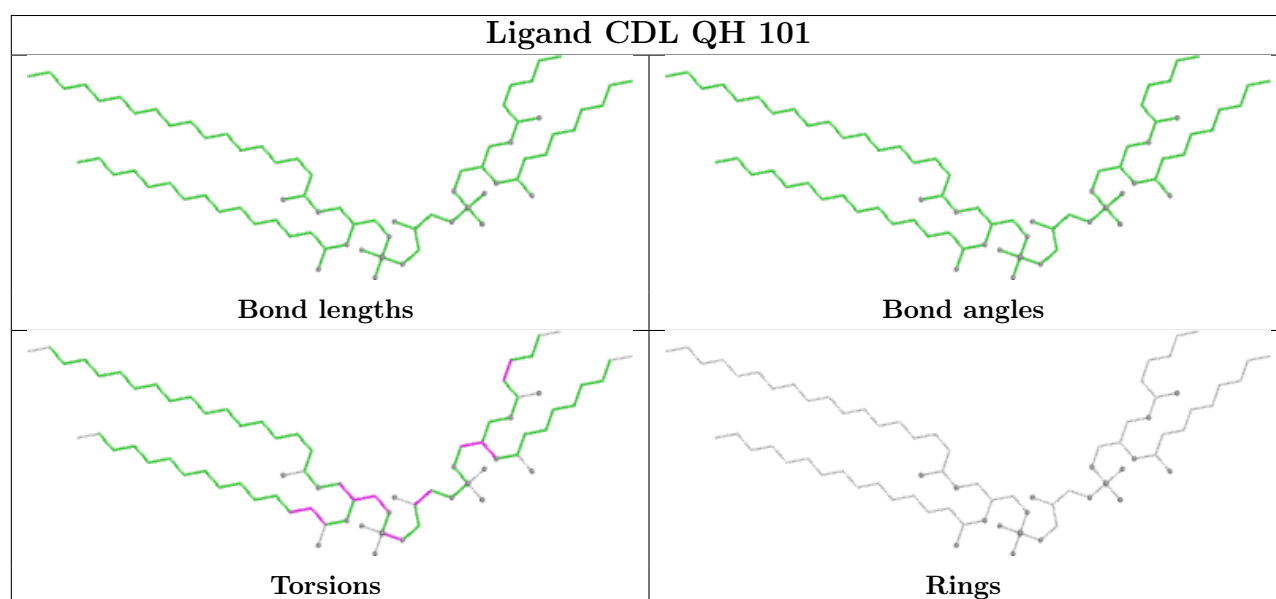
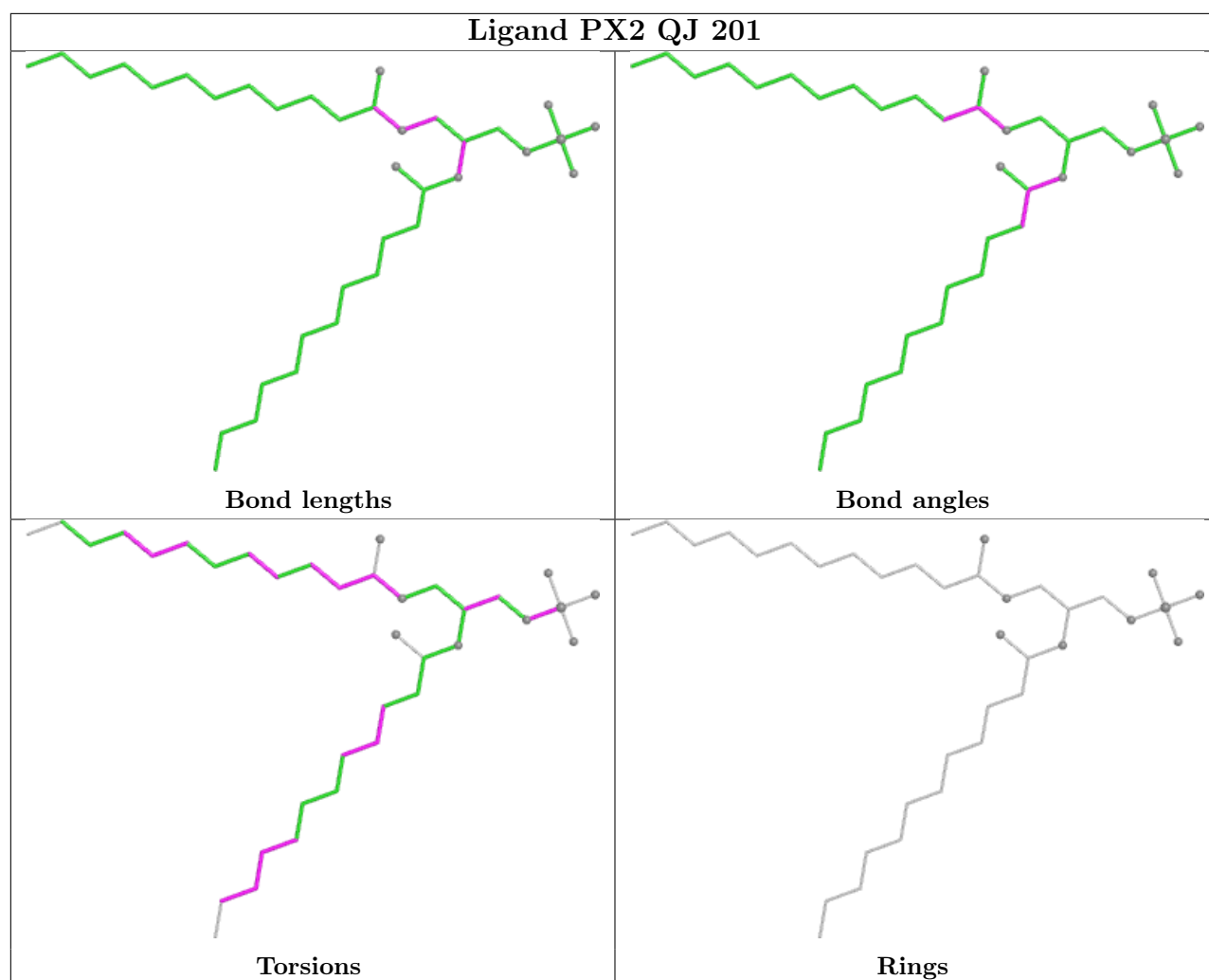


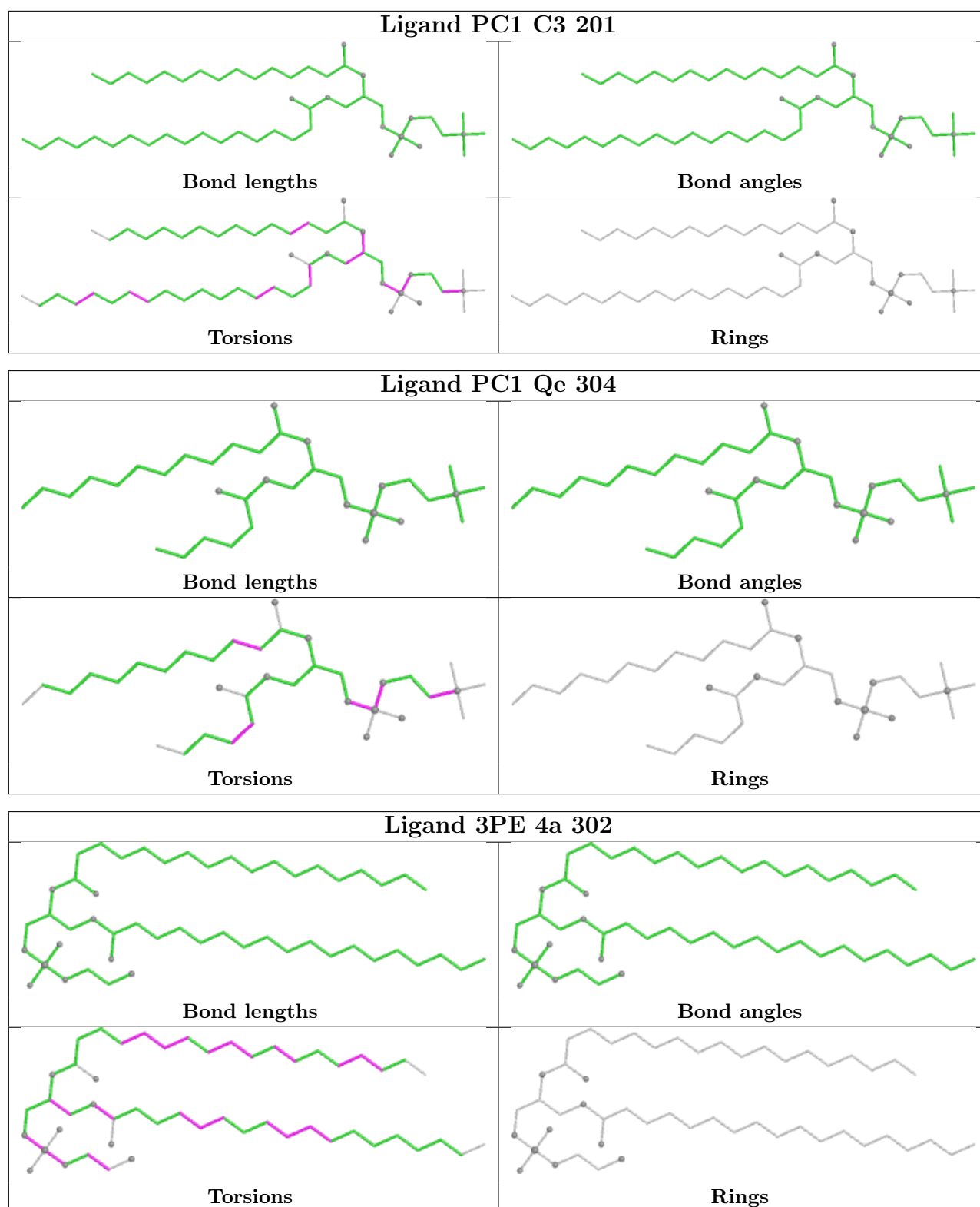


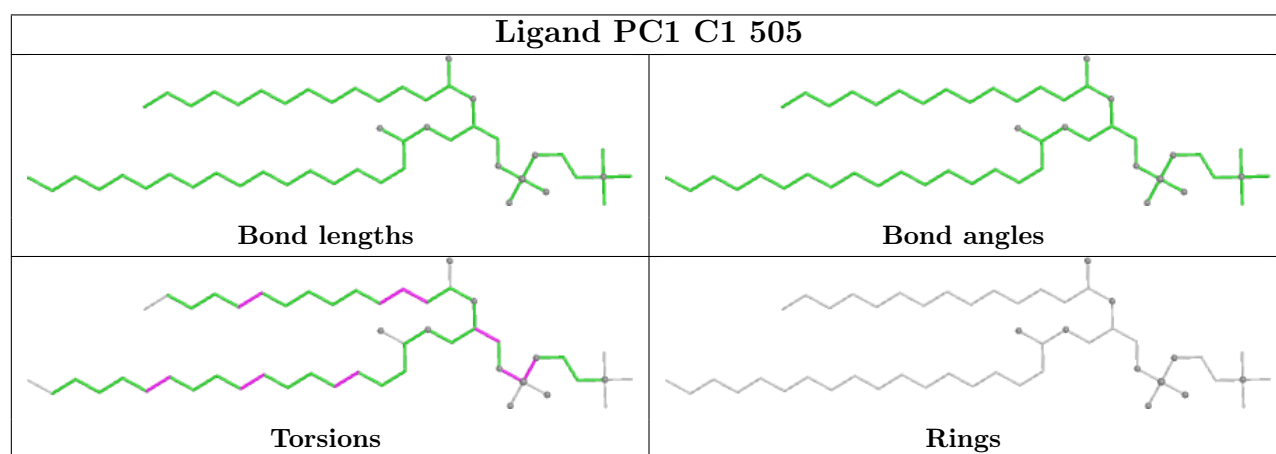
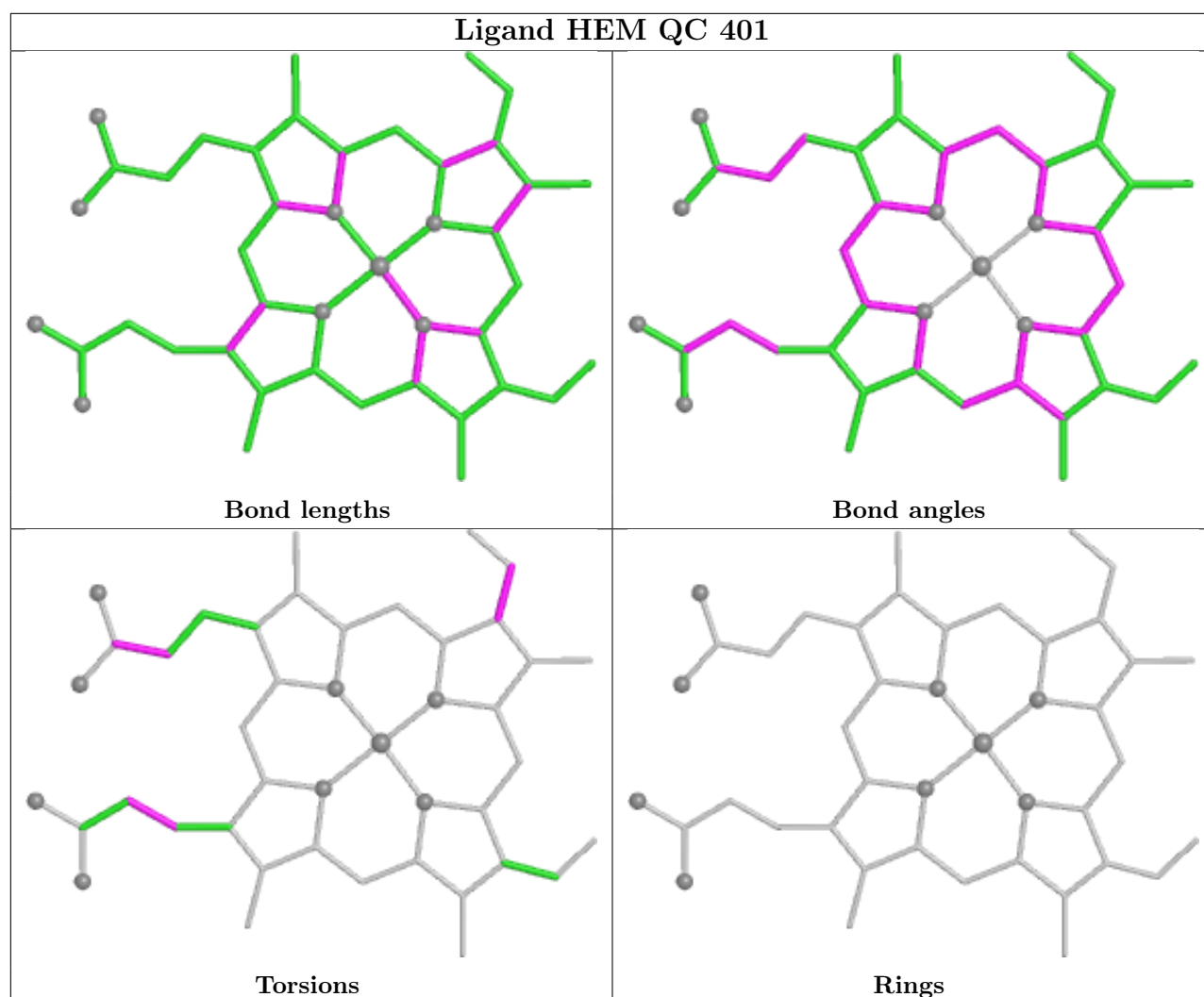


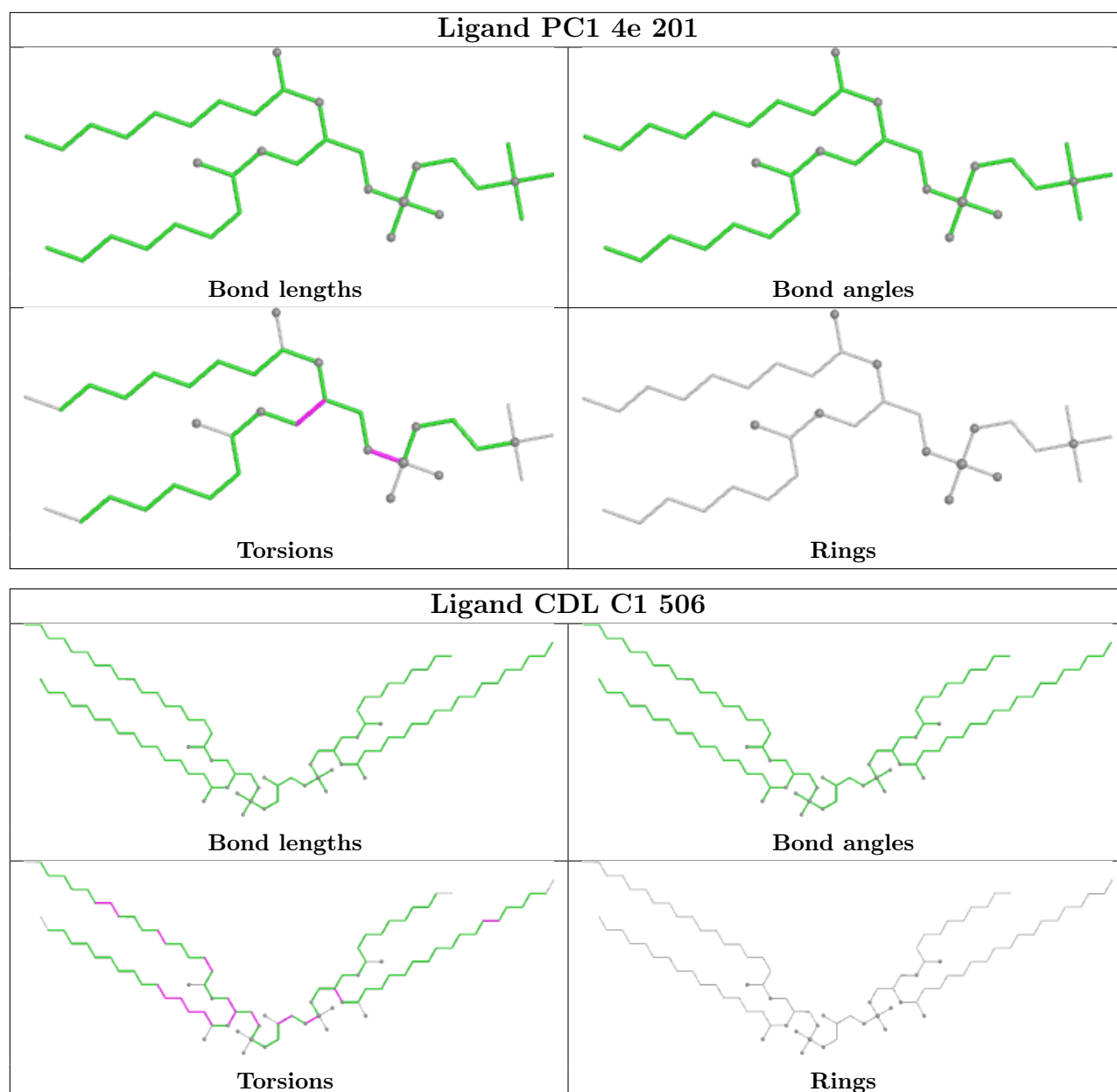


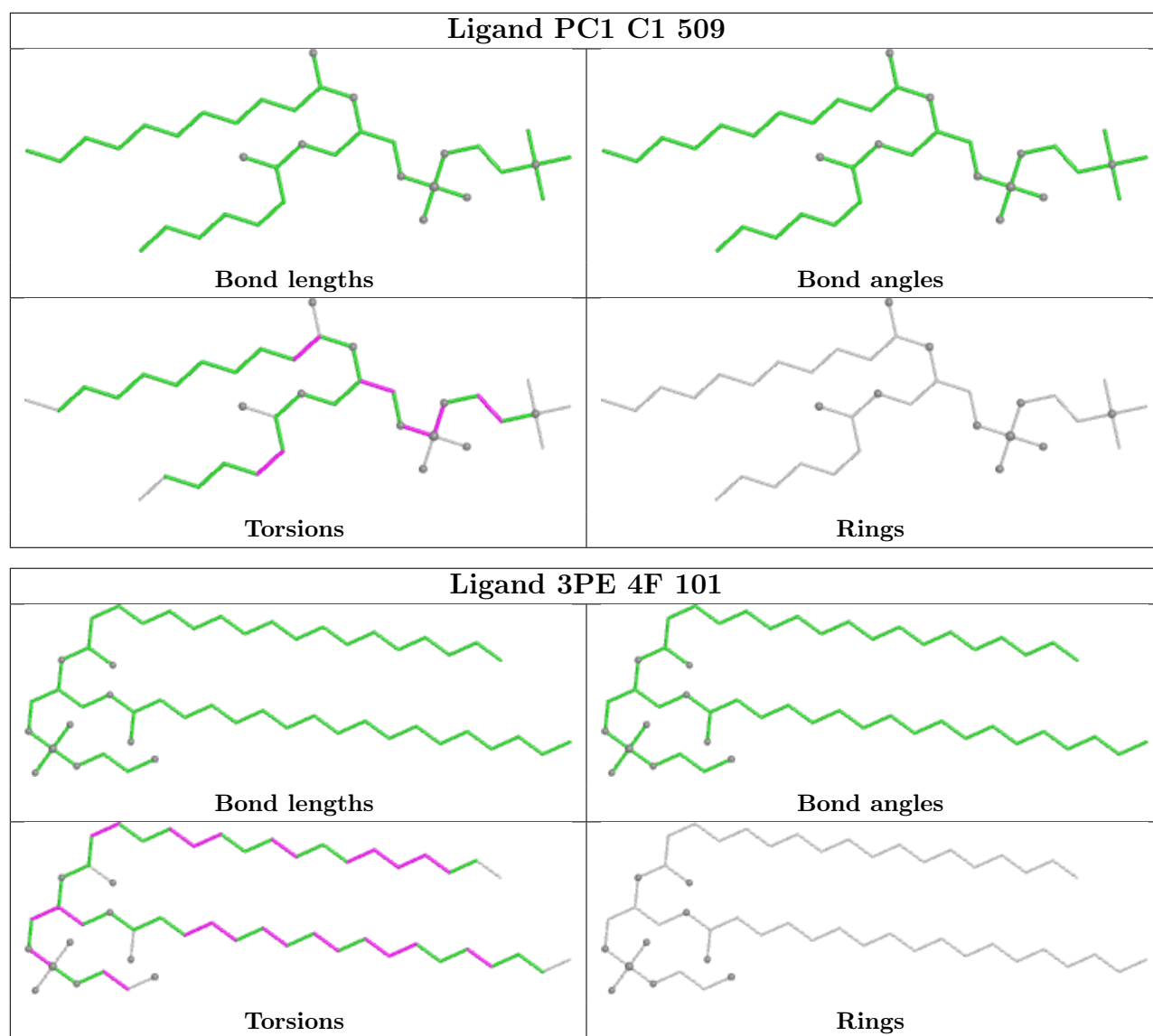




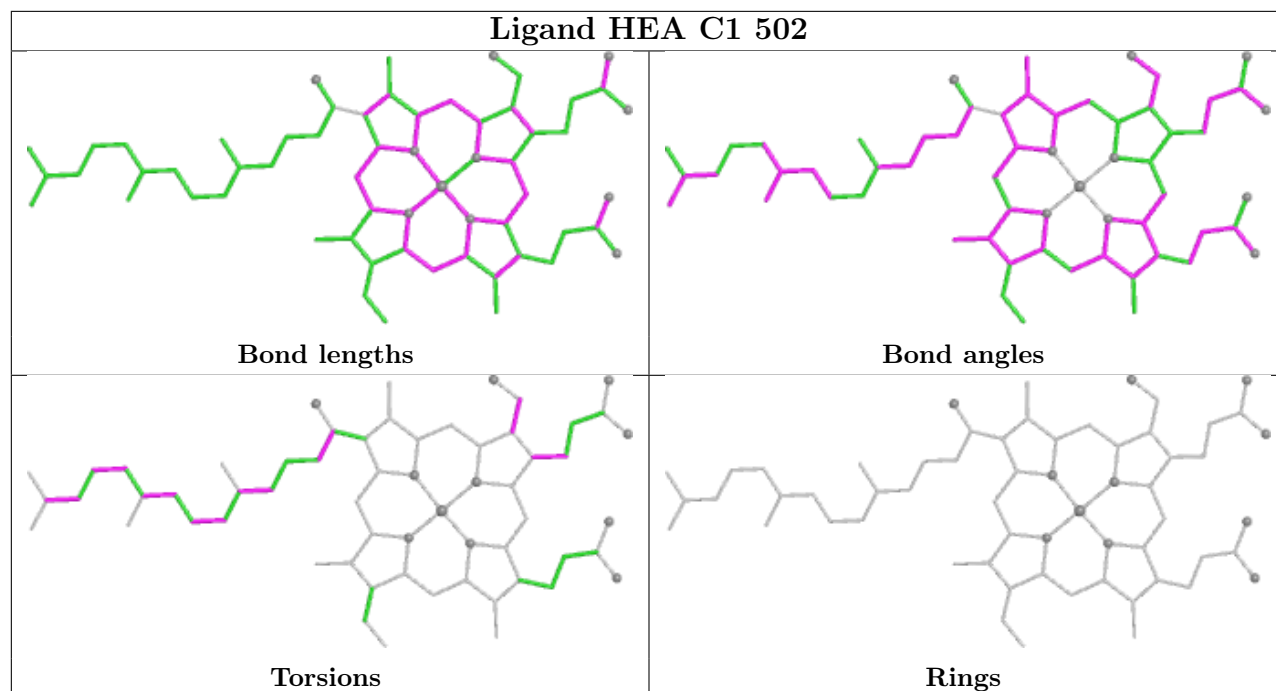




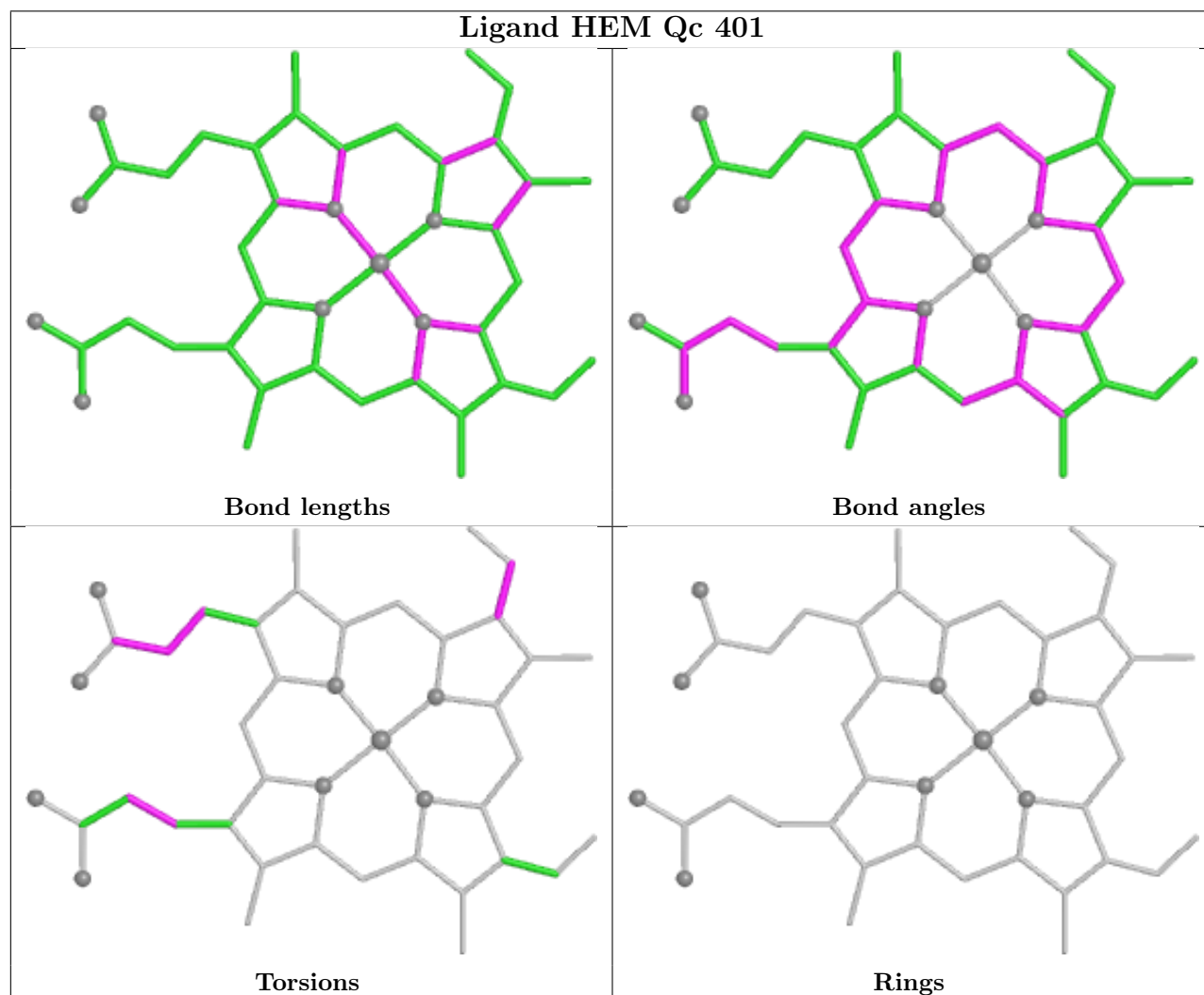


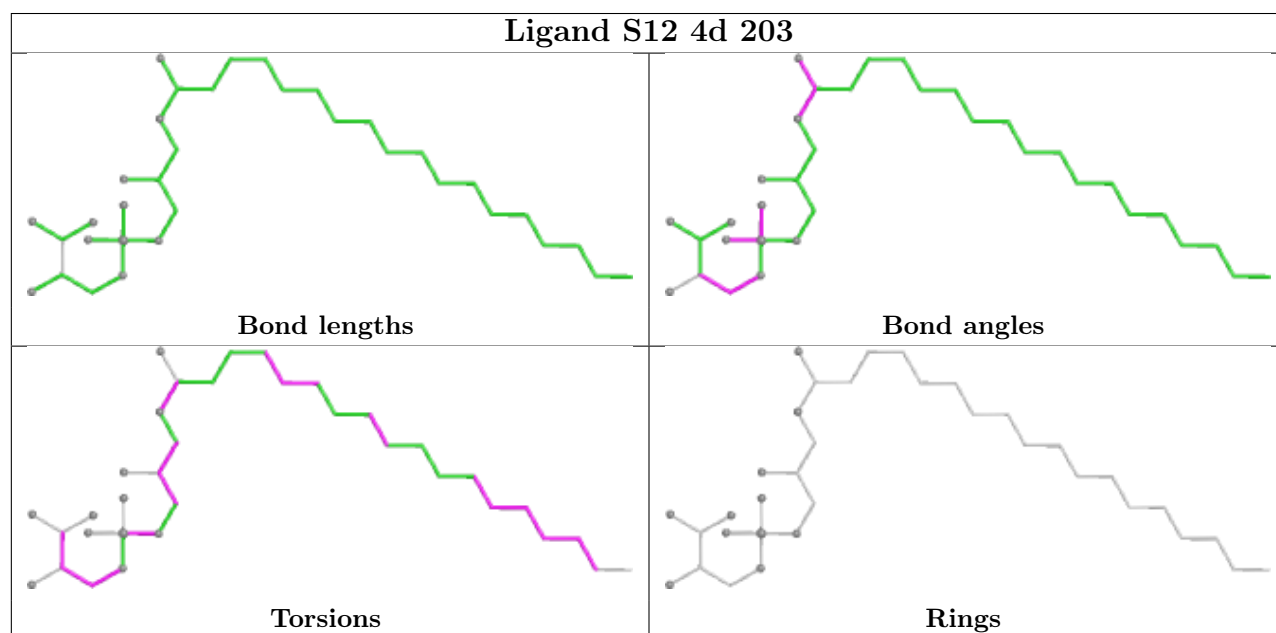
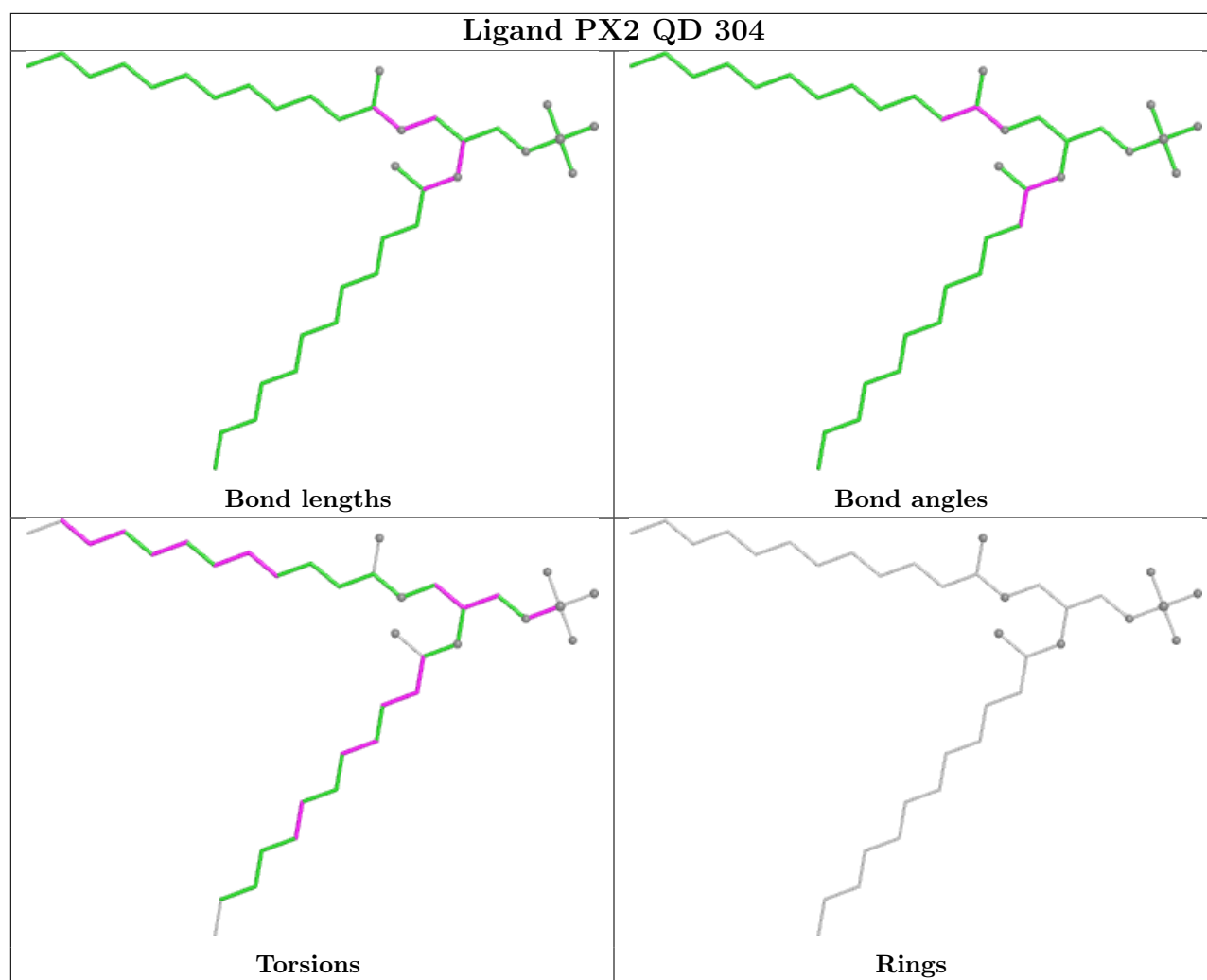


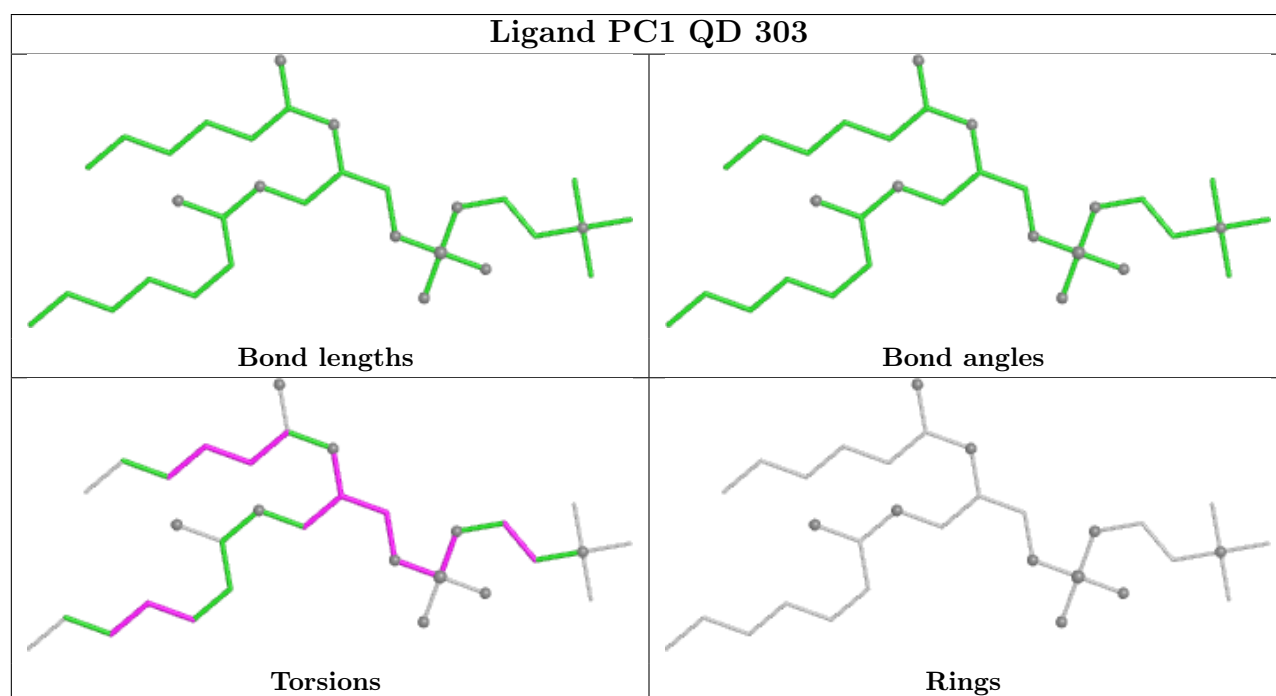
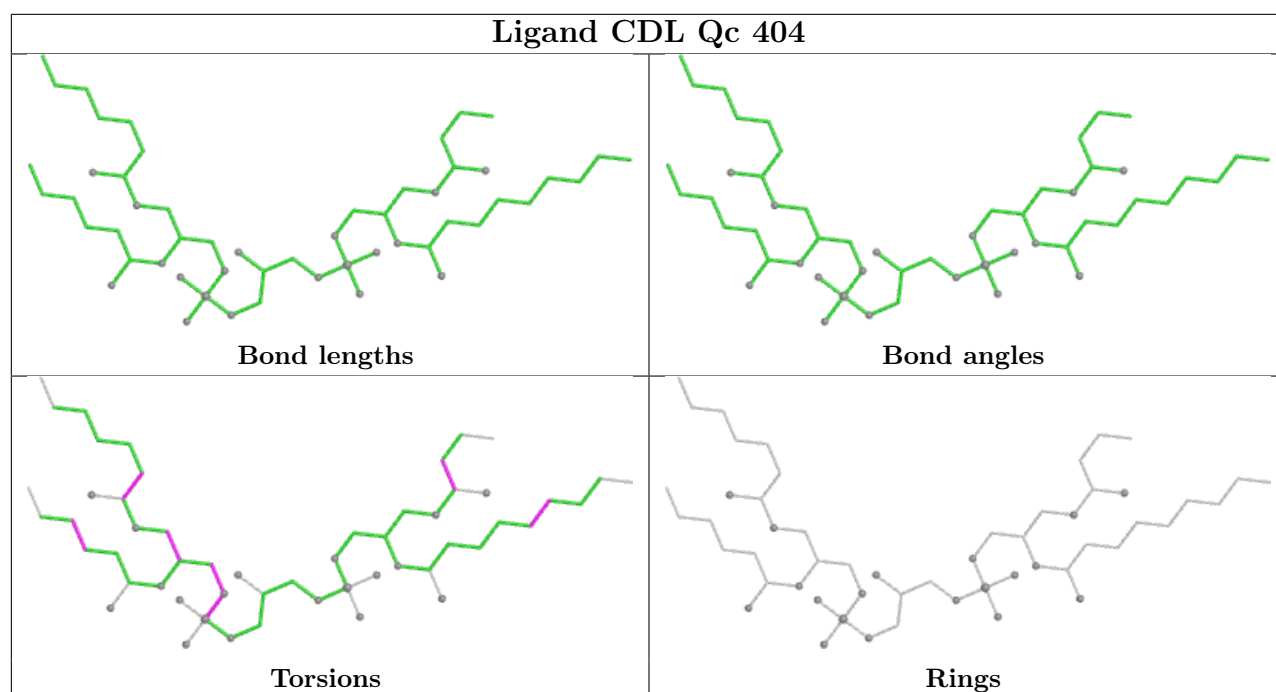
Ligand HEA C1 502

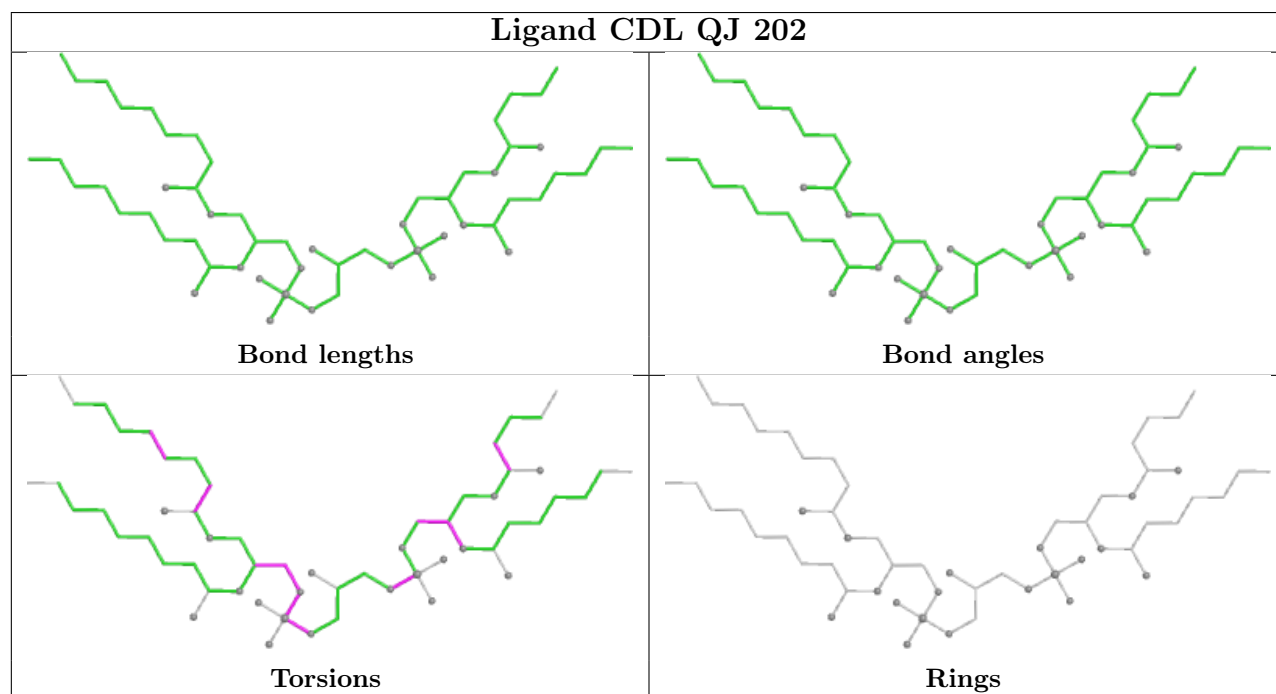
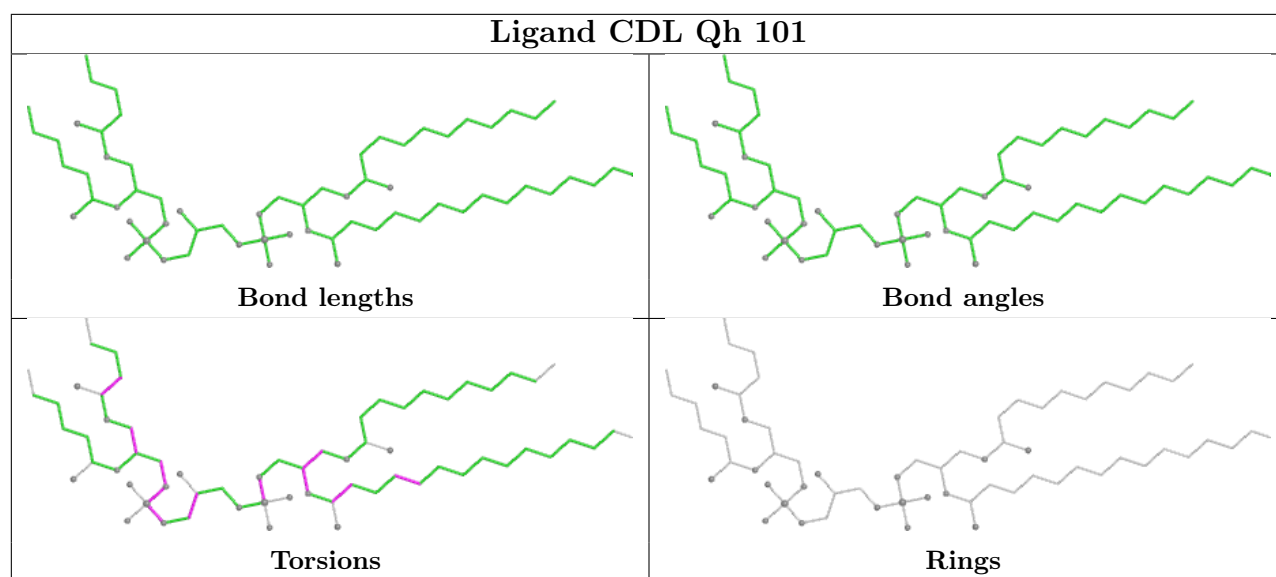


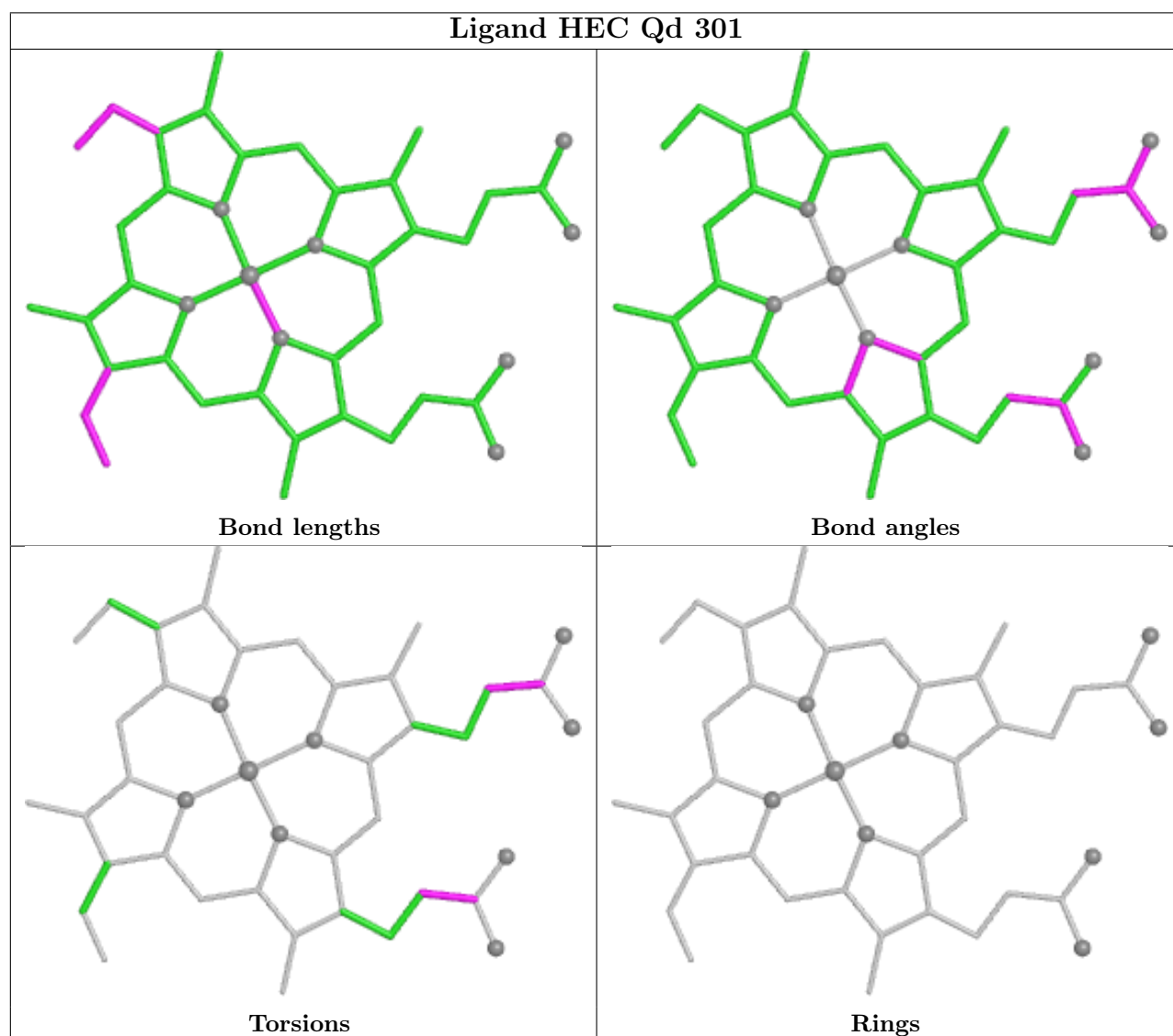
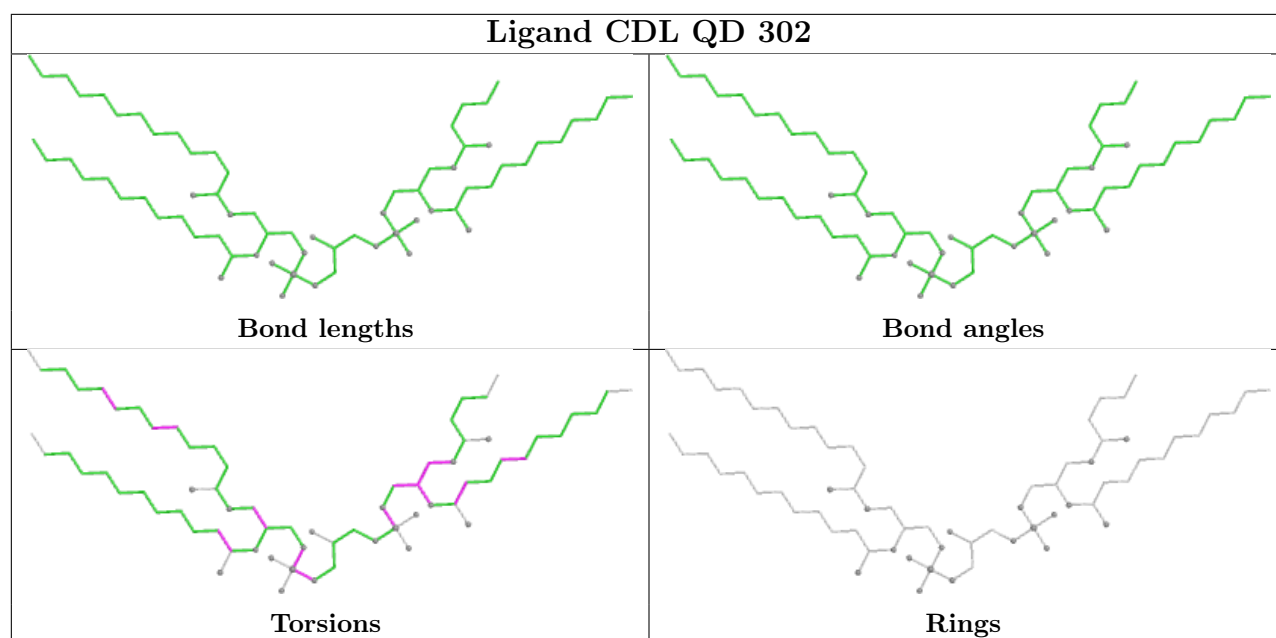
Ligand HEM Qc 401

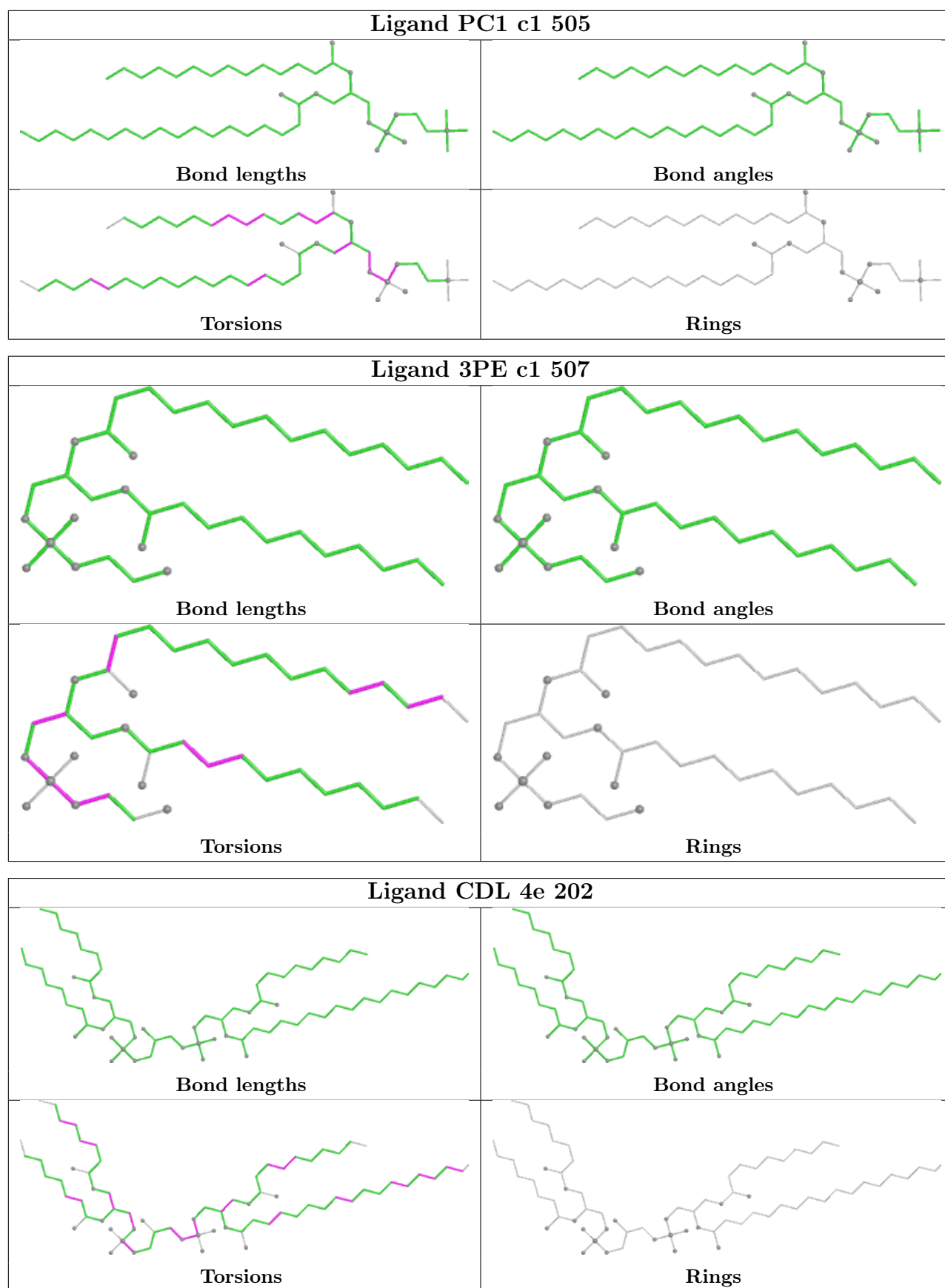


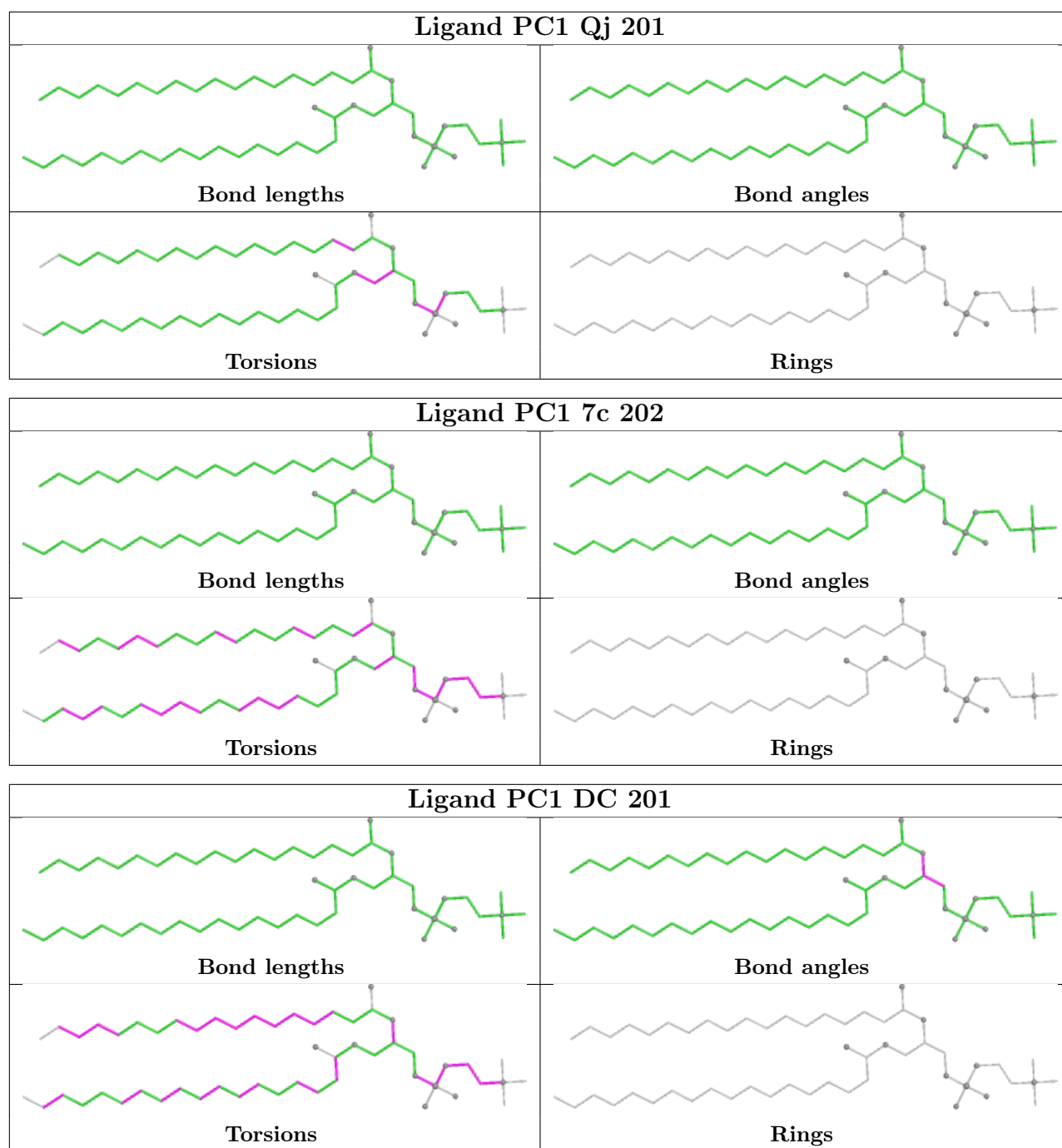


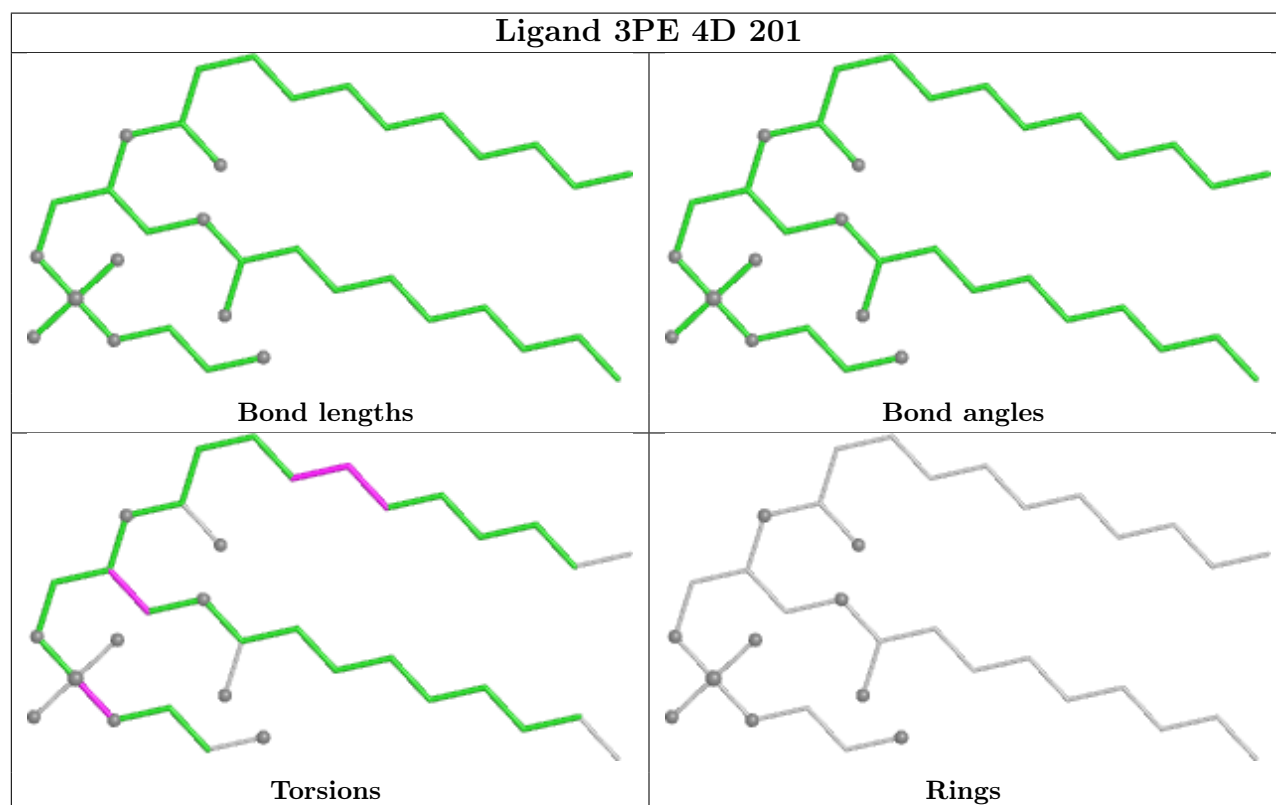
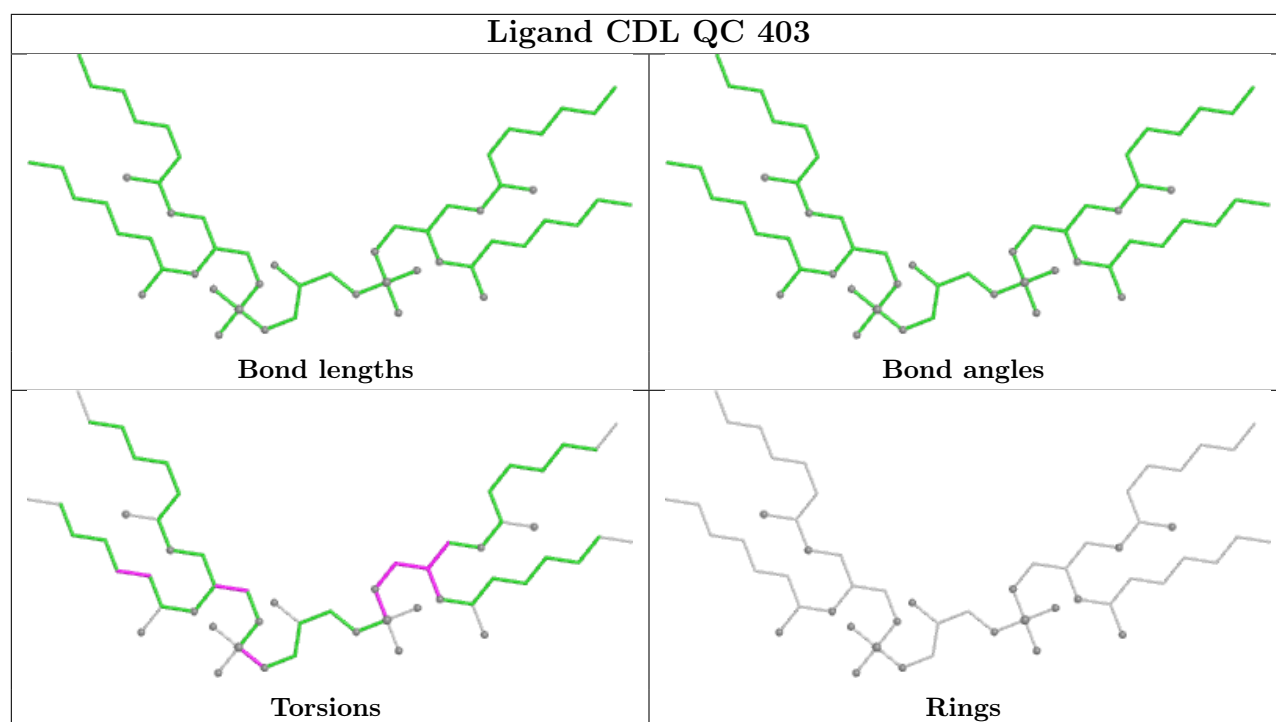












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

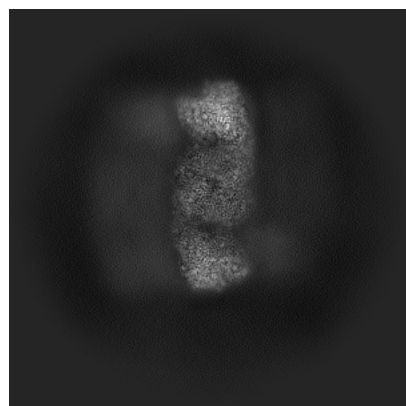
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35723. These allow visual inspection of the internal detail of the map and identification of artifacts.

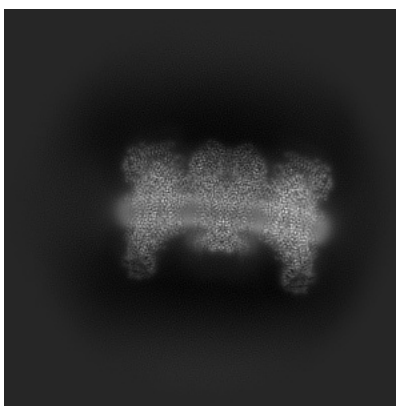
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

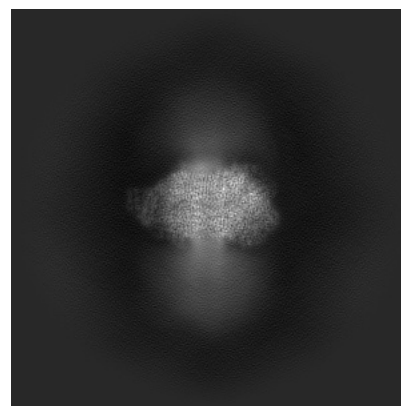
6.1.1 Primary map



X

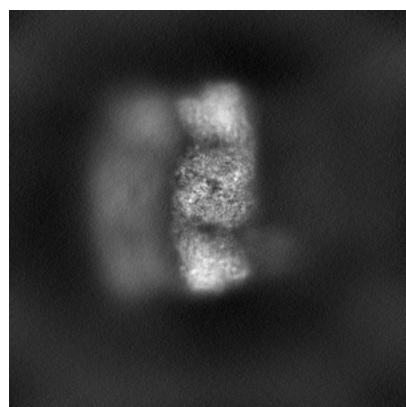


Y

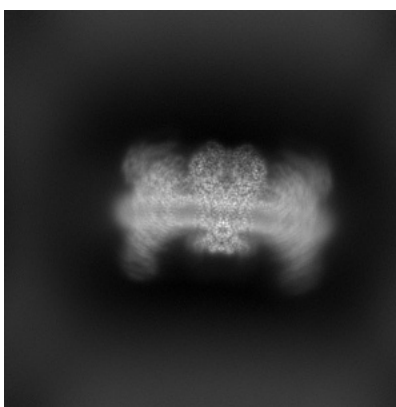


Z

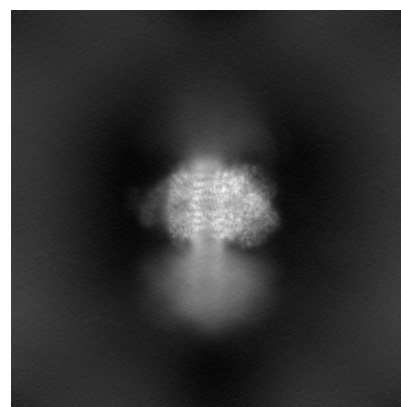
6.1.2 Raw map



X



Y

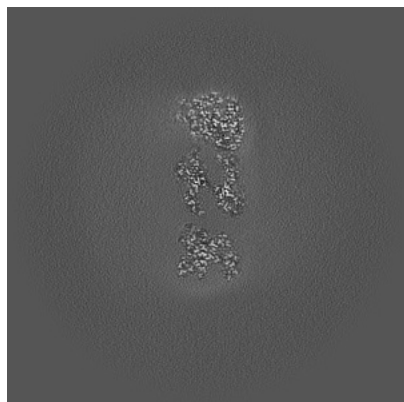


Z

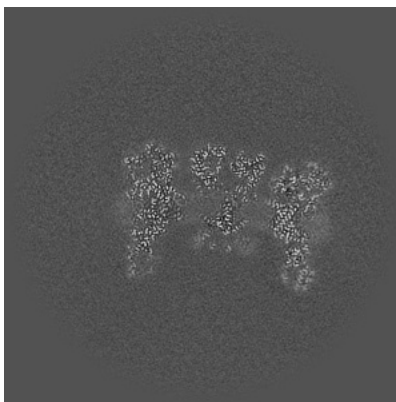
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

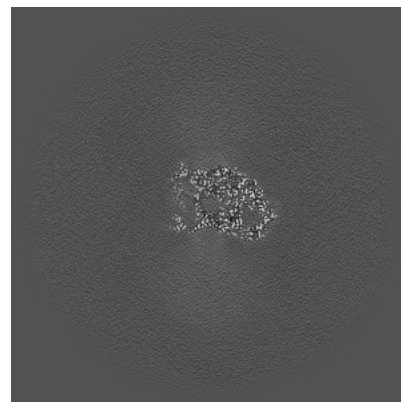
6.2.1 Primary map



X Index: 224

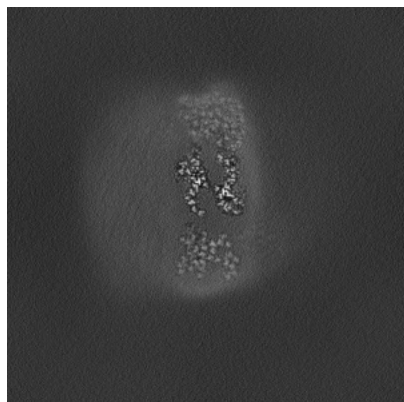


Y Index: 224

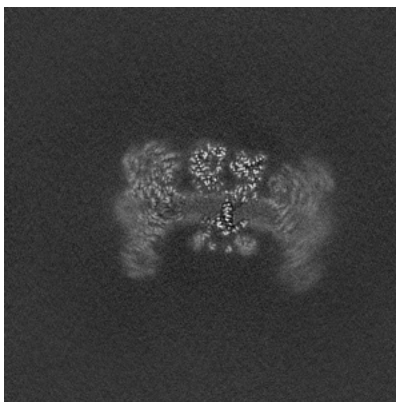


Z Index: 224

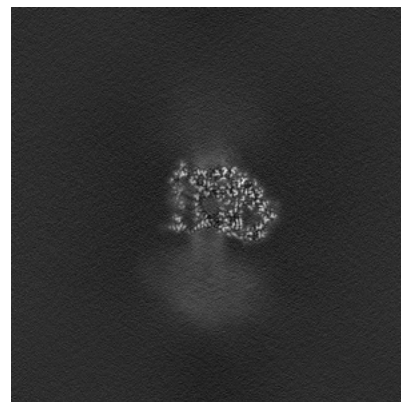
6.2.2 Raw map



X Index: 224



Y Index: 224

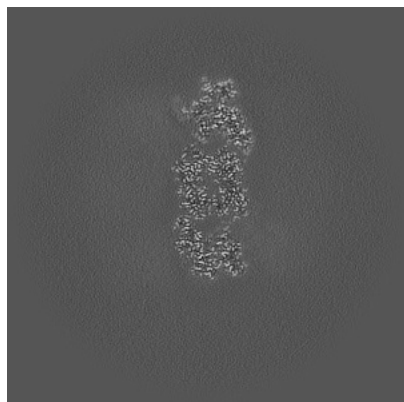


Z Index: 224

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

6.3 Largest variance slices [i](#)

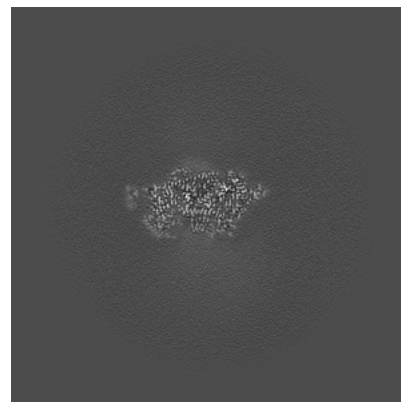
6.3.1 Primary map



X Index: 248

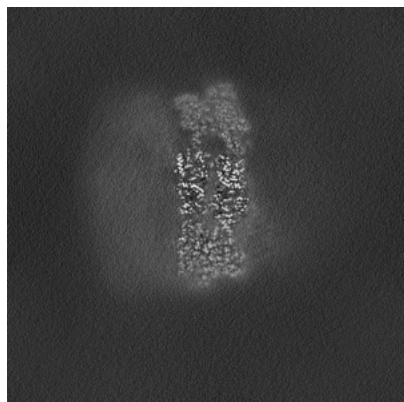


Y Index: 240

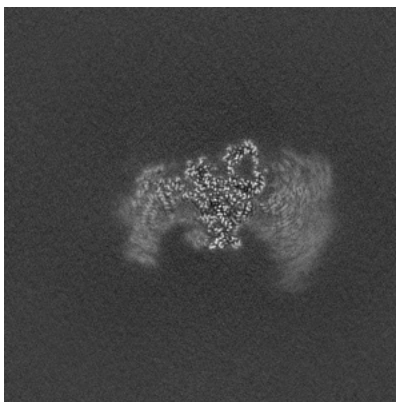


Z Index: 326

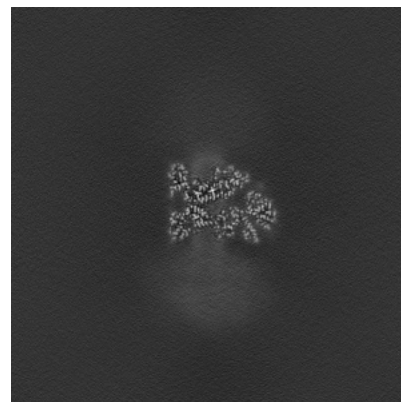
6.3.2 Raw map



X Index: 237



Y Index: 245

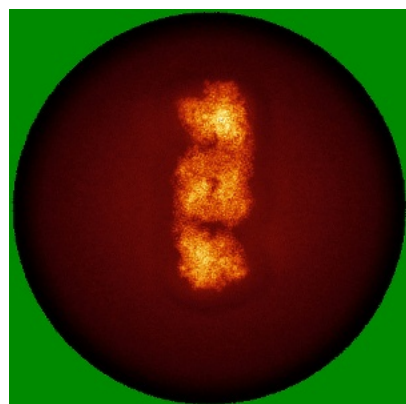


Z Index: 242

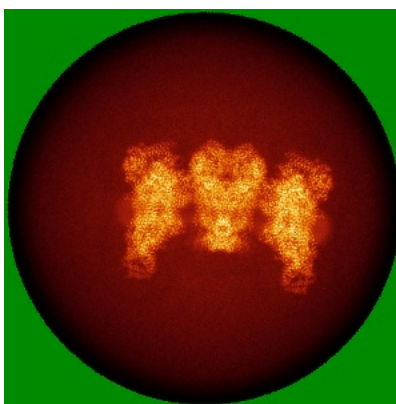
The images above show the largest variance slices of the map in three orthogonal directions.

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

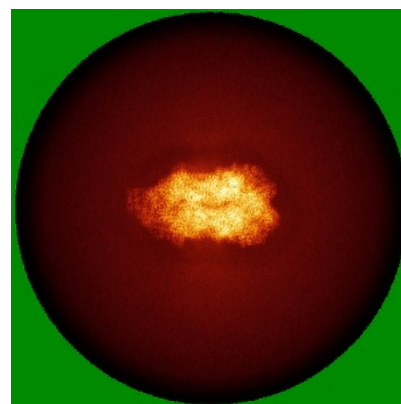
6.4.1 Primary map



X

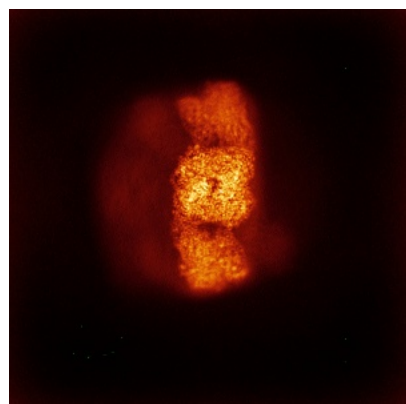


Y

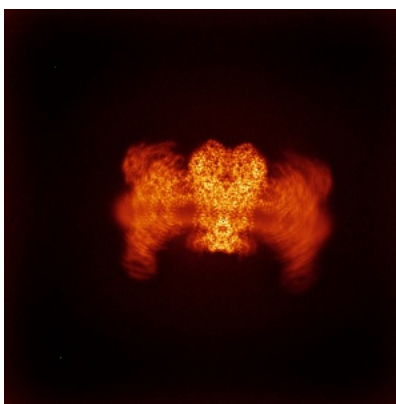


Z

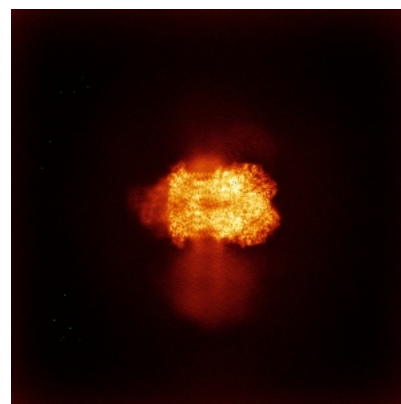
6.4.2 Raw map



X



Y

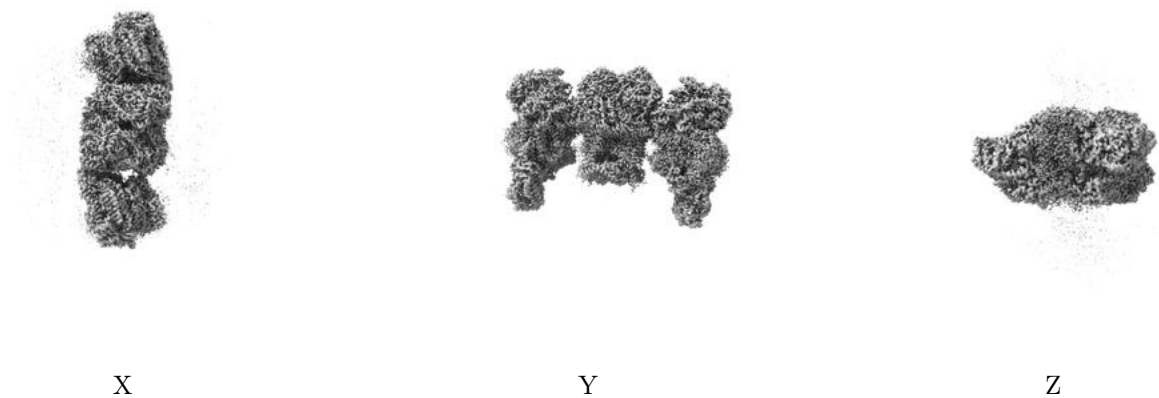


Z

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.

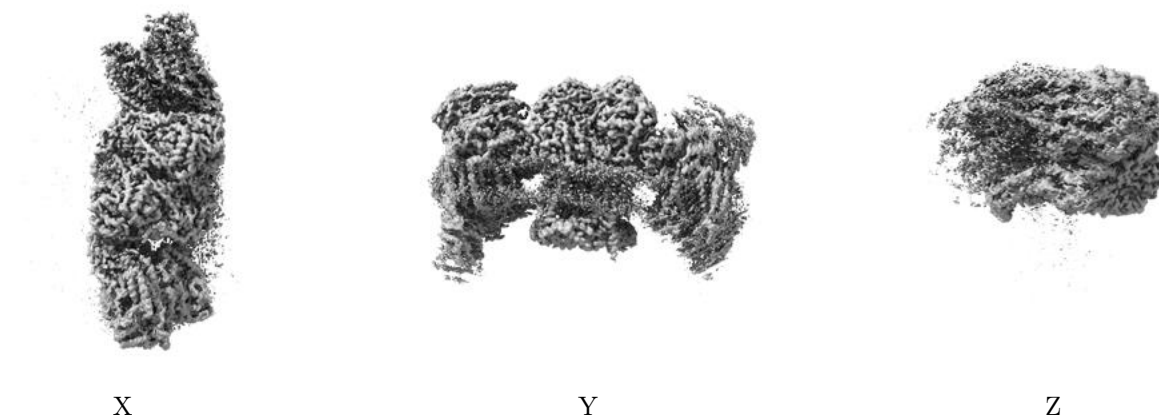
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

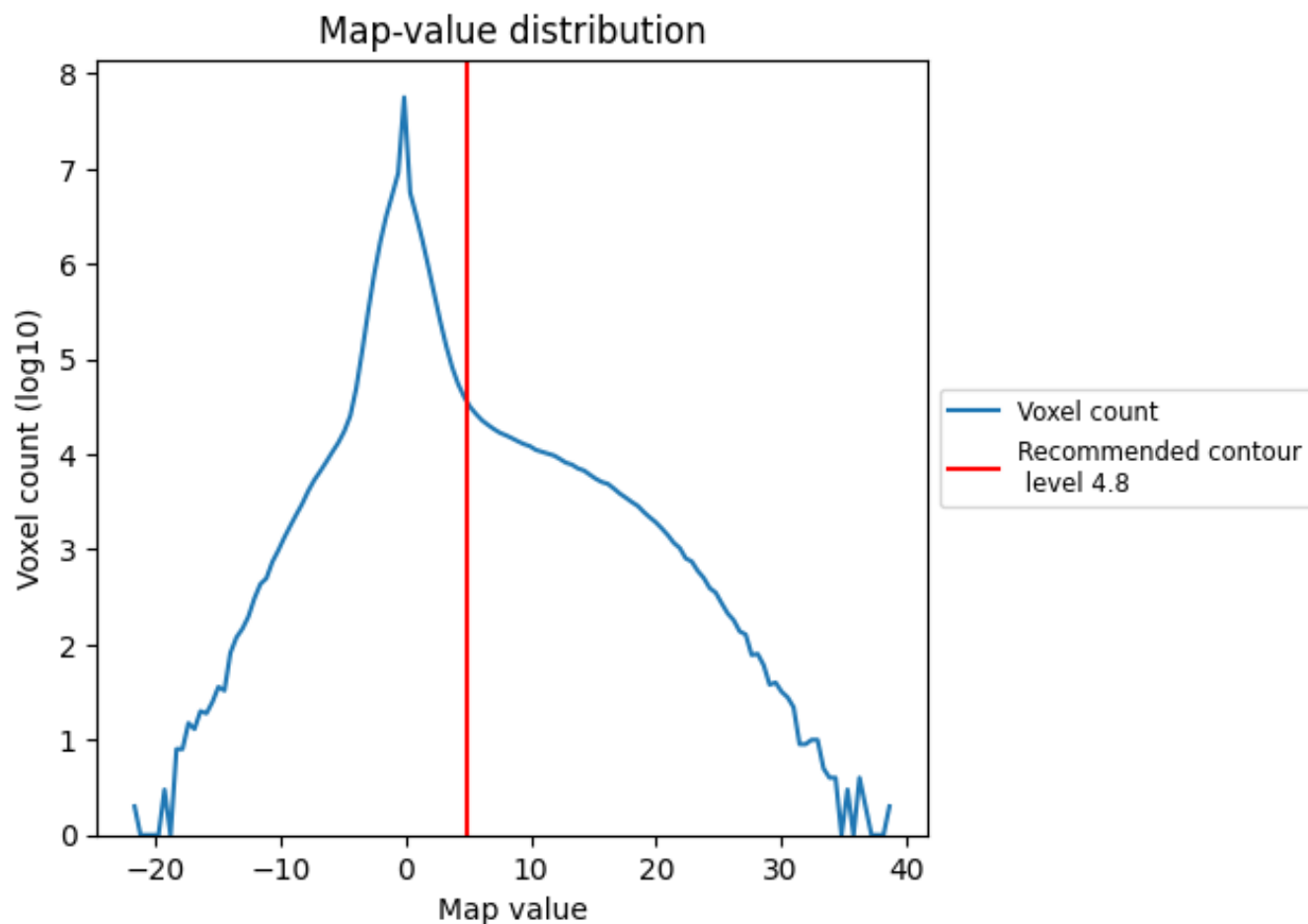
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

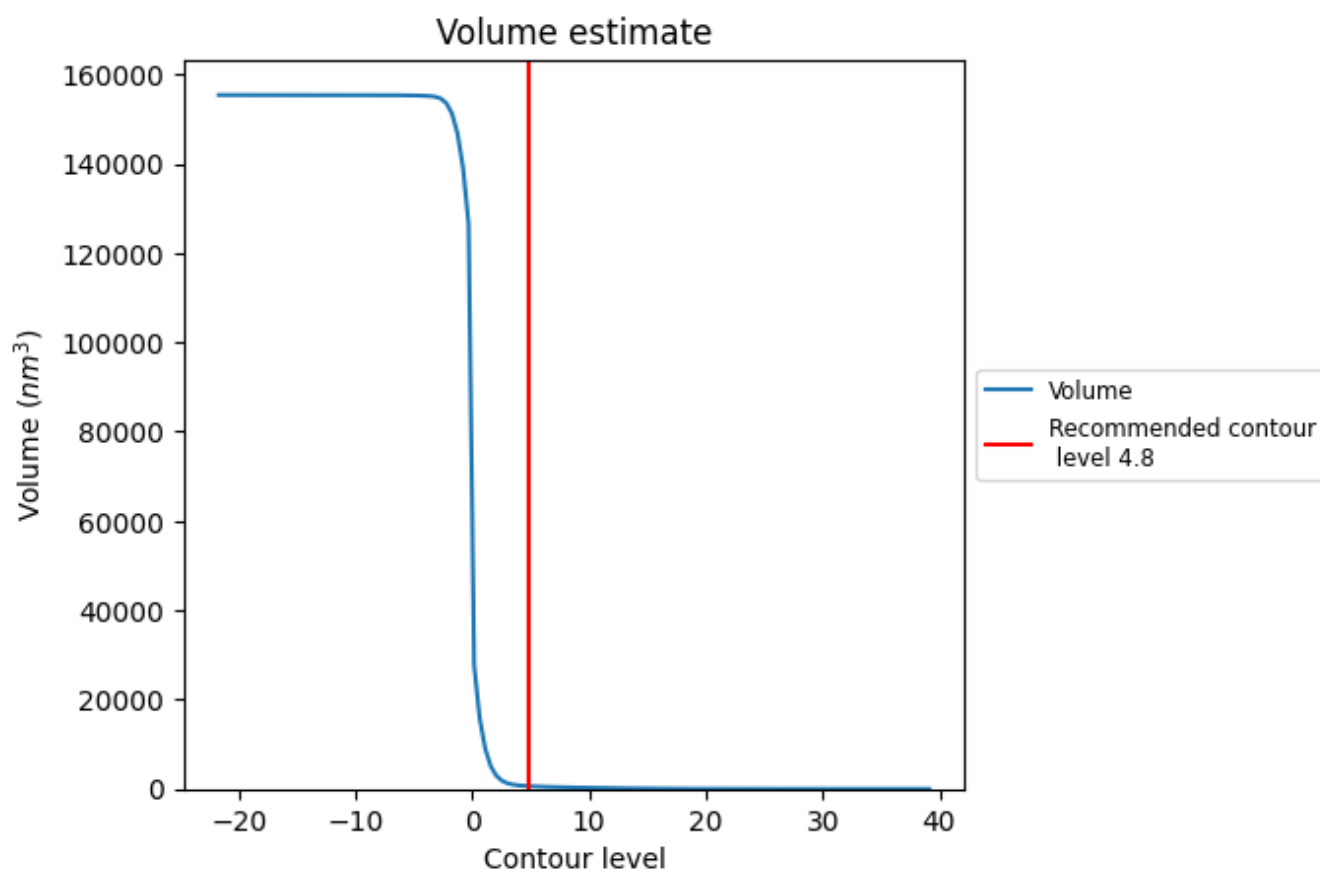
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

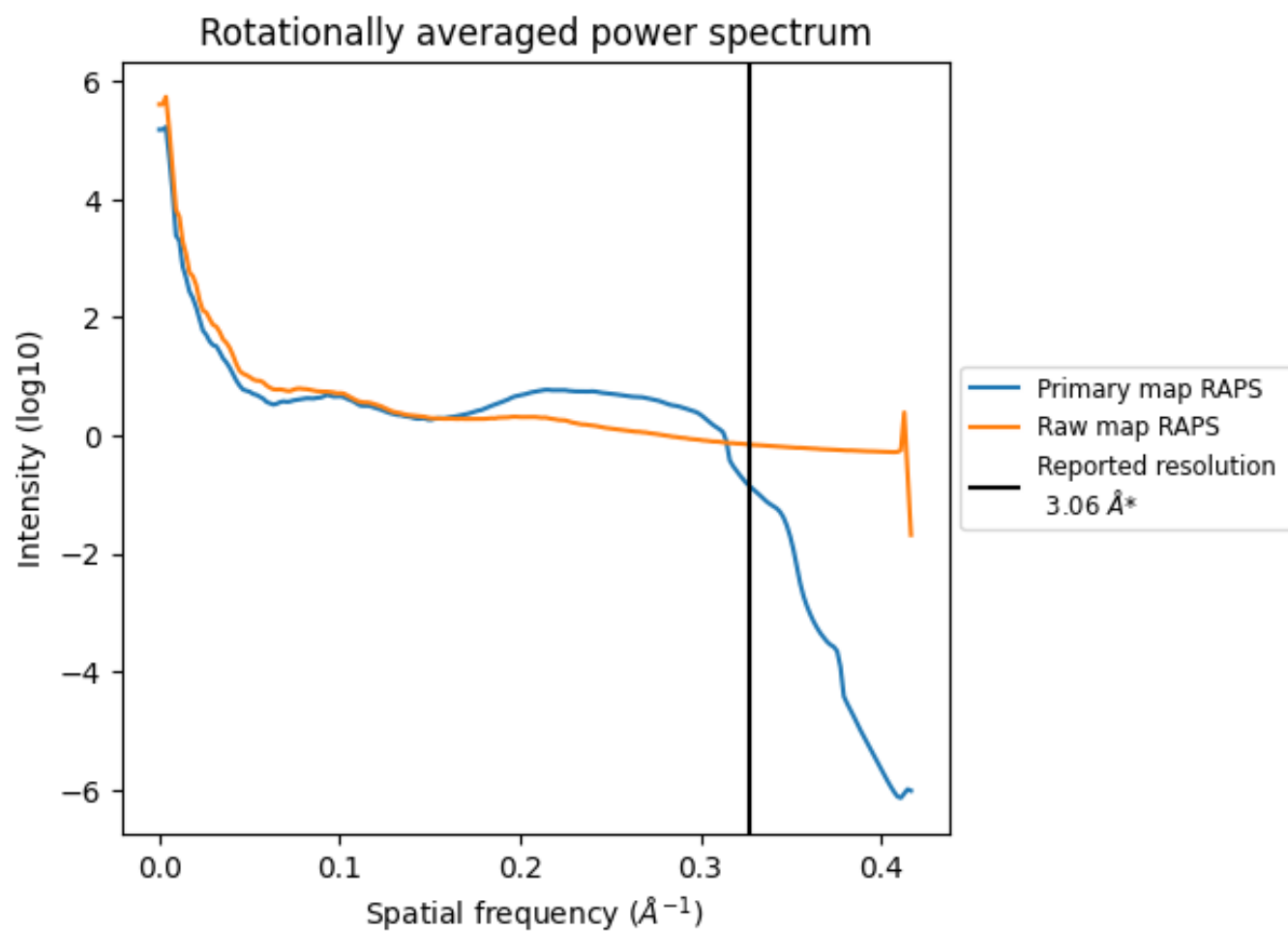
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm^3 ; this corresponds to an approximate mass of 577 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 ⓘ

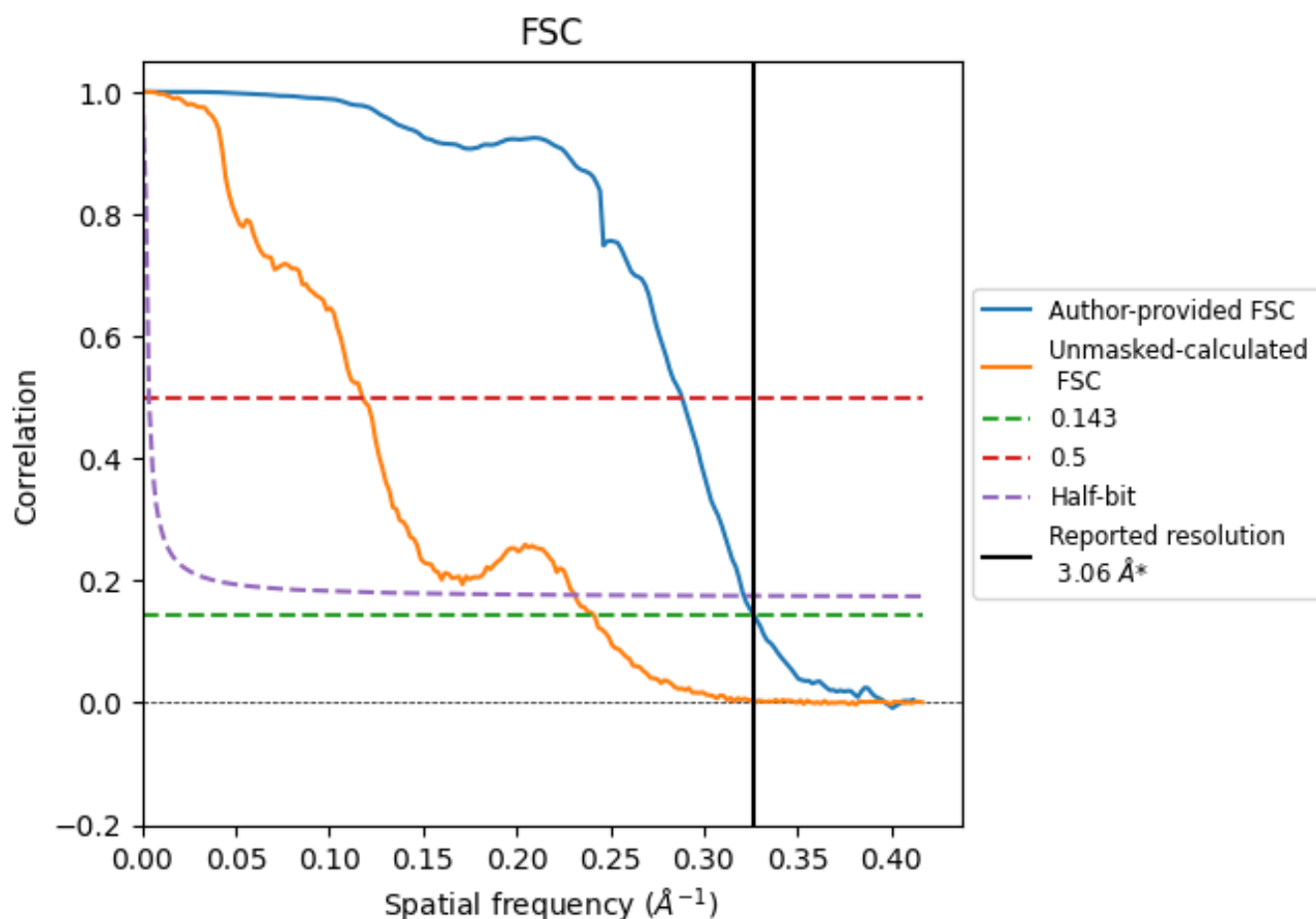


*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.327 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

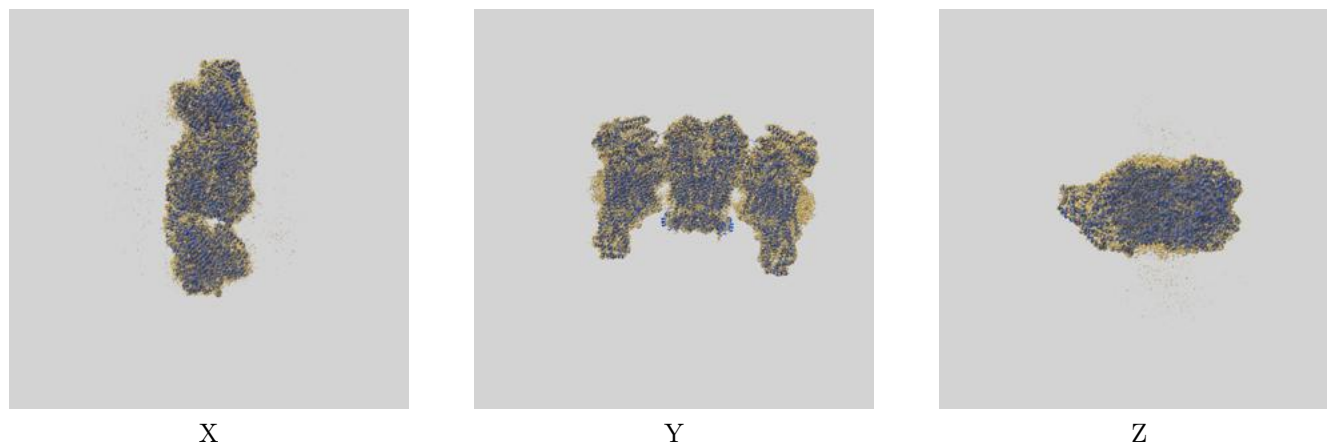
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.47	3.11
Unmasked-calculated*	4.14	8.49	4.33

*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 4.14 differs from the reported value 3.06 by more than 10 %

9 Map-model fit [i](#)

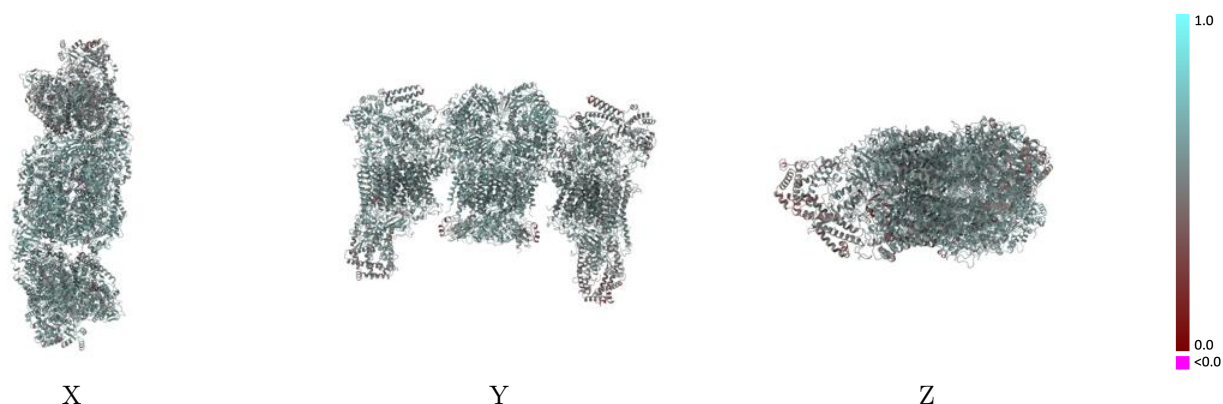
This section contains information regarding the fit between EMDB map EMD-35723 and PDB model 8IUJ. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



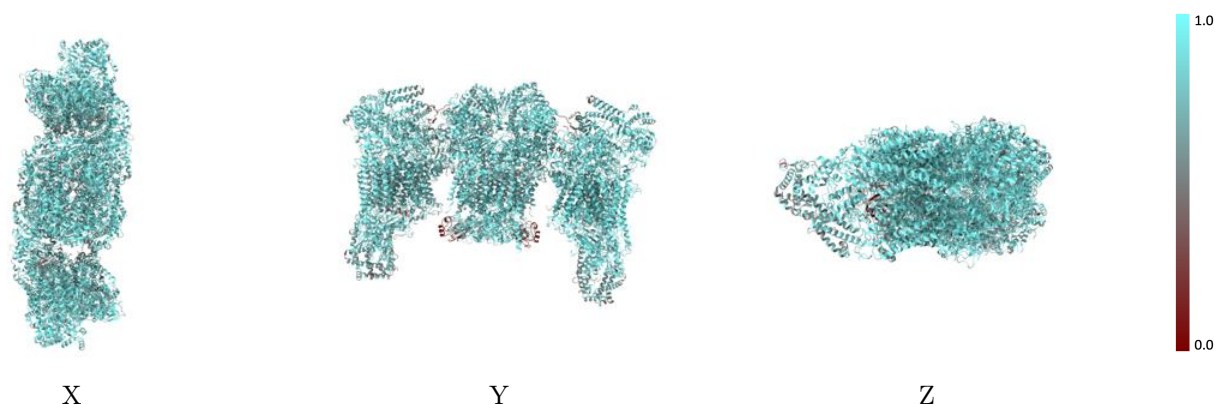
The images above show the 3D surface view of the map at the recommended contour level 4.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



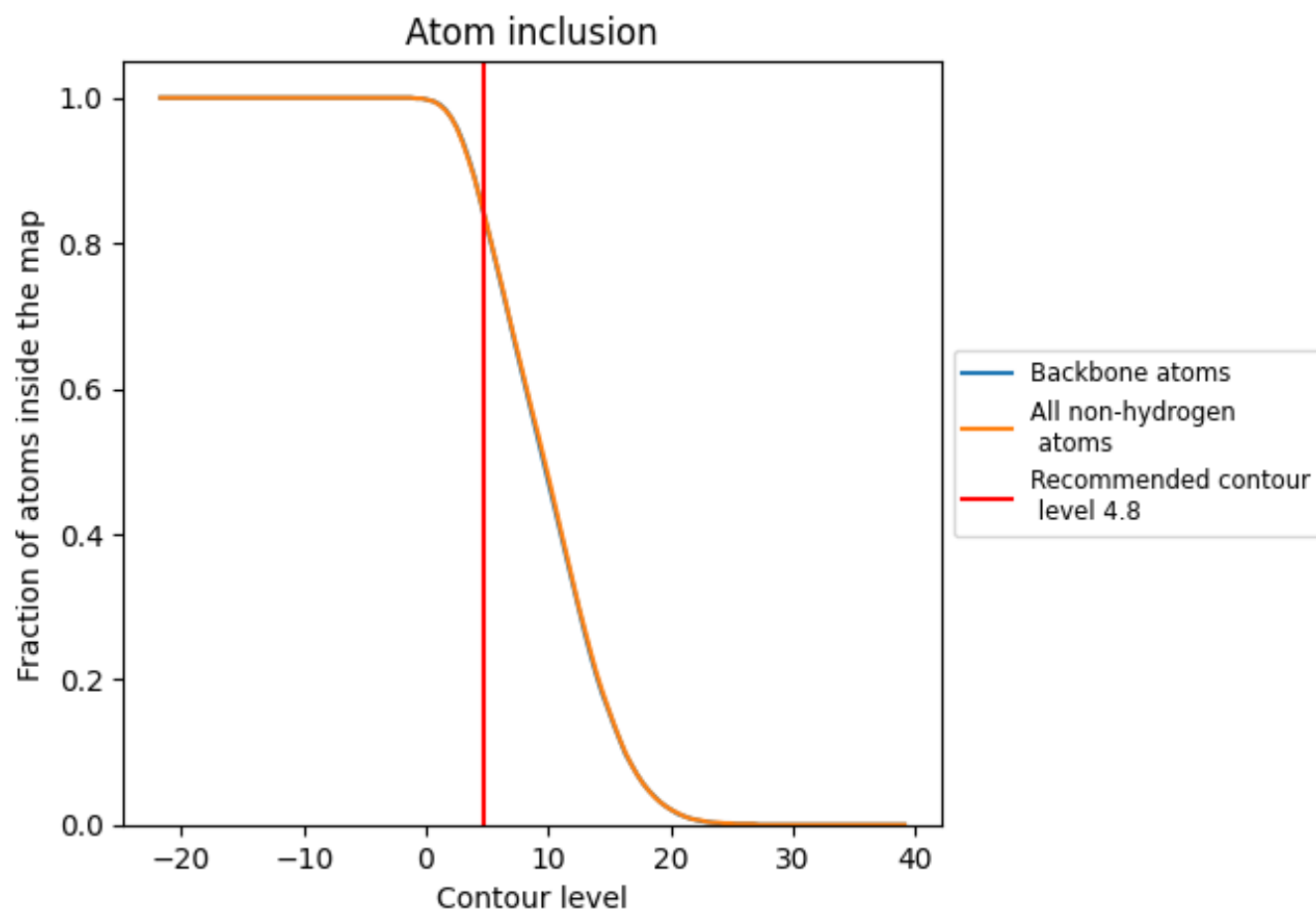
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.5610
4A	 0.7670	 0.5460
4C	 0.8170	 0.5460
4D	 0.8530	 0.5730
4E	 0.7640	 0.5250
4F	 0.8490	 0.5620
4G	 0.8070	 0.5490
4H	 0.8430	 0.5600
4I	 0.8950	 0.5910
4J	 0.8580	 0.5850
4a	 0.7740	 0.5010
4c	 0.8140	 0.4910
4d	 0.8570	 0.5230
4e	 0.7520	 0.4770
4f	 0.8630	 0.5130
4g	 0.8230	 0.5000
4h	 0.8320	 0.5110
4i	 0.9140	 0.5550
4j	 0.8530	 0.5390
5B	 0.9050	 0.5900
5C	 0.8750	 0.5800
5b	 0.9110	 0.5490
5c	 0.8900	 0.5410
6A	 0.7400	 0.5430
6B	 0.8050	 0.5460
6a	 0.8190	 0.4980
6b	 0.8040	 0.5050
7A	 0.8550	 0.5710
7C	 0.8630	 0.5810
7a	 0.8520	 0.5210
7c	 0.8730	 0.5500
C1	 0.8940	 0.5840
C2	 0.9060	 0.5890
C3	 0.8630	 0.5670
DC	 0.8480	 0.5830



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Chain	Atom inclusion	Q-score
QA	 0.8470	 0.5910
QB	 0.8490	 0.5930
QC	 0.8710	 0.5980
QD	 0.8720	 0.6000
QE	 0.5790	 0.5170
QF	 0.7130	 0.5470
QG	 0.8860	 0.6090
QH	 0.8410	 0.5910
QI	 0.8720	 0.5900
QJ	 0.7980	 0.5790
QK	 0.8320	 0.5860
Qa	 0.8590	 0.5900
Qb	 0.8300	 0.5760
Qc	 0.8740	 0.5930
Qd	 0.8690	 0.5900
Qe	 0.5830	 0.5140
Qf	 0.7320	 0.5380
Qg	 0.8890	 0.5990
Qh	 0.8180	 0.5870
Qi	 0.8790	 0.5770
Qj	 0.7820	 0.5710
Qk	 0.8440	 0.5880
c1	 0.9060	 0.5520
c2	 0.9140	 0.5570
c3	 0.8680	 0.5290
dc	 0.8820	 0.5440