



## wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 02:35 PM EST

PDB ID : 7JRP  
EMDB ID : EMD-22448  
Title : Plant Mitochondrial complex SC III2+IV from Vigna radiata  
Authors : Maldonado, M.; Letts, J.A.  
Deposited on : 2020-08-12  
Resolution : 3.80 Å(reported)  
Based on initial models : 6Q9E, 6HU9

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

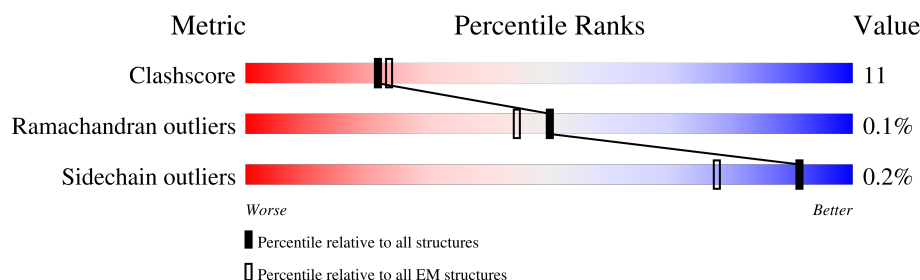
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.









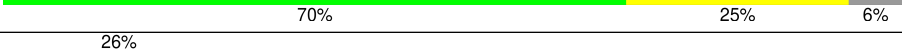
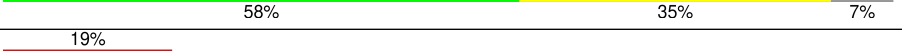
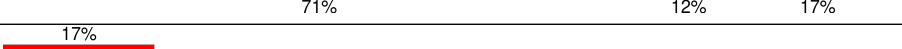
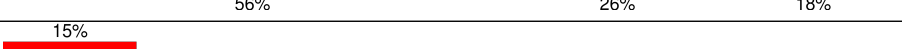


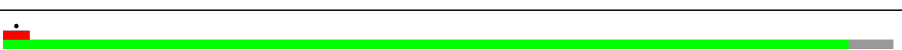

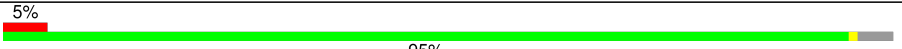




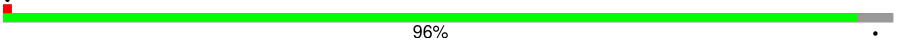


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	527	
1	M	527	
2	B	506	
2	N	506	
3	C	393	
3	O	393	
4	D	306	
4	P	306	

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Mol	Chain	Length	Quality of chain
5	E	271	
5	Q	271	
6	F	122	
6	R	122	
7	G	72	
7	S	72	
8	H	69	
8	T	69	
9	J	72	
9	V	72	
10	K	81	
10	W	81	
11	a	527	
12	b	251	
13	c	265	
14	d	79	
15	e	150	
16	f	100	
17	g	181	
18	h	64	
19	i	67	
20	j	96	

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 45166 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		
1	M	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		

- Molecule 2 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	457	Total	C	N	O	S	0	0
			3471	2196	588	675	12		
2	N	455	Total	C	N	O	S	0	0
			3456	2187	585	672	12		

- Molecule 3 is a protein called COB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		
3	O	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		

- Molecule 4 is a protein called cytochrome c1-2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		
4	P	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	74	Total	C	N	O	S	0	0
			574	375	97	101	1		
5	Q	74	Total	C	N	O	S	0	0
			574	375	97	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	116	Total	C	N	O	S	0	0
			965	616	173	172	4		
6	R	115	Total	C	N	O	S	0	0
			959	613	172	170	4		

- Molecule 7 is a protein called cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			578	382	97	98	1		
7	S	70	Total	C	N	O	S	0	0
			578	382	97	98	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			536	344	90	96	6		
8	T	64	Total	C	N	O	S	0	0
			527	339	89	93	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			480	313	83	83	1		
9	V	59	Total	C	N	O	S	0	0
			476	311	82	82	1		

- Molecule 10 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	31	Total	C	N	O	S	0	0
			218	144	35	38	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	32	Total	C	N	O	S	0	0
			226	150	36	39	1		

- Molecule 11 is a protein called COX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	524	Total	C	N	O	S	0	0
			4074	2726	640	684	24		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	239	Total	C	N	O	S	0	0
			1915	1249	308	348	10		

- Molecule 13 is a protein called COX3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	265	Total	C	N	O	S	0	0
			2134	1445	335	347	7		

- Molecule 14 is a protein called COX4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	76	Total	C	N	O	S	0	0
			595	387	97	109	2		

- Molecule 15 is a protein called cytochrome c oxidase subunit 5b-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	94	Total	C	N	O	S	0	0
			733	464	124	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	59	Total	C	N	O	S	0	0
			480	315	76	88	1		

- Molecule 17 is a protein called cytochrome c oxidase subunit 6b-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	74	Total	C	N	O	S	0	0
			612	385	110	113	4		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 5C.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	49	Total	C	N	O	S	0	0
			391	255	67	68	1		

- Molecule 19 is a protein called COX7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	64	Total	C	N	O	S	0	0
			510	331	91	87	1		

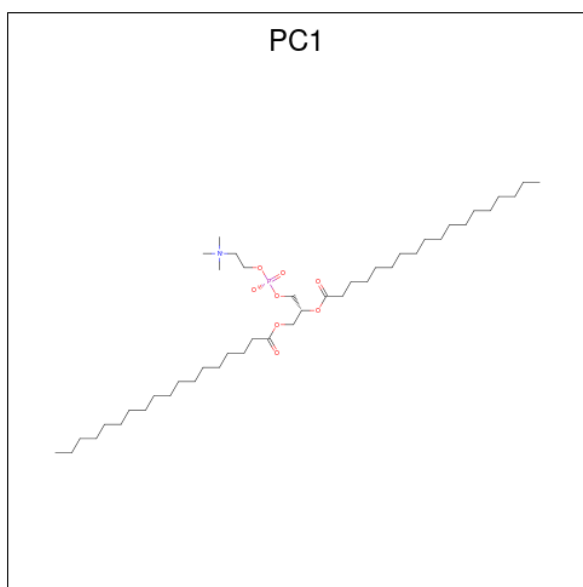
- Molecule 20 is a protein called COX7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	47	Total	C	N	O	S	0	0
			384	254	67	60	3		

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

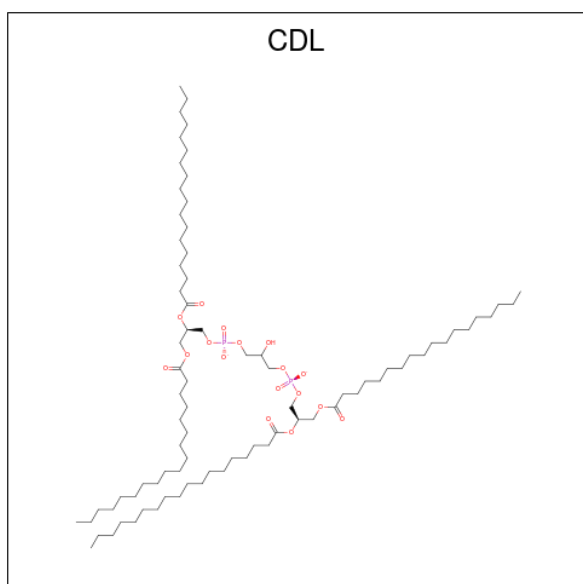
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Zn	0
			1	1	
21	M	1	Total	Zn	0
			1	1	
21	e	1	Total	Zn	0
			1	1	

- Molecule 22 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
22	M	1	Total	C	N	O	P	0
			27	17	1	8	1	
22	S	1	Total	C	N	O	P	0
			28	18	1	8	1	
22	a	1	Total	C	N	O	P	0
			39	29	1	8	1	
22	i	1	Total	C	N	O	P	0
			36	26	1	8	1	

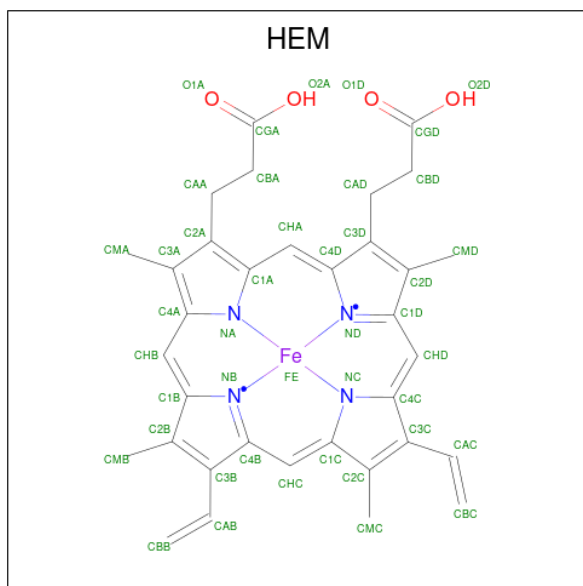
- Molecule 23 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).





Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			51	32	17	2	
23	C	1	Total	C	O	P	0
			54	35	17	2	
23	C	1	Total	C	O	P	0
			55	36	17	2	
23	D	1	Total	C	O	P	0
			41	22	17	2	
23	M	1	Total	C	O	P	0
			53	34	17	2	
23	O	1	Total	C	O	P	0
			54	35	17	2	
23	P	1	Total	C	O	P	0
			48	29	17	2	
23	S	1	Total	C	O	P	0
			50	31	17	2	
23	a	1	Total	C	O	P	0
			67	48	17	2	

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



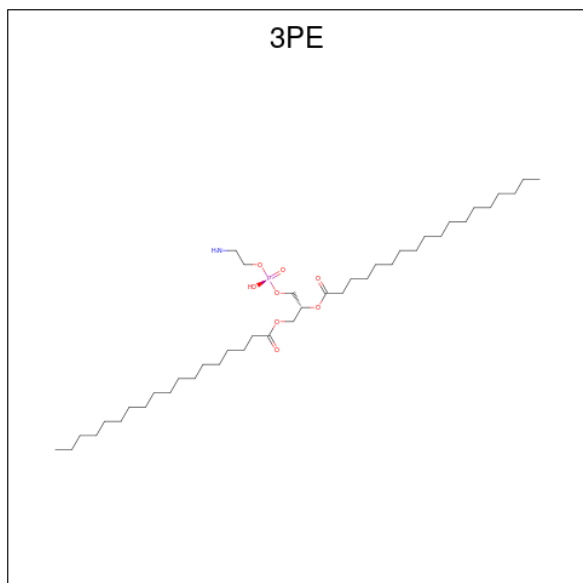
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	G	1	Total	C	N	O	P	0
			20	10	1	8	1	
25	O	1	Total	C	N	O	P	0
			24	14	1	8	1	
25	O	1	Total	C	N	O	P	0
			26	16	1	8	1	

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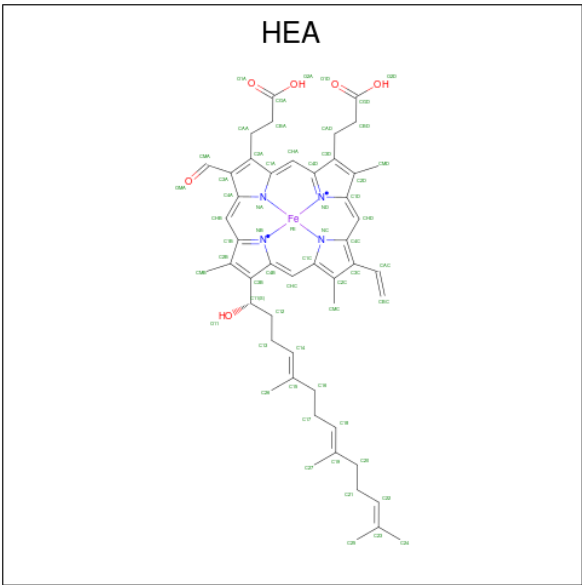
Mol	Chain	Residues	Atoms					AltConf
25	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
25	O	1	Total	C	N	O	P	0
			26	16	1	8	1	
25	P	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	a	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	a	1	Total	C	N	O	P	0
			39	29	1	8	1	
25	b	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	b	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	b	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	c	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	c	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	d	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	i	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 26 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 27 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).



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

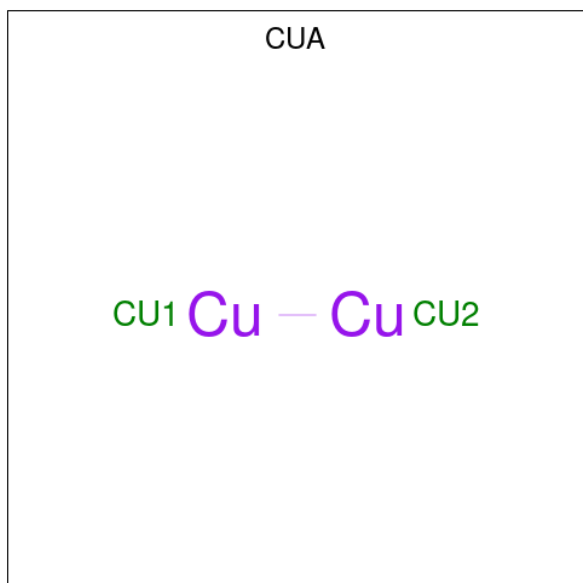
- Molecule 28 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
28	a	1	Total	Cu	0
			1	1	

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

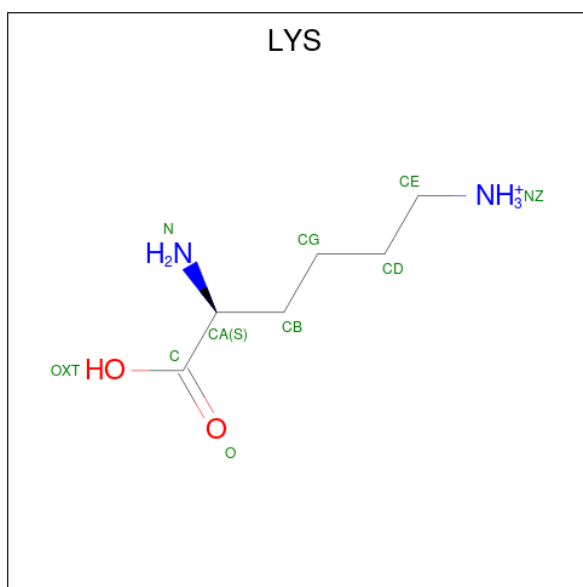
Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	Mg	0
			1	1	

- Molecule 30 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		AltConf
30	b	1	Total	Cu	0
			2	2	

- Molecule 31 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).



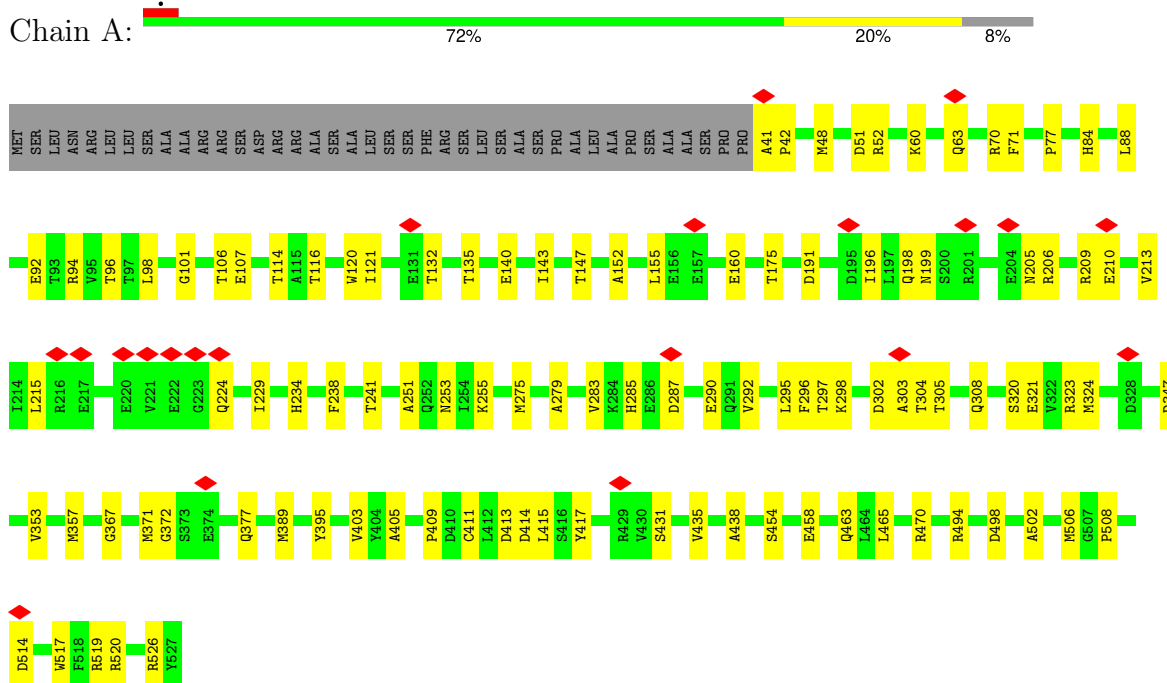
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	i	1	9	6	2	1	0

### 3 Residue-property plots

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

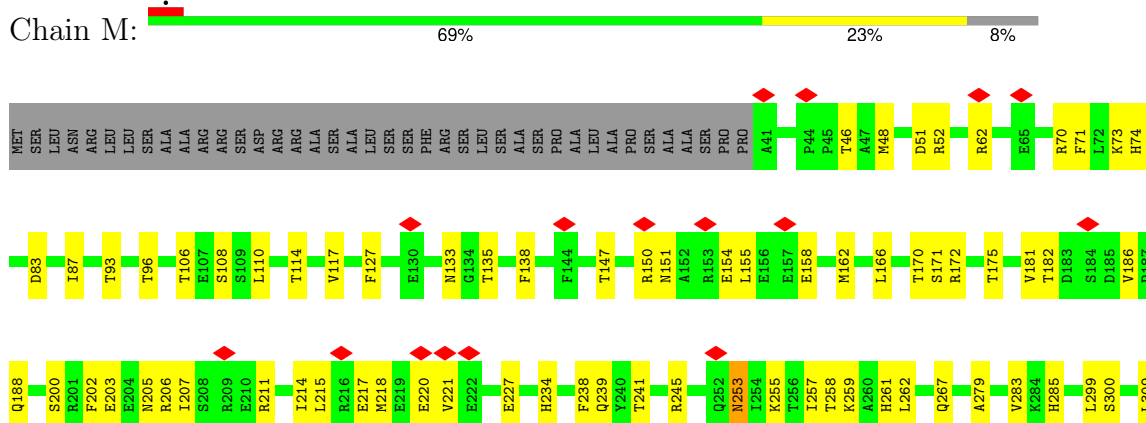
- Molecule 1: Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1

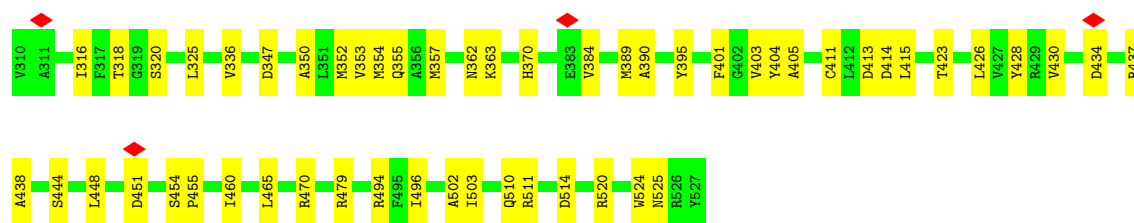
Chain A:



- Molecule 1: Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1

Chain M:

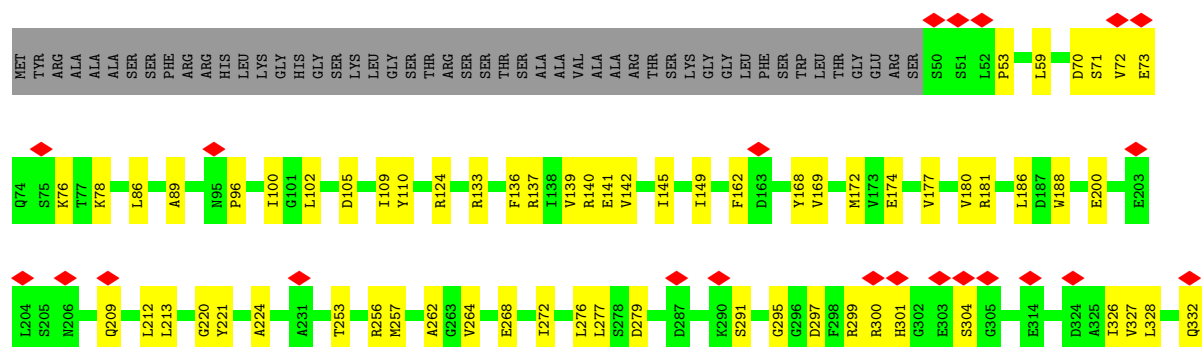




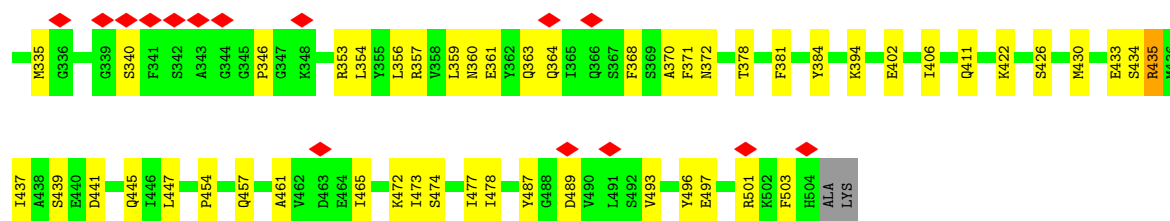
• Molecule 2: Alpha-MPP



• Molecule 2: Alpha-MPP

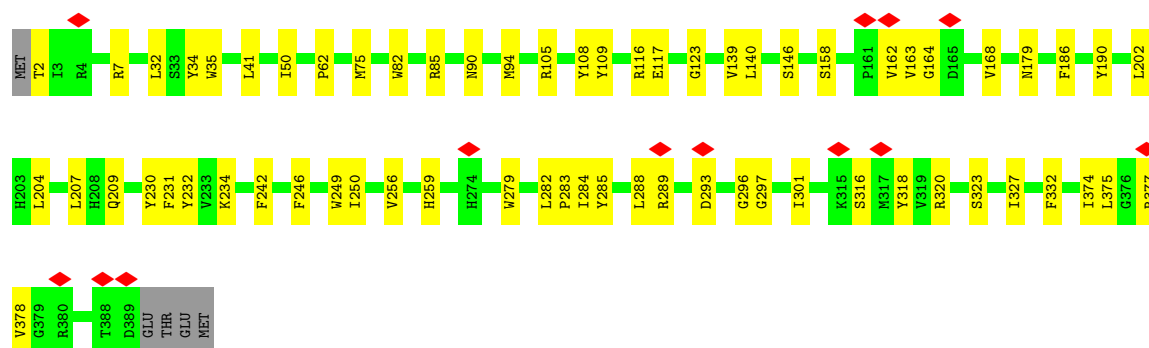






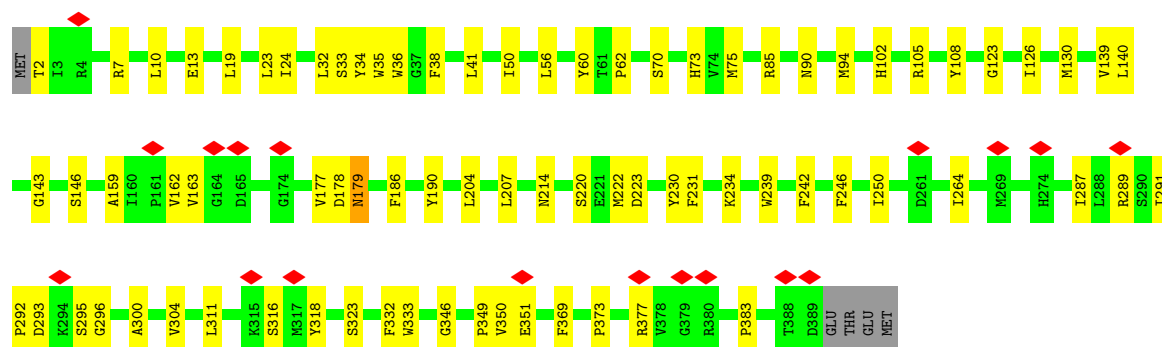
- Molecule 3: COB

Chain C: 82% 17%



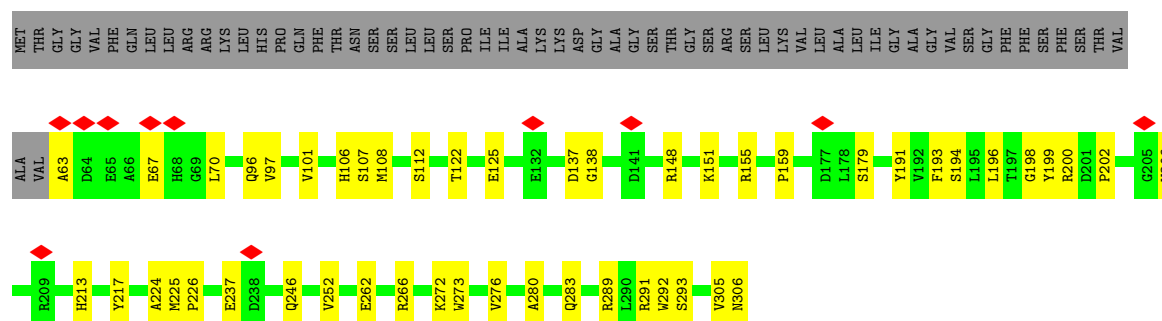
- Molecule 3: COB

Chain O: 5% 79% 20%



- Molecule 4: cytochrome c1-2, heme protein, mitochondrial

Chain D: 64% 16% 20%

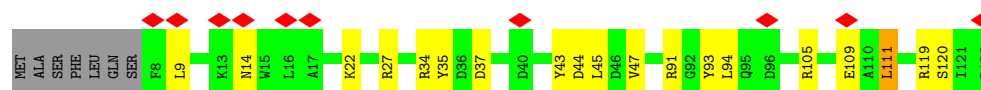
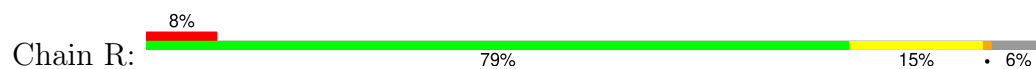


- Chain P: 

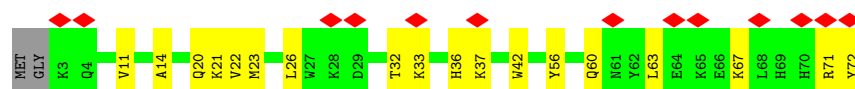




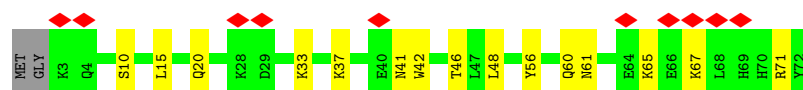
- Molecule 6: Cytochrome b-c1 complex subunit 7



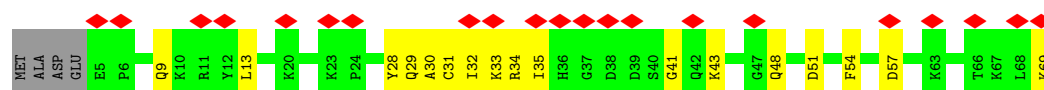
- Molecule 7: cytochrome b-c1 complex subunit 8



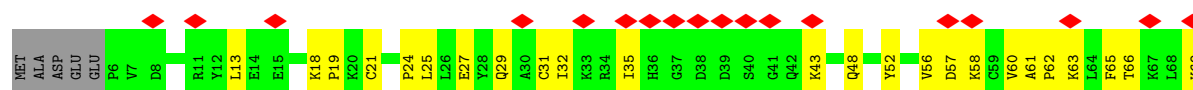
- Molecule 7: cytochrome b-c1 complex subunit 8



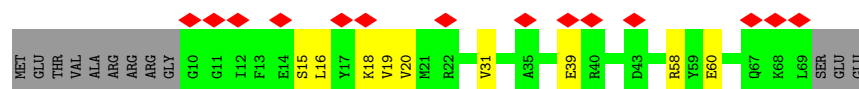
- Molecule 8: Cytochrome b-c1 complex subunit 6



- Molecule 8: Cytochrome b-c1 complex subunit 6



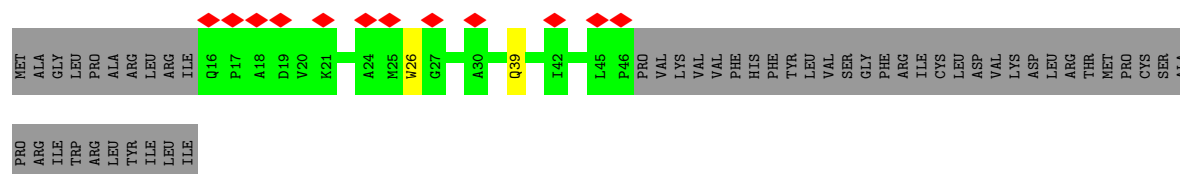
- Molecule 9: cytochrome b-c1 complex subunit 9



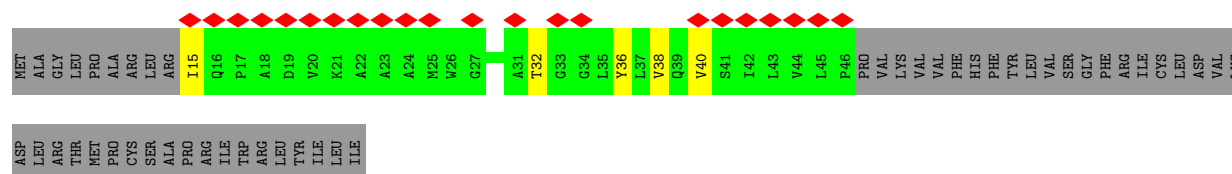
- Molecule 9: cytochrome b-c1 complex subunit 9



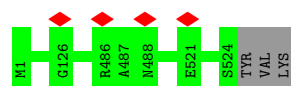
- Molecule 10: QCR10



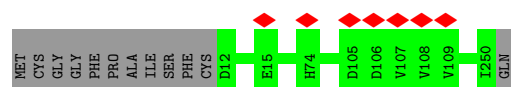
- Molecule 10: QCR10



- Molecule 11: COX1



- Molecule 12: Cytochrome c oxidase subunit 2



- Molecule 13: COX3



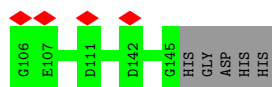
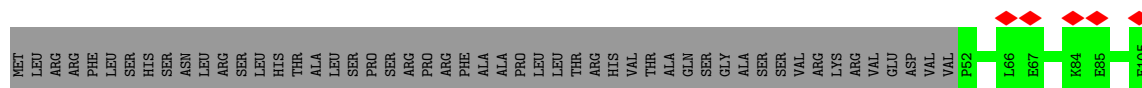
There are no outlier residues recorded for this chain.

- Molecule 14: COX4

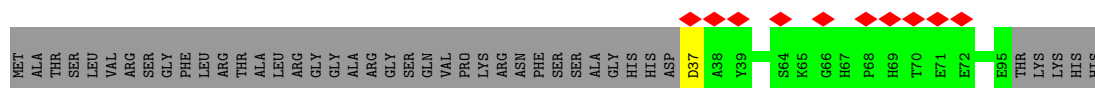




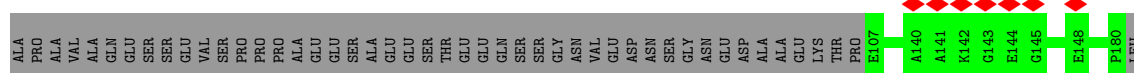
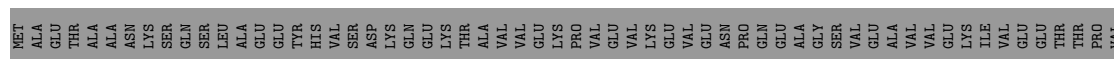
- Molecule 15: cytochrome c oxidase subunit 5b-2, mitochondrial



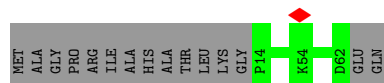
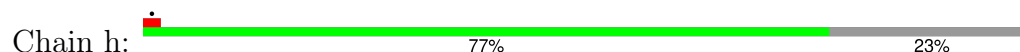
- Molecule 16: cytochrome c oxidase subunit 6a, mitochondrial



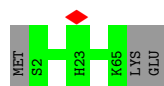
- Molecule 17: cytochrome c oxidase subunit 6b-1



- Molecule 18: Cytochrome c oxidase subunit 5C



- Molecule 19: COX7a



- Molecule 20: COX7c



MET	ALA	PHE	ASN	ASN	ALA	LEU	ARG	SER	ALA	ALA	LYS	LEU	ILE	ALA	SER	SER	GLU	SER	SER	ILE	SER	THR	SER	VAL	SER	ARG	GLY	PHE	HIS	SER	THR	PRO	MET	LYS	ARG	MET	GLY	GLY	GLY	HIS	GLY	HIS	ASP	GLU	PRO	Y47	R59	M60	K61	H62	R63	T93	ALA	SER	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29348	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 ( $e^-/\text{\AA}^2$ )	86.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60010	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.662	Depositor
Minimum map value	-36.912	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.159	Depositor
Recommended contour level	6	Depositor
Map size (Å)	426.5984, 426.5984, 426.5984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/3914	0.48	0/5309
1	M	0.32	0/3914	0.49	0/5309
2	B	0.30	0/3541	0.48	0/4803
2	N	0.30	0/3526	0.49	0/4785
3	C	0.38	0/3220	0.46	0/4413
3	O	0.38	0/3220	0.47	0/4413
4	D	0.33	0/1962	0.44	0/2663
4	P	0.34	0/1962	0.45	0/2663
5	E	0.33	0/588	0.45	0/797
5	Q	0.34	0/588	0.46	0/797
6	F	0.35	0/986	0.46	1/1326 (0.1%)
6	R	0.35	0/980	0.46	1/1318 (0.1%)
7	G	0.29	0/595	0.42	0/807
7	S	0.30	0/595	0.44	0/807
8	H	0.30	0/550	0.44	0/737
8	T	0.29	0/541	0.52	0/724
9	J	0.31	0/490	0.43	0/660
9	V	0.27	0/486	0.41	0/655
10	K	0.27	0/222	0.41	0/305
10	W	0.31	0/230	0.45	0/316
11	a	0.38	0/4214	0.52	0/5758
12	b	0.35	0/1971	0.53	0/2697
13	c	0.38	0/2217	0.46	0/3030
14	d	0.34	0/612	0.48	0/832
15	e	0.33	0/756	0.47	0/1026
16	f	0.29	0/499	0.50	1/682 (0.1%)
17	g	0.39	0/631	0.58	0/853
18	h	0.33	0/399	0.44	0/538
19	i	0.33	0/524	0.50	0/705
20	j	0.34	0/394	0.47	0/528
All	All	0.34	0/44327	0.48	3/60256 (0.0%)



There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	111	LEU	CA-CB-CG	5.49	127.92	115.30
6	R	111	LEU	CA-CB-CG	5.23	127.33	115.30
16	f	37	ASP	CB-CG-OD2	5.18	122.96	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3838	0	3797	71	0
1	M	3838	0	3797	94	0
2	B	3471	0	3471	95	0
2	N	3456	0	3453	87	0
3	C	3104	0	3070	61	0
3	O	3104	0	3070	67	0
4	D	1910	0	1843	43	0
4	P	1910	0	1843	47	0
5	E	574	0	591	15	0
5	Q	574	0	591	30	0
6	F	965	0	982	27	0
6	R	959	0	977	15	0
7	G	578	0	599	17	0
7	S	578	0	599	13	0
8	H	536	0	528	15	0
8	T	527	0	521	20	0
9	J	480	0	486	7	0
9	V	476	0	483	17	0
10	K	218	0	230	2	0
10	W	226	0	241	7	0
11	a	4074	0	4063	0	0
12	b	1915	0	1876	0	0
13	c	2134	0	2098	0	0
14	d	595	0	596	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	e	733	0	677	0	0
16	f	480	0	452	0	0
17	g	612	0	563	0	0
18	h	391	0	405	0	0
19	i	510	0	528	0	0
20	j	384	0	398	0	0
21	A	1	0	0	0	0
21	M	1	0	0	0	0
21	e	1	0	0	0	0
22	A	29	0	32	1	0
22	M	27	0	28	1	0
22	S	28	0	30	2	0
22	a	39	0	52	0	0
22	i	36	0	46	0	0
23	A	51	0	46	1	0
23	C	109	0	106	5	0
23	D	41	0	26	1	0
23	M	53	0	50	4	0
23	O	54	0	55	2	0
23	P	48	0	40	2	0
23	S	50	0	44	2	0
23	a	67	0	78	0	0
24	C	86	0	60	6	0
24	O	86	0	60	9	0
25	C	158	0	189	10	0
25	F	32	0	38	2	0
25	G	20	0	14	0	0
25	O	109	0	114	7	0
25	P	28	0	30	2	0
25	a	227	0	301	0	0
25	b	108	0	141	0	0
25	c	200	0	270	0	0
25	d	35	0	44	0	0
25	h	38	0	50	0	0
25	i	35	0	44	0	0
26	D	43	0	30	7	0
26	P	43	0	30	3	0
27	a	120	0	108	0	0
28	a	1	0	0	0	0
29	a	1	0	0	0	0
30	b	2	0	0	0	0
31	i	9	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	45166	0	44996	655	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 11.

The worst 5 of 655 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)
4:P:283:GLN:NE2	5:Q:115:LEU:CA	1.87	1.37
4:P:283:GLN:NE2	5:Q:115:LEU:HA	0.94	1.26
4:P:283:GLN:HE21	5:Q:115:LEU:CA	1.43	1.23
9:V:32:ILE:HG21	10:W:32:THR:HG22	1.25	1.10
3:C:374:ILE:HG12	3:C:377:ARG:NH2	1.72	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/527 (92%)	450 (93%)	35 (7%)	0	100	100
1	M	485/527 (92%)	451 (93%)	34 (7%)	0	100	100
2	B	455/506 (90%)	411 (90%)	42 (9%)	2 (0%)	30	63
2	N	453/506 (90%)	406 (90%)	47 (10%)	0	100	100
3	C	386/393 (98%)	365 (95%)	21 (5%)	0	100	100
3	O	386/393 (98%)	363 (94%)	23 (6%)	0	100	100
4	D	242/306 (79%)	234 (97%)	8 (3%)	0	100	100
4	P	242/306 (79%)	229 (95%)	13 (5%)	0	100	100
5	E	72/271 (27%)	68 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Q	72/271 (27%)	66 (92%)	6 (8%)	0	100	100
6	F	114/122 (93%)	111 (97%)	3 (3%)	0	100	100
6	R	113/122 (93%)	109 (96%)	4 (4%)	0	100	100
7	G	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
7	S	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
8	H	63/69 (91%)	59 (94%)	4 (6%)	0	100	100
8	T	62/69 (90%)	55 (89%)	7 (11%)	0	100	100
9	J	58/72 (81%)	54 (93%)	4 (7%)	0	100	100
9	V	57/72 (79%)	55 (96%)	2 (4%)	0	100	100
10	K	29/81 (36%)	25 (86%)	4 (14%)	0	100	100
10	W	30/81 (37%)	28 (93%)	2 (7%)	0	100	100
11	a	522/527 (99%)	471 (90%)	51 (10%)	0	100	100
12	b	237/251 (94%)	206 (87%)	31 (13%)	0	100	100
13	c	263/265 (99%)	249 (95%)	14 (5%)	0	100	100
14	d	74/79 (94%)	67 (90%)	7 (10%)	0	100	100
15	e	92/150 (61%)	83 (90%)	9 (10%)	0	100	100
16	f	57/100 (57%)	54 (95%)	3 (5%)	0	100	100
17	g	72/181 (40%)	63 (88%)	9 (12%)	0	100	100
18	h	47/64 (73%)	46 (98%)	1 (2%)	0	100	100
19	i	62/67 (92%)	57 (92%)	5 (8%)	0	100	100
20	j	45/96 (47%)	39 (87%)	5 (11%)	1 (2%)	5	30
All	All	5411/6618 (82%)	5007 (92%)	401 (7%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	j	63	ARG
2	B	435	ARG
2	B	113	PRO

### 5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/438 (93%)	405 (100%)	2 (0%)	86	90
1	M	407/438 (93%)	405 (100%)	2 (0%)	86	90
2	B	378/414 (91%)	378 (100%)	0	100	100
2	N	377/414 (91%)	376 (100%)	1 (0%)	91	92
3	C	333/338 (98%)	331 (99%)	2 (1%)	84	88
3	O	333/338 (98%)	332 (100%)	1 (0%)	91	92
4	D	198/247 (80%)	198 (100%)	0	100	100
4	P	198/247 (80%)	197 (100%)	1 (0%)	86	90
5	E	62/233 (27%)	62 (100%)	0	100	100
5	Q	62/233 (27%)	62 (100%)	0	100	100
6	F	102/107 (95%)	101 (99%)	1 (1%)	73	80
6	R	101/107 (94%)	101 (100%)	0	100	100
7	G	64/65 (98%)	64 (100%)	0	100	100
7	S	64/65 (98%)	64 (100%)	0	100	100
8	H	60/63 (95%)	60 (100%)	0	100	100
8	T	59/63 (94%)	59 (100%)	0	100	100
9	J	49/59 (83%)	49 (100%)	0	100	100
9	V	49/59 (83%)	49 (100%)	0	100	100
10	K	21/66 (32%)	21 (100%)	0	100	100
10	W	22/66 (33%)	22 (100%)	0	100	100
11	a	433/436 (99%)	433 (100%)	0	100	100
12	b	213/222 (96%)	213 (100%)	0	100	100
13	c	219/219 (100%)	219 (100%)	0	100	100
14	d	65/68 (96%)	64 (98%)	1 (2%)	60	74
15	e	77/126 (61%)	77 (100%)	0	100	100
16	f	50/82 (61%)	50 (100%)	0	100	100
17	g	63/153 (41%)	63 (100%)	0	100	100
18	h	42/52 (81%)	42 (100%)	0	100	100
19	i	55/58 (95%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	j	40/77 (52%)	40 (100%)	0	100	100
All	All	4603/5553 (83%)	4592 (100%)	11 (0%)	91	94

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	435	ARG
3	O	179	ASN
14	d	71	ASN
4	P	282	LEU
6	F	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
12	b	121	GLN
11	a	505	GLN
8	T	48	GLN
11	a	431	HIS
7	S	20	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 5 are monoatomic - leaving 53 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	3PE	C	408	-	27,27,50	0.40	0	30,32,55	0.37	0
23	CDL	A	603	-	50,50,99	0.38	0	56,62,111	0.36	0
25	3PE	F	201	-	31,31,50	0.39	0	34,36,55	0.55	0
24	HEM	C	403	3	42,50,50	1.28	5 (11%)	46,82,82	1.71	9 (19%)
25	3PE	a	607	-	39,39,50	0.34	0	42,44,55	0.33	0
25	3PE	C	404	-	37,37,50	0.35	0	40,42,55	0.37	0
22	PC1	S	101	-	27,27,53	1.13	2 (7%)	33,35,61	1.16	3 (9%)
25	3PE	i	103	-	34,34,50	0.36	0	37,39,55	0.30	0
25	3PE	C	405	-	27,27,50	1.26	2 (7%)	30,32,55	1.26	3 (10%)
25	3PE	a	612	-	38,38,50	0.34	0	41,43,55	0.32	0
25	3PE	c	304	-	42,42,50	0.35	0	45,47,55	0.46	0
26	HEC	P	402	4	32,50,50	2.00	4 (12%)	30,82,82	2.74	16 (53%)
25	3PE	a	606	-	31,31,50	0.37	0	34,36,55	0.39	0
25	3PE	a	609	-	37,37,50	0.35	0	40,42,55	0.41	0
27	HEA	a	601	11	58,67,67	1.21	5 (8%)	63,103,103	1.76	16 (25%)
25	3PE	d	101	-	34,34,50	0.36	0	37,39,55	0.33	0
24	HEM	C	402	3	42,50,50	1.28	5 (11%)	46,82,82	1.77	12 (26%)
25	3PE	b	302	-	35,35,50	0.36	0	38,40,55	0.34	0
23	CDL	a	608	-	66,66,99	0.36	0	72,78,111	0.37	0
22	PC1	A	602	-	28,28,53	1.39	2 (7%)	34,36,61	1.31	3 (8%)
25	3PE	a	611	-	37,37,50	0.35	0	40,42,55	0.31	0
25	3PE	b	303	-	28,28,50	0.40	0	31,33,55	0.44	0
25	3PE	h	101	-	37,37,50	0.35	0	40,42,55	0.33	0
24	HEM	O	403	3	42,50,50	1.32	5 (11%)	46,82,82	1.78	11 (23%)
22	PC1	i	101	-	35,35,53	0.35	0	41,43,61	0.42	0
22	PC1	M	603	-	26,26,53	0.38	0	32,34,61	0.41	0
25	3PE	c	305	-	39,39,50	0.34	0	42,44,55	0.33	0
27	HEA	a	602	11	58,67,67	1.23	5 (8%)	63,103,103	1.50	12 (19%)
25	3PE	O	401	-	23,23,50	1.17	2 (8%)	26,28,55	1.18	2 (7%)
25	3PE	c	301	-	39,39,50	0.35	0	42,44,55	0.38	0
23	CDL	P	403	-	47,47,99	0.40	0	53,59,111	0.50	0
25	3PE	O	405	-	25,25,50	1.30	2 (8%)	28,30,55	1.30	3 (10%)
25	3PE	b	304	-	42,42,50	0.32	0	45,47,55	0.33	0
25	3PE	C	407	-	34,34,50	0.34	0	37,39,55	0.47	0
25	3PE	c	302	-	39,39,50	0.35	0	42,44,55	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	3PE	a	610	-	39,39,50	0.34	0	42,44,55	0.32	0
23	CDL	C	409	-	54,54,99	0.38	0	60,66,111	0.35	0
23	CDL	M	602	-	52,52,99	0.39	0	58,64,111	0.43	0
23	CDL	S	102	-	49,49,99	0.41	0	55,61,111	0.40	0
22	PC1	a	605	-	38,38,53	0.35	0	44,46,61	0.38	0
25	3PE	G	101	-	19,19,50	1.27	2 (10%)	22,24,55	1.08	2 (9%)
25	3PE	O	406	-	32,32,50	0.37	0	35,37,55	0.35	0
25	3PE	P	401	-	27,27,50	1.08	2 (7%)	30,32,55	1.15	2 (6%)
25	3PE	c	303	-	36,36,50	0.35	0	39,41,55	0.35	0
30	CUA	b	301	12	0,1,1	-	-	-	-	-
25	3PE	C	406	-	28,28,50	0.40	0	31,33,55	0.41	0
26	HEC	D	501	4	32,50,50	2.04	4 (12%)	30,82,82	2.76	15 (50%)
31	LYS	i	102	-	7,8,9	0.48	0	3,8,10	0.39	0
23	CDL	D	502	-	40,40,99	0.43	0	46,52,111	0.44	0
23	CDL	O	402	-	53,53,99	0.38	0	59,65,111	0.47	0
24	HEM	O	404	3	42,50,50	1.31	5 (11%)	46,82,82	1.69	9 (19%)
25	3PE	O	407	-	25,25,50	0.41	0	28,30,55	0.43	0
23	CDL	C	401	-	53,53,99	0.40	0	59,65,111	0.36	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
25	3PE	C	408	-	-	5/31/31/54	-
23	CDL	A	603	-	-	13/59/59/110	-
25	3PE	F	201	-	-	9/35/35/54	-
24	HEM	C	403	3	-	6/12/54/54	-
25	3PE	a	607	-	-	4/43/43/54	-
25	3PE	C	404	-	-	9/41/41/54	-
22	PC1	S	101	-	-	12/30/30/57	-
25	3PE	i	103	-	-	9/38/38/54	-
25	3PE	C	405	-	-	14/31/31/54	-
25	3PE	a	612	-	-	5/42/42/54	-
25	3PE	c	304	-	-	12/46/46/54	-
26	HEC	P	402	4	-	2/10/54/54	-
25	3PE	a	606	-	-	10/35/35/54	-
25	3PE	a	609	-	-	14/41/41/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	HEA	a	601	11	-	8/32/76/76	-
25	3PE	d	101	-	-	15/38/38/54	-
24	HEM	C	402	3	-	3/12/54/54	-
25	3PE	b	302	-	-	8/39/39/54	-
23	CDL	a	608	-	-	14/77/77/110	-
22	PC1	A	602	-	-	5/31/31/57	-
25	3PE	a	611	-	-	5/41/41/54	-
25	3PE	b	303	-	-	9/32/32/54	-
25	3PE	h	101	-	-	2/41/41/54	-
24	HEM	O	403	3	-	8/12/54/54	-
22	PC1	i	101	-	-	5/39/39/57	-
22	PC1	M	603	-	-	1/29/29/57	-
25	3PE	c	305	-	-	7/43/43/54	-
27	HEA	a	602	11	-	8/32/76/76	-
25	3PE	O	401	-	-	1/26/26/54	-
25	3PE	c	301	-	-	11/43/43/54	-
23	CDL	P	403	-	-	14/56/56/110	-
25	3PE	O	405	-	-	9/29/29/54	-
25	3PE	b	304	-	-	6/46/46/54	-
25	3PE	C	407	-	-	12/37/37/54	-
25	3PE	c	302	-	-	8/43/43/54	-
25	3PE	a	610	-	-	10/43/43/54	-
23	CDL	C	409	-	-	7/64/64/110	-
23	CDL	M	602	-	-	7/62/62/110	-
23	CDL	S	102	-	-	13/60/60/110	-
22	PC1	a	605	-	-	14/42/42/57	-
25	3PE	G	101	-	-	6/22/22/54	-
25	3PE	O	406	-	-	7/36/36/54	-
25	3PE	P	401	-	-	9/30/30/54	-
25	3PE	c	303	-	-	8/40/40/54	-
25	3PE	C	406	-	-	6/32/32/54	-
26	HEC	D	501	4	-	2/10/54/54	-
31	LYS	i	102	-	-	1/6/7/9	-
23	CDL	D	502	-	-	14/49/49/110	-
23	CDL	O	402	-	-	14/62/62/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	HEM	O	404	3	-	7/12/54/54	-
25	3PE	O	407	-	-	2/29/29/54	-
23	CDL	C	401	-	-	11/64/64/110	-

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	501	HEC	C3C-C2C	-6.45	1.33	1.40
26	P	402	HEC	C3C-C2C	-6.31	1.33	1.40
26	D	501	HEC	C2B-C3B	-6.31	1.33	1.40
26	P	402	HEC	C2B-C3B	-6.20	1.33	1.40
22	A	602	PC1	O21-C21	4.96	1.46	1.35

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	501	HEC	CBB-CAB-C3B	-7.84	109.15	127.49
26	P	402	HEC	CBB-CAB-C3B	-7.53	109.86	127.49
26	P	402	HEC	CBC-CAC-C3C	-5.82	113.87	127.49
26	D	501	HEC	CBC-CAC-C3C	-5.48	114.67	127.49
24	O	403	HEM	CHC-C4B-NB	4.90	129.71	124.44

There are no chirality outliers.

5 of 421 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	602	PC1	C11-O13-P-O12
22	A	602	PC1	C11-O13-P-O14
22	A	602	PC1	C11-O13-P-O11
22	S	101	PC1	C1-O11-P-O12
22	S	101	PC1	C1-O11-P-O14

There are no ring outliers.

24 monomers are involved in 63 short contacts:

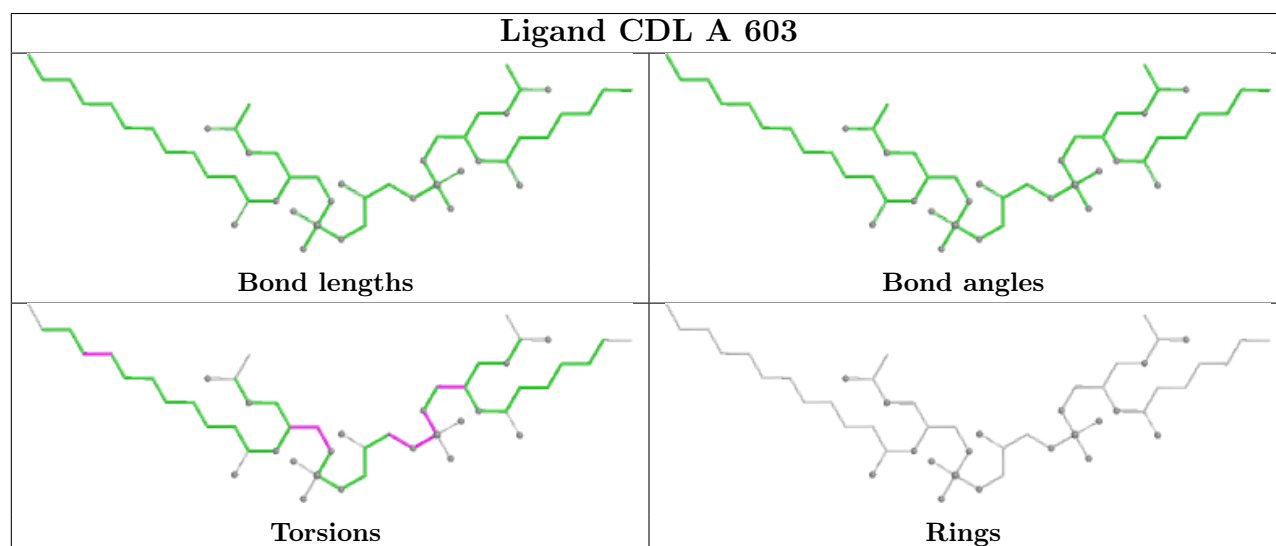
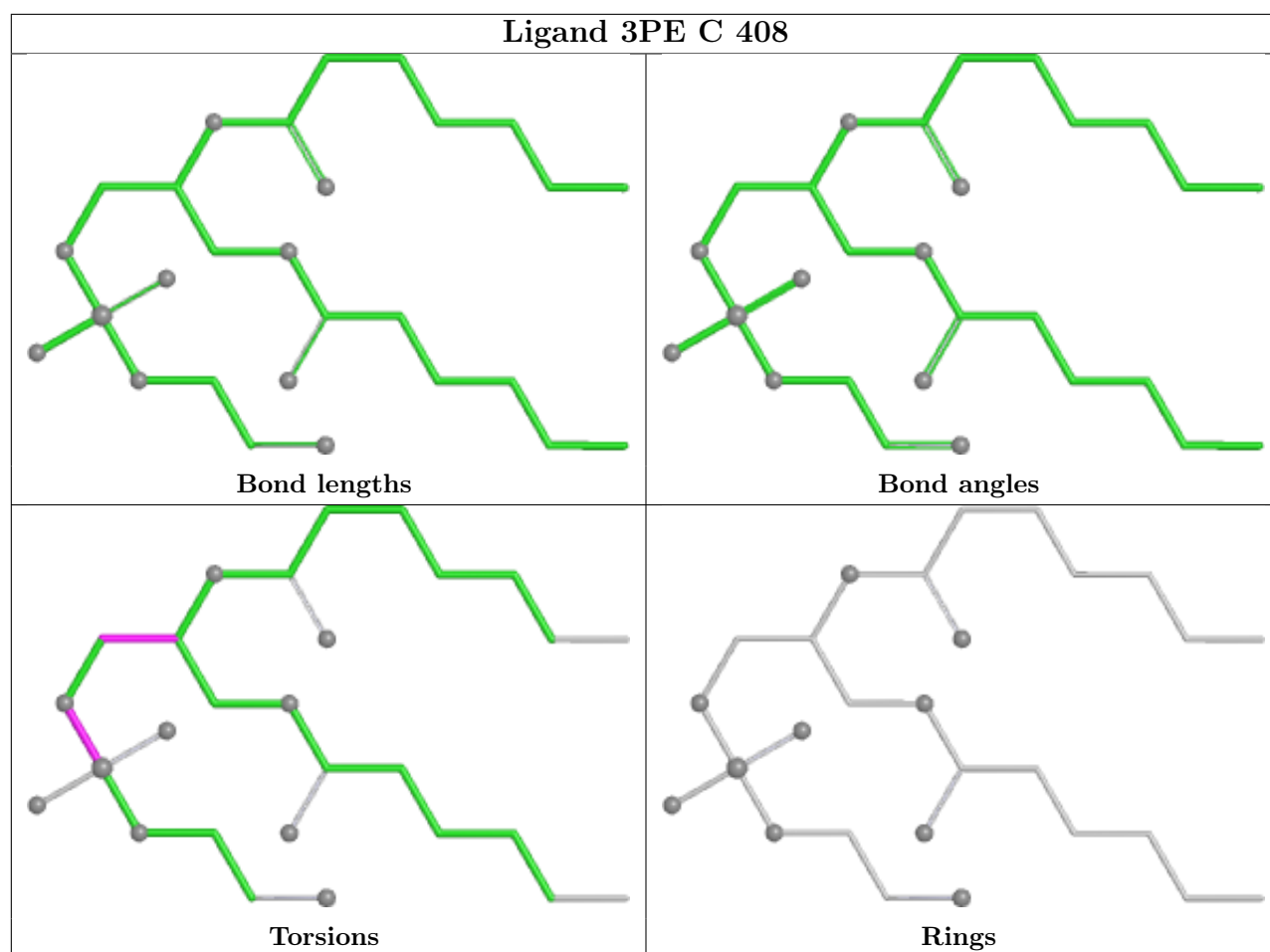
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	408	3PE	1	0
23	A	603	CDL	1	0
25	F	201	3PE	2	0
24	C	403	HEM	4	0

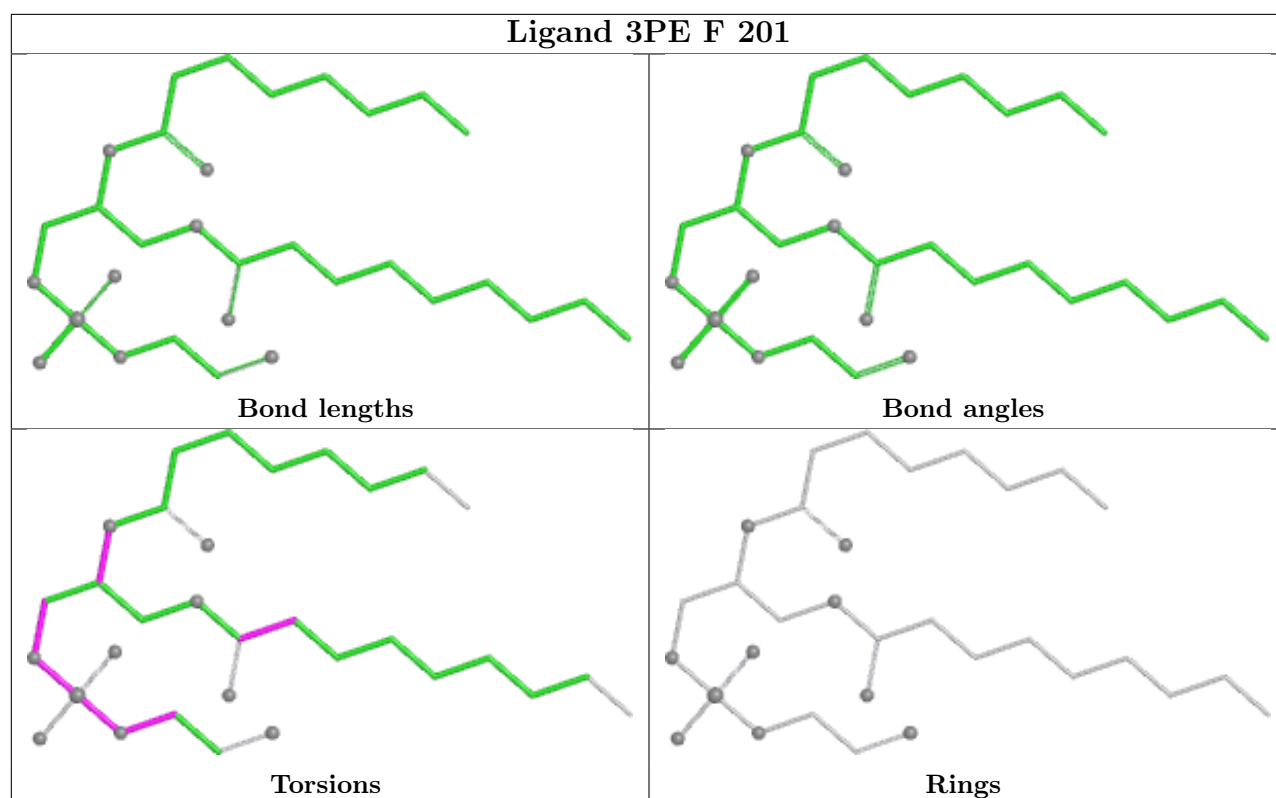
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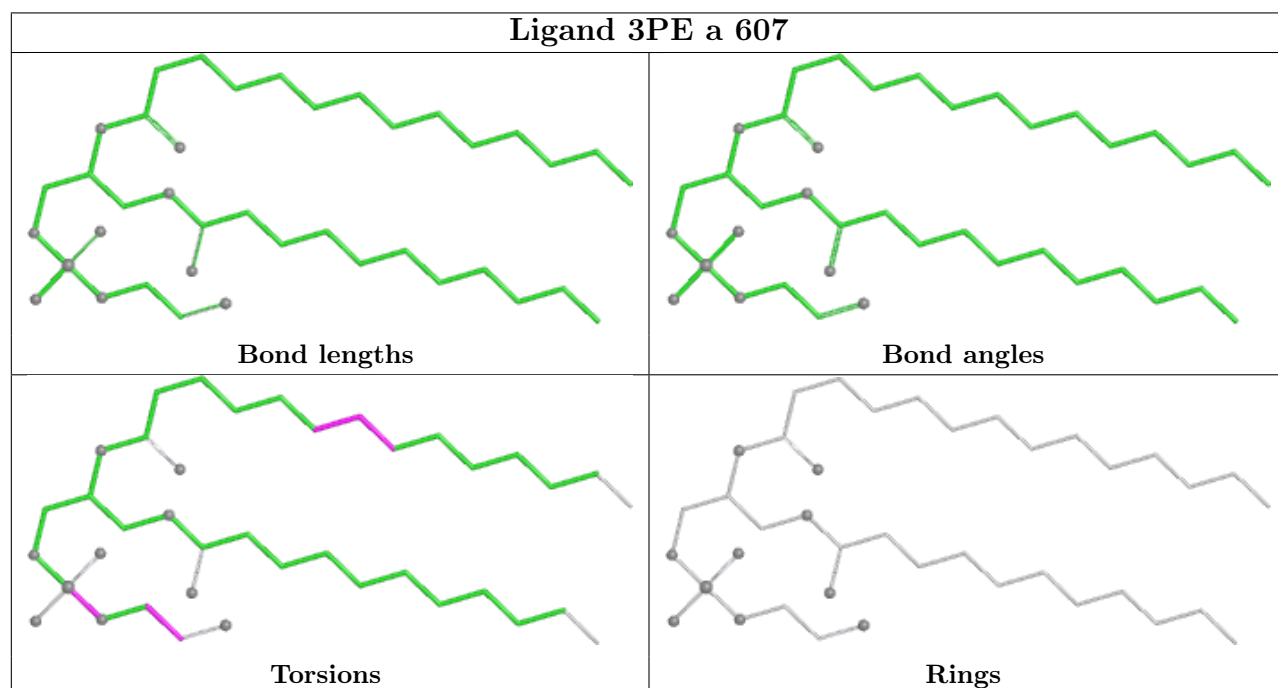
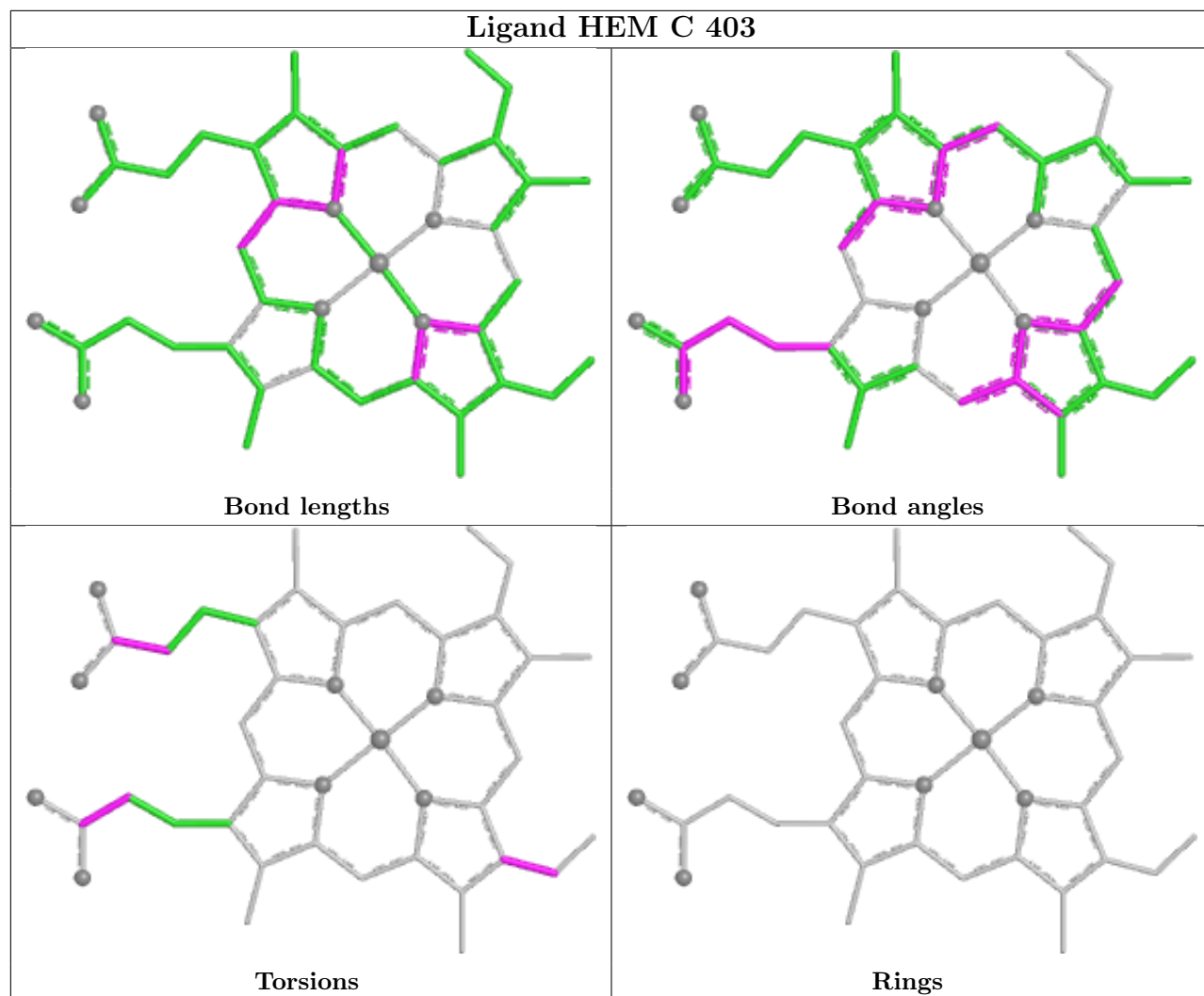
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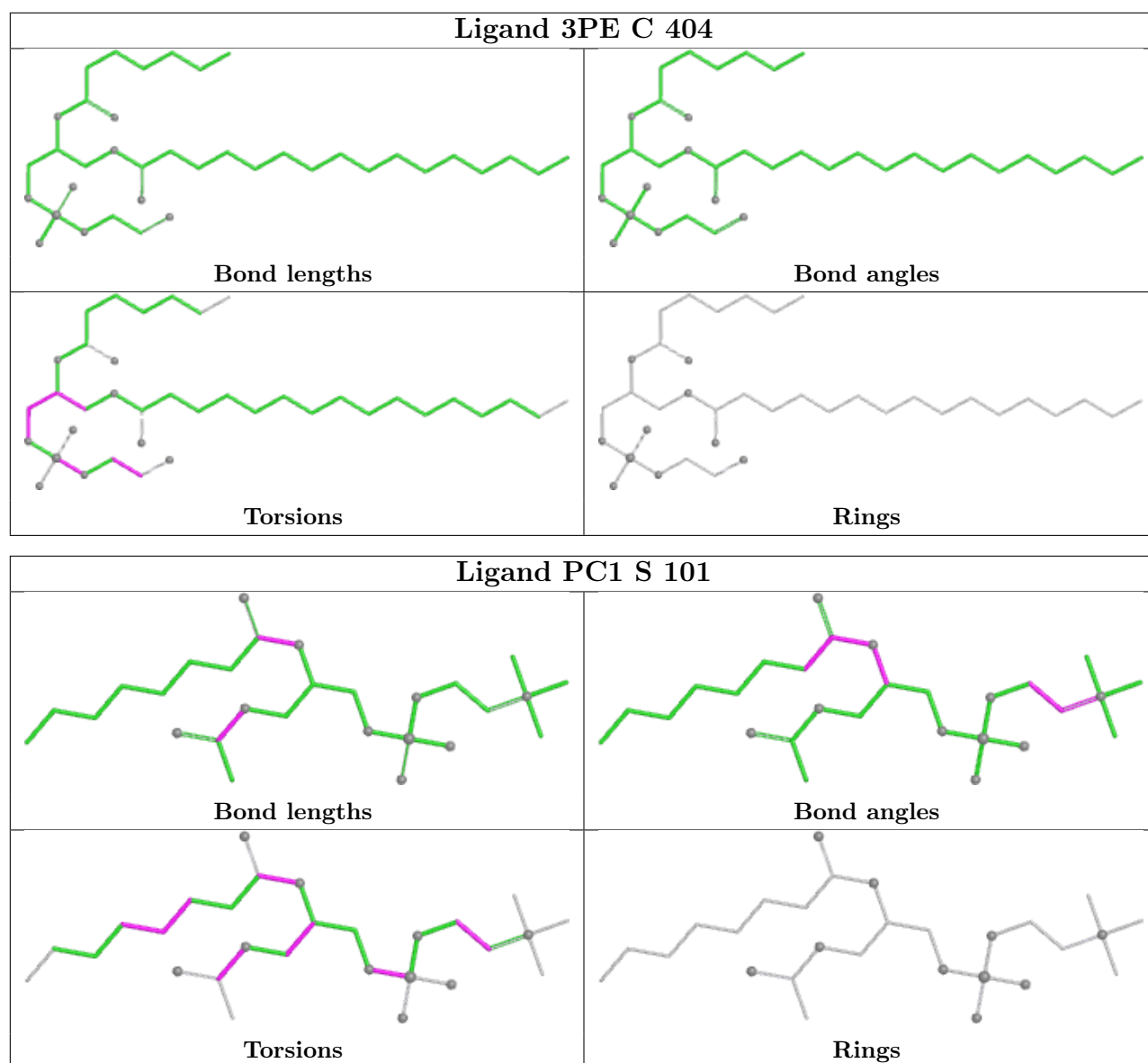
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	S	101	PC1	2	0
25	C	405	3PE	2	0
26	P	402	HEC	3	0
24	C	402	HEM	2	0
22	A	602	PC1	1	0
24	O	403	HEM	3	0
22	M	603	PC1	1	0
25	O	401	3PE	7	0
23	P	403	CDL	2	0
25	C	407	3PE	3	0
23	C	409	CDL	2	0
23	M	602	CDL	4	0
23	S	102	CDL	2	0
25	P	401	3PE	2	0
25	C	406	3PE	4	0
26	D	501	HEC	7	0
23	D	502	CDL	1	0
23	O	402	CDL	2	0
24	O	404	HEM	6	0
23	C	401	CDL	3	0

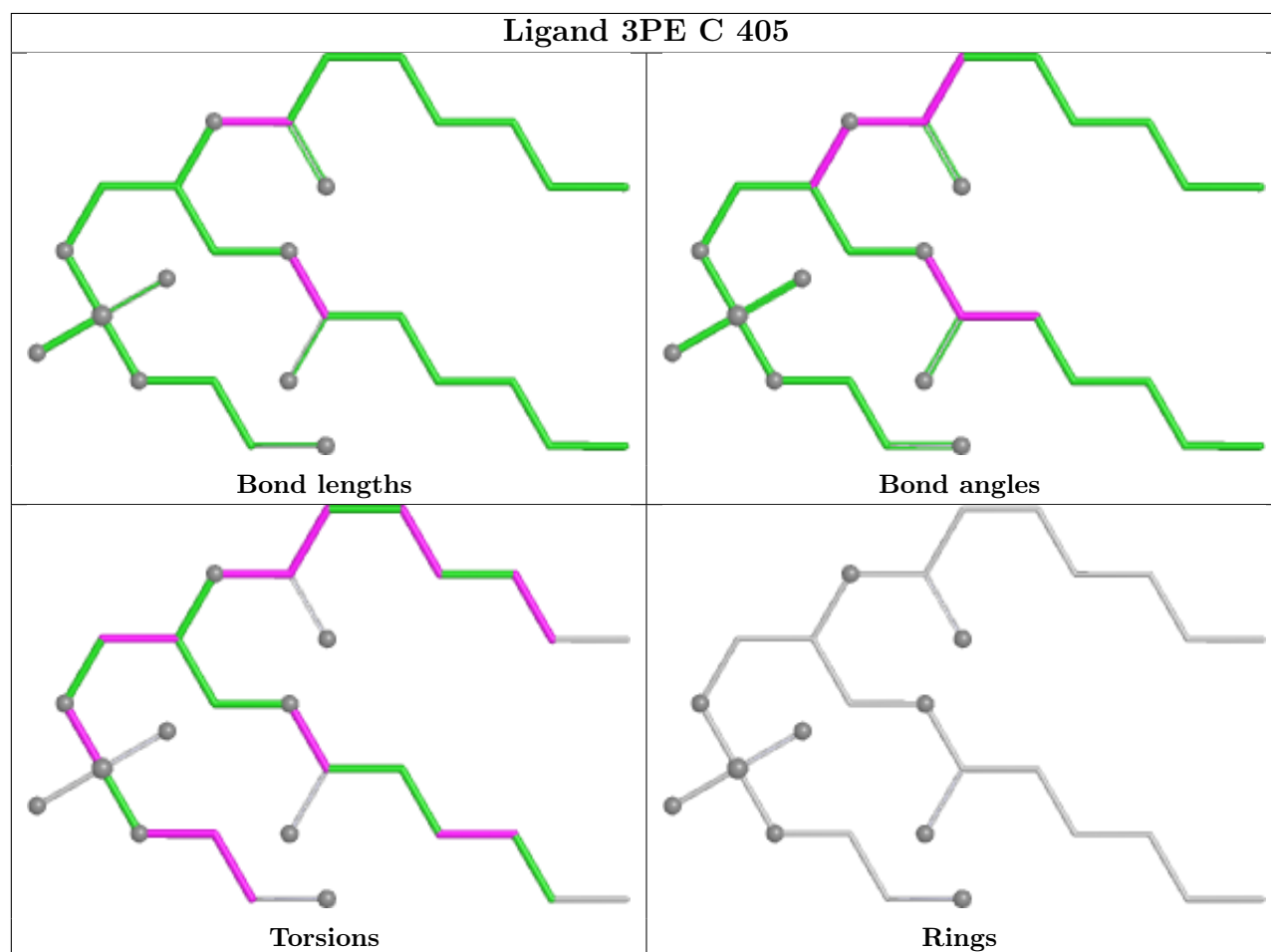
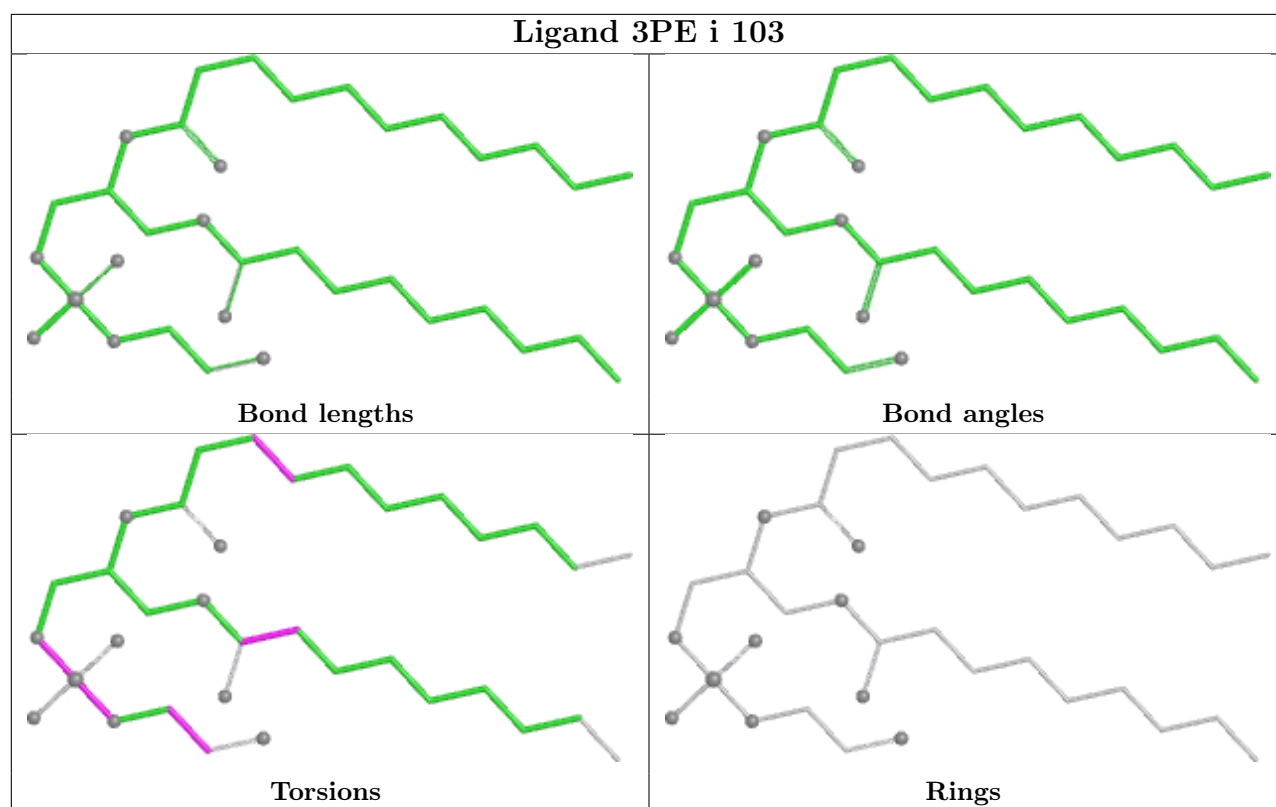
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



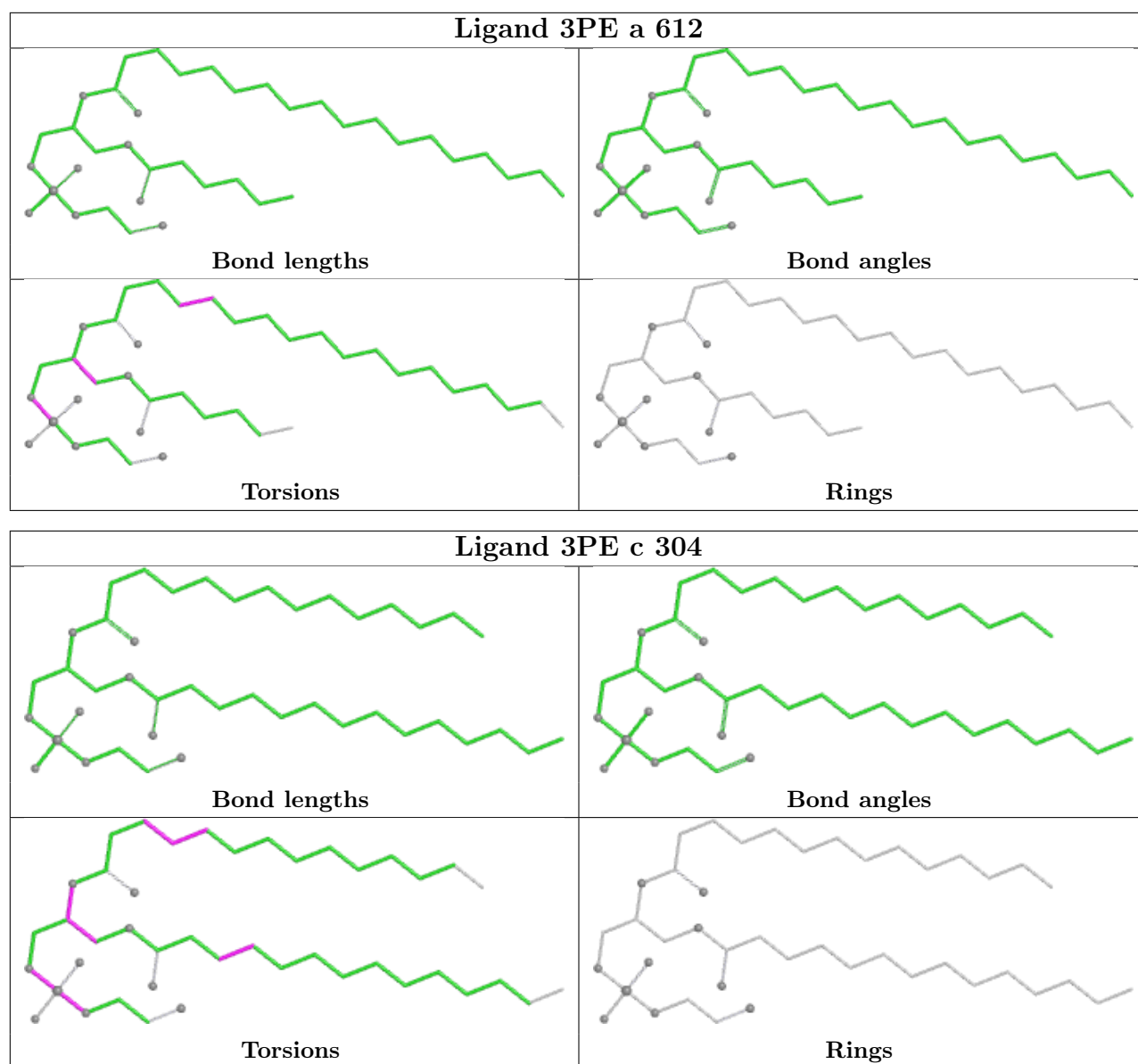


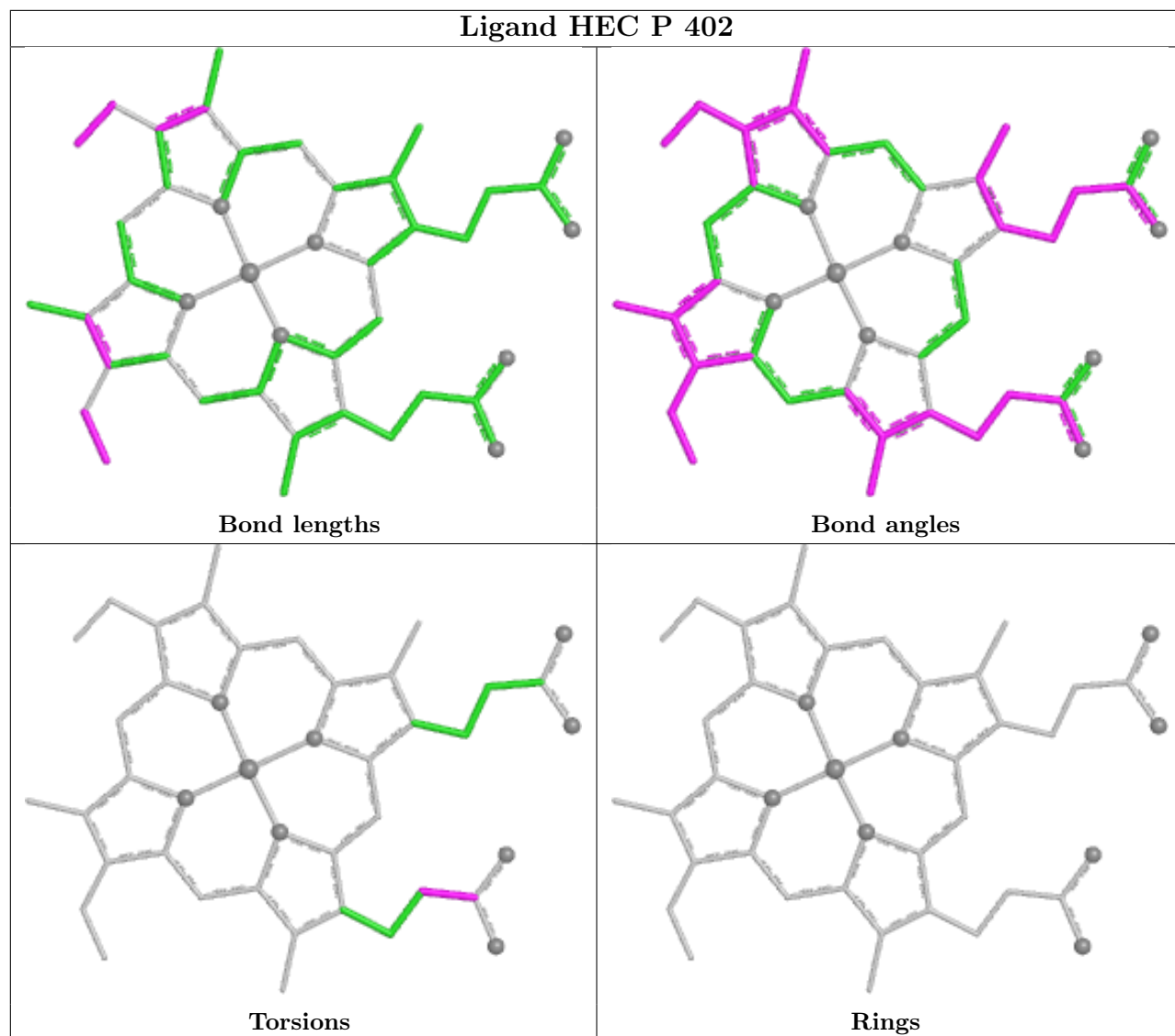


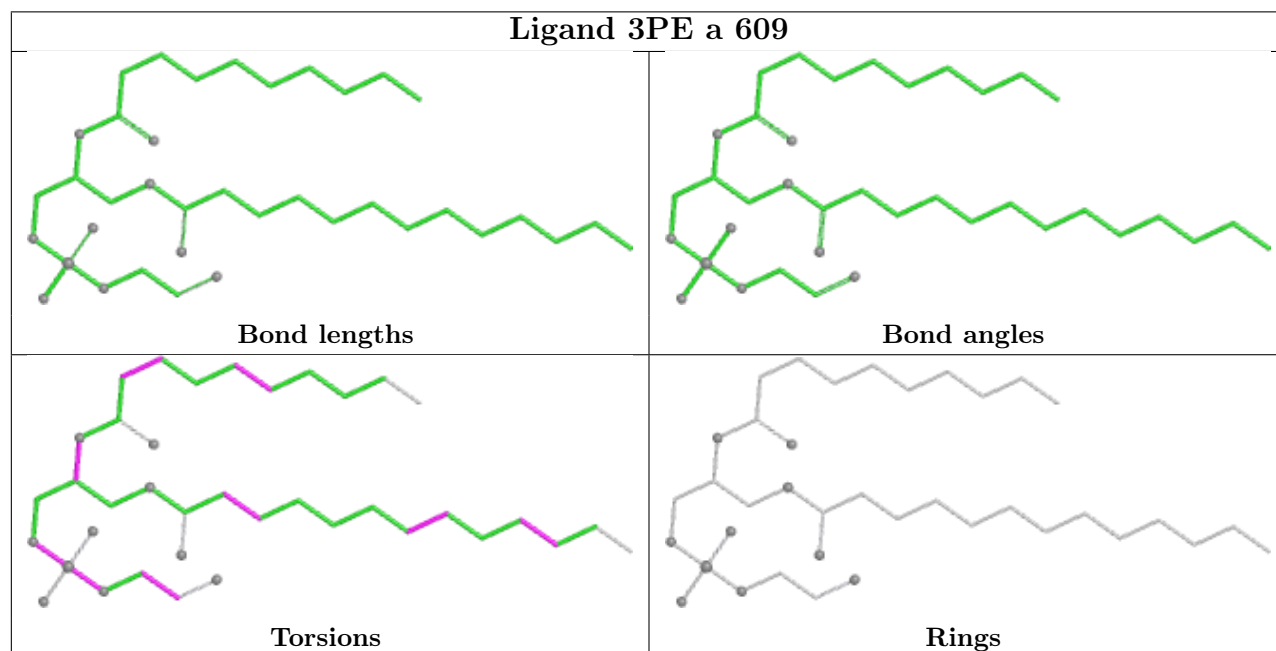
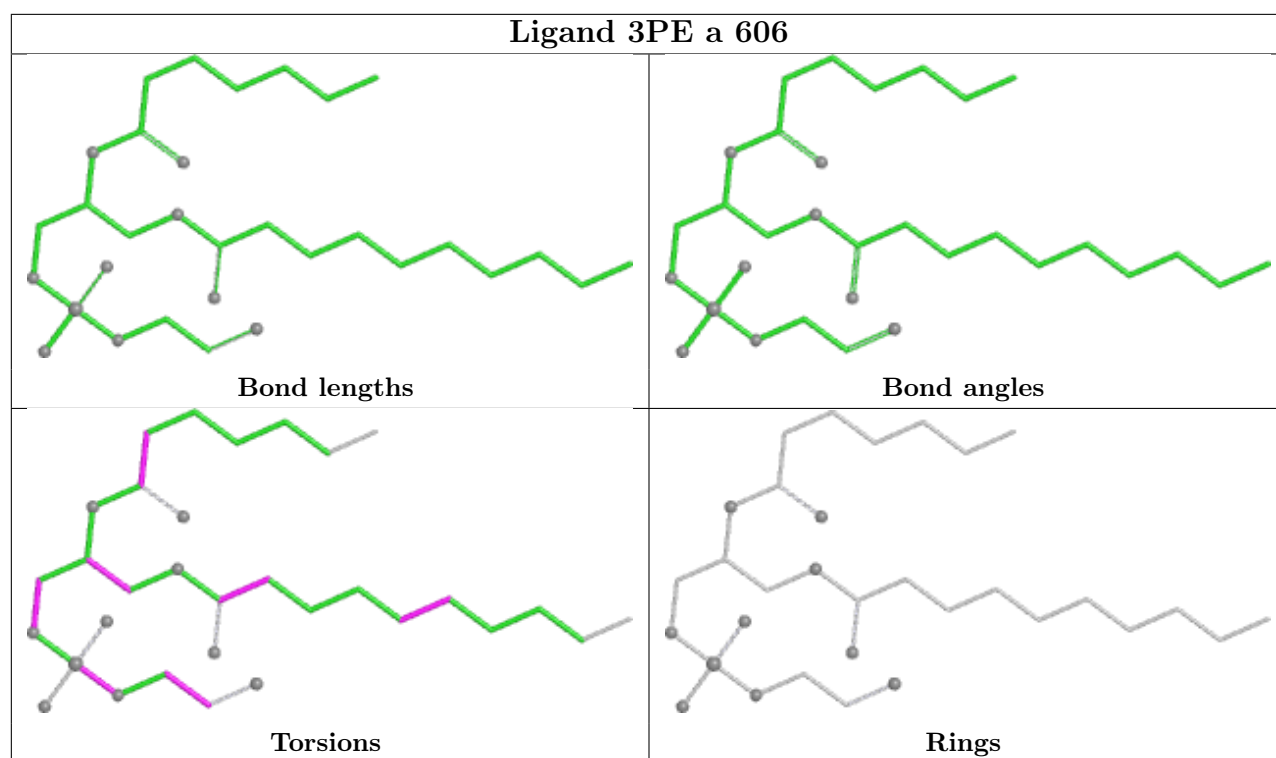


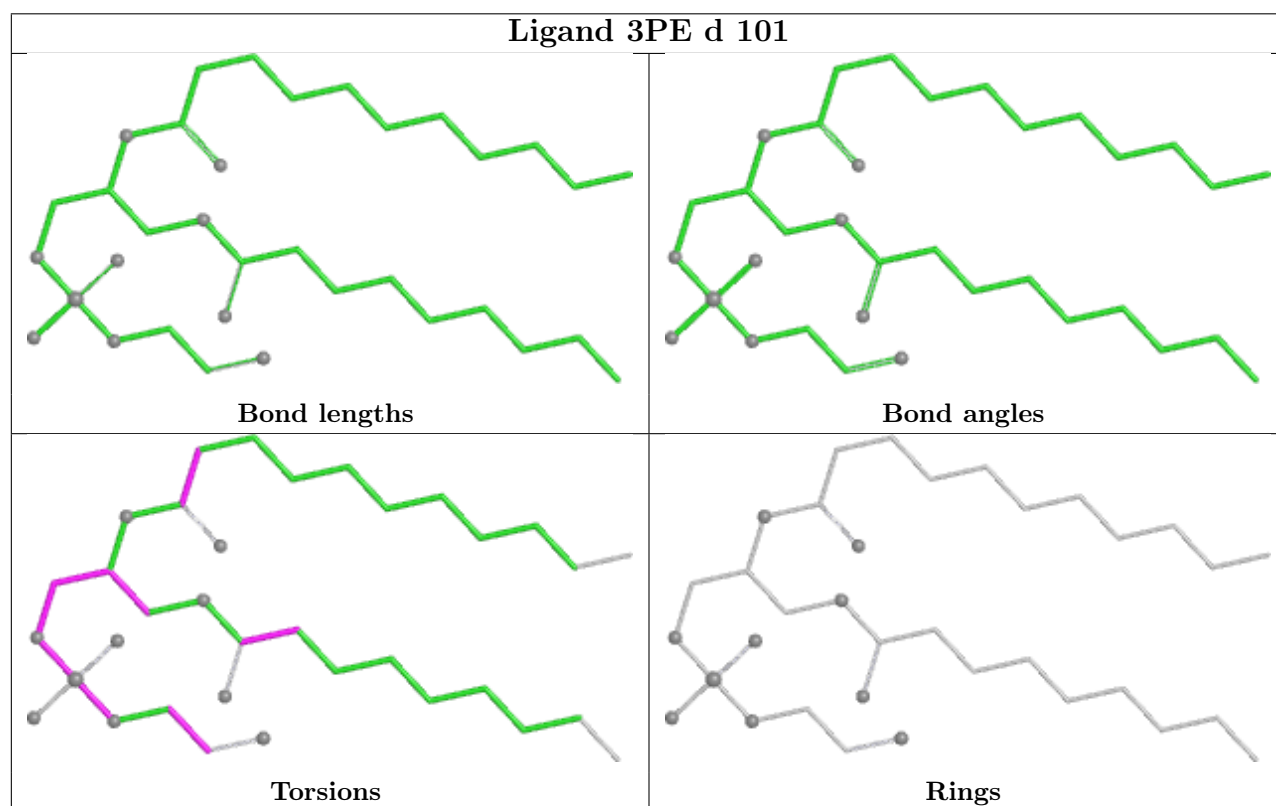
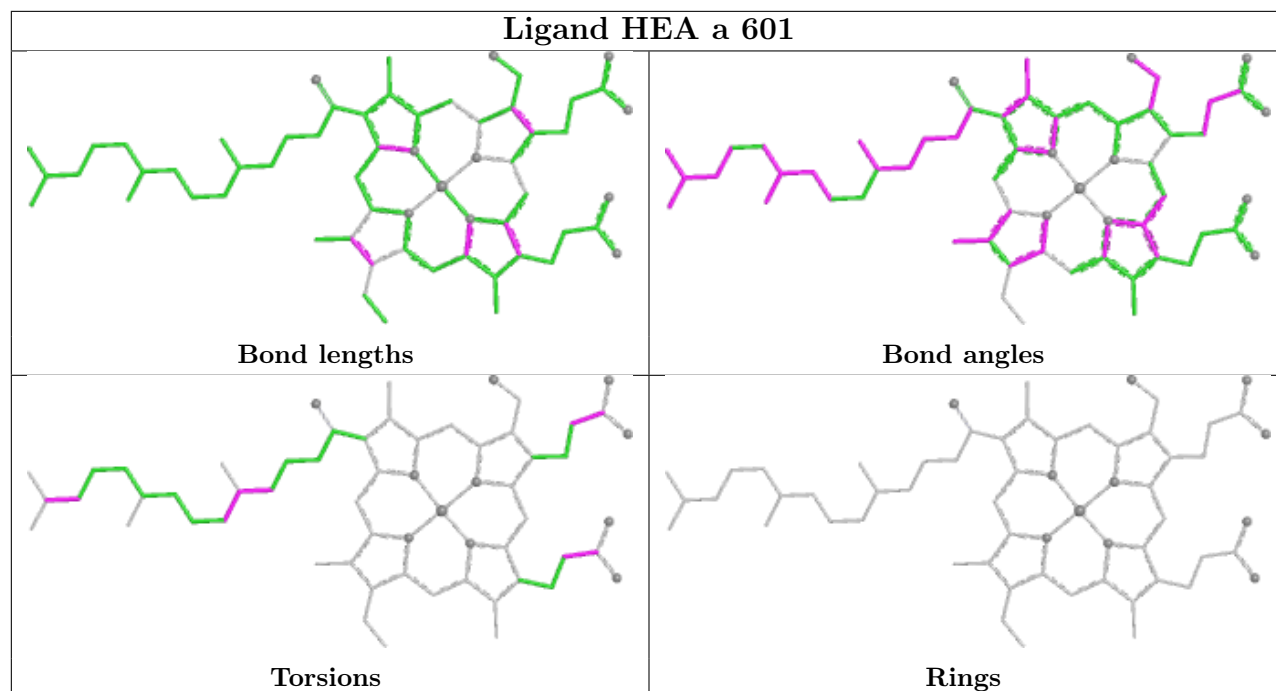


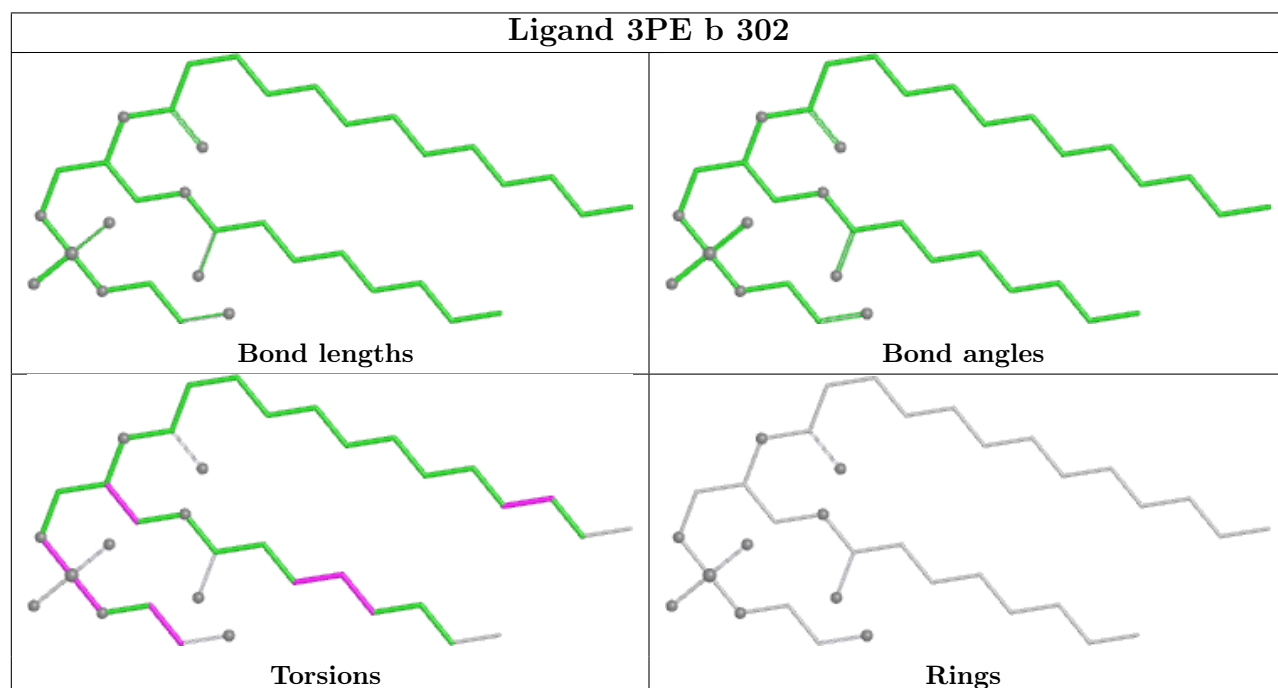
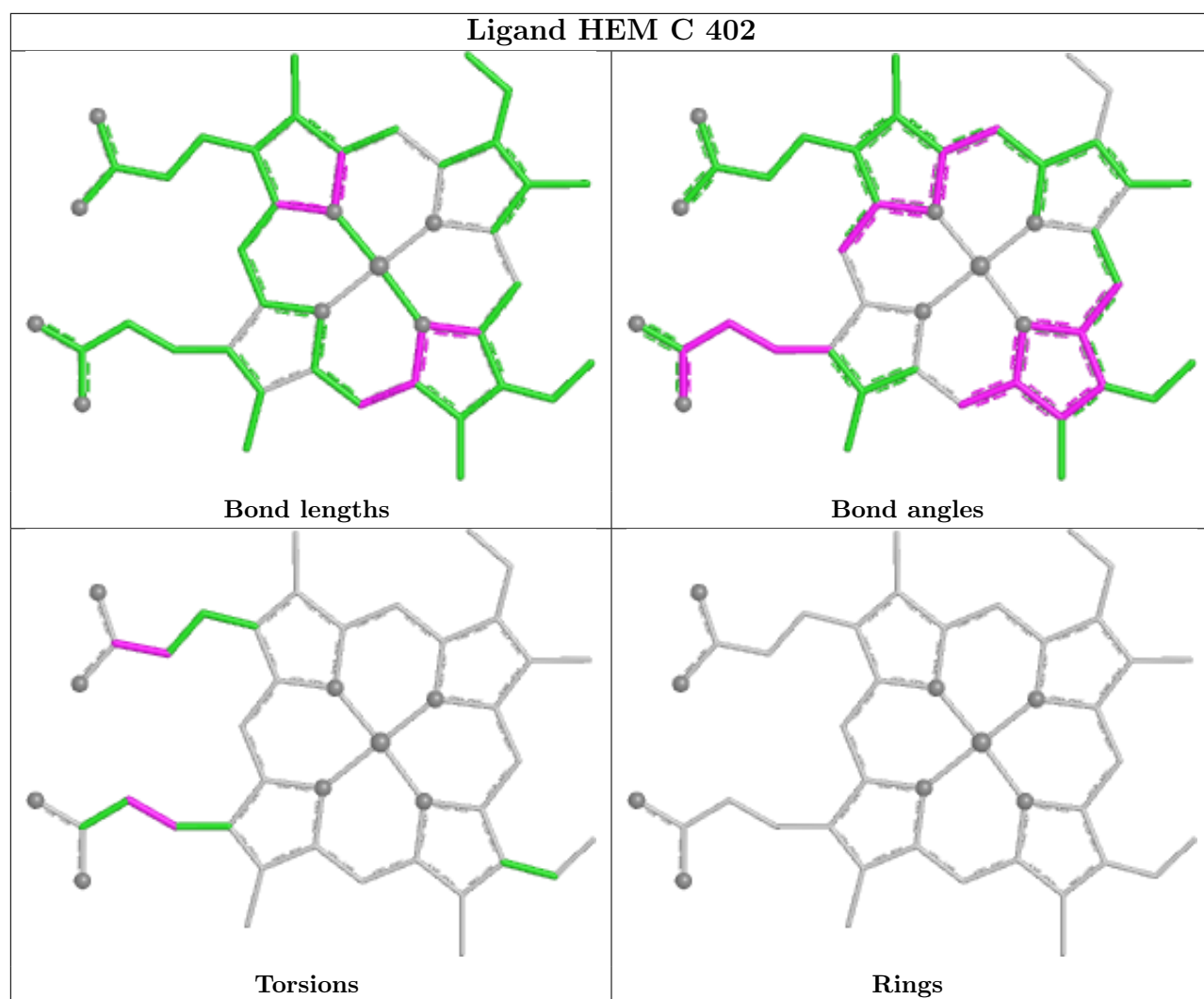


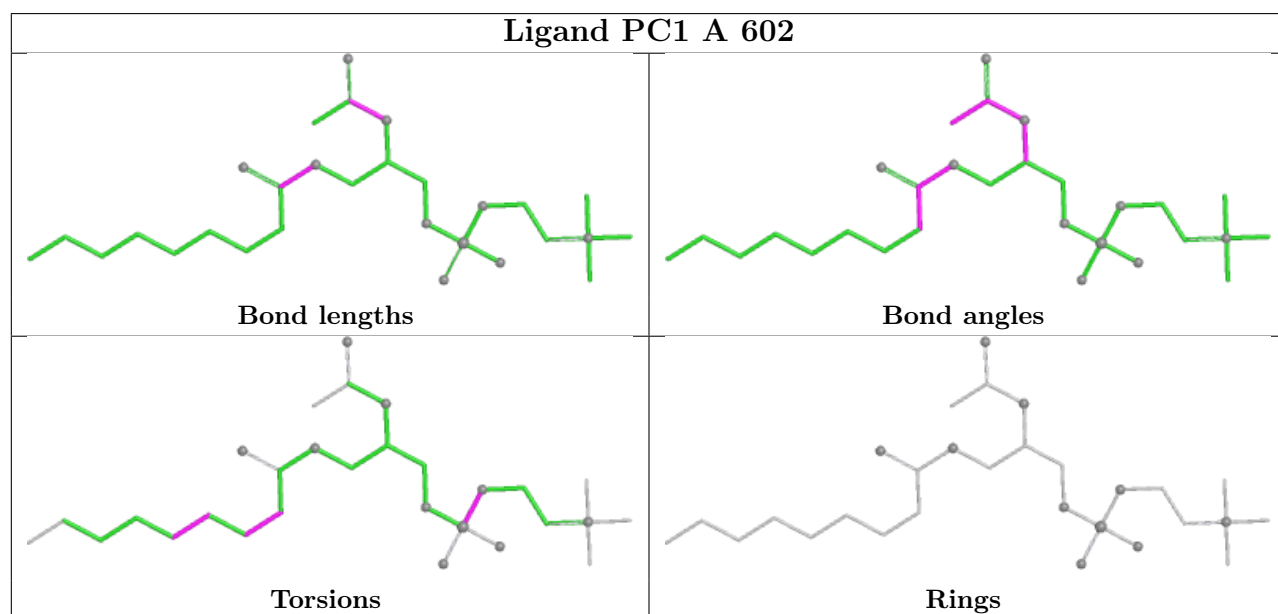
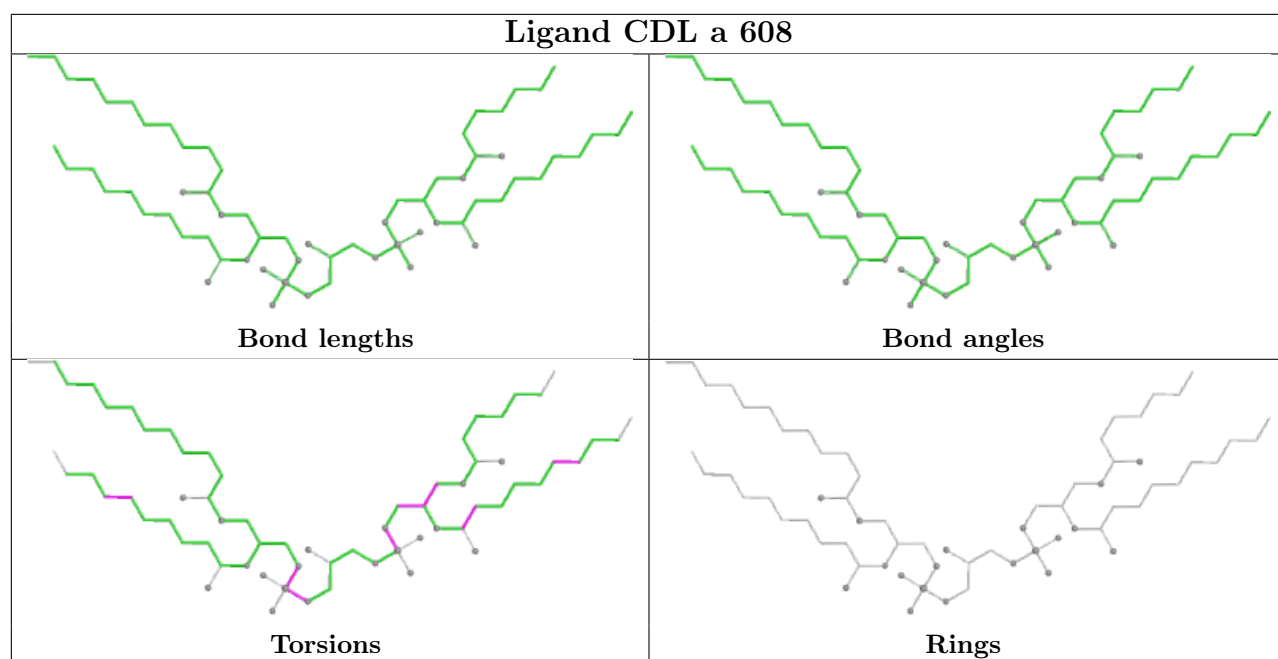


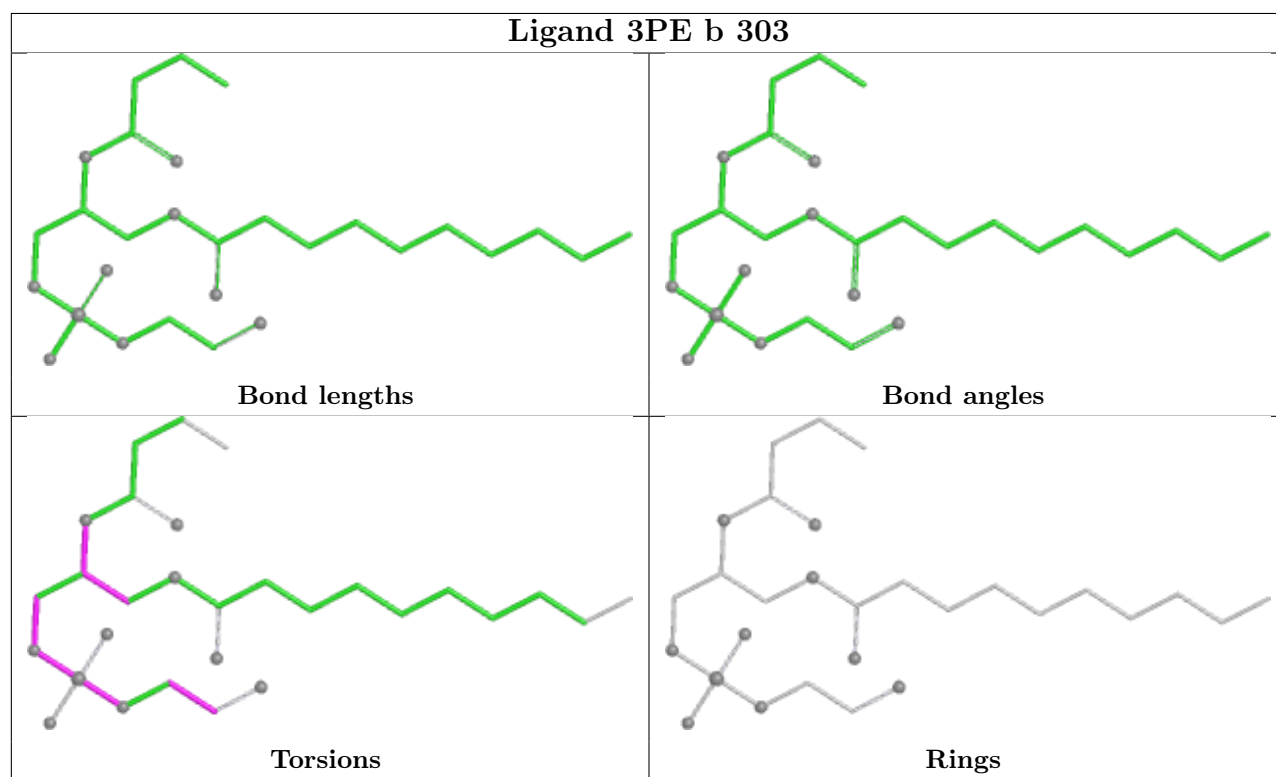
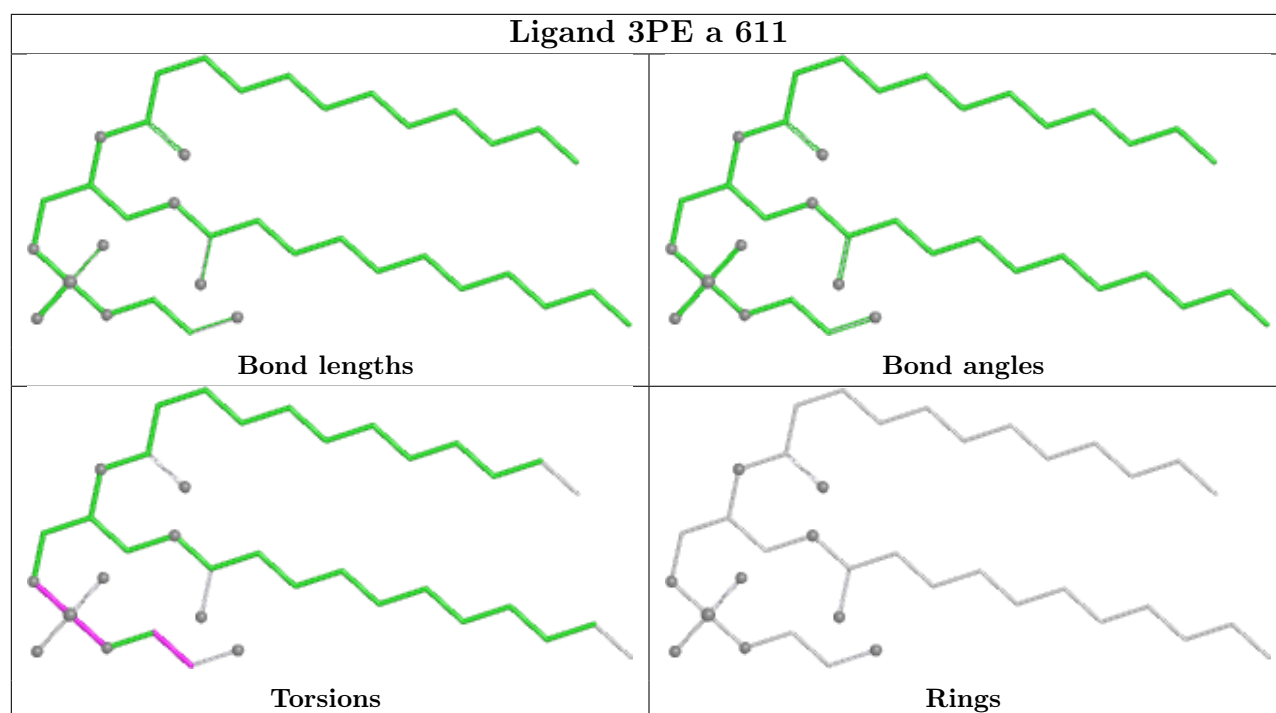


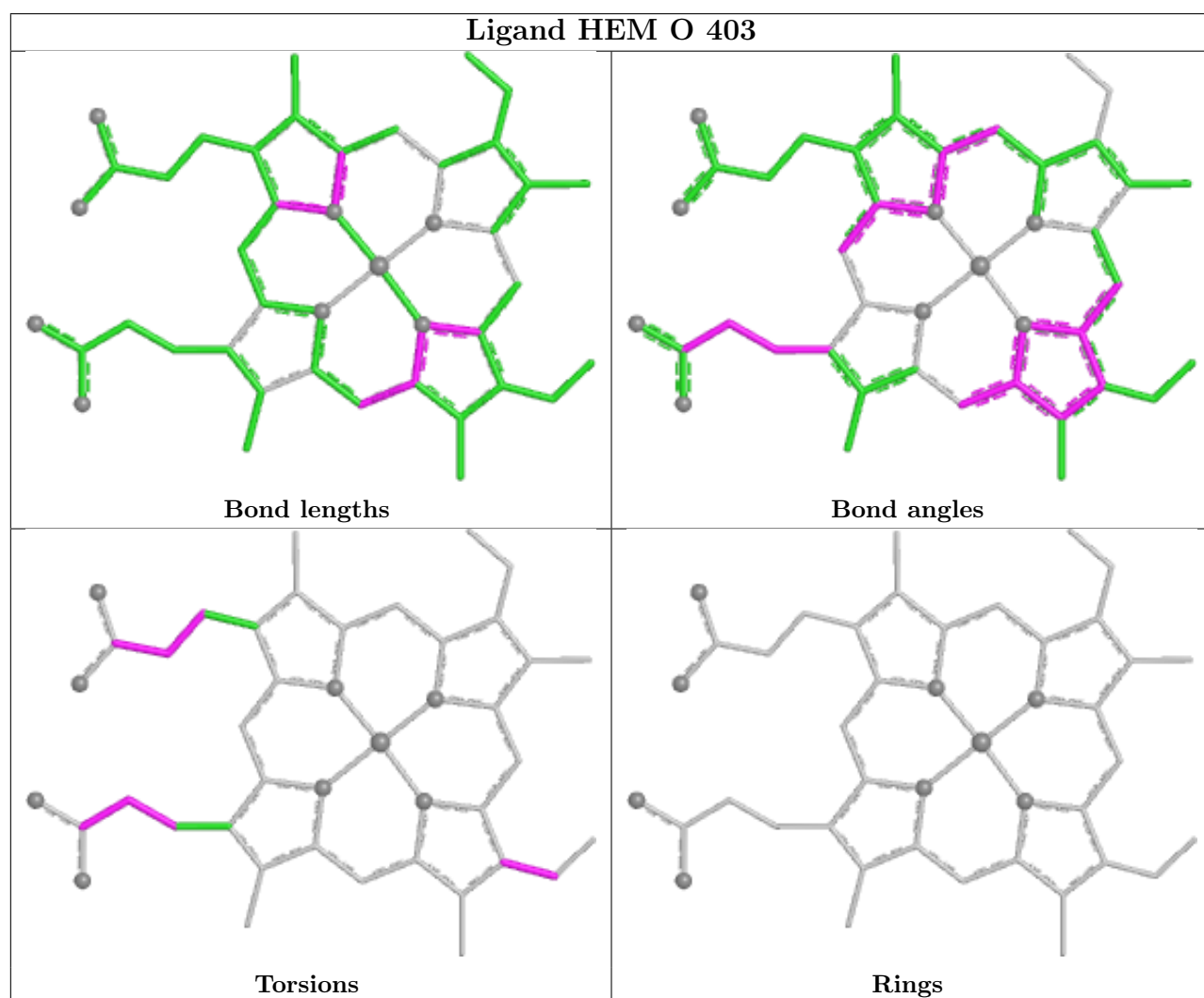
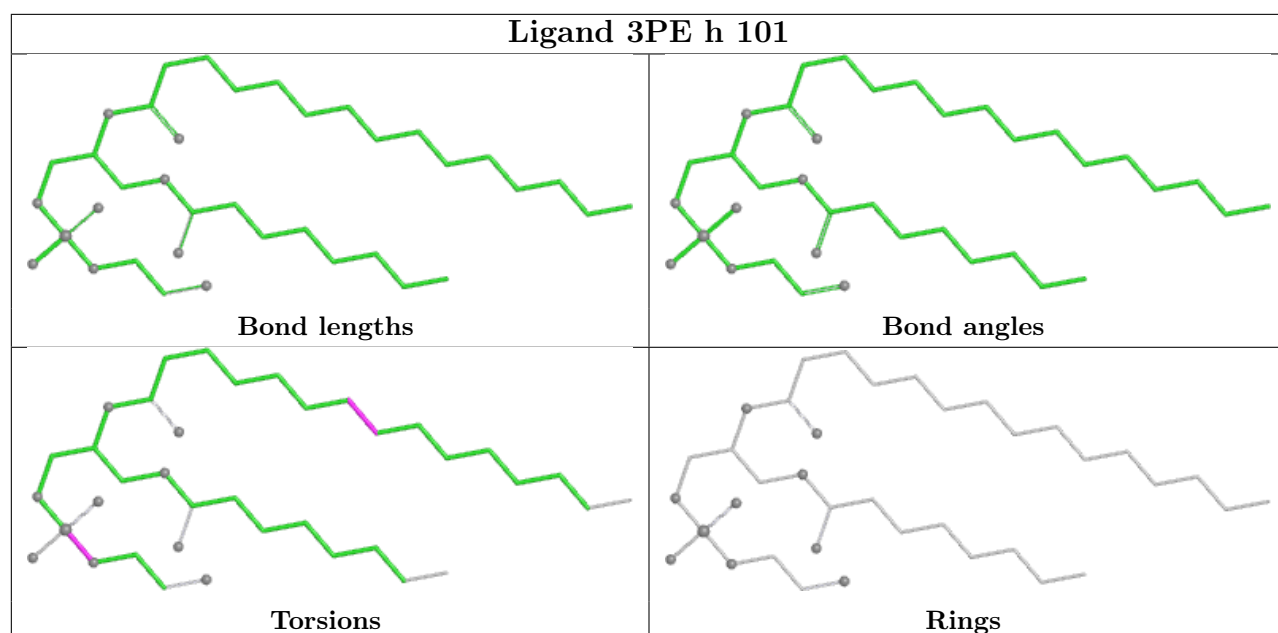




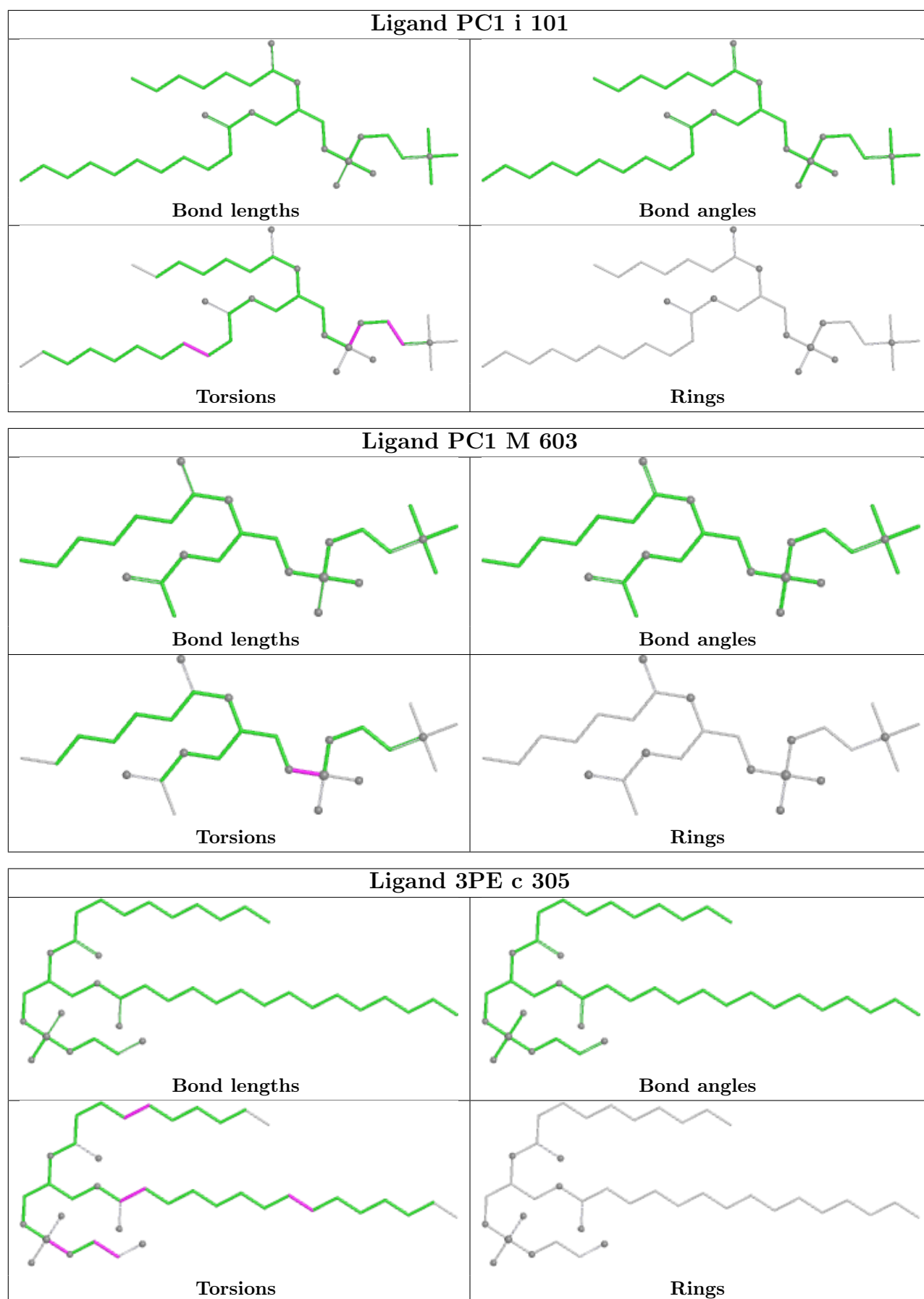


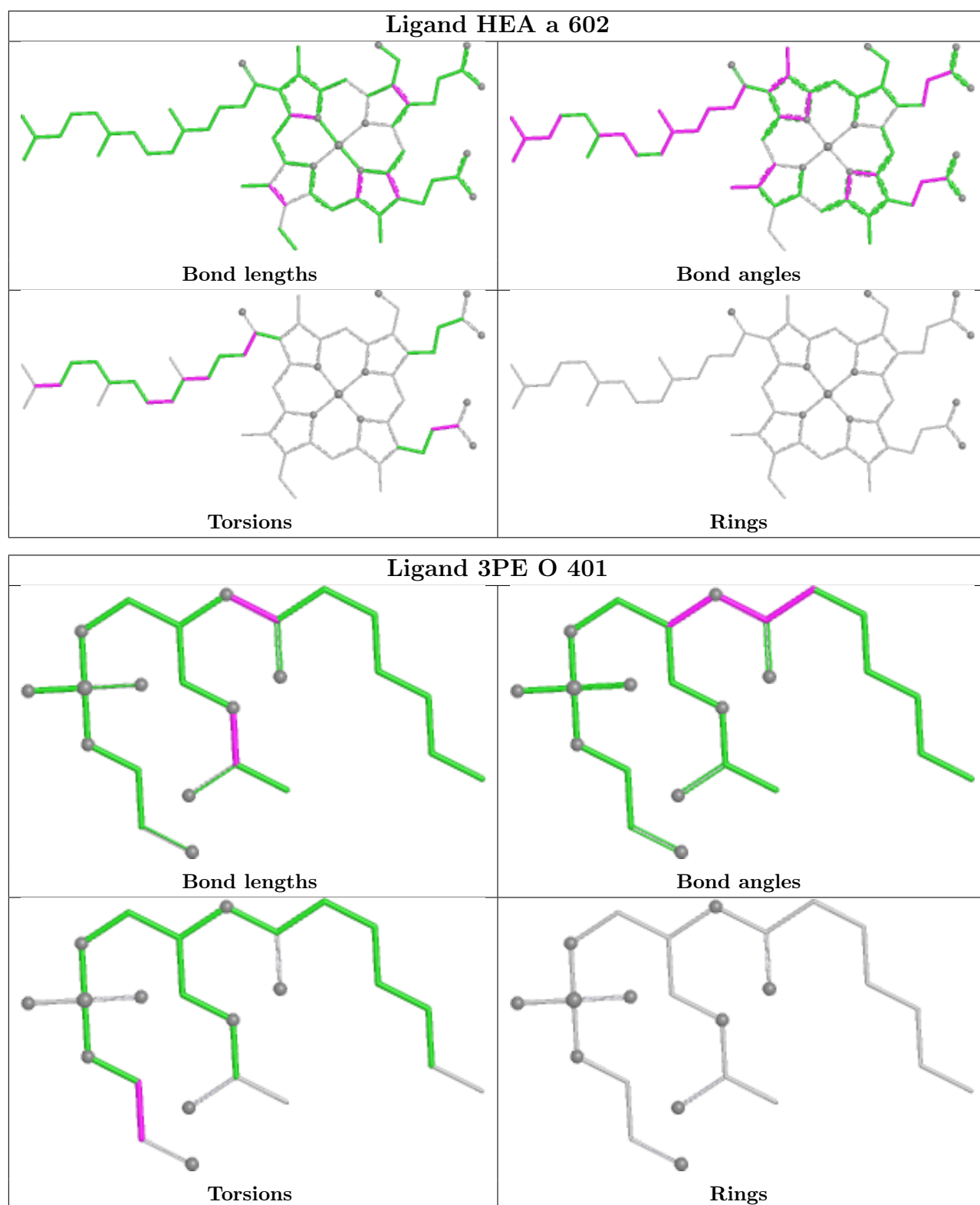


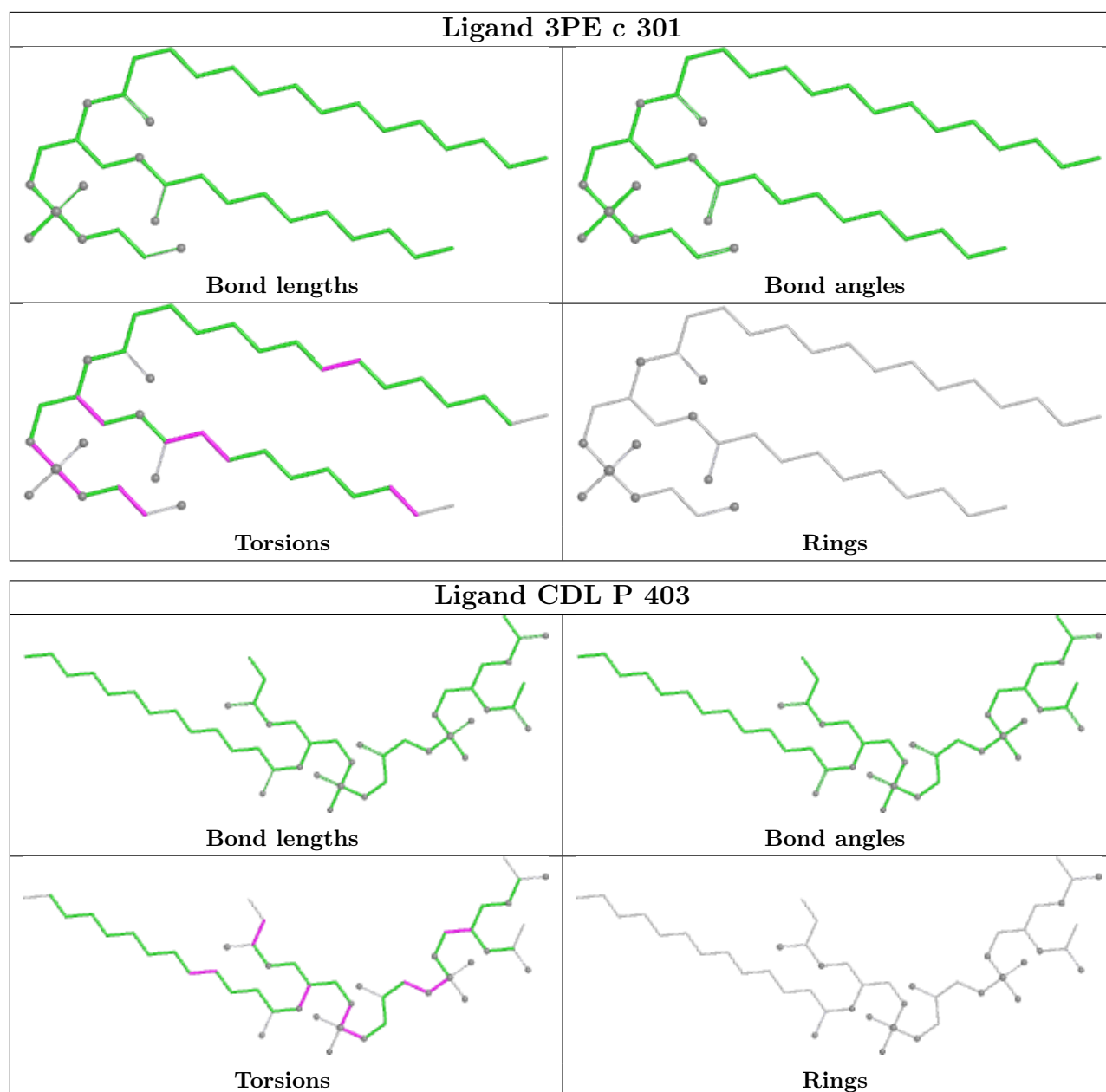


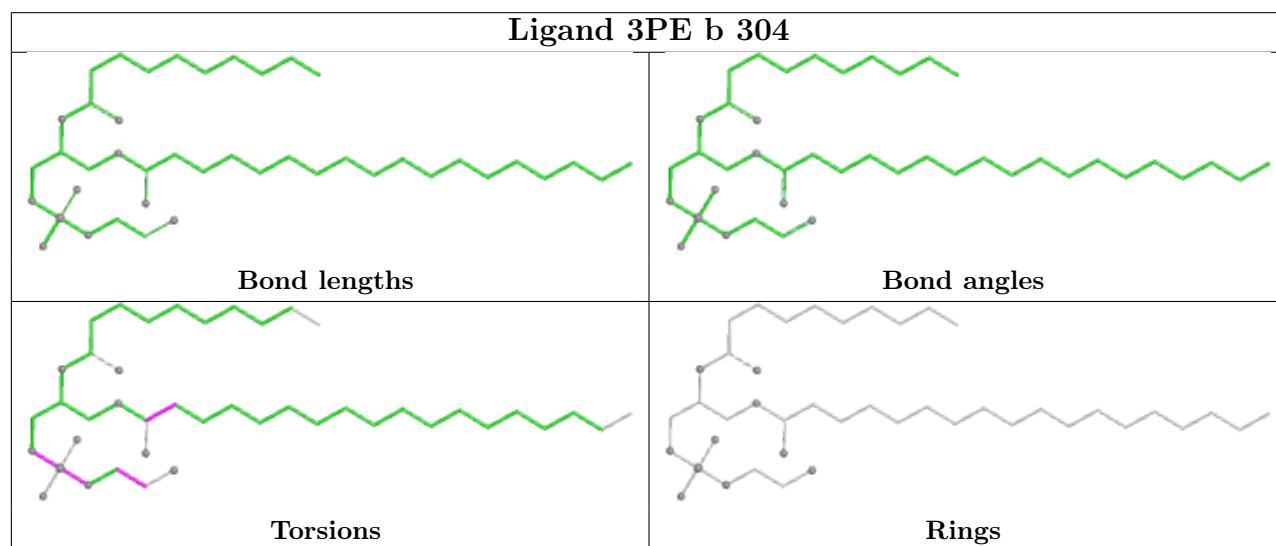
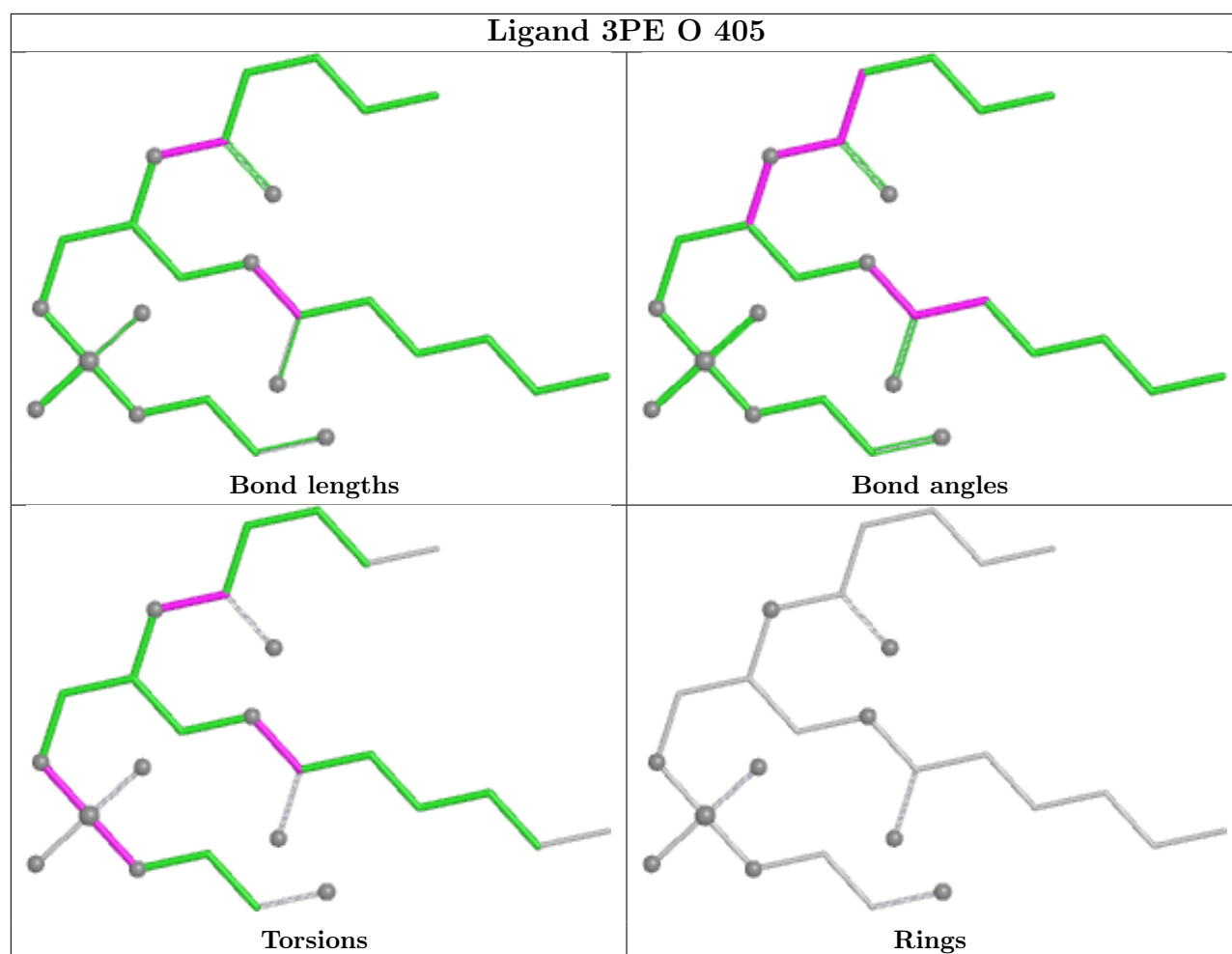


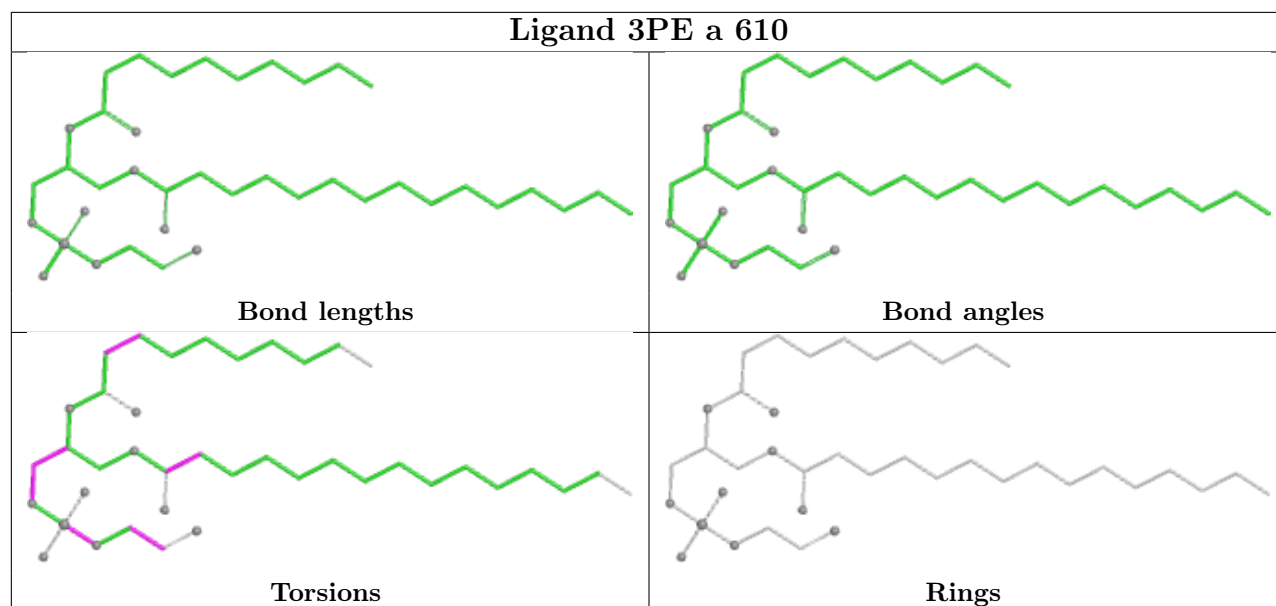
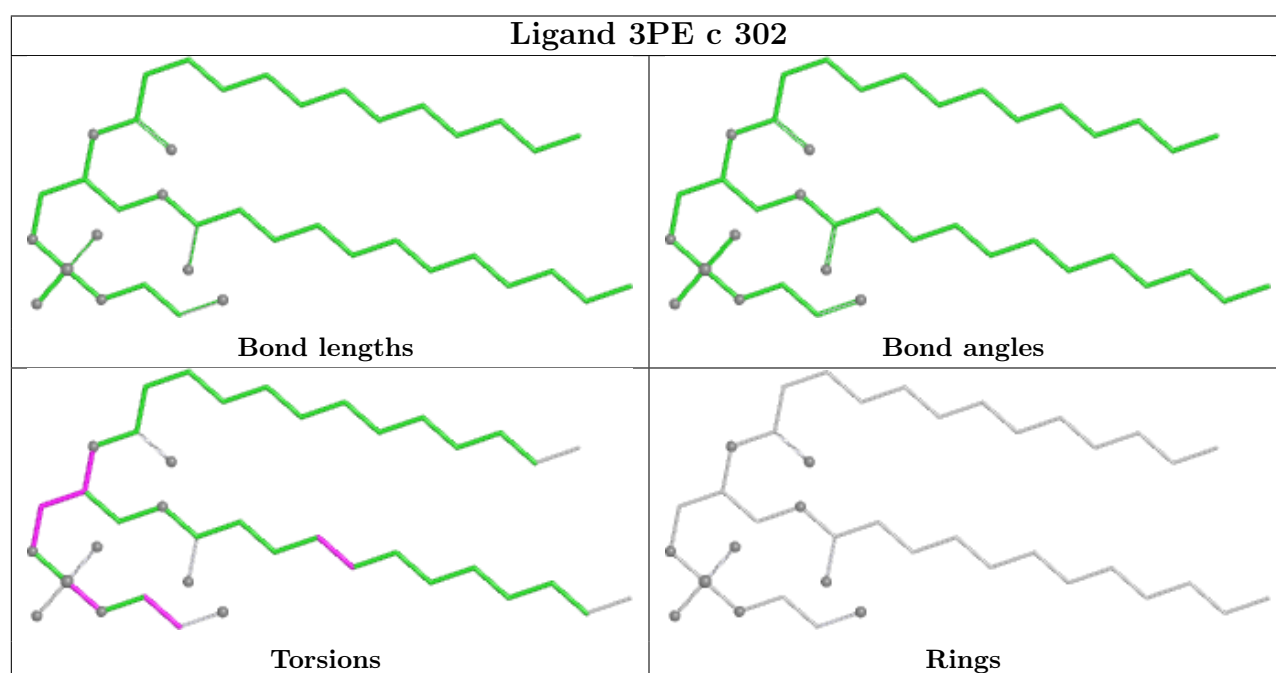
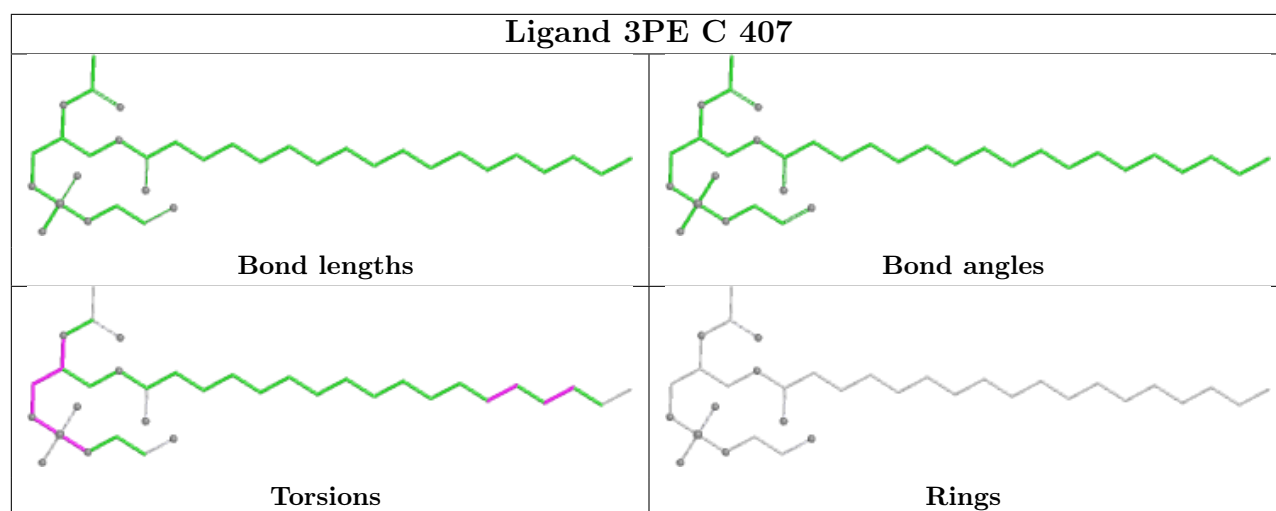


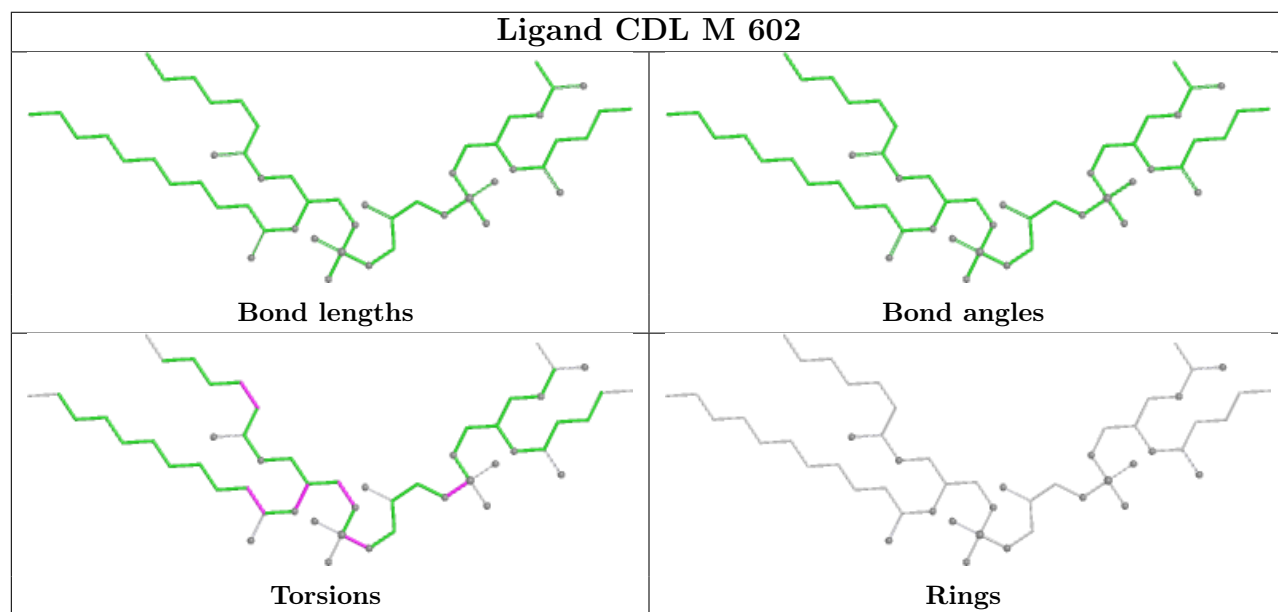
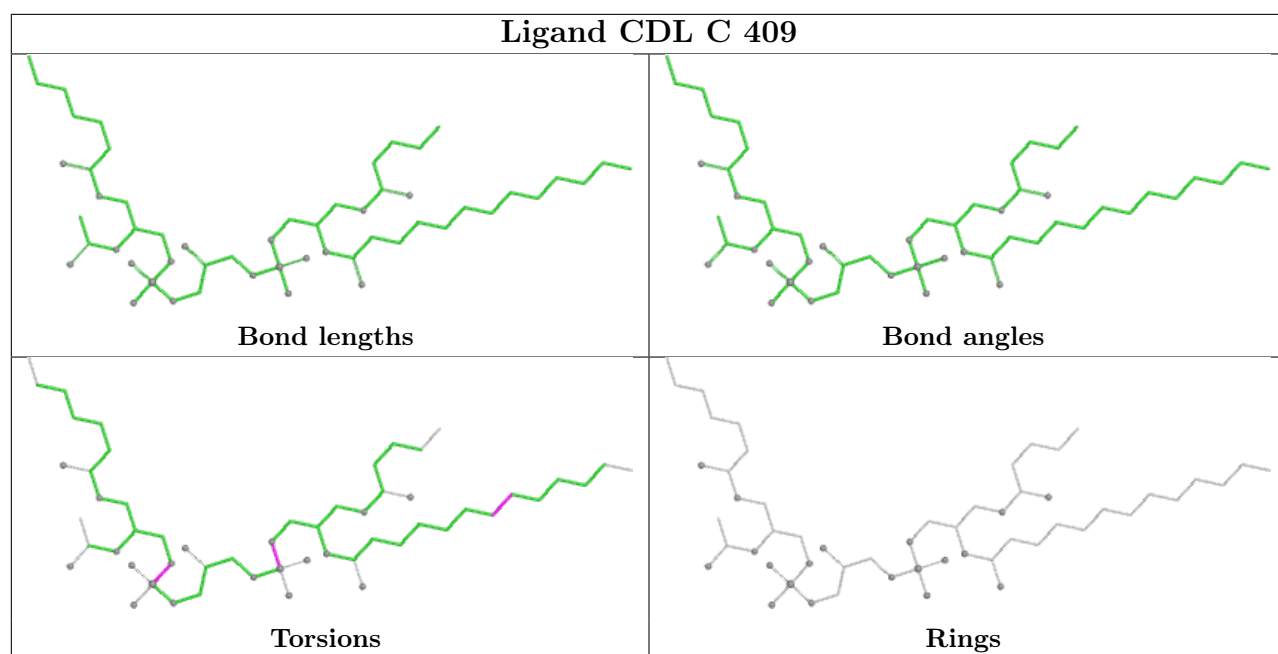


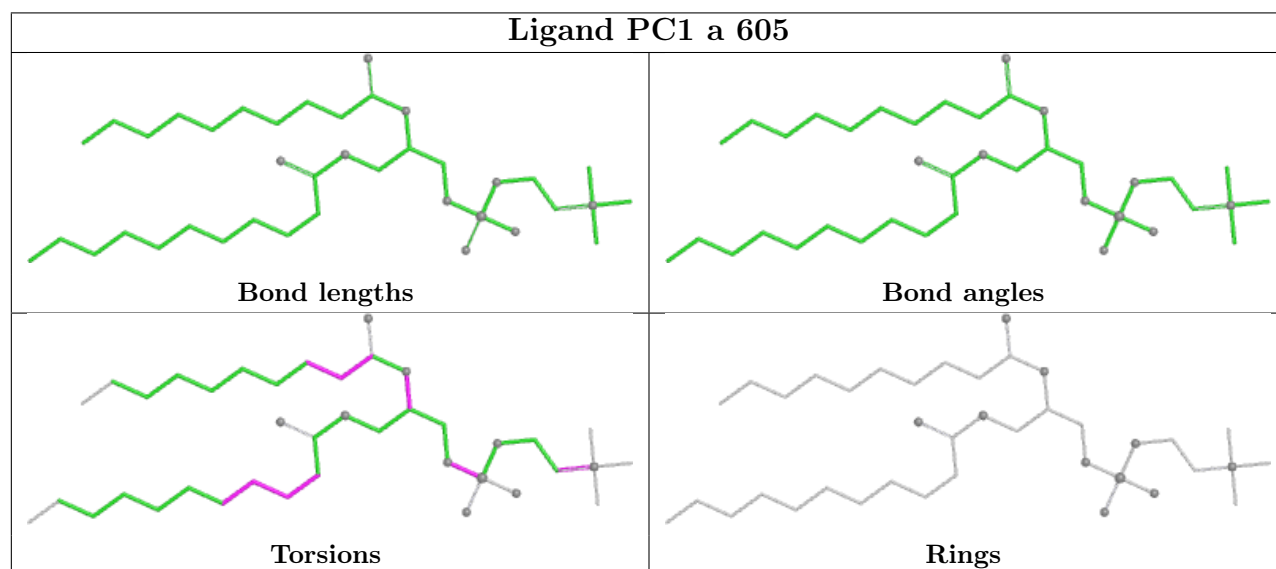
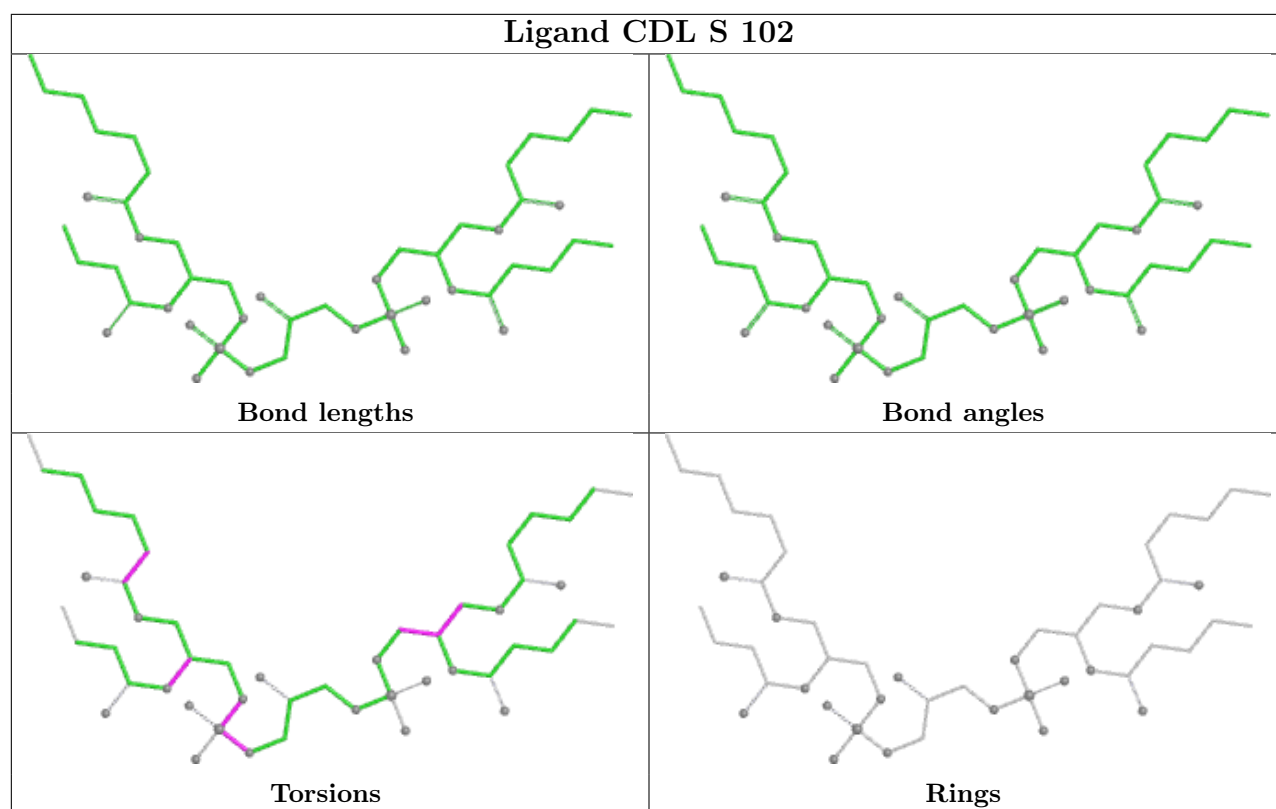


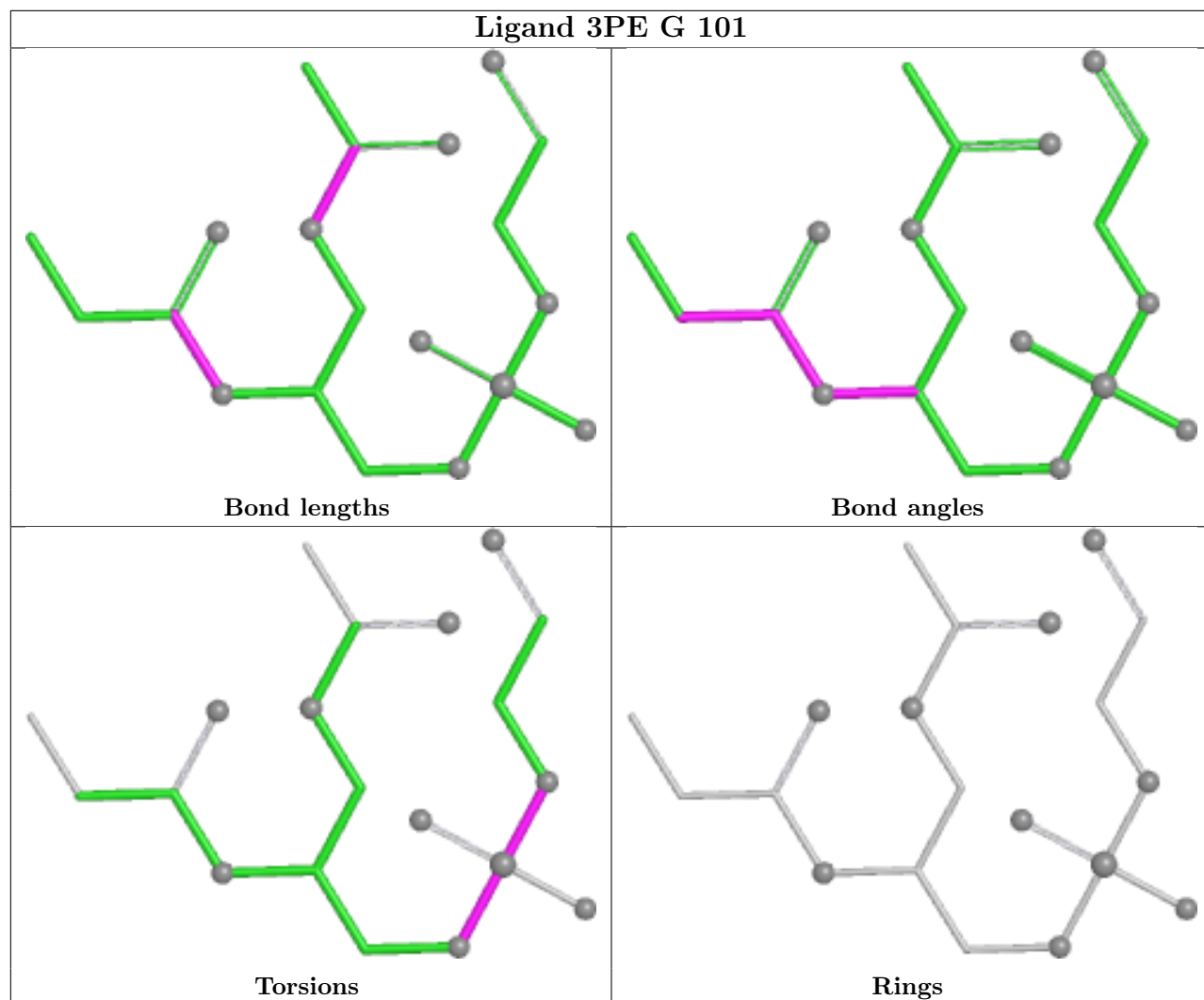




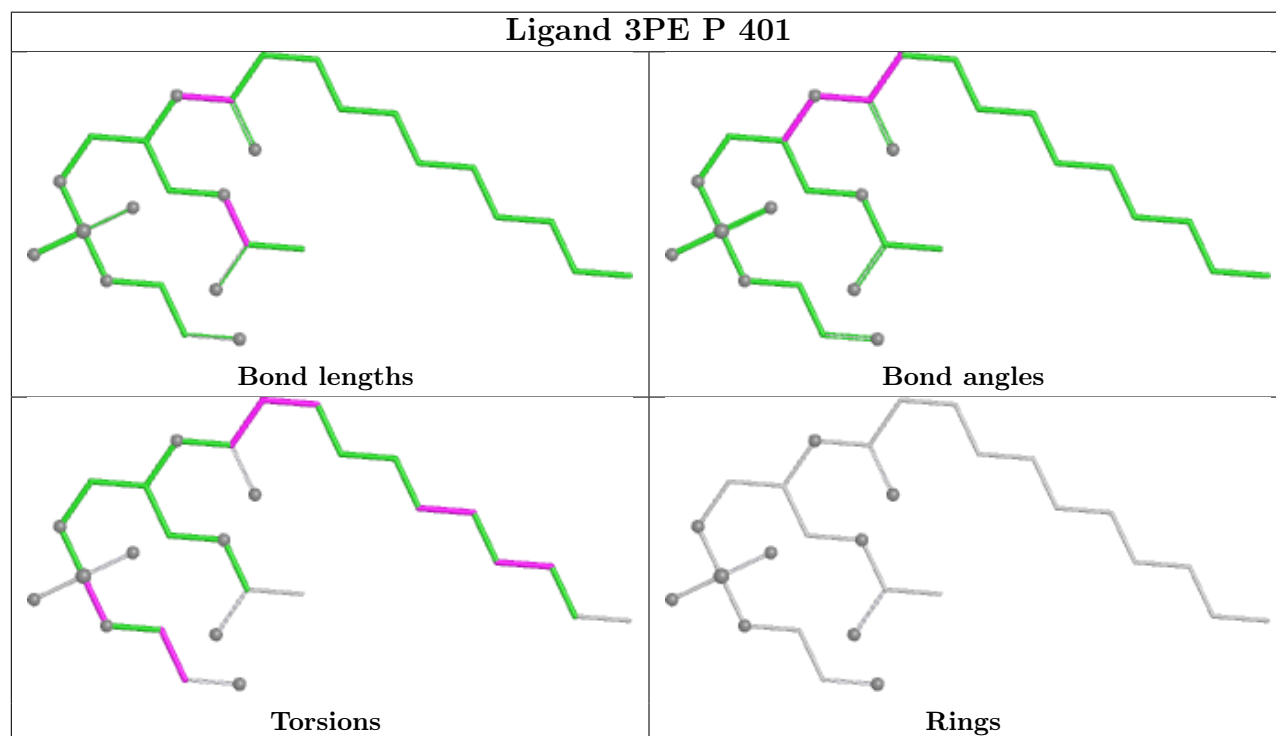
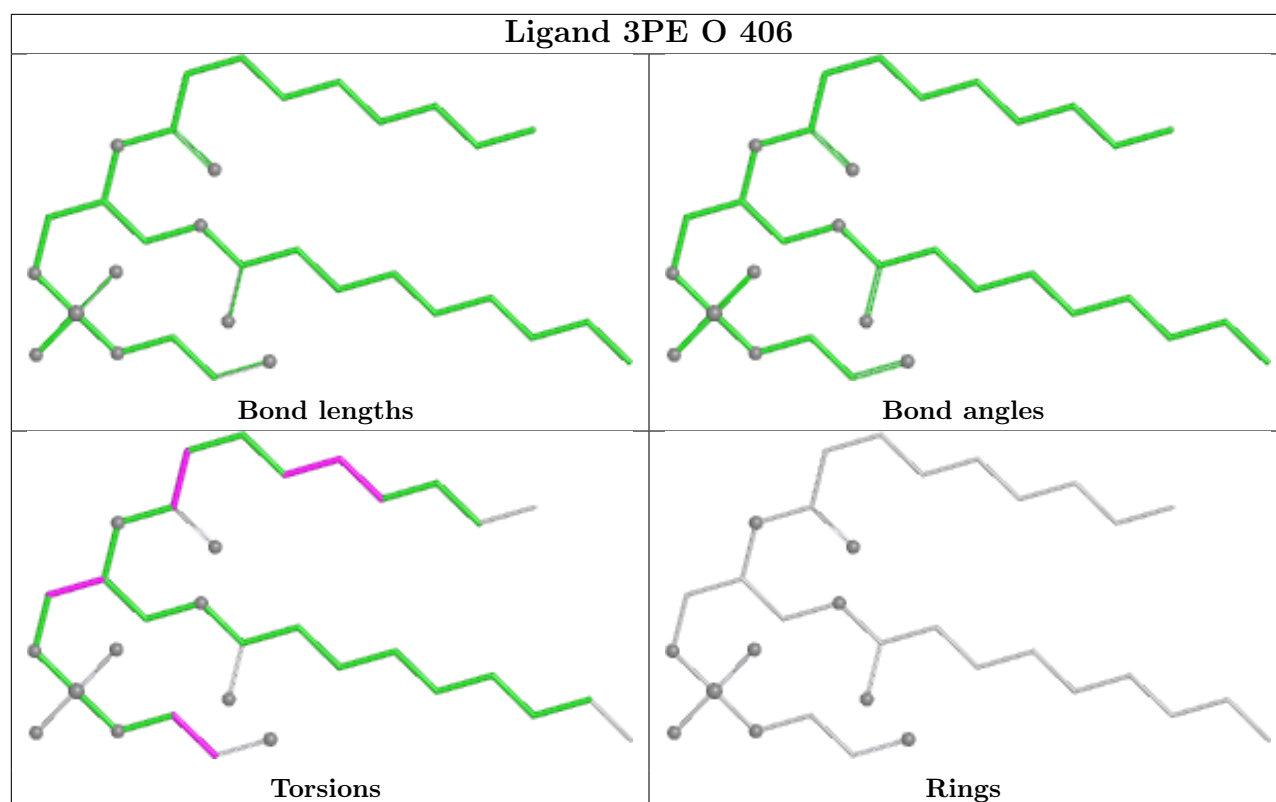


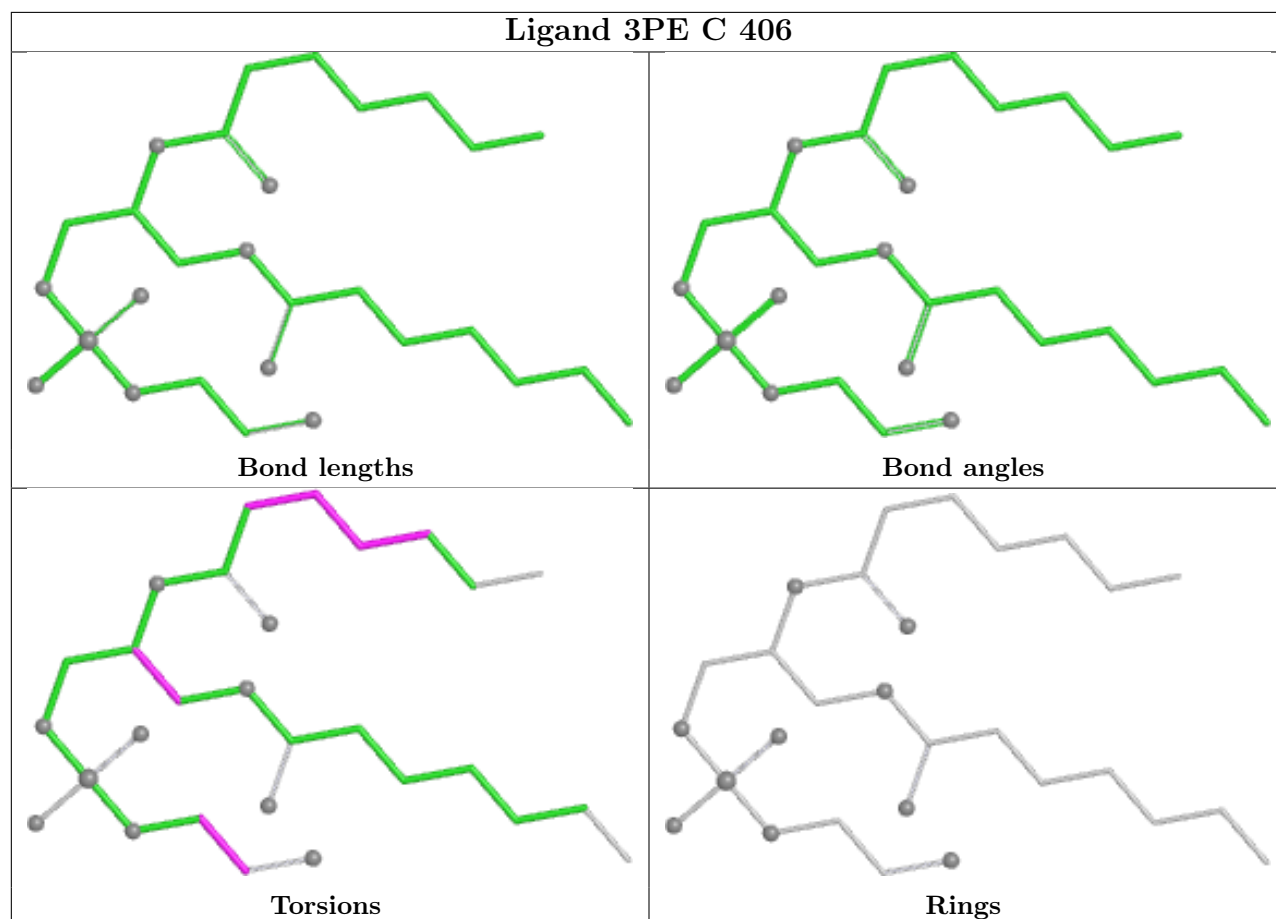
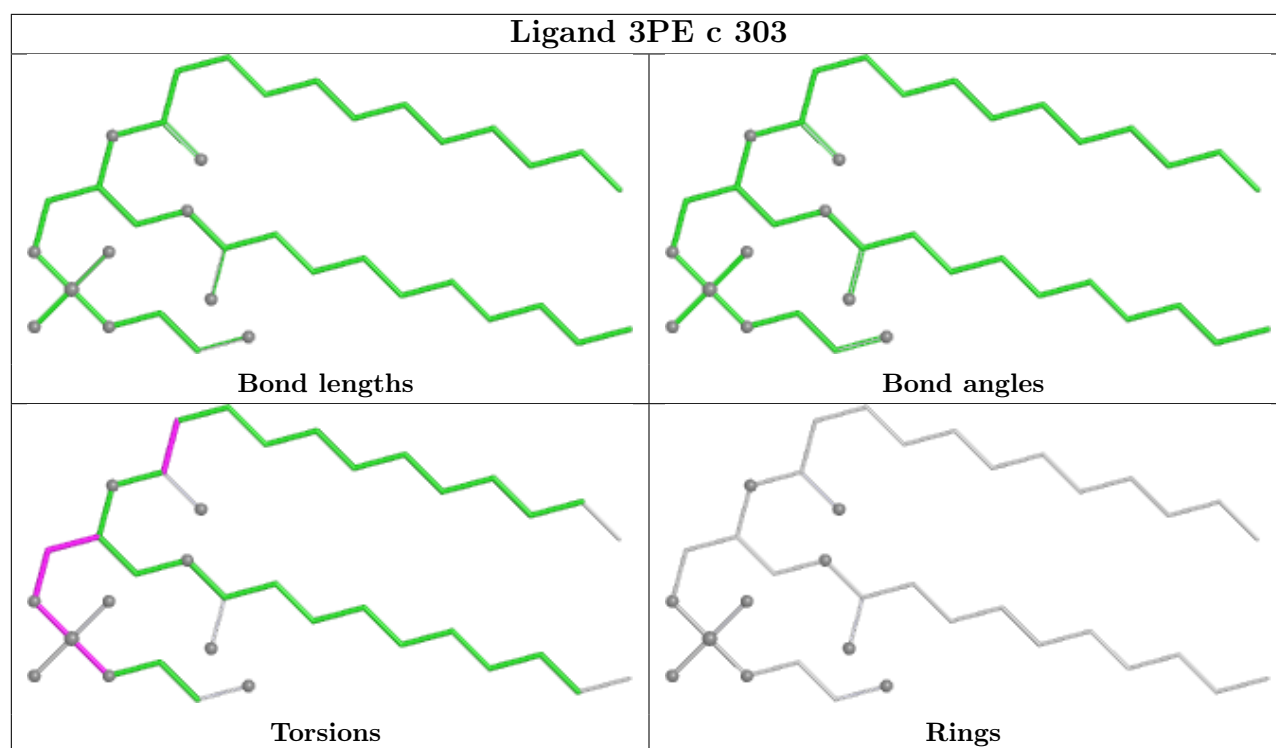


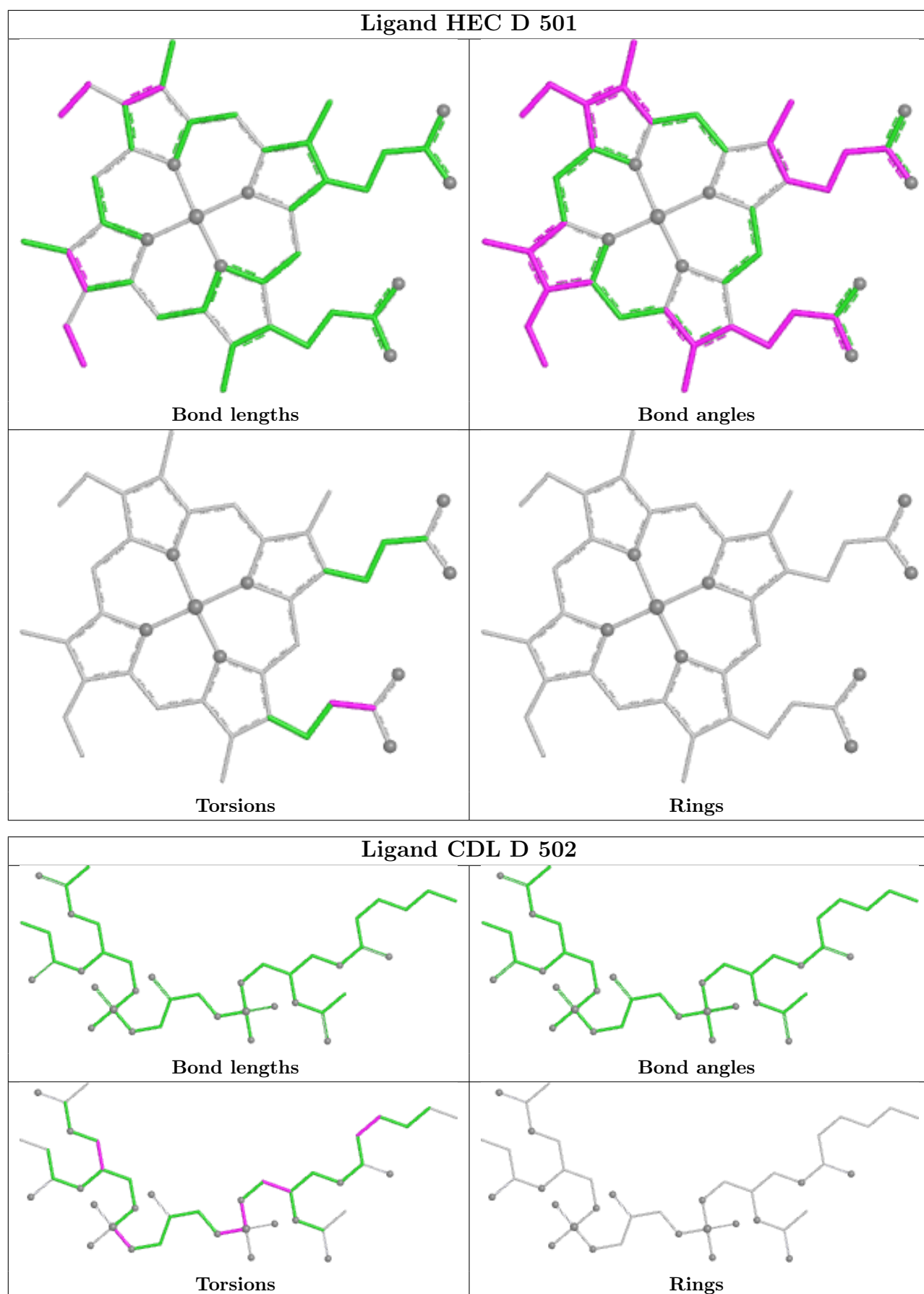


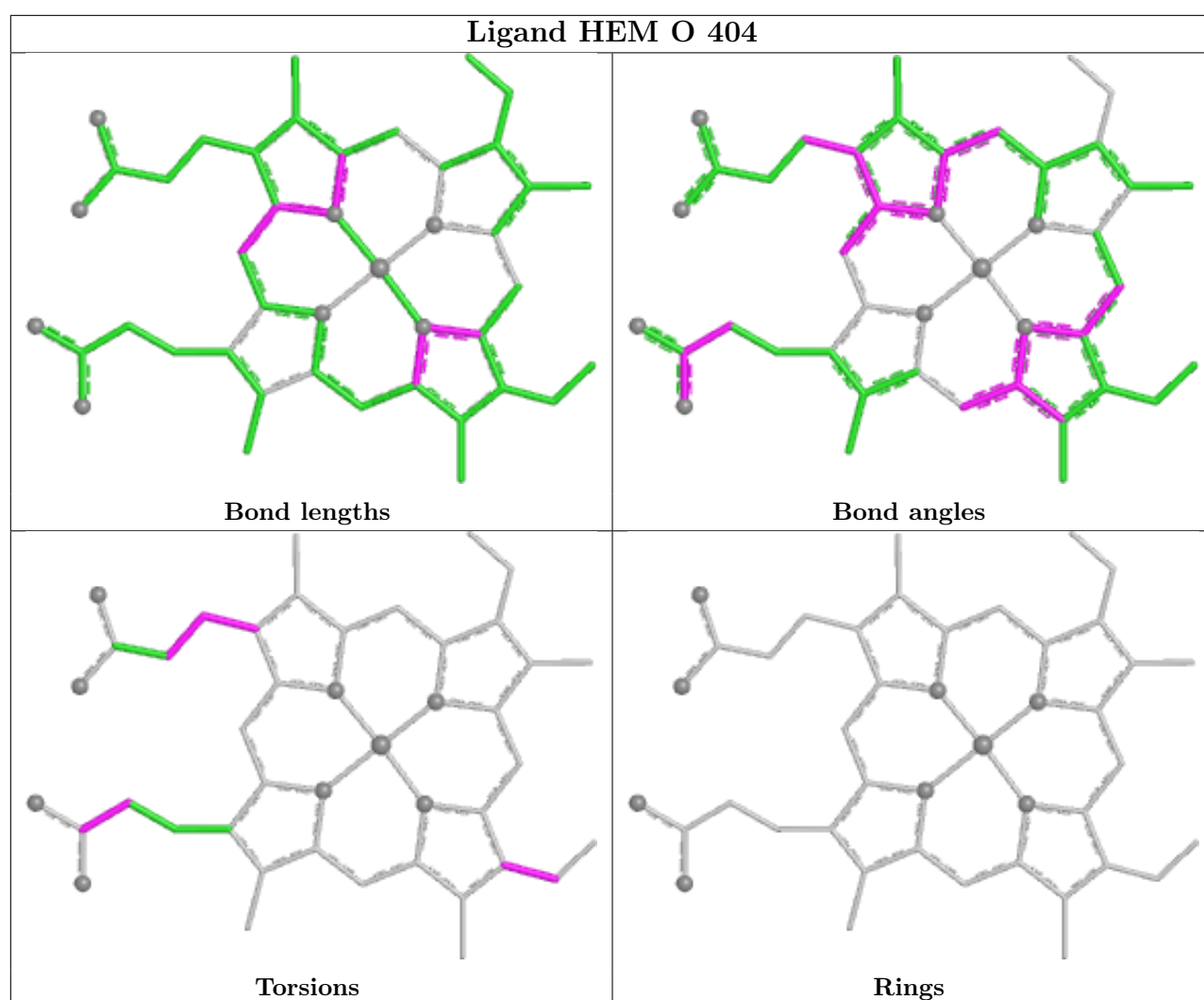
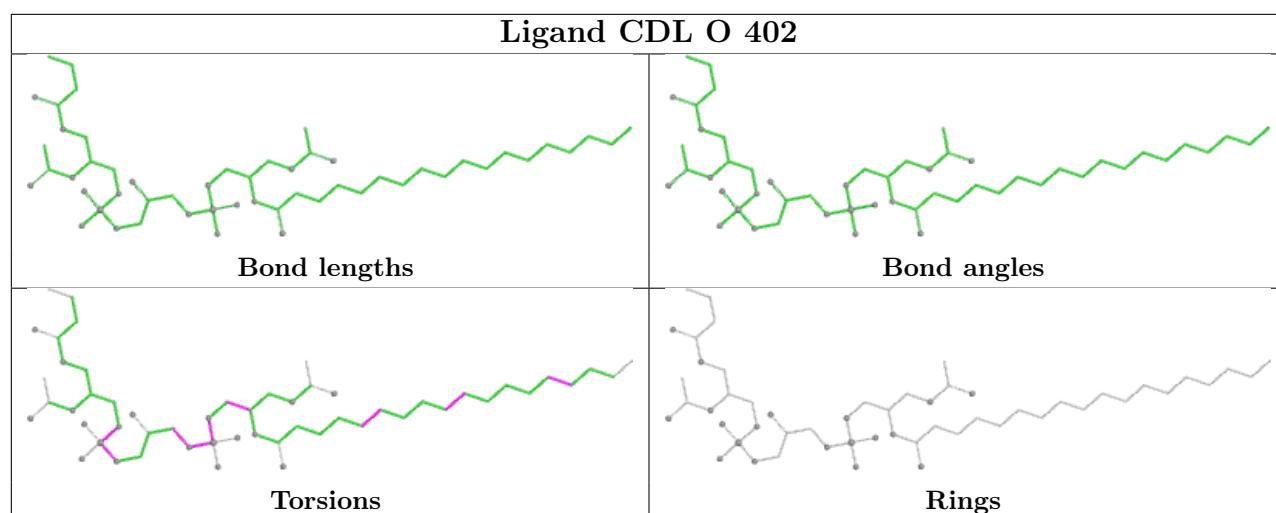


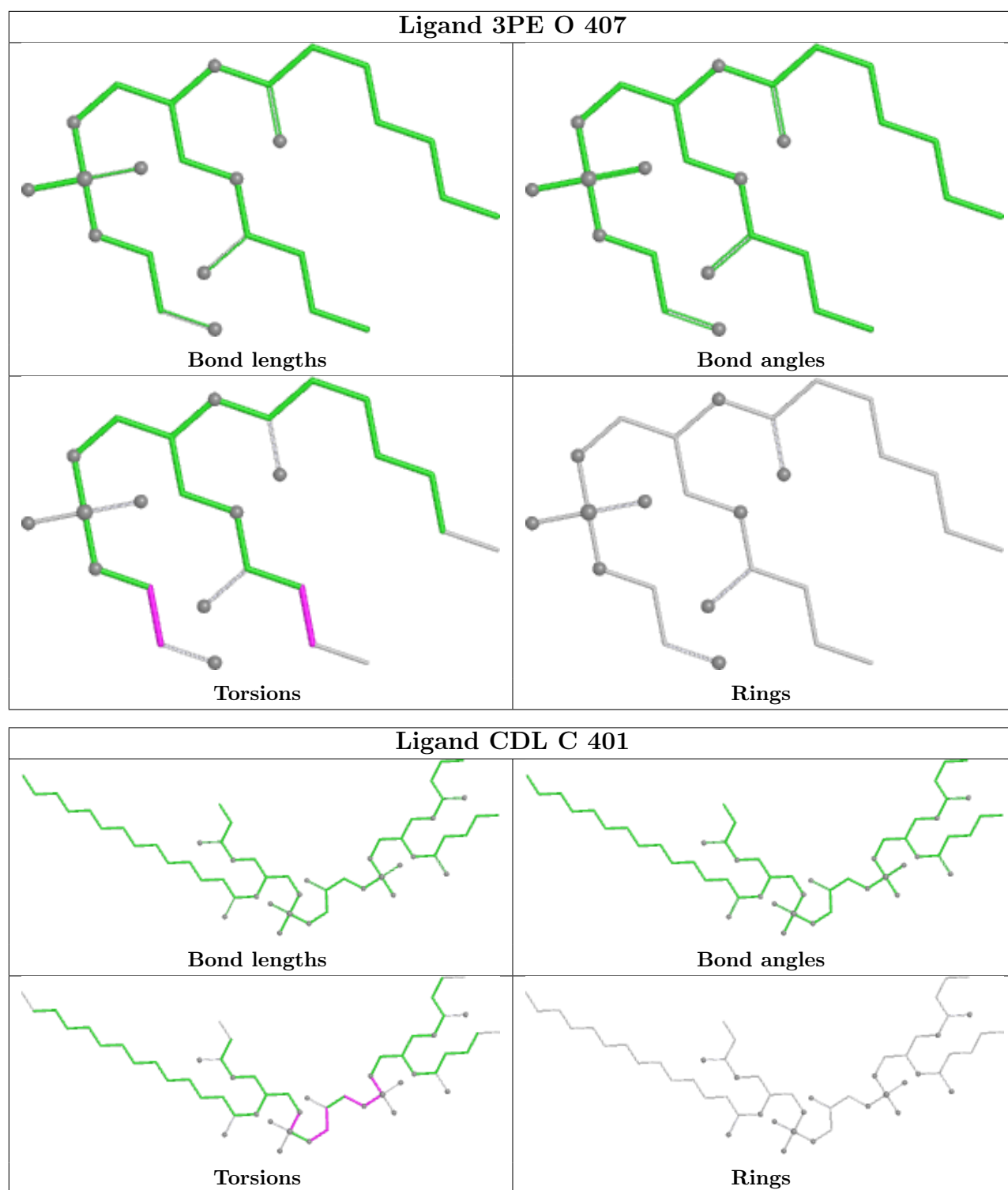












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

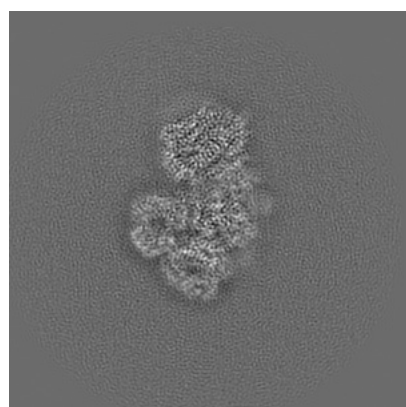
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22448. These allow visual inspection of the internal detail of the map and identification of artifacts.

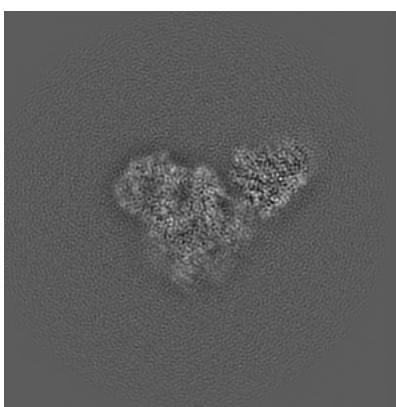
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

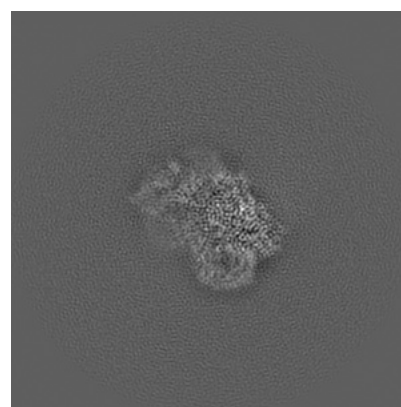
#### 6.1.1 Primary map



X



Y

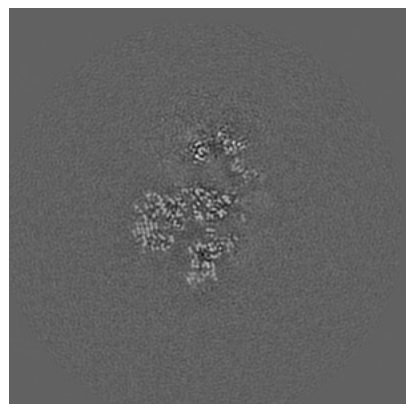


Z

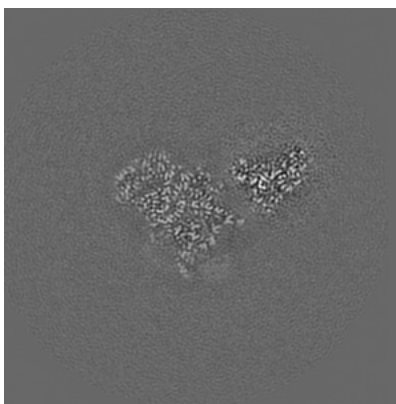
The images above show the map projected in three orthogonal directions.

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

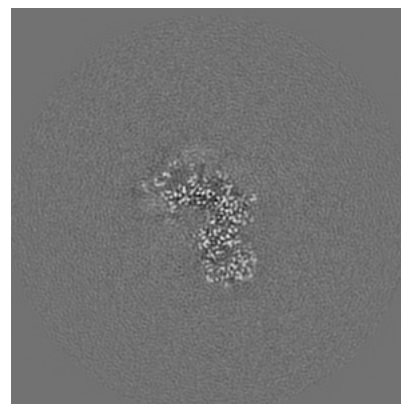
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

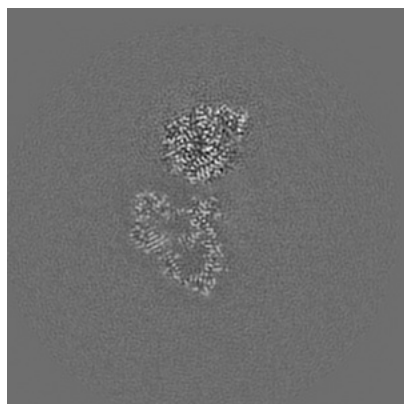


Z Index: 256

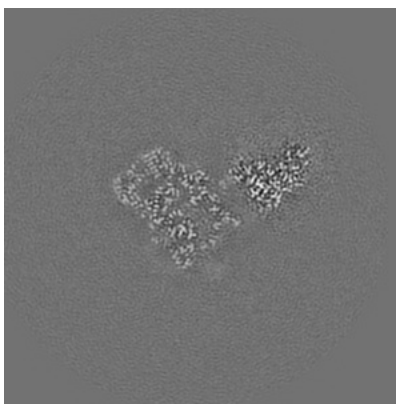
The images above show central slices of the map in three orthogonal directions.

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

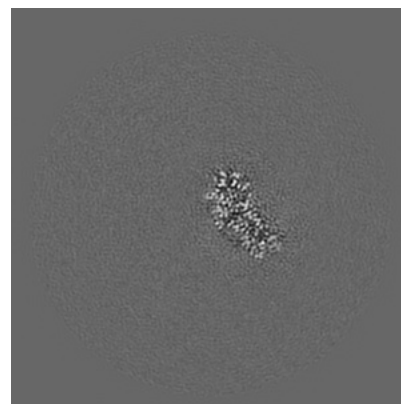
### 6.3.1 Primary map



X Index: 294



Y Index: 251

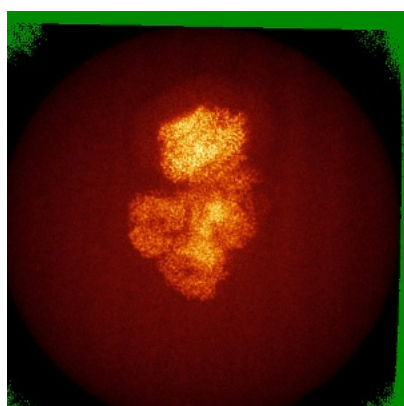


Z Index: 349

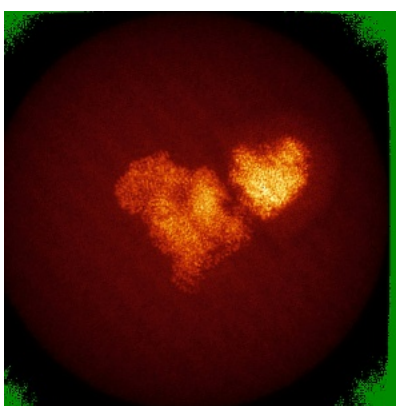
The images above show the largest variance slices of the map in three orthogonal directions.

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

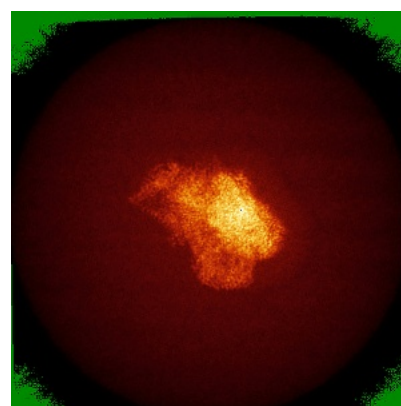
### 6.4.1 Primary map



X



Y



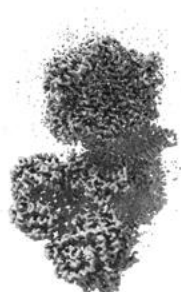
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

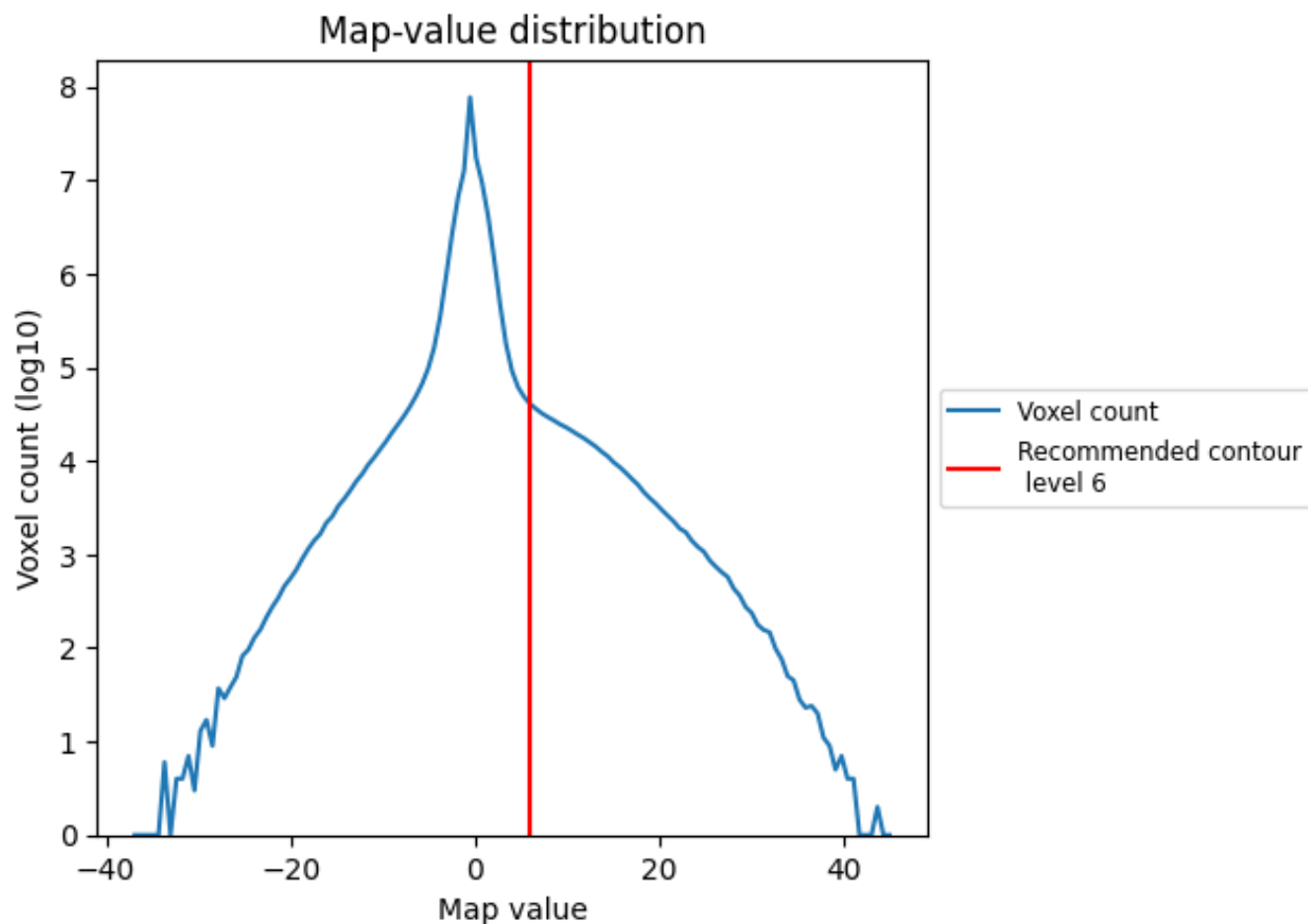
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

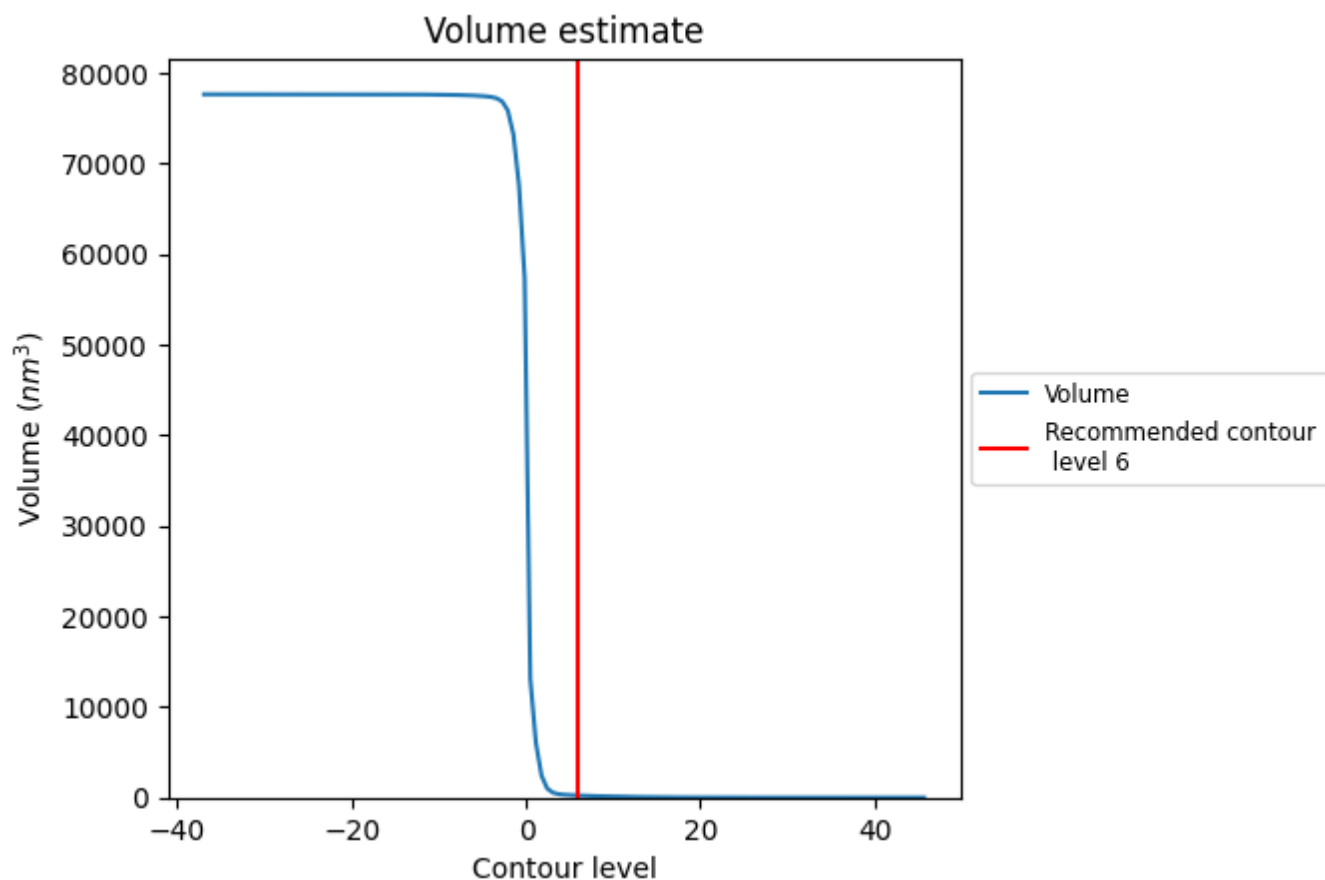
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

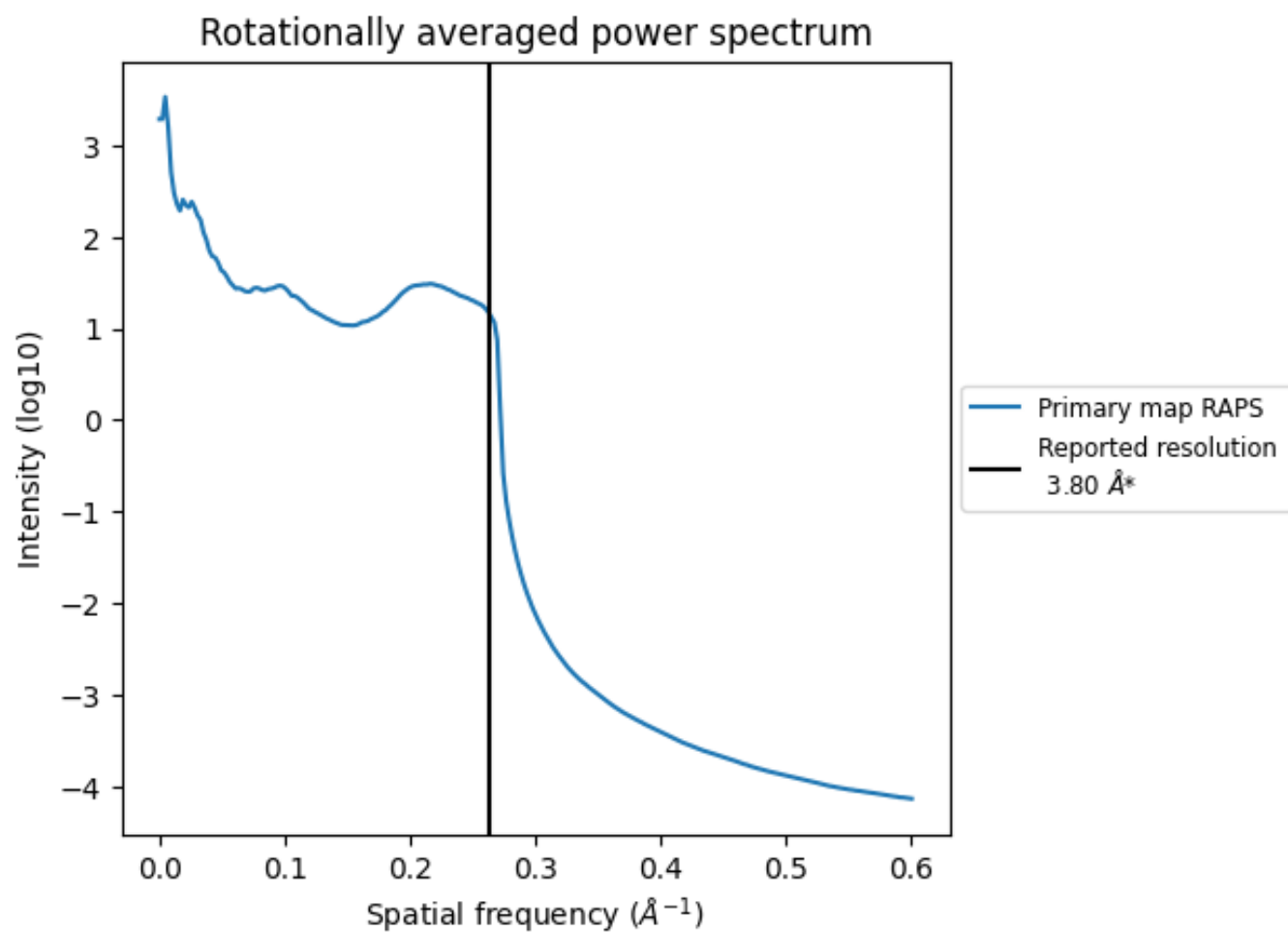
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228  $\text{nm}^3$ ; this corresponds to an approximate mass of 206 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 0.263 Å<sup>-1</sup>

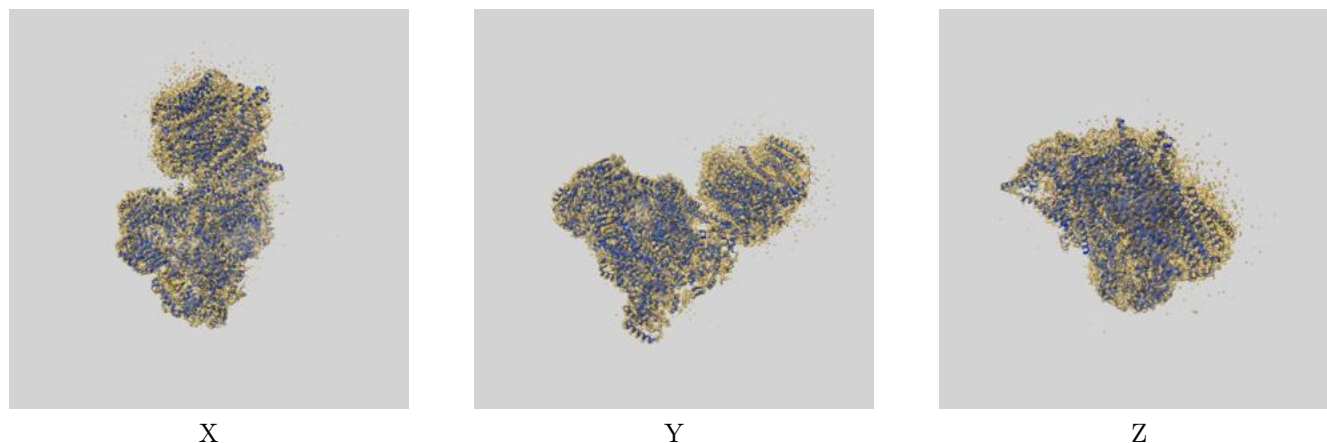
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

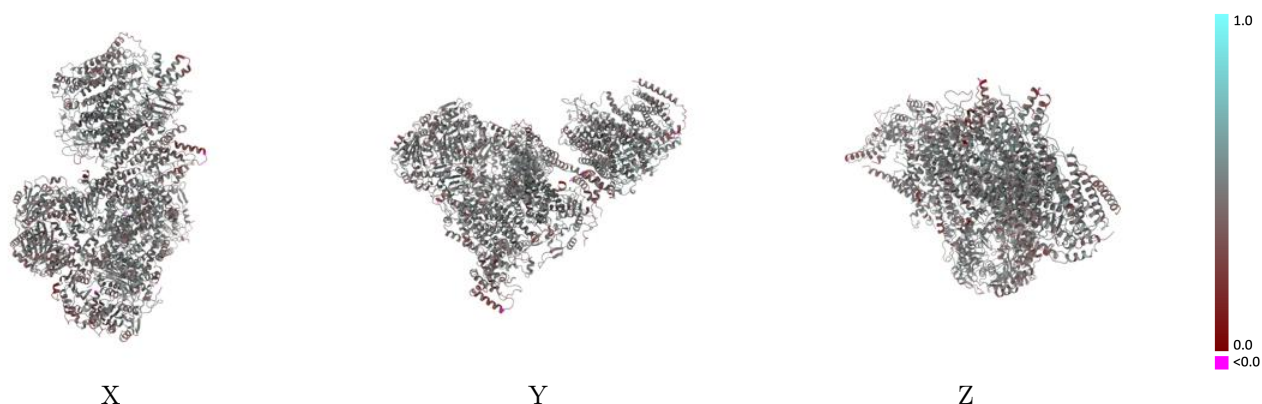
This section contains information regarding the fit between EMDB map EMD-22448 and PDB model 7JRP. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

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



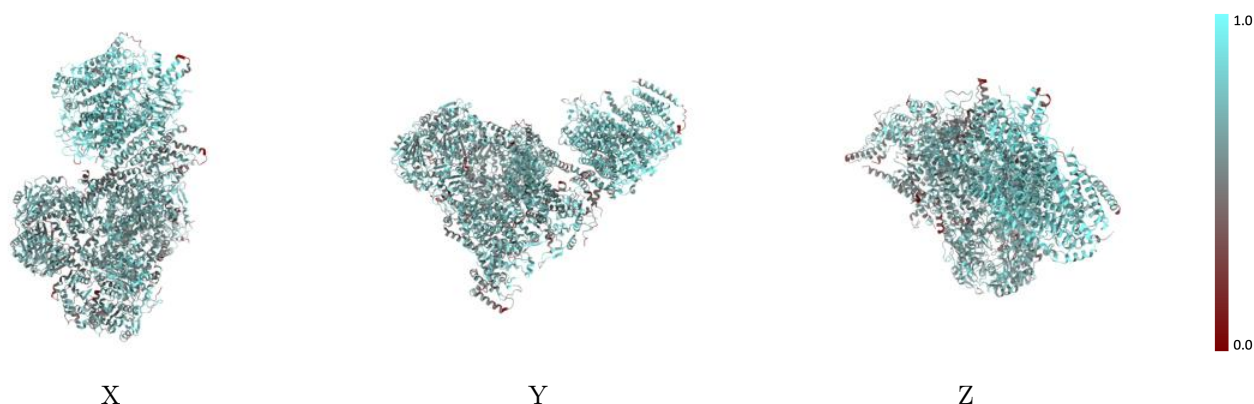
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



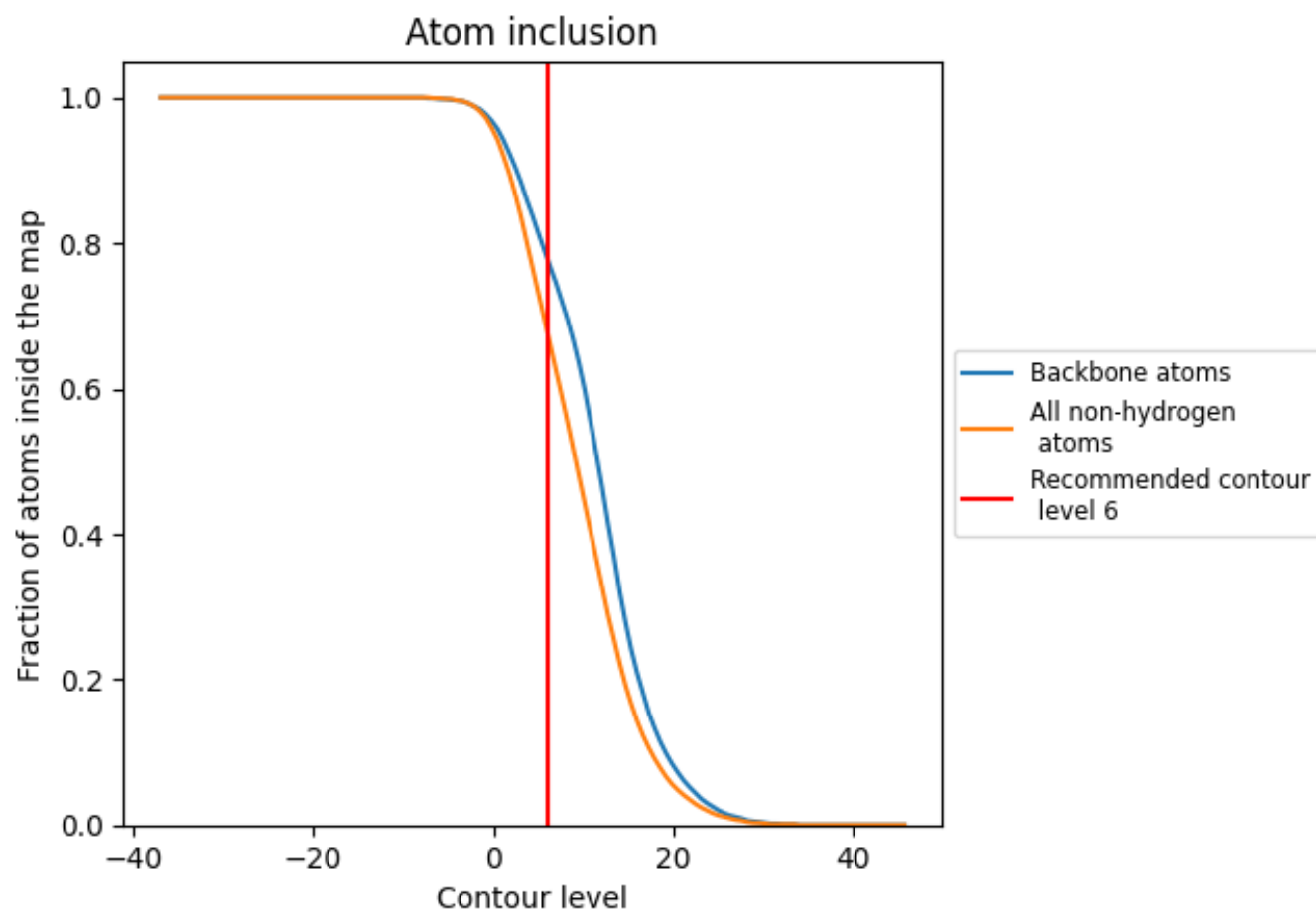
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

## 9.4 Atom inclusion [i](#)

































































At the recommended contour level, 78% of all backbone atoms, 68% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.4630
A	 0.6750	 0.4630
B	 0.6150	 0.4340
C	 0.6710	 0.4840
D	 0.6920	 0.4650
E	 0.6020	 0.4600
F	 0.6670	 0.4810
G	 0.5470	 0.4320
H	 0.4820	 0.3410
J	 0.5520	 0.4310
K	 0.4720	 0.3930
M	 0.6630	 0.4590
N	 0.6200	 0.4380
O	 0.6980	 0.4870
P	 0.6670	 0.4690
Q	 0.6000	 0.4640
R	 0.6690	 0.4740
S	 0.5660	 0.4600
T	 0.5000	 0.3520
V	 0.5510	 0.4110
W	 0.3480	 0.3550
a	 0.7970	 0.4960
b	 0.7670	 0.4900
c	 0.7920	 0.4890
d	 0.7210	 0.4550
e	 0.7490	 0.4440
f	 0.6790	 0.4400
g	 0.7650	 0.4530
h	 0.6820	 0.4370
i	 0.7530	 0.4730
j	 0.7500	 0.4690

